# Gas-Phase Ion and Neutral Thermochemistry

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David R. Lide, Jr., Editor

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# Gas-Phase Ion and Neutral Thermochemistry

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# Foreword

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David R. Lide, Jr., Editor
*Journal of Physical and Chemical Reference Data*

# Gas-Phase Ion and Neutral Thermochemistry

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Critically evaluated data on heats of formation of positive and negative ions in the gas phase are compiled and presented in these tables (GIANT tables), along with auxiliary information on ionization energies, proton affinities, electron affinities and acidities, as well as relevant thermochemistry of related neutral species. The literature coverage is through the middle of 1986. The criteria used in carrying out evaluations of data are described, and a short discussion is presented of special concerns for the thermochemistry of charged species.

Key words: acidity; anion; basicity; cation; Franck-Condon principle; electron affinity; heats of formation; ion/molecule equilibrium; ionization energy; negative ion; proton affinity.

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## Tables of Data

# 1. Introduction

## 1.1. History

This publication is the direct linear descendant of two earlier compilations of evaluated heats of formation of ions derived from ionization potential and appearance potential data, both carried out under the auspices of the National Bureau of Standards. The first such volume, "Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions" by J. L. Franklin, J. G. Dillard, H. M. Rosenstock, J. T. Herron, K. Draxl, and F. H. Field[1] appeared in 1969, and included all data on threshold energies for formation of positive ions which had appeared in the literature through mid-1966. That book, although woefully out-of-date now, is still occasionally referred to in the mass spectrometric literature, and is one of the most widely cited publications in the history of mass spectrometry. In 1977, H. M. Rosenstock, K. Draxl, B. W. Steiner, and J. T. Herron published an update, "Energetics of Gaseous Ions," which covered the literature through mid-1971[2]; the scope of the work was also extended to cover data on anions. In both of these books, the data for the threshold energies for formation of ions (ionization potentials and appearance potentials) were evaluated where possible, and where thermochemical data for relevant neutral species were available, values for heats of formation of the corresponding ions were derived.

In 1982, two of the present authors published an extensive compilation of *unevaluated* ionization potential and appearance potential data ("Ionization Potential and Appearance Potential Measurements, 1971–1981")[3] which covered the literature from the 1971 cut-off date of the 1977 book through mid-1981.

Since the mid-1970's, much information about ion thermochemistry has been derived from determinations of the equilibrium constants of ion/molecule reactions, a type of data which was not covered in the earlier compilations. Much of the work on equilibria of positive ions involves proton transfer reactions. These data have been compiled and evaluated by some of the present authors[4].

## 1.2. Definitions

The *heat of formation of a positive ion in the gas phase* is obtained by taking the heat of formation of the corresponding neutral species and adding the energy required to remove an electron, the so-called adiabatic ionization potential or, more correctly, the *adiabatic ionization energy*, $IP_a$ (sometimes designated IE, or, in the older literature, I):

$$\mathrm{M} \xrightarrow{IP_a} \mathrm{M}^+ + \mathrm{e} \qquad (1)$$

$$\Delta_f H(\mathrm{M}^+) = \Delta_f H^\circ(\mathrm{M}) + IP_a - \Delta_f H(\mathrm{e}) \qquad (2)$$

As discussed in Sec. 1.6.2., Eq. (2) is rigorously correct only at absolute zero. According to the convention adopted in this work for dealing with the thermochemistry of the electron (the "ion convention", sometimes called the "stationary electron convention", see Sec. 1.6.1.) "298 K heats of formation" of positive ions are often derived by simply adding the 0 K value for the ionization energy to the 298 K heat of formation of the molecule. The assumptions inherent in this treatment are discussed in Secs. 1.6.1. and 1.6.2. The user of these tables is cautioned that there is an alternate convention for dealing with the thermochemistry of the electron, which results in numerically different values for heats of formation for ions than those given here; details are discussed in Sec. 1.6.1.

The *vertical ionization energy* is the energy change corresponding to formation of the ion in a configuration which is effectively the same as that of the equilibrium geometry of the ground state neutral molecule. See Sec. 2.1. for a more complete discussion.

Accepting the simplifications described and justified in Sec. 1.6., determination of the heat of formation of a *molecular ion* is, in principle, straightforward, requiring only a value for the heat of formation of the corresponding neutral molecule and a reliable value for the adiabatic ionization energy. Many positive ions of interest, however, do not have stable neutral molecular counterparts. These include many of the ions which originate by fragmentation of a molecular ion, *fragment ions*:

$$\mathrm{AB}^+ \rightarrow \mathrm{A}^+ + \mathrm{B} + \mathrm{e} \qquad (3)$$

Heats of formation of fragment ions, $A^+$, are usually based on mass spectrometric determinations of the energy required to generate the ion from the neutral precursor molecule. This energy is called the "appearance potential" or, more correctly, the "*appearance energy*", *AP*:

$$\mathrm{AB} \xrightarrow{AP} \mathrm{A}^+ + \mathrm{B} + \mathrm{e} \qquad (4)$$

In the case that there is no potential barrier in the reaction coordinate, and little or no kinetic shift (see Sec. 2.2.), the onset energy for formation of $A^+$ corresponds approximately to the enthalpy change of reaction 4. Under these conditions, the heat of formation of $A^+$ is usually assumed to be given by:

$$\Delta_f H(\mathrm{A}^+) = \Delta_f H^\circ(\mathrm{AB}) - \Delta_f H^\circ(\mathrm{B}) + AP \qquad (5)$$

where, according to the ion convention, the term accounting for the electron has been taken to be zero. For a discussion of a more exact treatment of the energetics of ionic fragmentation processes, see Sec. 1.6.2.

Stable cations formed in the gas phase also include ions formed by protonating a neutral molecule:

$$\mathrm{BH}^+ + \mathrm{M} \rightarrow \mathrm{MH}^+ + \mathrm{B} \qquad (6)$$

In practice, heats of formation of most *protonated molecules* are derived from experiments in which the equilibrium constant of a proton transfer reaction such as 6 is determined (given that a heat of formation of a reference $BH^+$ ion is available from appearance potential determinations). Formally, the relationship between the heat of formation of $MH^+$ and its neutral counterpart, M, is defined in terms of a quantity called the *proton affinity, PA*. The proton affinity is the negative of the enthalpy change of the hypothetical protonation reaction:

$$M + H^+ \xrightarrow{-PA} MH^+ \tag{7}$$

$$\Delta_f H(MH^+) = \Delta_f H^\circ(M) + \Delta_f H(H^+) - PA \tag{8}$$

The term proton affinity, as universally used, is a quantity defined at 298 K (and therefore not strictly analogous to the adiabatic ionization energy, which is the 0 K enthalpy change of reaction 1). (The Gibbs energy change associated with reaction 7 is called the *gas basicity, GB*, of molecule M.) At 298 K, the heat of formation of the proton, using the ion ("stationary electron") convention, is 365.7 kcal/mol, 1530.0 kJ/mol.

The *electron affinity* (*EA*) of a molecule is, for *negative ions* or *anions*, the quantity which is analogous to the ionization energy for positive ions. That is, the electron affinity is equal to the energy difference between the heat of formation of a neutral species and the *heat of formation of the negative ion* of the same structure. The electron affinity is defined as the negative of the 0 K enthalpy change for the electron attachment reaction:

$$M + e \xrightarrow{-EA_a} M^- \tag{9}$$

The *gas phase acidity* (or merely, acidity) of a molecule AH, $\Delta_{acid}G(AH)$, is the Gibbs energy change of the reaction:

$$AH \rightarrow A^- + H^+ \tag{10}$$

usually defined at 298 K. The enthalpy change of reaction 10, $\Delta_{acid}H$, is, of course, the proton affinity of the anion. The Gibbs energy change of the reaction:

$$AH + B^- \rightarrow BH + A^- \tag{11}$$

is called the *relative acidity* of species AH and BH.

### 1.3. Scope, Limitations to Coverage, and Organization

The intent of the present effort is to give (a) the "best" available experimentally-determined values for ionization potentials, electron affinities, acidities or proton affinities of molecules or molecular fragments, and (b) the heats of formation of the corresponding positive and negative ions. Also included are values for the heats of formation of the relevant neutral species which were used to obtain the heats of formation of the ions. Appearance energies are not specifically listed here, although heats of formation of ions derived from such data are given where the accuracy is sufficiently great to warrant inclusion.

In evaluating heats of formation of ions for the present work, all data presented in the previous compilations[1,2,3,4] have been considered, along with data from the more recent literature, 1981–1986. In addition, thermochemical information about ions derived from ion/molecule equilibrium constant determinations has been fully utilized, both in evaluations of ionization potential/appearance potential, proton affinity, acidity, and electron affinity data, and in deriving values for heats of formation of ions for which no other information is available.

Because the values for the heats of formation of ions are, of course, dependent on the larger corpus of thermochemical data on uncharged species, the values for heats of formation of relevant neutral species which were utilized are included as an intrinsic part of the tables.

The user familiar with the previous compilations in this series will note that the format of the present work is considerably different from that of its predecessors. In all three previous volumes, *all* ionization energy or appearance energy data pertaining to a particular ionic species were displayed, so that the books served as complete summaries and guides to the literature. Because of the increasing volume of such an archive with time, such a display is no longer practical for the positive ion data. Furthermore, because the general quality of mass spectrometric measurements has increased greatly over the last decade, display of some of the now out-of-date early data is no longer even desirable for ionization potentials/appearance potentials.

On the other hand, there has been a tremendous increase in the number of anions for which some thermochemical information is known, and this publication presents the first extensive evaluated compilation of those data. The table of anion thermochemistry (Table 2), therefore, includes both as *complete* a collection as possible of the literature data, and an assignment where possible of the "best" value for the thermochemistry.

Because earlier volumes in this series[1,2] were devoted to deriving values for *heats of formation* of ions, this work has been defined in the same way. It should be emphasized that in Table 1 (the positive ion table) molecules for which heats of formation are not known or have not been estimated are not included, even if the corresponding ionization energies or proton affinities are known. On the other hand, Table 2 (the negative ion table) presents a complete archive of data on electron affinities and gas phase acidities, whether or not the thermochemistry of relevant neutral species is available; the evaluation of the scale of gas phase acidities will, however, be the subject of a separate publication[5]. The total archive of ionization energy and appearance energy data will be published separately[6], as will the updated scales of gas phase basicities/proton affinities[7].

Another consequence of defining this work in terms of thermochemical data is that the abundant data on excited states of ions from photoelectron spectroscopy are not included here. The combined bibliographies of this work and its predecessors, however, do include the entire corpus of literature of photoelectron spectroscopy, since values for the *lowest* ionization energy derived from photoelectron experiments are included. Also not included are data on multiply charged ions.

Thermochemical information about ion/molecule clusters has been published in a recent compilation[8], and is not specifically included here, although some information derived from the enthalpy changes associated with the association of the first solvent molecule have been used in evaluating certain heats of formation.

At this writing, publications are beginning to appear in increasing numbers giving quantum mechanical calculations of very high accuracy on the thermochemical properties of ions, especially small ions[9,10]. The present work includes *only* data derived from experimental determinations. However, conclusions derived from some high level calculations have been taken into account in the evaluation of data for particular species.

The solution phase reduction potentials of a variety of species have been correlated with gas phase electron affinities (EAs), and values for a large number of EAs have been extrapolated from such correlations. More recent determinations of accurate gas phase data have shown that such relationships hold only for limited classes of compounds, so that the solution phase data can be taken only as an approximate guide to predicting electron affinities. Thus, any electron affinity values derived from reduction potentials have been omitted from this compilation. Such values were included in a recent compilation of anion data[11].

This compilation also does not attempt to cover negative electron affinities — cases where the electron in the highest occupied molecular orbital is unbound (resonance states), and therefore the lifetime of the anion with respect to autodetachment is on the order of microseconds, at most. Electron transmission spectrometry[12] is used to determine thermochemical data for such species. Brief mention is made for certain small molecules and elements for which the anion is known to be unbound, to differentiate from cases for which there is just no data available.

The data on positive ions and on negative ions are not interdependent, and have been evaluated separately. Data on the positive ions were collected and evaluated at the National Bureau of Standards (ionization energies, equilibrium constant data) and the University of Ottawa (appearance energies), while information concerning the negative ions was handled at the University of Tennessee. The data on cations and anions are presented in two separate tables.

Since heats of formation of ions are derived using data on heats of formation of neutral molecules and radicals, data on the thermochemistry of uncharged species are an integral part of this work. Although only experimentally-determined values for heats of formation of neutral species were utilized in the 1977 evaluation, estimation schemes for arriving at thermochemical information are now widely accepted and used. Estimated heats of formation are included for many species for which no experimental data are available. These estimations, and a literature search for thermochemical data not available in compilations, were performed primarily at the University of Maryland, Baltimore County Campus.

## 1.4. Literature References

With respect to ionization energies, appearance energies, or proton affinities, the present publication gives specific citations only to publications which were not included in the previous compilations[1,2,3,4]. The bibliography includes *all* references which have appeared since the previous publications[1,2,3,4] even if the data from a particular paper are not given here because of a lack of information about the thermochemistry of relevant neutral molecules. When no literature reference is given for these kinds of data in the positive ion table, it should be assumed that the primary reference can be obtained from the secondary sources, references 1, 2, 3, or 4. When the source of the data on ion thermochemistry is a recent paper which was not included in any of these previous compilations, the reference is specifically cited in a footnote. The literature citations for which a specific column is provided in Table 1 refer only to the source of the data on the thermochemistry of the neutral species.

In Table 2, specific citations are given for the data on both the ion thermochemistry and the relevant neutral thermochemistry.

## 1.5. Units

Information is displayed in the tables using different units, dictated by the current practices for reporting data of a particular kind. For example, ionization energy and electron affinity values are usually reported in electron volts, and that is the unit used here for these data. Heats of formation of positive ions are given here in both kcal/mol and kJ/mol. The reason for this duplication is simply that both units are extensively used in the literature, and users of these tables will be about equally divided between those who prefer kilocalories and those who prefer kilojoules. Furthermore, because of the duplication in units, the data can always be displayed as they appeared in the original paper, a practice which helps in elimination of transcribing errors. While the same statements certainly apply to data on negative ions, the amount of information which needs to be displayed in Table 2 is sufficiently great that including the same information twice, in two sets of units, would crowd the page too much; therefore, the negative ion heats of formation and acidities are given only in the SI unit, kJ/mol.

The conversion factors which were used in this work are: 1 electron volt (eV) = 23.06036 kilocalories/mole = 96.4845 kilojoules/mole; 1 kilocalorie/mole = 4.184 kilojoules/mole.

## 1.6. Ion Thermochemistry at Finite Temperatures

The auxiliary thermochemical information required for citation of ion heats of formation—heats of formation of relevant neutral species—is available mostly for species at 298 K. These thermochemical data are correct for use in deriving ion heats of formation from equilibrium constant determinations, i.e., for treatment of data derived from processes occurring at temperatures other than 0 K. However, strictly speaking, the ionization energy and the electron affinity of a molecule are quantities which correspond to processes occurring at 0 K. As mentioned above in Sec. 1.2., a rigorously correct treatment of heats of formation of ions requires explicit treatment of the differences in thermochemical values at 0 K and at higher temperatures. This section describes the principles involved in such a correct treatment, considers the simplifications which are often made in the literature, and specifies how data have been treated in this work.

### 1.6.1. Thermochemical Conventions for the Electron

We are concerned with the way in which the enthalpies of formation of the chemical species, $M^+$ and $M^-$, are *defined*, particularly at temperatures other than 0 K. The enthalpy of formation of any chemical species is always taken as the difference between the enthalpy of the compound and the sum of the enthalpies of the elements of which it is composed. However, in the case of an ion, $M^+$ or $M^-$, a special problem arises—one must explicitly take into account the enthalpy of the electron in some way.

There are two conventions for dealing with the thermochemistry of the electron, one used predominantly by thermodynamicists[13,14,15] and one adopted by scientists studying ion physics/chemistry[16,17]. The thermodynamicists' convention, commonly called the "thermal electron convention" or merely the "electron convention", defines the electron as a standard *chemical element* and treats its thermochemistry accordingly. The mass spectrometrists' convention, known as the "stationary electron convention" or the "ion convention", defines the electron as a *sub-atomic particle.* Because of differences in the treatment of the thermochemistry under these two definitions, except at absolute zero values cited for the enthalpies of formation of ions in certain thermochemical compilations such as the JANAF tables[13] or the NBS Tables of Chemical Thermodynamic Properties[14] differ from those cited here, or in most mass spectrometric literature, by 1.481 kcal/mol, 6.197 kJ/mol. Our values are lower for positive ions and higher for negative ions. Problems arise when users unknowingly mix inconsistent values for heats of formation in the same equation.

There is considerable confusion and misunderstanding of the basic assumptions and treatment of the thermochemistry of the electron in the two approaches. Many scientists who regularly use one or the other convention in their work can not clearly explain the differences. Indeed, some hold that the two ways of dealing with the thermochemistry of the electron are not merely two conventions, but two scientifically different concepts, one of which must be incorrect. The discussion which follows is an attempt to present the question of how the electron is treated in a thermochemical equation in as simple and straightforward a manner as possible, in the hope that some of the confusion will be dispelled and the identity of the two treatments as *conventions* will become clear. This discussion is also intended to justify the choice of the usual mass spectrometrists' convention for use in these tables.

The relationships between the various quantities which must be considered are shown in the thermochemical cycles:

$$\begin{array}{ccccc} M_{0\,K} & \xrightarrow{IP} & M^+{}_{0\,K} & + & e_{0\,K} \\ A\downarrow & & B\downarrow & & C\downarrow \end{array} \tag{12a}$$

$$M_{298\,K} \xrightarrow{\Delta H_I} M^+{}_{298\,K} + e_{298\,K} \tag{12b}$$

and

$$\begin{array}{ccccc} M_{0\,K} & + & e_{0\,K} & \xrightarrow{-EA} & M^-{}_{0\,K} \\ A\downarrow & & C\downarrow & & D\downarrow \end{array} \tag{13a}$$

$$M_{298\,K} + e_{298\,K} \xrightarrow{\Delta H_{EA}} M^-{}_{298\,K} \tag{13b}$$

where $A$, $B$, $C$, and $D$ are the integrated heat capacities for the various indicated species, e.g., $A$ is the energy required to raise M from 0 K to 298 K, and $\Delta H_I$ and $\Delta H_{EA}$ are the 298 K enthalpies of reaction. This discussion will be concerned with the standard temperature, 298 K, but the arguments can obviously be extended to any other temperature.

At 0 K, the heat of formation of the electron is zero and the heats of formation of the ions are exactly equal to the 0 K heat of formation of the molecule M plus the energy difference between M and the corresponding ion:

$$\Delta_f H(M^+)_{0\,K} = \Delta_f H^\circ(M)_{0\,K} + IP, \tag{14}$$

$$\Delta_f H(M^-)_{0\,K} = \Delta_f H^\circ(M)_{0\,K} - EA \tag{15}$$

At absolute zero, there is no difference between the two conventions.

When the temperature is raised to 298 K, the heats of formation of $M^+$ and $M^-$ will be related to the heat of formation of M at 298 K through the enthalpy changes of reactions 12b and 13b:

$$\Delta_f H(M^+)_{298\,K} = \Delta_f H^\circ(M)_{298\,K} - \Delta_f H(e)_{298\,K} + \Delta H_I \tag{16}$$

$$\Delta_f H(M^-)_{298\,K} = \Delta_f H^\circ(M)_{298\,K} + \Delta_f H(e)_{298\,K} + \Delta H_{EA} \tag{17}$$

The enthalpy changes of reaction at 298 K are related to the 0 K ionization energy and electron affinity through the relationships:

$$\Delta H_I = IP_a + (C + B - A) \tag{18}$$

$$\Delta H_{EA} = -EA - (C + A - D) \tag{19}$$

If the electron is defined to be a chemical element (the "electron convention"), its heat of formation by definition is zero at all temperatures in its standard state. Thermodynamicists start from this assumption and then make a second one, that an electron gas can be treated as an ideal gas following Boltzmann statistics; this second assumption is used to calculate the integrated heat capacity of the electron, $C$. In many thermodynamics data compilations, the integrated heat capacity terms for M and the corresponding ion, $M^+$ or $M^-$, are taken to be approximately equal for many ions, i.e. $A = B = D$. (See Sec. 1.6.2. for a discussion of this assumption.) Under this set of assumptions, Eqs. (16) and (17) can be written:

$$\Delta_f H(M^+)_{298\ K} = \Delta_f H°(M)_{298\ K} + [IP_a + C] \tag{20}$$

$$\Delta_f H(M^-)_{298\ K} = \Delta_f H°(M)_{298\ K} - [EA - C] \tag{21}$$

(where the term $\Delta_f H(e)_{298\ K}$ has been taken to be equal to zero and the quantity in brackets is the assumed enthalpy change of reaction at 298 K). What most often causes confusion for non-thermodynamicists is the de facto assignment of the integrated heat capacity of the electron, $C$, to the ion $M^+$ or $M^-$, rather than to the electron in going from 0 K to 298 K. This is required if the heat of formation of the electron is constrained to be zero at all temperatures. It is questionable whether an ion is any more "ideal" than an electron, due to the Coulombic forces between the particles, but this assignment is a necessity if the original assumptions are carried through the argument.

In contrast, the standard treatment of ion heats of formation followed in almost the entire corpus of literature on ion physics/chemistry essentially assumes that:

$$\Delta_f H(M^+)_{298\ K} = \Delta_f H°(M)_{298\ K} + [IP_a + B - A] \tag{22}$$

$$\Delta_f H(M^-)_{298\ K} = \Delta_f H°(M)_{298\ K} + [-EA - A + D] \tag{23}$$

(where the expressions in brackets are assumed to be equal to the enthalpy change of reaction at 298 K, and the quantities $A$, $B$, and $D$ are often, but not always, taken to be equal). Since this is equivalent to taking a value of zero for the integrated heat capacity of the electron (the term $C$ in Eqs. (18) and (19)), this way of treating the thermochemistry of the electron has come to be known as the "stationary electron" convention. The use of this term has unfortunately led to the widespread conception that this convention defines the ionization process as producing an electron which has no thermal energy at 298 K. Since this is not the case, it is preferable to choose another designation for the convention. In this publication we will adopt the term originally suggested by Syverud[18] for the mass spectrometrists' convention, "ion convention".

At 298 K, the integrated heat capacity of an ideal Boltzmann gas is 1.481 kcal/mol, 6.197 kJ/mol. The relationship between 298 K heats of formation of ions in the ion convention (IC) and the thermodynamicists' convention (TC) is:

$$\Delta_f H(M^+)_{298\ K}(IC) = \Delta_f H(M^+)_{298\ K}(TC) - 6.197\ \text{kJ/mol} \tag{24}$$

$$\Delta_f H(M^-)_{298\ K}(IC) = \Delta_f H(M^-)_{298\ K}(TC) + 6.197\ \text{kJ/mol} \tag{25}$$

Table 1.6.1.1. summarizes the assumptions made in the two conventions and the data compilations where they are used.

TABLE 1.6.1.1. Summary of assumptions about electron thermochemistry in data compilations.

| Convention | Compilation | Convention Includes $H_T - H_0$ for Species: M | $M^+$ or $M^-$ | e | Value of $C$, kJ/mol |
|---|---|---|---|---|---|
| Thermal electron | JANAF Tables[13] | Yes[a] | Yes[a] | Yes | 6.197 |
| Thermal electron | Gurvich et al[15] | Yes[a] | Yes[a] | Yes | 6.197 |
| Thermal electron (Modified) | TN270[14] | No | No | Yes | 6.197 |
| Ion convention | This work, Refs. 1–4 | Yes[a] | Yes[a] | No | 0 |
| Ion convention | Some papers | No | No | No | 0 |

[a]When sufficient information is available. See discussion in Sec. 1.6.2.

The objection has been made that the mass spectrometrists' convention is scientifically incorrect because the electron actually does have thermal energy at 298 K. Note, however, that the values derived in the mass spectrometrists' convention for the heats of formation of the ions are numerically identical to those one would obtain if one assigned the thermal energy of the electron *to the electron* rather than to the enthalpy of formation of the accompanying ion (as is done in the thermodynamicists' convention). That is, in Eqs. (16) and (17) if one assigns a value of $C$ to $\Delta_f H(e)_{298\ K}$ and takes the value for the enthalpy change of reaction from Eqs. (18) and (19), one obtains:

$$\Delta_f H(M^+)_{298\ K} = \Delta_f H°(M)_{298\ K} - C + IP_a + (C + B - A) \tag{26}$$

$$\Delta_f H(M^-)_{298\ K} = \Delta_f H°(M)_{298\ K} + C - EA - (C + A - D) \tag{27}$$

which are identical to expressions 22 and 23. Although this is a nonstandard treatment, it is possible to justify using a special convention for the thermochemical properties of the electron, since this species is not normally considered to be a chemical element; a stronger justification is found by considering that the use of the standard treatment for an element in this case results in heats of formation for a large body of molecular species — ions — which reflect an arbitrary temperature dependence which can not be experimentally measured or verified at the present time.

In fact, the mass spectrometrists' convention for treating the electron was not derived from a conscious treatment of the electron as having a non-zero heat of formation at 298 K. Indeed, earlier discussions of this convention[16,17,18] have centered mainly on the reluctance to assign a purely arbitrary temperature dependence to ionization or electron attachment events and a recognition that absolute values of the various parameters, $\Delta H_I$, $\Delta H_{EA}$, $B$, $D$, and especially $C$ were not available. The enthalpy changes of reactions 12b and 13b are not directly measured by any currently-available experimental techniques, and can not be said to be known within $\pm 6.197$ kJ/mol. As will be discussed below, accurate values for the integrated heat capacities of ions $M^+$ and $M^-$ are not available except for a few small species, and the assumption that $(B - A)$ and $(A - D)$ are exactly equal to zero is often not warranted (see Sec. 1.6.2.). Most important, however, the value chosen for the integrated heat capacity of the electron, $C$, is completely arbitrary. To quote from the 1985 edition of the JANAF thermochemical tables[13c]:

> "As shown by Sommerfeld[19], the electron gas is a degenerate Fermi-Dirac gas and its properties will differ from the classical (Boltzmann) gas. These deviations will increase as the temperature decreases or as the density increases. Due to the low mass of the electron, these departures from classical behavior will persist to higher temperatures and lower densities than for atomic systems. Under conditions of 1 atm pressure, Gordon[20] showed that the deviation of the Fermi-Dirac gas from the Boltzmann gas is negligible above 1250 K. Below this temperature the deviation between classical and quantum statistics will be significant.
>
> Despite these known deviations we have chosen to present the classical (Boltzmann) values here since the primary purpose of this table is to serve as a reference state for the calculation of tables of thermodynamic properties for atomic and molecular ions..... Therefore, although this ideal-gas table has the formalism of 1 bar as the standard reference state, it should not be applied to real systems where the electron partial pressure exceeds $10^{-6}$ bar."

That is, the authors of the JANAF tables[13] recognize that the standard thermodynamicists' convention for dealing with the electron does involve a completely arbitrary assumption about the value assigned to the enthalpy of the electron (as does the mass spectrometrists' convention when expressed by Eqs. (22) and (23)—but not in the assumptions built into the equivalent Eqs. (26) and (27)). Syverud[18], in an unpublished discussion of conventions for treating the thermochemical properties of the electron, cites a value of approximately 3.3 kJ/mol, 0.8 kcal/mol for the value of $C$ derived from a quantum chemical calculation (source not quoted). Furthermore, while the rationale for the thermodynamicists' convention is that the values "correspond to a meaningful thermal process"[21], the use of that convention is excluded for a substantial set of possible thermal conditions.

The mass spectrometrists' approach to the problem recognizes that the specific inclusion of the term for the enthalpy of the electron in deriving ion heats of formation is not physically meaningful if it is based on the assumption that an electron gas can be treated like an ideal gas. In fact, at this time neither the enthalpy changes of reactions 12b and 13b nor the enthalpy of the electron are established; a solution is to adopt a convention (the "ion convention") which sidesteps the problem, that is, in which the enthalpy change of reaction and the enthalpy of the electron need not be known or assumed. If, in the future, information about the integrated heat capacities of the electron and the ions does become available, the values for heats of formation of ions can be fine-tuned; however, in the meantime, there is no real problem with using data in the present form as long as internal consistency is maintained.

It will be noted that in the tables, the symbol $\Delta_f H$ rather than $\Delta_f H^\circ$ is used to denote the standard heats of formation of the ions. This convention has been adopted here to emphasize that the heats of formation are referred to the ion convention rather than the electron convention used by thermodynamicists.

#### 1.6.2. Thermochemistry of Positive Ions at Finite Temperatures

*Molecular ions*. Using the ion convention (also known as the stationary electron convention, see Sec. 1.6.1.) the heat of formation of molecular ion $M^+$ at temperature $T$ can be defined in terms of the heat of formation of the corresponding neutral species, M, at temperature $T$, and a quantity labelled $\Delta H_I$, the gas phase enthalpy change of ionization, which represents the energy required to bring about ionization at temperature $T$:

$$\Delta_f H(M^+)_T = \Delta_f H^\circ(M)_T + \Delta H_I \qquad (28)$$

In applying Eq. (28), the value for $\Delta H_I$ is usually taken to be exactly equal to the adiabatic ionization potential. Although the use of the ion convention obviates the necessity of assigning an exact value to the increase in the ionization energy at temperature $T$ due to energy imparted to the electron, the assumption that $\Delta H_I$ is the same as $IP_a$ is still not correct. The adiabatic ionization energy of a molecule is the energy difference between the lowest rotational and vibrational levels of the ground state of the molecule and the lowest rotational and vibrational levels of the electronic ground state of the ion, i.e., the difference between the heats of formation of the molecule and the corresponding ion at absolute zero. The adiabatic ionization energy—the quantity obtained from analysis of a Rydberg series (Sec. 2.3.1.) or from determinations of an ionization onset energy (Sec. 2.3.3.) — is a measure of the $0 \rightarrow 0$ transition, and does not depend on the temperature at which the determination is made.

However, it is a common practice to derive "298 K heats of formation" of positive ions by simply adding the 0 K value for the ionization energy to the 298 K heat of formation of the molecule. This practice probably gains impetus from the fact that much of the available thermochemical data for chemical compounds (particularly for organic and other large polyatomic compounds) correspond to values for heats of formation at 298 K.

The relationship between the enthalpy change associated with ionization at temperature $T$, $\Delta H_I$, and the adiabatic ionization energy is shown in thermochemical cycle 12, and given explicitly in Eq. 18. When using the ion convention for dealing with thermochemistry of the electron (Sec. 1.6.1.), the integrated heat capacity of the electron (the quantity $C$ in the cycle) can be ignored, and the relationship between the adiabatic ionization energy and the enthalpy change of ionization at temperature $T$ is given by:

$$\Delta H_I = IP_a + B - A \qquad (29)$$

That is, $IP_a$ and $\Delta H_I$ are the same only when the integrated heat capacities of the neutral molecule, M, and the ion, $M^+$, are identical over this temperature range. An analysis[22] of the differences between integrated heat capacities of M and $M^+$ for various molecules demonstrated that (a) there will be no discernable differences between the translational and rotational heat capacities of M and $M^+$, (b) that differences arising from a splitting of degenerate energy levels in multiplet ground states of M or $M^+$ will never be larger than 0.009 eV at temperatures in the 300−400 K range, and (c) when the frequency of a particular vibration changes upon ionization, there will be a difference between the integrated heat capacities of M and $M^+$. However, even this contribution will usually be sufficiently small that a significant error will not be introduced if it is ignored. For example, the lowest ionization energy of ethylene corresponds to removal of an electron from the C–C pi bond, which leads to a lowering of the frequency of the symmetric C–C stretch from 1623 to 1230 $cm^{-1}$ and a reduction in the frequency of the twisting around the C–C bond from 1027 to 430 $cm^{-1}$. Although these differences in vibrational frequencies are significant, the predicted effect on the 298 K enthalpy of ionization is to raise it above the value for the adiabatic ionization potential by only 0.0069 eV, i.e. only the most accurate experimental measurements would detect an increment of this size. Thus for most species, the simplifying assumption that the adiabatic ionization energy and the 298 K enthalpy of ionization, $\Delta H_I$, are approximately the same:

$$IP_a \sim \Delta H_I \qquad (30)$$

will not introduce significant errors in the 298 K heats of formation of molecular radical cations.

In this compilation, most values of heats of formation of molecular ions correspond to 298 K. Most of these were obtained by simply adding the value for the adiabatic ionization energy to the 298 K heat of formation of the neutral species, that is, the assumption stated in Eq. (30) was usually made. Of course, a rigorously correct treatment would require calculating exact values for integrated heat capacities $A$ and $B$ from complete sets of vibrational frequencies for the molecule and the ion. This complete procedure has been applied to only a few of the species listed in this compilation. Vibrational frequencies for most of the ions are not available, and the correction would simply cancel out if one made the often-used assumption that the vibrational frequencies of the ion and its neutral counterpart are the same. Whenever the original authors carried out such a complete analysis (a routine procedure only for photoelectron-photoion coincidence studies), the results of that analysis are included here, and both 0 K and 298 K values for the ion heat of formation are given. In addition, for those diatomic and triatomic and other small molecules for which values for the 0 K heats of formation as well as the vibrational frequencies of the molecule[23] and the ion[24] were readily available, the heats of formation of the ion at absolute zero and at 298 K were derived by the more correct procedure. In the course of this work, we did not, however, carry out a comprehensive literature search for sets of vibrational frequencies, but only made use of readily available compilations[23,24].

*Fragment ions*. Analogous arguments can be applied to the use of appearance energies for the derivation of heats of formation of fragment ions, $A^+$, at temperature $T$ in Eq. (5). If there are no complicating factors (see Sec. 2.2.), the appearance energy, $AP$, corresponds to the enthalpy change for the fragmentation reaction 4, and can be used to derive a value for the heat of formation of the fragment ion, $A^+$. Correctly, a 0 K heat of formation of $A^+$ must be obtained using 0 K heats of formation of AB and B in the calculation, and this heat of formation can then be corrected to some other temperature, $T$, taking into account the vibrational frequencies of the ion and appropriate thermodynamic functions of the elements.

For the most common experimental techniques (energy selected electron impact, photoionization mass spectroscopy, etc.) for measuring the appearance energy of a fragment ion starting from a molecule or radical at temperature, $T$, the major problem is to identify the internal energies of the reaction products. This matter has been discussed at length by Traeger and McLaughlin[25]. At *onset* the products of the unimolecular decomposition will be formed with zero translational energy with respect to the center of mass (provided that the fragmentation does not involve a reverse energy barrier) and a center of mass translational energy the same as that of the precursor molecule. The products thus are at a translational quasi-temperature, $T^*$. In principle, if the observational time scale of the experiment and the sensitivity of the ion detector are great enough, then the observed appearance energy approaches that for products having 0 K internal energy (i.e., all internal energy modes have contributed to reaching the transition state). Traeger and McLaughlin[25] showed that for the molecule AB:

$$AP_T(\mathrm{exp}) = \Delta_f H[\mathrm{A}^+ + \mathrm{B} + \mathrm{e}]_T - \Delta_f H^\circ[\mathrm{AB}]_T + 5/2RT - \int C_p[\mathrm{A}^+ + \mathrm{B} + \mathrm{e}]\mathrm{d}T \quad (31)$$

In effect, this equation corrects the observed threshold energy for the fragmentation process to an effective 0 K value by adding the thermal rotational and vibrational energy contained in AB to the onset.

Most heats of formation of fragment ions are derived making the simplifying assumption that the last two terms of Eq. (31) will cancel one another. That is, values for heats of formation of fragment ions at 298 K derived from appearance potential data are more often obtained by simply using an observed onset energy and 298 K heats of formation of relevant neutral species in Eq. (5). When such a value for a heat of formation has been reported in the literature, the value is given here as it appeared in the original paper, with only the imposed requirement that the thermochemistry of the relevant neutral species employed must be internally consistent with the values of those species used in this publication. Where the original authors have used a more sophisticated analysis, such as that represented by Eq. (31), or that routinely used in the interpretation of photoelectron-photoion data, both 0 K and 298 K values of the ion are cited. The user should be cautioned that the 298 K value assigned to a heat of formation of a fragment ion may differ by as much as 3 or 4 kcal/mol, 12–18 kJ/mol, depending on which of these treatments has been used. For example, Baer and Brand[26], and Lossing[27] determined the appearance energies for formation of $C_4H_7^+$ ions in $C_5H_{10}$ isomers. Although the appearance energies reported in the two studies were almost identical, the 298 K values for heats of formation of the $C_4H_7^+$ ions derived by Baer and Brand[26], using a complete treatment of the temperature dependence of the heat of formation, are higher than the values derived by Lossing[27] by 4.3 kcal/mol, 18 kJ/mol.

#### 1.6.3. Thermochemistry of Negative Ions at Finite Temperatures

The electron affinity is a quantity which is analogous to the ionization energy. That is, the electron affinity is a 0 K quantity which corresponds to the transition from the ground state of the neutral species to the ground state of the anion. Thus, the heat of formation of an anion at 298 K can not rigorously be taken as the heat of formation of the corresponding neutral species (298 K) minus the (positive) electron affinity (0 K) without some estimate of the temperature dependence of the electron affinity. Although the use of the ion convention ("stationary electron" convention) allows one to ignore the integrated heat capacity of the electron, a term for correcting for the integrated heat capacity of the anion from 0 K to 298 K is required. Statistical mechanics permits a calculation of this quantity if the structure and vibrational frequencies of the anion are known. However, at present the necessary data are not readily available for most anions, and therefore this correction is generally ignored in this work.

Under the assumption that the temperature dependence of the electron affinity and that of the ionization energy of the H atom are equal, one can relate the (298 K) gas phase acidity, Eq. (10), to the (0 K) electron affinity:

$$\Delta_{\mathrm{acid}}H(\mathrm{AH}) = D(\mathrm{A{-}H}) - EA_{0\,\mathrm{K}}(\mathrm{A}) + IP_{0\,\mathrm{K}}(\mathrm{H}) \quad (32)$$

There is not extensive data on the validity of this assumption, although it appears to hold[13] to ±2 kJ/mol for $Cl^-$ and $OH^-$.

## 2. Positive Ions

In the discussion which follows, a brief description of the Franck-Condon principle along with a discussion of the implications for an analysis of data obtained from experimental determinations of ionization energies will be given in Sec. 2.1. In Sec. 2.2., special problems in the interpretation of appearance potential data will be summarized, followed in Sec. 2.3. by short descriptions of the various experimental techniques used in obtaining the data given here, with attention to intrinsic experimental problems which may affect the reliability of data. Section 2.4. will give a discussion of the rationale used in evaluating ionization energy and appearance energy data from the various approaches, and a description of the conventions and symbols used in the tables. Finally, Sec. 2.5. summarizes a few of the regular trends observed in the data, and describes schemes for estimating data on heats of formation of positive ions.

Detailed discussions of the ionization process and of the experimental techniques used in studying ion chemistry, as well as of thermodynamics, are available in many books and reviews. Therefore, no attempt will be made to present a comprehensive discussion or review of these subjects. Rather, attention will be given only to those aspects which have a bearing on the evaluation of data on ionization energies, appearance energies, or ion/molecule equilibrium constants.

### 2.1. The Evaluation of Experimentally-Determined Ionization Energies:

#### The Franck-Condon Principle

Ionization of a molecule by photoionization or by electron impact is governed by the Franck-Condon principle, which states that the most probable ionizing transition will be that in which the positions and momenta of the nuclei are unchanged[28,29]. Thus, when the equilibrium geometries of an ion and its corresponding neutral species are closely similar, the energy dependence of the onset of ionization will be a sharp step function leading to the ion vibrational ground state. However, when the equilibrium geometry of the ion involves a significant change in one or more bond lengths/angles from that of the neutral species, the transition to the lowest vibrational level of the ion is no longer the most intense, and the maximum transition probability (the vertical ionization energy) will favor population of a higher vibrational level of the ion; if the geometry change is great, it is possible that the transition to the lowest vibrational level of the ion will not even be observed. These situations are illustrated for hypothetical diatomic species in Fig. 1.

In evaluating ionization energy data, the shapes of photoelectron bands are useful indicators as to which of the situations pictured in Fig. 1 prevails for the particular molecule. A sharp onset indicates that the equilibrium geometries of ion and neutral are quite similar, and that photoionization or electron impact determinations of the ionization threshold are likely to be free of complications. When an ionization process proceeds according to the second situation pictured in the figure, the *onset* of the photoelectron band is observed approximately at the adiabatic ionization energy; adiabatic ionization energies derived from observation of the onsets of photoelectron bands are usually in excellent agreement with adiabatic ionization energies obtained from analyses of Rydberg series or from the most reliable threshold determinations.

When the equilibrium geometry of the ion is very different from that of the corresponding neutral molecule and the lowest vibrational level is not populated in ionization by photon absorption or electron impact, it has been shown that values for the adiabatic ionization energies can be obtained by determining the equilibrium constant for charge transfer to another molecule of known ionization energy:

$$A^+ + B \rightleftharpoons B^+ + A \qquad (33)$$

The enthalpy change for this reaction, which (Sec. 2.3.5.) is obtained from the equilibrium constant determination, is just the difference between the enthalpies of ionization, $\Delta H_I$, of species A and B. As shown above (Sec. 1.6.) this difference is likely to be quite close to the difference in the adiabatic ionization energies:

$$\Delta H(33) = [\Delta H_I(B) - \Delta H_I(A)] \sim [IP_a(B) - IP_a(A)] \qquad (34)$$

In such determinations, the ions are at thermal equilibrium with their surroundings, and one measures the thermochemical properties of the ions in their equilibrium geometries.

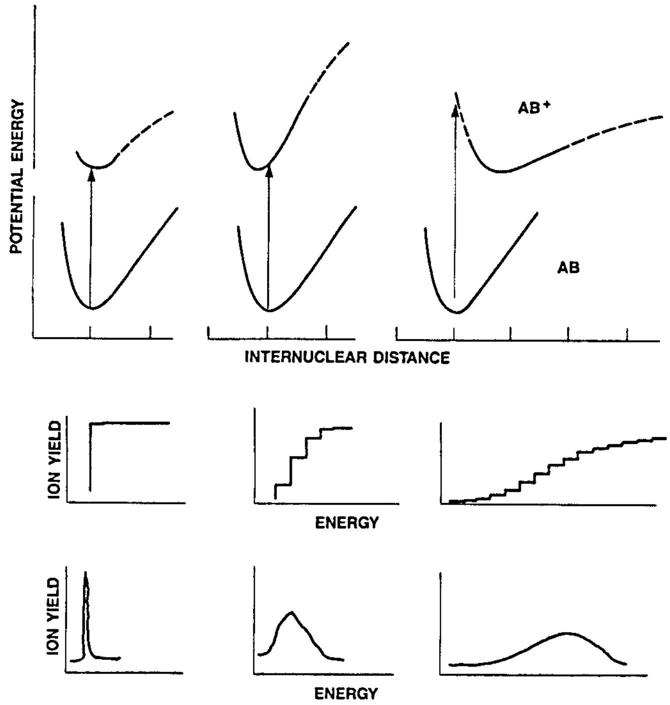


Fig. 1. Potential energy curves for hypothetical diatomic molecule AB, and the corresponding positive ion, $AB^+$ for the cases in which the equilibrium internuclear distance is (a) the same, (b) slightly different, or (c) greatly different. Below the potential energy curves are hypothetical probabilities for ionization as a function of energy for cases (a), (b), and (c), and, at bottom, shapes of observed photoelectron bands for the three corresponding cases.

## 2.2. Interpretation of Appearance Energies

In the discussion above, the appearance energy for formation of a fragment ion (reaction 4) was defined, and Eqs. (5) and (31), for obtaining values for the heat of formation of the fragment ion, were derived, with the proviso that the equations were valid only when there is no potential barrier in the reaction coordinate, and no significant "kinetic shift" associated with the determination.

The "kinetic shift"[2,30,31] is the term applied to describe the experimental observation of ionization onsets which are higher than the thermodynamic onset energy due to the fact that the apparatus samples the (fragmenting) ions at a certain time (usually around $10^{-5}$ s) after ionization has occurred, when ions undergoing a slow fragmentation process have not yet had time to dissociate. One approach for getting around this problem is an analysis based on the determination of the so-called rate-energy curve for a given fragmentation, in which the rate constant of the dissociating ion is derived as a function of energy. This kind of information is derived by analysis of the data from an elegant technique which is, moreover, capable of delivering very accurate thermochemical information for fragmentation processes, photoelectron-photoion coincidence spectroscopy (PEPICO)[32]. Another approach to detecting a barrier in the reaction coordinate is the determination of the kinetic energy carried off by the fragment ion. Studies of metastable peaks, for example, permit such an evaluation[33].

## 2.3. Experimental Techniques

The 1977 evaluated compilation included an extensive review of the experimental techniques which provide ionization energy and appearance energy data, along with a detailed description of how the data derived from each type of experiment are interpreted to give ionization energies[2,31]. Although technological advances have been made in mass spectrometric instrumentation since that review was written, the detailed presentation given there is still recommended reading for anyone interested in an in-depth description of the basic principles of the various approaches. For the present purposes, it will suffice to summarize briefly the different types of experiments from which the data presented here originate, and to give some general indications of the strengths and limitations of the different techniques, and how these influence the evaluator in arriving at a recommended value for an ionization energy.

### 2.3.1. Optical Spectroscopy

The identification of a Rydberg series in an atomic or molecular spectrum leads to a value for the ionization energy; in cases where the analysis of the spectrum is straightforward, the spectroscopic ionization energy values are highly accurate. The determination of atomic ionization energies through optical spectroscopy is a highly developed field which has been extensively reviewed. A large fraction of atomic ionization energies listed here are from expert evaluations of atomic spectra[34]. In the evaluation of ionization energies of atoms and diatomic molecules, spectroscopic ionization energies have been chosen where they are available. For polyatomic species, a value derived from an analysis of the optical spectrum has been given great weight, unless several determinations from other highly reliable techniques are in conflict with the spectroscopic value. As pointed out by Rosenstock[2,31], the evaluation of molecular Rydberg series is not always straightforward, and reported spectroscopic ionization energies of polyatomic species may disagree with values derived from ionization onset determinations or the onsets of photoelectron bands due to complications in the analysis of vibrational and rotational structure.

### 2.3.2. Beam Studies Involving Laser Photoionization

In the years since the cut-off date of the literature search for the previous volume of this series[2], several highly accurate ionization energy values have been reported based on multi-photon ionization of vibrationally-cooled species in a molecular beam[35]. In these studies, a vibrationally and rotationally cooled beam of molecules is raised to a specific excited state by irradiation with a tunable laser; while this excitation energy is held constant, a second independently tunable laser is used to ionize the beam of excited molecules, with the photon energy being tuned through the ionization onset. The excitation laser is then tuned to a different transition, and the ionization scan is repeated. In this way, the entire Franck-Condon accessible region of the intermediate electronic state is mapped out, insuring that the molecular geometry corresponding to the adiabatic ionization energy is accessed. Since every intermediate vibronic state leads to an independent value of the ionization threshold, the experiment contains an internal consistency check.

### 2.3.3. Determination of Ionization/Appearance Energies by Threshold Techniques

In the several techniques which fall under this heading, the onset of ionization or of the appearance of a particular fragment ion is detected as a function of the energy of the ionizing agent, either photons or an electron beam. The most obvious problem which must be considered with regard to this technique is the accurate characterization of the energy of the ionizing medium, photons or electrons. When ionization is brought about by photon absorption, this is usually not a problem; monochromators capable of delivering photons with a high energy resolution are available. The most sophisticated photoionization experiments involve detection of energy-selected electrons; in the so-called "threshold photoelectron spectroscopy" technique, only those photoelectrons which correspond to essentially zero energy of ejection are detected.

In the past, many experimental determinations of ionization onsets were carried out in instruments in which ionization was effected by bombarding the sample of interest with an electron beam in which the electrons had a known energy. This technique, called "electron ionization" or in the older literature, "electron impact", resulted in many determinations which were unreliable because of the energy spread of the electrons in a conventional beam. Several approaches have been utilized to overcome this problem; the most successful has been the use of a so-called "electron monochromator", in which the energy of the electron beam is narrowly defined by passing the beam through electron energy selectors of various designs[31,36,37,38,39]. Results obtained using electron beams with well-defined energies are in excellent agreement with analogous results derived from determinations of photoionization thresholds. At this writing, reliable data on ion thermochemistry are being obtained from experiments of this sort. Although studies are still being published which report ionization energy and appearance energy data from less accurate electron ionization techniques, the intent of the authors of those studies is rarely to examine the thermochemistry of the ionization process.

In the powerful threshold technique known as photoelectron-photoion coincidence (PEPICO)[32], the thermochemistry and detailed mechanism of an ionic fragmentation process can be mapped out very accurately. Ejected electrons which originated with "zero" kinetic energy are matched with their corresponding positive ions. At energies where parent ions, $M^+$, are undergoing dissociation to form one or more fragment ions, one obtains the relative probabilities for the formation of the daughter ions from parent ions of known energy (i.e. the breakdown curve). The ions can be detected at differing times after the ionization event for the determination of the time dependence of the dissociation process. The complete interpretation of such data requires a modeling of the dissociation using statistical theories of unimolecular decomposition (i.e. quasi-equilibrium/RRKM theory)[40,41]. As pointed out by Dannacher in a recent review[32], in spite of its great strengths, this technique has not been widely utilized, possibly because of the intricate instrumentation required, the complexity of the data analysis, and the fact that each determination requires the investment of a great amount of time on the part of the experimentalist.

To summarize, intrinsic problems associated with threshold determinations of ionization energies are: a) the difficulty of detecting the onset when there is a large change of molecular geometry in the ionization process, as discussed in Sec. 2.1.; and, b) the observation of ionization at energies below the adiabatic ionization energy when there is a significant population of vibrationally excited molecules in the system ("hot bands").

#### 2.3.4. Photoelectron Spectroscopy

It is also possible to determine the energy change associated with ionization process 1 by effecting ionization with a photon of well-defined energy and measuring the energy of the ejected electrons:

$$M + h\nu \rightarrow M^+ + e \qquad (35)$$

where

$$KE(e) = h\nu - I - E^*(\text{vib,rot}) \qquad (36)$$

(where $E^*$(vib,rot) is the internal energy of $M^+$ and $I$ is the binding energy of the electron).

The most widely-used technique of this type is conventional photoelectron spectroscopy[42] in which the photon sources are usually the helium resonance lines of 58.4331 nm (21.218 eV) or 30.3781 nm (40.813 eV); some work is done with neon resonance lines (73.589 nm and 74.370 nm, 16.848 and 16.671 eV) or other intense monochromatic sources. In such an experiment, the ejected electrons will have differing energies depending on the distribution of energy levels in the $M^+$ ions formed; a map of the abundances of the electron as a function of energy is called the photoelectron *spectrum*. As described in Sec. 2.1., the shapes of the photoelectron bands will reflect not only the energy differences in the different states of $M^+$ but the $M \rightarrow M^+$ transition probabilities as governed by the Franck-Condon principle. In cases where the equilibrium geometry of the ion and the corresponding neutral are the same or are similar, it is found that the observed onset of the first photoelectron band is usually a reliable indicator of the adiabatic ionization potential (see Fig. 1).

#### 2.3.5. Ion/Molecule Equilibrium Constant Determinations

This evaluation takes into account (although previous works in the series did not) all information on ion thermochemistry generated by ion/molecule equilibrium constant determinations.

An ion/molecule equilibrium:

$$A^+ + B \rightleftharpoons C^+ + D \qquad (37)$$

is established in a high pressure mass spectrometer[43], flow tube[44], or ion cyclotron resonance spectrometer[45], and the equilibrium constant is determined by observing the relative abundances of the two ions, $A^+$ and $C^+$, after a large number of collisions:

$$K_{eq} = \frac{[C^+][D]}{[A^+][B]} \qquad (38)$$

The neutral reactants, B and D, are present in great abundance compared to the ionic reactants, and therefore, the ratio [D]/[B] does not change as equilibrium is established. A single measurement leads to a value for the Gibbs energy change of reaction 37 at the temperature of the measurement, while a series of measurements at different temperatures permits an experimental evaluation of the entropy and enthalpy changes associated with the reaction:

$$-RT \ln K_{eq} = \Delta G = \Delta H - T\Delta S \qquad (39)$$

In practice, many studies have been published in which measurements were made at a single temperature, the (usually small) entropy change for the reaction was estimated from statistical mechanical considerations (usually just from consideration of changes in symmetry numbers), and the corresponding enthalpy change was derived from these two pieces of information.

Published ion/molecule equilibrium studies involving cations provide data on charge transfer (reaction 33), proton transfer (reaction 6), and hydride or halide transfer equilibria:

$$R_1^+ + R_2X \rightleftharpoons R_2^+ + R_1X \qquad (40)$$

(where X is H, F, Cl, Br, or I). Studies of hydride transfer and halide transfer equilibria have led to quantitative information about the relative heats of formation of alkyl carbocations. These data were used to supplement information from appearance potential determinations in evaluating heats of formation of alkyl carbocations.

Most ion/molecule equilibrium studies involving positive ions have been devoted to the derivation of an extensive (more than 100 kcal/mol in length) scale of relative proton affinities (see Eqs. (7) and (8)). The results were mainly derived from interlocking ladders of enthalpy changes for reaction 6. These data have recently been evaluated to establish internal consistency[4]. Most of the values for heats of formation of protonated molecules given in this evaluation are taken from that publication. When this is the case, no specific literature reference is given, it being understood that the source is the evaluated compilation[4].

As noted above (reaction 33), in determinations of charge transfer equilibrium constants, the difference in the ionization energies of two reacting molecules is obtained. A thermochemical ladder of relative ionization energies determined in this way[22] closely reproduces the equivalent scale of spectroscopic ionization energies, thus demonstrating the reliability of the approach for deriving information on relative ionization energies. The most useful application of this approach for ionization energy data has proved to be the determination of ionization energies for species which undergo a large change of geometry upon ionization (case 3 in Fig. 1), and which therefore exhibit very slow onsets of ionization as a function of energy. For example, the only reliable data on the adiabatic ionization energies of n-alkanes[46] and of alkyl hydrazines[47,48] come from thermochemical ladders established through equilibrium constant determinations.

The main uncertainty associated with this technique, aside from the necessity of relating the thermochemical ladder to a reliable comparison standard, is the temperature of the reacting system. However, the reproduction of relative spectroscopic ionization energies through equilibrium measurements[22] demonstrates that this is not a serious problem.

#### 2.3.6. Ion/Molecule Bracketing Experiments

There are some ion/molecule systems for which an equilibrium can not be established in an ion source, either because one of the relevant neutral species is unstable (e.g. a radical or unstable molecule) or because of competing reactions in the system. In such cases, it is sometimes possible to obtain an experimental estimate of the enthalpy change of a particular reaction (charge transfer, proton transfer, hydride transfer, etc.) by use of a technique known as "bracketing" in which the ion of interest is reacted with a series of molecules chosen for variations in the relevant thermochemical parameter (proton affinity, ionization energy, etc.). The occurrence, and sometimes the rate constant, of reaction is monitored as a function of the parameter of interest; the approximate onset energy is usually assumed to lie on the energy scale at a point where the rate of reaction becomes very slow. Few data in this work are derived from such measurements, but in cases where heats of formation are derived from this kind of experiment, a specific comment describes the experiment.

#### 2.3.7. Onsets of Endothermic Reactions

Several pieces of data given here have been derived from an analysis of the enthalpy changes of endothermic ion/molecule reactions. Although some such information has been obtained from straightforward kinetic treatments (Arrhenius plots) of the temperature dependences of the rate constants of endothermic ion/molecule reactions[49,50] recent quantitative studies[51,52,53] cover a much broader energy range by generating a beam of energy- and mass-selected ions which is focussed into a collision chamber containing the reactant gas; product ions are detected as a function of the energy of the ions in the beam.

#### 2.3.8. Other Techniques

Essentially all of the ionization potentials and heats of formation of positive ions included in this evaluation have been derived from results obtained using the experimental approaches listed above. Several additional techniques (Auger electron spectroscopy, Penning ionization, Born-Haber cycle calculations, and analyses of so-called charge transfer spectra) were described in the Introduction to the 1977 compilation[2,31] but are not widely used for the quantitative determination of data of interest to this compilation. Such data, when available, have been taken into account in the evaluation, except for ionization energies derived from charge transfer spectra. The latter technique is mainly used for obtaining values for ionization potentials of compounds of low vapor pressure. Since the cut-off date for inclusion of literature in the 1977 volume, numerous quantitative determinations of ionization energies for such species, mainly by photoelectron spectroscopy or by ion/molecule equilibrium constant determinations, have appeared in the literature. These have made the charge transfer spectra data obsolete for many species. Since it is generally seen that the gas phase ionization potentials derived from charge transfer spectra may be very inaccurate, all these data have been ignored in the present volume.

### 2.4. Reliability of Ionization Energy Data and Criteria for Evaluation

#### 2.4.1. Comparisons between Results of Different Techniques

The data on ionization energies summarized here are derived from the different types of measurements described above, and are consequently of widely varying quality, not only because the accuracies of the measurement techniques differ, but also because of differences in the focusses of the research in which the measurements were made. For example, many of the ionization energies reported for inorganic species were never intended by the original authors to be quantitative ionization energy measurements, but are simply qualitative indicators of whether or not a given ion observed in the vapor over a heated Knudsen cell has been formed by electron impact ionization of the corresponding neutral species (in which case it exhibits an onset at a relatively low energy) or through fragmentation of a molecular ion (which would correspond to a higher onset energy). In these experiments, error limits of 0.5 to 1 eV are commonly cited by the original authors. Similarly, most photoelectron spectroscopic studies are carried out for the purpose of examining molecular orbital energy levels; thermochemistry is not a concern, and often, although the accuracy of the measurements is very high, only vertical ionization energies, which are not necessarily related to thermochemical onsets, are reported.

Because many of the values for ionization energies given here are derived from evaluations of several different determinations carried out using different techniques, there is no specific indication in Table 1 of an experimental method associated with a particular value. In carrying out the evaluation, an attempt was made to integrate the entire corpus of information about any given ion, giving weight to various determinations depending on the nature of the ionization onset, the measurement techniques used, the attention to detail by the original authors, and so forth. Usually (but not always) a spectroscopically-determined ionization energy was considered more reliable than a contradictory value obtained by observation of an ionization threshold. A value obtained from an observed ionization onset using photoionization or an electron monochromator was considered more reliable than an onset obtained using less accurate techniques. In all of these cases, an observed onset of a photoelectron band was given great weight in carrying out the analysis, with values from any of the above three techniques being downgraded if they did not match the photoelectron onset (unless, of course, the differences could be rationalized in terms of the principles outlined above).

As mentioned above, many photoelectron spectroscopy studies do not cite values for adiabatic ionization potentials. In these cases, where the authors have provided a figure showing the photoelectron spectrum, it is usually possible to estimate from the figure the value for the adiabatic onset; where adiabatic ionization energies have been obtained in this way, a specific comment to that effect is made.

Data derived from ion/molecule equilibrium constant determinations have been utilized as an aid in evaluating information obtained from other sources. For example, where scales of relative ionization energies were available from equilibrium constant determinations, internal consistency with these scales was required in the assigned ionization energy or heat of formation values. Where this was not possible, a specific comment spells out the discrepancy. As described in Sec. 2.3.5., ionization energy values derived from equilibrium constant determinations provide the only values for ionization energies of species which undergo large changes of geometry upon ionization such as normal alkanes with six or more C–atoms[46], or hydrazines[47,48]. When an ionization energy has been obtained solely from this approach, the source of the data is indicated in a comment, and the identity of the reference compound is given.

Heats of formation of protonated molecules derived from the evaluated proton affinity scale[4] are taken from that publication. More recent data are included, with the internal consistency requirement rigorously maintained. The value for the corresponding proton affinity of the molecule is given in a comment. Note that to locate a value for a *proton affinity*, one must look under the empirical formula of the corresponding *protonated molecule*, i.e. the proton affinity of methane is located by looking under $CH_5$. When data from recent publications are given, the literature source is specifically cited.

#### 2.4.2. Reliability of Data; Error Limits

*Ionization Energies*. The experimentally-determined ionization energies collected here display widely varying uncertainties, ranging from $\pm 0.0001$ eV or smaller for some spectroscopic or multiphoton-laser determinations to $\pm 1$ eV for measurements carried out on the vapor above a heated Knudsen cell. The error limits associated with a particular ionization energy are specifically listed when the original work(s) gave an estimate of this quantity. In other cases, the error limits are indicated by the number of significant figures displayed; in these cases, it can be assumed that the error limits are five times the last significant figure displayed.

Some of the ionization energy values are shown enclosed in parentheses. Data enclosed in parentheses are considered not to be firmly established for one of three reasons:

(1) The measurement itself must be considered unreliable (as in, for example, threshold determinations in which the energy spread of the electrons was not well defined).

(2) The relevant ionization energy has been determined more than once but with poor agreement between the different results, and there is no auxiliary information available which allows a choice between the divergent values. In such cases, the evaluation gives either (a) the value determined by the most reliable technique, or (b) an average of two or more values determined by the same technique, with error limits indicating the scatter in the data. In a very few cases where the scatter in the reported values is very great or where the value obtained by the "most reliable" technique appears to be specious, no evaluated ionization energy is cited, but a note is included which lists the various determined values.

(3) Parentheses are also used to indicate data which are unevaluated. That is, when a particular molecule has been studied only once, and additional information which would permit one to judge the reliability of the data is unavailable, the ionization energy is given exactly as it appears in the original reference but is enclosed in

parentheses. Many of these untested determinations are undoubtedly reliable; the cited error limits and the number of significant figures shown in the table will give an indication of the probable reliability of the technique by which such a value was obtained.

As described above, some ionization energy values were obtained by reading onsets of photoelectron bands in figures reproduced in papers, where the original authors did not assign a numerical value to the band onset. In every such case, a specific comment is made indicating that the value has been derived from a figure. The accuracy with which such onsets can be read should be assumed to be not better than 0.1–0.2 eV, except where the authors have given an enlarged view of the band onset, in which case, an additional significant figure is cited. When a figure was not given, the lowest vertical ionization potential from the original paper is cited as the upper limit to the adiabatic ionization energy.

*Heats of Formation.* The cited heats of formation of ions necessarily reflect both the uncertainties in the ionization (or appearance) energy values and the uncertainties in the heats of formation of the relevant neutral species. Values of ionic heats of formation which are not firmly established - either because of a poorly established ionization/appearance energy or because of large uncertainties in the heat of formation of the neutral species - are shown enclosed in parentheses.

Although the values which were used for heats of formation of neutral species will be discussed separately in Sec. 4, it should be emphasized here that many of these data are based on estimates. Some of the estimation schemes for particular classes of compounds are sophisticated and well-documented, and can be considered to lead to values for heats of formation which are as reliable as most experimental data. Other estimations have been carried out by various authors with varying degrees of attention to complexities, or in some cases, with little or no documentation about how the estimate was accomplished. A large fraction of the estimates used were made specifically for this publication, and even among this fraction, there is a broad spectrum of quality depending on the size of the network of related information which was available. Rather than try to sort out and make judgments about the quality of each estimate of the heat of formation of a neutral molecule, the policy has been followed of enclosing in parentheses each ion heat of formation based on an estimated value for the heat of formation of relevant neutral molecules or radicals; this practice is not meant to disparage the quality of the estimated data, but simply to alert the reader to the fact that it is being used. As a first approximation, the user can assume that the reliability of an estimate varies inversely with the complexity of the molecule.

## 2.5. Trends in the Data

### 2.5.1. Estimation Schemes for Heats of Formation of Cations

Within the past few years, a sufficient amount of reliable information on ionization energies and heats of formation of many classes of positive ions has become available so that regular trends as a function of molecular size and structure can be discerned. These can be used to develop empirical schemes for estimating ionization energies and/or heats of formation of cations. Since ionization energies for a homologous series do not have a linear dependence on molecular size, values for heats of formation of ions can not be reproduced satisfactorily by simple additivity systems like those in widespread use for the prediction of thermochemical data for neutral molecules. The predictive schemes put forward to date utilize equations which are empirical.

One series of several papers[54,55,56,57] presents a scheme which is designed to predict values for the heat of formation of positive ions at 298 K from equations of the form:

$$\Delta_f H(M^+) = A - Bn + C/n \qquad (41)$$

where $A$, $B$, and $C$ are constants derived from the data for any particular series, and $n$ is the total number of *atoms* in the molecule. The parameters derived in the paper of Holmes, Fingas, and Lossing[54] for predicting heats of formation of the parent ions of several common classes of compounds are listed in Table 2.5.1.1.

This method works because to an excellent approximation, the ionization energies of a homologous series vary linearly as $n^{-1}$, as expressed in the term $C/n$ in Eq. (41). The other two terms, $A$ and $Bn$, reflect the additive nature of heats of formation of neutral molecules. Also, for molecules in which there is multiple substitution by characteristic groups on charge-bearing atoms or at the position of charge delocalized pi-electron systems, good straight-line relationships exist between ionic heats of formation and the logarithm of the number of atoms (i.e. ion size). Such correlations permit reasonably accurate estimates of ion enthalpies of formation[54,55,56,57].

Bachiri, Mouvier, Carlier, and DuBois[58] have advanced a scheme for the estimation of ionization energies of alkenes, alkynes, aldehydes, ketones, alcohols, ethers, mercaptans, and thioethers. Their empirical equation takes the form:

$$\log_{10} \frac{IP(R_1XR_2) - IP_\infty}{IP_0 - IP_\infty} = 0.106[I(R_1) + I(R_2)] \qquad (42)$$

where X is a functional group (i.e. $-CH{=}CH-$ or $>C{=}CH_2$ for alkenes, -O- for alcohols and ethers, $>C{=}O$ for aldehydes and ketones, etc.), $R_1$ and $R_2$ are the attached alkyl groups, $IP_0$ is the ionization potential of the reference compound for which $R_1 = R_2 = H$. $IP_\infty$ in Eq. (42) is a constant for each compound type. (A modification of this scheme which does away with the need for the parameter $IP_\infty$ has also been put forward recently[59]). Table 2.5.1.2. lists the constants for the alkyl substituent groups and the different compound types (modified slightly from the values given in the original publication to predict adiabatic rather than vertical ionization energies).

TABLE 2.5.1.1. Estimation scheme[c] of Holmes, Fingas, and Lossing[54]: $\Delta_f H(M^+)$kcal/mol $= A - Bn + C/n$

| Compound Type | A | kcal/mol[a] B | C | Correction Terms |
|---|---|---|---|---|
| Alkanes | 224 | 2.2 | 298 | For each branch: −3 |
| 1-Alkenes | 231.6 | 1.61 | 110 | For each branch on C-2: −13 |
| | | | | For each remote branch: −2.5 |
| x-Alkenes | 219.6 | 1.61 | 110 | For each branch on =C: −13 |
| | | | | For each branch elsewhere: −2.5 |
| | | | | One cis correction: +1 |
| | | | | Two cis corrections at one double bond: +3 |
| | | | | If one group is t-butyl: +4 |
| | | | | If both groups are t-butyl: +10 |
| 1-Alkynes | 278 | 1.57 | 110 | For each branch: −4 |
| 2-Alkynes | 260 | 1.58 | 110 | For each branch: −4 |
| 3-Alkynes | 257 | 1.57 | 110 | For each branch: −4 |
| 4-Alkynes | 257 | 1.57 | 110 | For each branch: −4 |
| 5-Alkynes | 256 | 1.57 | 110 | For each branch: −4 |
| Alkanols | 175 | 1.59 | 216 | For each branch adjacent to −OH: −6 |
| | | | | For each branch elsewhere: −2 |
| Aliphatic ethers | 157 | 1.41 | 368 | For each branch adjacent to −O−: −6 |
| | | | | For each branch elsewhere: −3 |
| | | | | [b]Asymmetry correction per carbon: +1 |
| Aliphatic | 188 | 1.65 | 135 | For each branch adjacent to C=O: −5 |
| | | | | For each branch elsewhere: −3 |
| Aliphatic ketones | 166 | 1.78 | 252 | For each branch adjacent to C=OD: −3.5 |
| | | | | [b]Asymmetry correction per carbon: +1.5 |
| Alkanoic acids | 142 | 1.90 | 112 | For each branch adjacent to C=O: −3.5 |
| | | | | For each branch elsewhere: −1.5 |
| Chloroalkanes | 236 | 1.98 | 57 | For each branch adjacent to halogen: −5 |
| | | | | For each branch elsewhere: −3 |
| Bromoalkanes | 219 | 1.40 | 115 | For each branch adjacent to halogen: −5 |
| | | | | For each branch elsewhere: −3 |
| Iodoalkanes | 222 | 1.69 | 44 | For each branch adjacent to halogen: −5 |

[a]Constants are given here in the units used in the original paper[54].
[b]Asymmetry correction for ethers and ketones having different numbers of C-atoms on either side of the functional group is based on the smallest numbers of C-atoms which must be transferred to give the most symmetrical species, e.g. for methyl pentyl ketone, +3 kcal/mol.
[c]$n$ is the total number of atoms in the molecule.

A comparison of ionization energy values[58] or heats of formation of cations[54] predicted from expressions 41 or 42 with the corresponding evaluated experimental values is given in Table 2.5.1.3. For both predictive schemes, the agreement between estimated values and experiment is generally quite good — good enough to inspire confidence in the use of the equations for filling in blanks in the data series.

As pointed out in one of the papers advancing these empirical estimation schemes[54] the equations are "not only useful for predicting new $\Delta_f H$ values, but also for revealing misfits which could indicate incorrect values for $\Delta_f H°$(Neutral) or the ionization energy, or, more interestingly, an ion structure having special stabilizing or destabilizing properties." In fact, the trends described by these equations were routinely examined in evaluating the data for just these reasons.

#### 2.5.2. Correlations of Ionization Energies with Proton Affinities or Substituent Constants

The proton affinity of molecule M, defined by Eq. 7, is equal to the M–H$^+$ bond energy of the MH$^+$ ion. The M$^+$–H bond energy is called the *hydrogen affinity* (*HA*) of M$^+$:

$$M^+ + H \xrightarrow{-HA} MH^+ \qquad (43)$$

Consider the thermodynamic cycle, constructed from reactions 7 and 43:

$$\begin{array}{ccccc} M & + & H^+ & \xrightarrow{-PA} & MH^+ \\ \downarrow IP(M) & & \downarrow -IP(H) & & \downarrow \\ M^+ & + & H & \xrightarrow{-HA} & MH^+ \end{array} \qquad (44)$$

From cycle 44 we write:

$$\begin{aligned} PA(M) &= HA(M^+) + IP(H) - IP(M) \\ &= HA(M^+) + 13.6\,\text{eV} - IP(M) \end{aligned} \qquad (45)$$

If the hydrogen affinity were a constant for a given compound type, the proton affinity values would vary linearly with the ionization potentials for a homologous

TABLE 2.5 1.2 Estimation scheme of Bachiri, Mouvier, Carlier, and DuBois[58]:

$$\log_{10} \frac{IP(R_1XR_2) - IP_\infty}{IP_0 - IP_\infty} = 0.106[I(R_1) + I(R_2)]$$

| X | | $IP_0$(eV) | $IP_\infty$(eV) |
|---|---|---|---|
| -C≡C- | (Alkynes) | 11.400 | 6.577 |
| -HC=CH- | (Alkenes) | 10.507 | 6.849 |
| >C=$CH_2$ | (Alkenes, gem) | 10.737 | 6.814 |
| -(C=O)-H | (Aldehydes except $CH_2O$) | 12.063 | 3.575 |
| >C=O | (Ketones) | 13.334 | 3.936 |
| -OH | (Alcohols) | 12.607 | (3.7) |
| -O- | (Ethers) | 12.612 | 5.483 |
| -S- | ($H_2S$, Thiols, Thioethers) | 10.473 | 5.725 |

| R | I |
|---|---|
| H | 0 (Convention) |
| Methyl | 1 (Convention) |
| Ethyl | 1.166 |
| n-Propyl | 1.271 |
| i-Propyl | 1.291 |
| n-Butyl | 1.330 |
| s-Butyl | 1.400 |
| i-Butyl | 1.358 |
| t-Butyl | 1.394 |
| n-Pentyl | 1.340 |
| i-Pentyl | 1.389 |
| neo-Pentyl | 1.369 |
| t-Pentyl | 1.479 |
| s-Pentyl [-CH($C_2H_5$)$_2$] | 1.462 |
| n-Hexyl | 1.355 |
| t-Hexyl [-C($CH_3$)$_2$(n-$C_3H_7$)] | 1.524 |
| t-Hexyl [-C($CH_3$)$_2$(i-$C_3H_7$)] | 1.570 |
| neo-Hexyl [-$CH_2CH_2C(CH_3)_3$] | 1.360 |

TABLE 2.5 1 3. Comparison of ionization energies/heats of formation with estimated values predicted from estimation schemes[a]

| Compound | IP (eV) | $\Delta_fH$/(Ion) (kJ/mol) | Holmes et al.[54] IP (eV) | Holmes et al.[54] $\Delta_fH$(Ion) (kJ/mol) | Bachiri et al.[58] IP (eV) | Bachiri et al.[58] $\Delta_fH$(Ion) (kJ/mol) |
|---|---|---|---|---|---|---|
| **Alkynes** | | | | | | |
| $CH_3C≡CH$ | 10.36 | 1186 | [10.34] | 1184 | 10.36 | [1184] |
| $C_2H_5C≡CH$ | 10.178 | 1147 | [10.13] | 1142 | 10.21 | [1151] |
| n-$C_3H_7C≡CH$ | 10.05 | 1113 | [10.04] | 1113 | 10.11 | [1121] |
| n-$C_4H_9C≡CH$ | (9.95) | (1079) | [10.02] | 1088 | 10.06 | [1092] |
| n-$C_5H_{11}C≡CH$ | (10.04) | (1071) | [ 9.93] | 1063 | 10.06 | [1075] |
| n-$C_6H_{13}C≡CH$ | (9.95) | (1038) | [ 9.93] | 1038 | 10.04 | [1046] |
| i-$C_3H_7C≡CH$ | 9.97 | 1096 | [ 9.95] | 1096 | 10.10 | [1109] |
| i-$C_3H_7C≡CCH_3$ | 9.31 | 996 | [ 9.32] | 996 | 9.33 | [ 996] |
| t-$C_4H_9C≡CH$ | (9.80) | (1050) | [ 9.80] | 1050 | 10.01 | [1071] |
| $CH_3C≡CCH_3$ | 9.562 | 1068 | [ 9.55] | 1067 | 9.54 | [1067] |
| $C_2H_5C≡CCH_3$ | 9.44 | 1038 | [ 9.43] | 1038 | 9.42 | [1038] |
| n-$C_3H_7C≡CCH_3$ | 9.366 | 1013 | [ 9.37] | 1013 | 9.35 | [1013] |
| n-$C_4H_9C≡CCH_3$ | (9.33) | (983) | [ 9.37] | 987 | 9.31 | [ 983] |
| n-$C_5H_{11}C≡CCH_3$ | 9.31 | 962 | [ 9.32] | 962 | 9.30 | [ 958] |
| n-$C_6H_{11}C≡CCH_3$ | (9.30) | (941) | [ 9.28] | 941 | 9.29 | [ 941] |
| $C_2H_5C≡CC_2H_5$ | 9.323 | 1004 | [ 9.28] | 1000 | 9.31 | [1004] |
| n-$C_3H_7C≡C_2H_5$ | (9.26) | 975) | [ 9.24] | 975 | 9.24 | [ 975] |
| n-$C_4H_9C≡CC_2H_5$ | 9.22 | 954 | [ 9.19] | 950 | 9.20 | [ 950] |
| n-$C_5H_{11}C≡CC_2H_5$ | 9.20 | 929 | [ 9.19] | 929 | 9.19 | [ 929] |
| n-$C_6H_{13}C≡CC_2H_5$ | 9.19 | 908 | [ 9.19] | 908 | 9.18 | [ 908] |

TABLE 2.5.1.3. Comparison of ionization energies/heats of formation with estimated values[a] — Continued

| Compound | $IP$ (eV) | $\Delta_f H$/(Ion) (kJ/mol) | Holmes *et al.*[54] $IP$ (eV) | Holmes *et al.*[54] $\Delta_f H$(Ion) (kJ/mol) | Bachiri *et al.*[58] $IP$ (eV) | Bachiri *et al.*[58] $\Delta_f H$(Ion) (kJ/mol) |
|---|---|---|---|---|---|---|
| **Alkenes** | | | | | | |
| $CH_3CH=CH_2$ | 9.73 | 958 | [ 9.73] | 958 | 9.71 | [958] |
| $C_2H_5CH=CH_2$ | 9.58 | 925 | [ 9.59] | 925 | 9.60 | [925] |
| n-$C_3H_7CH=CH_2$ | 9.52 | 895 | [ 9.54] | 900 | 9.53 | [895] |
| n-$C_4H_9CH=CH_2$ | 9.44 | 870 | [ 9.48] | 874 | 9.49 | [874] |
| n-$C_5H_{11}CH=CH_2$ | 9.44 | 849 | [ 9.45] | 849 | 9.49 | [853] |
| n-$C_6H_{13}CH=CH_2$ | 9.43 | 828 | [ 9.41] | 828 | 9.48 | [833] |
| i-$C_3H_7CH=CH_2$ | 8.96 | 812 | [ 8.94] | 812 | 8.92 | [808] |
| t-$C_4H_9CH=CH_2$ | 9.45 | 849 | [ 9.43] | 853 | 9.45 | [853] |
| $(C_2H_5)_2C=CH_2$ | 9.06 | 820 | [ 9.06] | 820 | 9.03 | [816] |
| E-$CH_3CH=CHCH_3$ | 9.100 | 866 | [ 9.12] | 866 | 9.09 | [866] |
| E-$C_2H_5CH=CHCH_3$ | 9.036 | 840 | [ 9.05] | 841 | 9.00 | [837] |
| E-n-$C_3H_7CH=CHCH_3$ | (8.97) | (812) | [ 8.99] | 816 | 8.95 | [812] |
| i-$C_3H_7CH=CHCH_3$ | 8.97 | 803 | [ 8.96] | 803 | 8.94 | [803] |
| E/Z-n-$C_4H_9CH=CHCH_3$ | (8.84) | (782) | [ 8.92] | 791 | 8.92 | [791] |
| E-n-$C_5H_{11}CH=CHCH_3$ | 8.85 | 757 | [ 8.97] | 766 | 8.91 | [761] |
| $C_2H_5CH=CHC_2H_5$ | 8.96 | 812 | [ 8.94] | 812 | 8.92 | [808] |
| $(CH_3)_2C=C(CH_3)_2$ | 8.27 | 728 | [ 8.04] | 707 | 8.23 | [724] |
| **Alcohols** | | | | | | |
| $CH_3OH$ | 10.85 | 845 | [10.82] | 845 | 10.68 | [828] |
| $C_2H_5OH$ | 10.47 | 774 | [10.45] | 774 | 10.40 | [770] |
| n-$C_3H_7OH$ | 10.22 | 732 | [10.20] | 728 | 10.23 | [732] |
| n-$C_4H_9OH$ | 10.06 | 695 | [10.03] | 695 | 10.14 | [703] |
| n-$C_5H_{11}OH$ | 10.00 | 669 | [ 9.96] | 661 | 10.12 | [678] |
| n-$C_6H_{13}OH$ | (9.89) | (640) | [ 9.86] | 636 | 10.10 | [661] |
| i-$C_3H_7OH$ | 10.12 | 703 | [10.10] | 703 | 10.20 | [711] |
| s-$C_4H_9OH$ | 9.88 | 661 | [ 9.96] | 669 | 10.03 | [674] |
| i-$C_4H_9OH$ | 10.09 | 690 | [10.03] | 686 | 10.09 | [690] |
| t-$C_4H_9OH$ | 9.97 | 648 | [9.90] | 644 | 10.09 | [661] |
| **Ethers** | | | | | | |
| $CH_3OCH_3$ | 10.025 | 782 | [ 9.94] | 774 | 9.86 | [766] |
| $C_2H_5OCH_3$ | 9.72 | 720 | [ 9.77] | 715 | 9.69 | [717] |
| n-$C_3H_7OCH_3$ | — | — | 9.58 | | | |
| i-$C_3H_7OCH_3$ | (9.42) | 657 | [ 9.41] | 657 | 9.56 | [669] |
| n-$C_4H_9OCH_3$ | (9.54) | (661) | [ 9.32] | 640 | 9.52 | [661] |
| n-$C_3H_7OC_2H_5$ | (9.45) | (640) | [ 9.46] | 640 | 9.42 | [636] |
| $C_2H_5OC_2H_5$ | 9.51 | 665 | [ 9.56] | 669 | 9.52 | [665] |
| n-$C_4H_9OC_2H_5$ | 9.36 | 611 | [ 9.36] | 611 | 9.36 | [611] |
| t-$C_4H_9OCH_3$ | 9.41 | 619 | [ 9.26] | 602 | 9.46 | [623] |
| **Aldehydes** | | | | | | |
| $CH_3CHO$ | 10.229 | 821 | [10.21] | 820 | 10.23 | [820] |
| $C_2H_5CHO$ | 9.953 | 773 | [ 9.97] | 774 | 9.96 | [774] |
| n-$C_3H_7CHO$ | 9.84 | 741 | [ 9.82] | 741 | 9.80 | [736] |
| n-$C_4H_9CHO$ | 9.74 | 711 | [ 9.76] | 711 | 9.71 | [707] |
| n-$C_5H_{11}CHO$ | 9.67 | 686 | [ 9.66] | 685 | 9.69 | [688] |
| i-$C_3H_7CHO$ | 9.705 | 721 | [ 9.69] | 719 | 9.77 | [727] |
| i-$C_4H_9CHO$ | 9.70 | 699 | [ 9.71] | 700 | 9.67 | [695] |
| s-$C_4H_9CHO$ | (9.59) | (690) | [ 9.58] | 690 | 9.61 | [692] |
| t-$C_4H_9CHO$ | 9.50 | 674 | [ 9.45] | 669 | 9.62 | [686] |
| neo-$C_5H_{11}CHO$ | (9.61) | (661) | [ 9.61] | 661 | 9.65 | [665] |
| **Ketones** | | | | | | |
| $CH_3COCH_3$ | 9.705 | 719 | [ 9.77] | 724 | 9.704 | [761] |
| $C_2H_5COCH_3$ | 9.51 | 678 | [ 9.53] | 680 | 9.48 | [675] |
| n-$C_3H_7COCH_3$ | 9.38 | 644 | [ 9.40] | 646 | 9.33 | [639] |
| n-$C_4H_9COCH_3$ | 9.35 | 628 | [ 9.26] | 619 | 9.26 | [619] |
| $C_2H_5COC_2H_5$ | 9.31 | 640 | [ 9.32] | 642 | 9.26 | [636] |

TABLE 2.5.1.3. Comparison of ionization energies/heats of formation with estimated values[a] — Continued

| Compound | IP (eV) | $\Delta_f H$/(Ion) (kJ/mol) | Holmes et al.[54] IP (eV) | Holmes et al.[54] $\Delta_f H$(Ion) (kJ/mol) | Bachiri et al.[58] IP (eV) | Bachiri et al.[58] $\Delta_f H$(Ion) (kJ/mol) |
|---|---|---|---|---|---|---|
| Ketones - Continued | | | | | | |
| n-$C_3H_7COC_2H_5$ | 9.12 | 598 | [ 9.25] | 611 | 9.12 | [598] |
| n-$C_4H_9COC_2H_5$ | (9.02) | (573) | [ 9.14] | 586 | 9.05 | [577] |
| i-$C_3H_7COCH_3$ | 9.30 | 636 | [ 9.21] | 628 | 9.31 | [636] |
| i-$C_3H_7COC_2H_5$ | (9.10) | (594) | [ 9.15] | 598 | 9.10 | [590] |
| $(i-C_3H_7)_2CO$ | 8 95 | 552 | [ 8.92] | 548 | 8.94 | [552] |
| s-$C_4H_9COCH_3$ | 9.21 | 598 | [ 9.24] | 602 | 9.17 | [594] |
| i-$C_4H_9COCH_3$ | 9.30 | 607 | [ 9.43] | 619 | 9.22 | [602] |
| t-$C_4H_9COCH_3$ | 9.11 | 590 | [ 9.14] | 590 | 9.17 | [594] |
| neo-$C_5H_{11}COCH_3$ | (9.23) | (573) | [ 9.29] | 577 | 9.21 | [569] |

[a]In these lists, values obtained through the use of the estimation scheme of Holmes et al[58] are *heats of formation* of ions at 298 K. The scheme of Bachiri et al[58] predicts *ionization energies*. For purposes of comparison, both quantities are given here, the conversion being made using standard heats of formation of corresponding neutral molecules from Table 1. The derived quantity is enclosed in brackets. Parentheses indicate a quantity which is not well established (see conventions for Table 1).

series, the slope of the plot would be $-1$ and the intercept would be $[HA(M^+) + 13.6\ \text{eV}]$.

It has been observed[45a,60,61] that the value which can be assigned to the $M^+$–H bond strength (i.e. the $HA$) is indeed often approximately constant for a homologous series, at least over a limited range. For instance, it was reported[62] that linear plots of $PA$ versus $IP$ for primary, secondary, and tertiary amines display the same slope, but have different intercepts (i.e. different values of $HA$). However, a detailed statistical analysis[63] of the relationships between proton affinities and ionization potentials for many different compound types (alcohols, ethers, primary-, secondary- and tertiary-amines, nitriles, mercaptans, sulfides, aldehydes, ketones, carboxylic acids, esters, amides, and atoms) demonstrated that only the parent radical cations of sulfides and mercaptans displayed a characteristic (constant) value of the hydrogen affinity. For other compound types, it was concluded that the hydrogen affinity itself varies linearly with the ionization energy:

$$HA(M^+) = c + \Delta IP(M) \qquad (46)$$

Several series of compounds for which reliable evaluated ionization energy and proton affinity data are both available are summarized in Table 2.5.2.1. along with values for the hydrogen affinities. The published analysis utilized vertical ionization energies corresponding to the orbital of the site of protonation, and a proton affinity scale which, although internally consistent, was constricted in length (due to the incorrect assumption in early equilibrium studies using ICR that the operating temperature was 300 K rather than 320 K) and related to an absolute standard whose proton affinity value has now been revised downward by 3 kcal/mol. Repeating that statistical analysis, but using instead the thermochemically more meaningful adiabatic ionization energies which relate to the $M^+$–H bond strengths, and the evaluated scale of proton affinities[4], it is seen that Eq. (46) does hold for alcohols, aldehydes, ketones, primary amines, cyclic ethers and esters. In the series of aliphatic ethers, thioethers, and secondary and tertiary amines, values of the hydrogen affinity appear to decrease slightly with decreasing ionization energy, but the differences are too small to be meaningful (i.e. the slope of a plot of Eq. (46) is $-0.7$ or greater), and the assumption that the hydrogen affinity is constant will be approximately valid. The hydrogen affinities of mercaptans and of aromatic amines are indeed constant. Substituting Eq. (46) into Eq. (45), we derive an expression which permits the estimation of an unknown proton affinity/ionization energy when one of these two parameters is known:

$$PA_1—PA_2 = (d—1)(IP_1—IP_2) = K(IP_1—IP_2) \qquad (47)$$

where $K = (d—1)$ is the slope of a plot of $PA$ versus $IP$ for a compound series:

$$PA_x = C + KIP_x \qquad (48)$$

Values for $C$ and $K$ derived from the statistical analysis of the data are given in Table 2.5.2.1. for those compound types for which sufficient information was available to make a meaningful analysis.

Attention has also been given to relating ionization energies and proton affinities of various series of compounds to the appropriate Taft substituent constants[64,65,66,67]. It has been shown that the adiabatic ionization energies of compounds RX (where R is an alkyl group) correlate linearly with $\sigma^*(R)$ and $\sigma_I(R)$ (measures of the polarizability and electron-releasing and donating ability of R) for constant electron-withdrawing group X. This is easily understood in terms of a lowering of the energy required to remove an electron with increasing electron-donating ability of the groups, R.

TABLE 2.5.2.1 The relationship between proton affinity, ionization energy, and hydrogen affinity for homologous series

$$PA(\mathrm{M}) = C + K{\cdot}IP(\mathrm{M})$$
$$HA(\mathrm{M}^+) = c + d{\cdot}IP(\mathrm{M})$$
$$(C - c = 1312\ \mathrm{kJ/mol},\ d - K = 1.00)$$

| | kJ/mol | | |
|---|---|---|---|
| | *IP* | *PA* | *HA* |
| **Alcohols:** $K = -0.54$, $C = 1335$ kJ/mol | | | |
| $CH_3OH$ | 1047 | 761 | 494 |
| $C_2H_5OH$ | 1010 | 788 | 485 |
| n-$C_3H_7OH$ | 986 | 798 | 472 |
| n-$C_4H_9OH$ | 971 | 800 | 456 |
| i-$C_4H_9OH$ | 974 | 805 | 464 |
| i-$C_3H_7OH$ | 976 | 800 | 464 |
| s-$C_4H_9OH$ | 953 | 799 | 439 |
| t-$C_4H_9OH$ | 958 | 810 | 460 |
| **Acyclic Ethers:** ($K = -0.77$, $C = 1548$ kJ/mol) | | | |
| $CH_3OCH_3$ | 967 | 804 | 460 |
| $C_2H_5OCH_3$ | 938 | 822 | 448 |
| $C_2H_5OC_2H_5$ | 918 | 838 | 444 |
| (n-$C_3H_7)_2O$ | 895 | 846 | 427 |
| (n-$C_4H_9)_2O$ | 910 | 852 | 448 |
| (s-$C_4H_9)_2O$ | 879 | 874 | 439 |
| t-$C_4H_9OCH_3$ | <908 | 846 | <444 |
| **Cyclic Ethers:** ($K = -0.40$, $C = 1192$ kJ/mol) | | | |
| c-$C_2H_4O$ | 1020 | 786 | 494 |
| c-$C_3H_6O$ | 933 | 824 | 448 |
| c-$C_4H_8O$ | 908 | 832 | 427 |
| c-$C_5H_{10}O$ | 892 | 836 | 414 |
| **Aldehydes:** ($K = -0.50$, $C = 1276$ kJ/mol) | | | |
| $CH_3CHO$ | 987 | 781 | 456 |
| $C_2H_5CHO$ | 960 | 793 | 444 |
| n-$C_3H_7CHO$ | 949 | 801 | 439 |
| i-$C_3H_7CHO$ | 936 | 806 | 431 |
| i-$C_4H_9CHO$ | 936 | 806 | 431 |
| **Ketones:** ($K = -0.39$, $C = 1188$ kJ/mol) | | | |
| $CH_3COCH_3$ | 936 | 823 | 448 |
| $C_2H_5COCH_3$ | 917 | 836 | 444 |
| $C_2H_5COC_2H_5$ | 898 | 843 | 427 |
| i-$C_3H_7COCH_3$ | 897 | 851 | 435 |
| (i-$C_3H_7)_2CO$ | 864 | 857 | 410 |
| t-$C_4H_9COCH_3$ | 879 | 846 | 414 |
| (t-$C_4H_9)_2CO$ | 836 | 864 | 389 |
| **Primary Amines:** ($K = -0.59$, $C = 1406$ kJ/mol) | | | |
| $CH_3NH_2$ | 866 | 896 | 448 |
| $C_2H_5NH_2$ | 855 | 908 | 452 |
| n-$C_3H_7NH_2$ | 847 | 912 | 448 |
| i-$C_3H_7NH_2$ | 841 | 915 | 444 |
| n-$C_4H_9NH_2$ | 841 | 914 | 444 |
| s-$C_4H_9NH_2$ | 839 | 923 | 448 |
| i-$C_4H_9NH_2$ | 839 | 915 | 444 |
| t-$C_4H_9NH_2$ | 833 | 924 | 444 |
| n-$C_5H_{11}NH_2$ | 836 | 916 | 439 |

TABLE 2 5 2 1 The relationship between proton affinity, ionization energy, and hydrogen affinity for homologous series—Continued

$$PA(M) = C + C \cdot IP(M)$$
$$HA(M^+) = c + d \cdot IP(M)$$
$$(C - c = 1312 \text{ kJ/mol}, d - K = 1.00)$$

| | kJ/mol | | |
|---|---|---|---|
| | *IP* | *PA* | *HA* |
| **Secondary Amines:** ($K = -0.72$, $C = 1502$ kJ/mol, $HA = 397$ kJ/mol) | | | |
| $(CH_3)_2NH$ | 794 | 923 | 406 |
| $(CH_3)(C_2H_5)NH$ | 786 | 932 | 406 |
| $(C_2H_5)_2NH$ | 773 | 945 | 406 |
| $(n\text{-}C_3H_7)_2NH$ | 756 | 952 | 397 |
| $(i\text{-}C_3H_7)_2NH$ | 746 | 963 | 397 |
| $(n\text{-}C_4H_9)_2NH$ | 742 | 956 | 385 |
| $(s\text{-}C_4H_9)_2NH$ | 736 | 966 | 389 |
| $(i\text{-}C_4H_9)_2NH$ | 754 | 956 | 397 |
| **Tertiary Amines:** ($K = -0.83$, $C = 1573$ kJ/mol, $HA = 385$ kJ/mol) | | | |
| $(CH_3)_3N$ | 754 | 942 | 385 |
| $(CH_3)_2(C_2H_5)N$ | 747 | 952 | 385 |
| $(CH_3)(C_2H_5)_2N$ | 723 | 962 | 372 |
| $(C_2H_5)_3N$ | 723 | 972 | 385 |
| $(n\text{-}C_3H_7)_3N$ | 715 | 979 | 381 |
| **Aromatic Amines:** ($K = -1.0$, $C = 1636$ kJ/mol, $HA = 305$ kJ/mol) | | | |
| $C_6H_5NH_2$ | 741 | 877 | 305 |
| $C_6H_5N(CH_3)_2$ | 687 | 935 | 310 |
| $3\text{-}(CH_3)C_6H_4N(CH_3)_2$ | 677 | 939 | 305 |
| $4\text{-}(CH_3)C_6H_4N(CH_3)_2$ | 669 | 944 | 301 |
| $3,5\text{-}(CH_3)_2C_6H_3N(CH_3)_2$ | 671 | 950 | 301 |
| $C_6H_5N(C_2H_5)_2$ | 674 | 952 | 314 |
| **Mercaptans:** ($K = -0.98$, $C = 1678$ kJ/mol, $HA = 381$ kJ/mol) | | | |
| $CH_3SH$ | 911 | 784 | 381 |
| $C_2H_5SH$ | 896 | 798 | 381 |
| $n\text{-}C_3H_7SH$ | 887 | 802 | 377 |
| $i\text{-}C_3H_7SH$ | 882 | 812 | 381 |
| $t\text{-}C_4H_9SH$ | 871 | 824 | 381 |
| **Thioethers:** ($K = -0.83$, $C = 1531$ kJ/mol, $HA = 360$ kJ/mol) | | | |
| $CH_3SCH_3$ | 838 | 839 | 364 |
| $C_2H_5SCH_3$ | 824 | 851 | 364 |
| $(C_2H_5)_2S$ | 813 | 858 | 360 |
| $(n\text{-}C_3H_7)_2S$ | 801 | 864 | 351 |
| $(i\text{-}C_3H_7)_2S$ | 796 | 877 | 360 |
| $(n\text{-}C_4H_9)_2S$ | 793 | 873 | 356 |
| $(t\text{-}C_4H_9)_2S$ | 779 | 890 | 356 |
| **Nitriles:** | | | |
| $CH_3CN$ | 1177 | 788 | 653 |
| $C_2H_5CN$ | 1142 | 806 | 636 |
| $n\text{-}C_3H_7CN$ | 1129 | 810 | 628 |
| $i\text{-}C_3H_7CN$ | 1133 | 813 | 632 |
| **Esters:** ($K = -0.58$, $C = 1401$ kJ/mol) | | | |
| $HCOOCH_3$ | 1043 | 790 | 523 |
| $HCOOC_2H_5$ | 1024 | 808 | 519 |
| $HCOO(n\text{-}C_3H_7)$ | 1015 | 813 | 515 |
| $HCOO(i\text{-}C_3H_7)$ | 1008 | 820 | 515 |
| $HCOO(n\text{-}C_4H_9)$ | 1013 | 815 | 515 |
| $CH_3COOCH_3$ | 991 | 828 | 506 |
| $CH_3COOC_2H_5$ | 966 | 840 | 494 |
| $CH_3COO(n\text{-}C_3H_7)$ | 969 | 839 | 494 |

TABLE 2.5.2.1. The relationship between proton affinity, ionization energy, and hydrogen affinity for homologous series—Continued

$$PA(\mathrm{M}) = C + K \cdot IP(\mathrm{M})$$
$$HA(\mathrm{M}^+) = c + d \cdot IP(\mathrm{M})$$
$$(C - c = 1312\ \mathrm{kJ/mol},\ d - K = 1.00)$$

| | kJ/mol | | |
|---|---|---|---|
| | *IP* | *PA* | *HA* |
| **Esters:** ($K = -0.58$, $C = 1401$ kJ/mol) | | | |
| $C_2H_5COOCH_3$ | 979 | 838 | 506 |
| n-$C_3H_7COOCH_3$ | 971 | 837 | 498 |
| i-$C_3H_7COOCH_3$ | 951 | 843 | 481 |
| t-$C_4H_9COOCH_3$ | 955 | 849 | 490 |
| **Acids:** | | | |
| $CH_3COOH$ | 1028 | 796 | 510 |
| $C_2H_5COOH$ | 1015 | 802 | 506 |

# 3. Negative Ions

The previous publication of evaluated heats of formation of ions, "Energetics of Gaseous Ions"[2], contains ionization/appearance potential data for over 4000 species leading to evaluated heats of formation for more than 600 positive ions. By contrast, that volume contains thermochemical data for only 117 anions, including only 12 organic (C, H containing) anions. These statistics reflect the relative importance of studies on cation versus anion thermochemistry at the time of the cut-off for the literature search for that volume, 1971.

The large discrepancy in the numbers of early studies on anions as compared to cations is easy to rationalize. Most neutral species display a much lower cross section for production of anions than for cation production, with the necessary consequence that conventional electron impact mass spectrometry is much more adaptable to studies of positive ions. Similarly, the presence of excess energy in a cation can cause fragmentation, with the identities of the fragment cations providing useful structural information. In contrast, loss of an electron from a bound anion to form the corresponding neutral species is often energetically preferred to a dissociation process producing a fragment anion. Thus, the "cation bias" of much of gaseous ion thermochemistry until the last decade is understandable.

The renaissance in gas phase anion chemistry and thermochemistry came about with the development of chemical ionization mass spectrometry as a commonly-used technique. Anions are often more useful than cations for analytical work in that they can originate with less internal energy. In a proton transfer reaction leading to an anion product, the new bond which is formed—with its share of the excess energy of reaction—is in the departing neutral species (reaction 11) while in the analogous reaction involving cations (reaction 6), the new bond is in the ion. Likewise, thermal electron attachment to those species which form stable radical anions is considerably faster than particle transfer, so that the chemical ionization step can be much more sensitive.

## 3.1. Aims

The compilation of anion thermochemistry in this work has slightly different aims than the companion cation compilation, in that the latter presents only the "best" available values for the ionization energy/heat of formation of a given structure. A complete archive of the literature having to do with cations has not been given, because the previous compilations[1,2,3,4] have summarized the literature exhaustively. Although there have been a number of compilations concerned with the thermochemistry of anions in the last few years[11,68-75] these have not presented data which are critically evaluated, i.e., the best values are not assigned, save for atomic ions[70]. The advances in the last decade in ion/molecule chemistry and in such techniques as photoelectron and photodetachment spectrometry have resulted in a tremendous increase in the number of chemical structures for which some anionic thermochemistry is known. This publication therefore includes a collection of the literature data which is as complete as possible, and an assignment of the "best" value for the thermochemistry where sufficient information is available.

The thermochemical parameters of critical interest in this compilation are the heat of formation of the anion and the electron affinity of the radical or neutral molecule corresponding to the anion. In order to properly evaluate these, however, data on the energetics of chemical processes involving the anions (Brønsted basicity of the anion, parameters for solvation by neutral species, etc.) are also included. The extensive thermochemical ladders of relative acidities, electron affinities, solvation thermochemistry, and similar data derived from chemical equilibria have provided a powerful tool for evaluating the thermochemistry of anions: chemical intuition. The use of structure-reactivity relationships allows the examination of the structure of an acid and a prediction about what its acidity, and therefore anion heat of formation, should be. The extra thermodynamic techniques such as linear free energy and enthalpy relationships often allow prediction of expected values accurate to better than a kJ/mol. Although results derived from such relationships can not always be trusted in cases of unusual structures, they nevertheless provide a reasonable rationale for assigning "best" values in many cases.

A problem that has become increasingly important recently is the question of the thermochemistry of the allied neutral species. As indicated below in the section on thermochemical relationships, the limiting factor in deriving anion thermochemical data is often the reliability of the data on the related thermochemistry of the neutral species (heats of formation, bond strengths). The information generated by the field of ion chemistry has outpaced the availability of neutral thermochemical data in recent years. In many cases, the best values for certain bond strengths are derived from data on the thermochemical properties of ions, rather than the other way around.

## 3.2. Experimental Techniques

Detailed descriptions of the various techniques used to obtain anion thermochemical data will not be presented here, since these are well documented in the literature by their practitioners. Brief descriptions of each technique follow, with comments about accuracy and limitations. The phrase in square brackets following the name is the acronym used in the database to refer to the method.

#### 3.2.1. Laser Photoelectron Spectroscopy [LPES]

A fixed frequency laser (commonly 2.54 eV photons) is used to irradiate a beam of anions, and the energies of the detached electrons are analyzed[70]. The method often provides information on the vibrational states of the neutral and ionic species as well. However, the assignment of the (0–0) threshold can be complicated by these states. The precision is commonly better than 0.2 kJ/mol, and can be much better.

#### 3.2.2. Laser Photodetachment [LPD]

In this technique, which may be considered the converse of photoelectron spectroscopy, the laser wavelength is varied to determine the threshold for detachment of a (presumably) thermal electron[71] from an anion. This experiment has usually been carried out in an ICR ion trap, with the decrease in the ICR signal of the ion as the detected quantity; the lower power of variable wavelength lasers often requires a longer irradiation period than with the ion beam in photoelectron spectroscopy. Precision is ca. 1-4 kJ/mol. The detection of the true threshold is often complicated by a gradual onset, although the general theory of the onset has been worked out[68,69]. This method actually yields the vertical detachment energy, which is equated with the electron affinity. This assumption is usually valid, but fails for molecules for which the geometries of the anion and neutral are considerably different (i.e., for which there is poor Franck-Condon overlap). A notable case is $CF_3^-$, where the photodetachment value is larger than the adiabatic value by 0.8 eV[77].

A recent determination of the spectrum of the hydroxide anion is at a resolution of ca. 2 J/mol[70] while coaxial LPD for $O^-$ furnishes a resolution of 0.006 $cm^{-1}$, or 0.07 J/mol[76]!

#### 3.2.3. Photodetachment [PD]

Early photodetachment experiments were carried out using an arc lamp and a monochromator to irradiate the ICR cell[71]. Precision was lower than with the laser experiment.

#### 3.2.4. Photodissociation [PDis]

Irradiation of anions does not always yield electron detachment as the first threshold process since bond cleavage may also be an allowed process. The wavelength threshold for such a process can provide information on the heat of formation of the anion, if the heats of formation of the products are known.

#### 3.2.5. Ion/Molecule Equilibrium Constant Determinations [IMRE,Kine,TDEq,TDAs]

As discussed in Sec. 2.3.5., this evaluation takes into account (although previous works in the series did not) all information on ion thermochemistry generated by ion/molecule equilibrium constant determinations. In the case of anions, ion/molecule equilibrium studies on electron transfer reactions:

$$A^- + B \rightleftharpoons B^- + A \tag{49}$$

lead to scales of relative electron affinities.

$$K_{eq} = \frac{[B^-][A]}{[A^-][B]} \tag{50}$$

while equilibrium constants for hydride or halide transfer reactions:

$$A + BY^- \rightleftharpoons B + AY^- \tag{51}$$

(where Y is H, F, Cl, Br, or I) lead to thermochemical ladders of relative acidities or halide affinities. Other scales of anionic thermochemistry are derived from equilibrium constants for solvation equilibria:

$$Y^- + X \rightleftharpoons [X{\cdot\cdot}Y^-] \tag{52}$$

Further, if the forward and reverse rate constants for a reaction are known, then the equilibrium constant, and thus $\Delta G$, can be calculated from kinetic data [Kine].

The bulk of the available data on anion thermochemistry in the past decade has been derived from ion/molecule equilibrium constant determinations and photoelectron/photodetachment spectroscopy. Extensive scales, spanning an energy range of nearly 400 kJ/mol, have been determined for proton transfer (leading to relative Brønsted acidities of molecules), electron transfer, and halide transfer reactions.

In general, the free energy changes associated with such equilibria are measured to a precision of ca. 0.5 kJ/mol. The absolute uncertainty of anion heats of formation derived from such results is usually on the order of 5–10 kJ/mol, and depends on the accuracy of the method of "anchoring" the resulting scales of relative thermochemical values.

There remain at present several points of uncertainty regarding these data. There is an active debate[78] about the actual temperature of the ions in an ICR cell. Although some early results indicated that effective ion temperatures could be as much as several hundred degrees above ambient[78], the accuracy of the kinetic rate constant "thermometer" used as the basis of that judgement was not established. Comparisons of equilibrium constant data obtained in ICR cells with data derived from other sources indicate that the effective ion temperatures in ICR cells are not more than 10 degrees higher than measured gas temperatures in the cells[22,78].

The measured equilibrium constant data lead directly to values of free energies, which require some knowledge of the entropy changes of the processes under consideration in order to derive the desired enthalpy changes. Entropy changes have been obtained either through statistical mechanical calculations[79,80], or by measuring equilibrium constants as a function of temperature [TDEq = temperature dependent equilibrium constant], leading through a van't Hoff treatment of the results to experimental values for the entropy and enthalpy changes. Finally, the dynamic range (i.e. ion trapping time) of all the mass spectrometric techniques now in use for ion/molecule equilibrium constant determinations is such that the maximum free energy change which can be determined for particle transfer reactions is no greater than ca. 30–40 kJ/mol at most, and often only 10 kJ/mol at room temperature. The dynamic range for determinations of thermochemical parameters of association reactions is much greater [TDAs = temperature dependent association].

There have been questions raised regarding the accuracy of this method, since alcohol bond strengths derived in this way were consistently 9 kJ/mol smaller than accepted values. It was originally thought that this discrepancy was due to the temperature problem alluded to above[78], because the acidity scale measured in the ICR spectrometer[80] was compressed relative to that determined by pulsed high pressure mass spectrometry[79]. If the equilibria established in the reaction cell of the ICR spectrometer were actually at a higher temperature than the value which was used to convert $K_{eq}$ to $\Delta(\Delta_{acid}G)$, then the calculated free energy scale from ICR experiments would be compressed. However, the gas phase basicity scales measured by ICR and by high pressure mass spectrometric methods agree quite well[4]. In addition, Taft[81] has recently redetermined many of the relative acidities that make up the thermochemical ladder, and finds that the region of the acidity scale from trifluoroethanol to acetone has a larger range than the original work indicated. These results have been confirmed in the laboratory of one of the present authors[82]. The region of the acidity scale from trifluoroethanol up to methanol has therefore been adjusted to include these new data. The data affected by this revision are still referred to by the original literature reference, e.g. 79BAR/SCO, and the original values are still displayed, but the method is denoted IMRE°. The revised values are *preferred* in the evaluation.

#### 3.2.6. Ion/Molecule Reaction Bracketing [IMRB]

For most of the techniques currently used for studying thermal ion/molecule reaction equilibria and kinetics, ions can only be examined for, at most, several thousand collisions with the reactive neutral gas. Thus, any reaction more endothermic than a few kcal/mol can not be observed on the time scale of the presently used techniques. In the observation of a series of reactions for which the functional groups present at the reactive site of the molecule are always the same, and the energy of the reaction is being varied by changing some distant substituent, then if the rate constant falls to less than the observable rate over some small energy range, it is a fair assumption that the reaction pathway has become endothermic at that point. From this, an estimate of the thermoneutral (equilibrium) point may be made. This technique must be applied with caution, because the mechanism of the observed reaction may not be the same for the entire series of molecules, so that apparent variations in reactivity may not actually reflect the thermochemistry of the assumed reaction.

#### 3.2.7. Electron Impact Appearance Potentials [EIAP]

Since a bound anion must be thermochemically more stable than the combined energies of the free electron plus the neutral species, simple attachment of electrons, even thermal ones, in general results in rapid autodetachment. In certain cases, however, the excited anion state can fragment to yield either an anion plus a neutral species (dissociative attachment), or an anion plus a cation (ion pair production). The latter process has not been well studied save for relatively small species, and is not at present a source of much thermochemical data. On the other hand, a considerable amount of thermochemical data has been derived from experiments in which the onset energy for dissociative attachment is measured. A complication in the interpretation of such onsets involves the unknown internal energy of both the anionic and neutral fragments. A particularly useful case is where two onsets are observed, with the fragments differing only in the identity of the species associated with the electron:

$$AB + e \rightarrow A^- + B\cdot \quad (53)$$

$$\rightarrow A\cdot + B^- \quad (54)$$

If the electron affinity of one of the product species is known, that of the other can be inferred from the known electron affinity and the difference in the onset energies for the two channels.

Most workers have not used monoenergetic electron beams, so the precision in the energy onsets is generally larger than 0.1 eV (10 kJ/mol). The resulting anion heats of formation include that uncertainty plus the uncertainties in the heats of formation of the associated reactant and neutral species. A few retarding potential difference measurements have been carried out, to improve the accuracy of such results.

#### 3.2.8. Neutral Beam Ionization/Appearance Potentials [NBIP/NBAP]

Collision of a neutral species with an energetic particle of low ionization potential, such as an alkali atom, can result in electron transfer, giving an alkali cation and an anion[83]. The electron affinity of the neutral species is equal to the translational energy of the alkali atom less its ionization potential. Determinations of electron affinities by this method have the advantage that one obtains values for the true electron affinity: electron attachment to a neutral species, rather than detachment from an anion. Certain anions can be produced by this technique which are not accessible via electron impact due to low energy exit channels, e.g. $CCl_4^-$. Due to the limited energy resolution of the neutral alkali beam, the precision of this technique is not high, typically 20 kJ/mol. The onset energies of fragment ions can also provide useful thermochemical information, if the thermochemistry of the co-produced neutral species is known.

Normally this technique results in a determination of the adiabatic electron affinity, but for a sufficiently fast beam of neutral species, the onset corresponds to the vertical attachment energy of the electron, which, in contrast to detachment methods, is smaller than the adiabatic value.

#### 3.2.9. Photoionization [PI]

This technique involves production of cation-anion pairs by vacuum ultraviolet photons. It has been used primarily for small molecules ($O_2$, $F_2$, etc.). The difference in onset for dissociative ion pair production and dissociative ionization

$$AB + h\nu \rightarrow A^- + B^+ \quad (55)$$

$$AB + h\nu \rightarrow A\cdot + B^+ + e \quad (56)$$

corresponds to the electron affinity of A.

#### 3.2.10. Endothermic Reaction Energy, Including Charge Transfer [Endo,EnCT,CIDT]

If an ion/molecule reaction is appreciably endothermic at thermal (room temperature) energies, it is not observable by present techniques. For some processes it is possible to increase the rate by increasing the translational energy of the reactants so that products can be observed. Assuming that all the translational energy is available to bring about the reaction through the intermediacy of a long-lived complex in which energy is statistically distributed, the onset energy for observation of a given reaction can be taken as the threshold for the process, and thermochemistry assigned accordingly. Here the acronym "Endo" describes the use of such onset energies for deriving thermochemical data, "EnCT" the use of such onsets in charge transfer processes.

A variant is the case of collision of a *non-reactive* species, which serves only to provide the energy necessary for the negative ion to fragment or detach the electron. This is termed the "Collision Induced Dissociation Threshold" method [CIDT].

#### 3.2.11. Surface Ionization (Magnetron) [SI]

The production of ions on a surface can yield thermochemical data if a number of parameters are known, including the work function of the surface. A common version of this experiment, the Magnetron technique[84] [Surface Ionization, SI], lacks mass analysis, and therefore many of the values for thermochemical parameters resulting from this method correspond to anions of uncertain identity. Precision is thought to be several tenths of a volt (>20 kJ/mol).

#### 3.2.12. Electron Swarm [ES]

In this technique[85], the electron affinity of a neutral species (usually a closed shell molecule) is calculated by a statistical method, using the rate of electron attachment, the autodetachment lifetime, and the vibrational frequencies of the species. The attachment rate is measured in a drift tube — electron swarm experiment, and extrapolated to thermal energy. The autodetachment lifetime is taken from results of beam experiments. The precision is probably a few tenths of an eV (30-40 kJ/mol) at best.

#### 3.2.13. Lattice energy [Latt]

The heat of formation of an anion can be derived from a Born-Haber cycle using the lattice energy and heat of formation of a crystal and the thermochemistry of the appropriate gas phase cation. This method is not especially accurate relative to more recent techniques, but for some singly charged inorganic anions it provides the only data available.

#### 3.2.14. Kinetic Branching Methods [Bran, CIDC]

If certain ion/molecule complexes are subjected to collision induced dissociation (CID), the weakest bond between the two species in the complex is the most likely one to break. If the functional groups forming the bond are identical, with the acids differing only in distant substitution, then either species has a chance to acquire the proton on breakup of the complex. The branching ratio in the reaction:

$$ROH\cdot\cdot{}^-OR' \xrightarrow{M} ROH + R'O^- \quad (57a)$$

$$\xrightarrow{M} RO^- + R'OH \quad (57b)$$

has been shown to reflect the relative acidities of the two species[87]. Once the sensitivity of this branching ratio for compounds of known acidity has been established, then CID of clusters with one compound of known acidity and one unknown can lead to an estimate for the acidity of the unknown species. This appears to be reliable to 1–2 kJ/mol in determining relative acidities. This approach has some limitations. First, values for the gas phase acidities for several members of the series must first be known from other sources for proper calibration. Further, the temperature of the reacting system is not defined, and so problems may arise in interpretation for systems with significant entropy changes. The general method has also been applied to the estimation of relative electron affinities[87] for complexes of aromatic radical anions with aromatic molecules.

The excited intermediate complex can be prepared other ways than by collision. If an ion/molecule reaction is sufficiently exothermic, and has more than one available reaction channel, then the branching ratio of products formed on breakup of the complex can reflect product stabilities. This assumption has been used to estimate the acidities of the simple alkanes[88] since many of the localized carbanions from those compounds do not appear to be bound with respect to electron loss. Such ions exist only in ion/molecule complexes, where the cluster energy may serve to prevent electron detachment before reaction.

#### 3.2.15. Electron Transmission Spectroscopy [ETS]

In this technique, the scattering angles of a monoenergetic electron beam impacting on a gas at less than the ionization threshold are determined. The presence of resonances in the spectrum implies electron capture to produce a temporary state, followed by autodetachment. This is the principal technique for measurement of negative electron affinities. Occasionally, a series of resonances can be extrapolated to below zero electron energy to give an estimate of a positive electron affinity[11].

#### 3.2.16. Electron Capture Detector [ECD]

An electron capture detector for a gas chromatograph, when operated in a variable temperature pulse sampling mode, can provide data on electron capture/detachment ratios. These can be converted into electron affinities. Use of the method is limited to the determination of electron affinities in the 0.2-0.8 eV (20–80 kJ/mol) range. The precision of such measurements is commonly quoted as less than 1 kJ/mol[89].

#### 3.2.17. Mobility of Ions in a Gas [Mobl]

If the mobility of an ion in a gas can be measured in response to a weak electric field, the potential well depth, corresponding to $\Delta_{aff}H$, for the ion associating with the neutral gas can be determined.

#### 3.2.18. Laser Optogalvanic Photodetachment Spectroscopy [LOG]

The gas of interest is subjected to an electrical discharge, and the discharge region is probed by a laser. The LOG[90] spectrum is recorded by scanning the wavelength of the laser, and monitoring laser-induced changes in the discharge impedance. The spectrum produced will be similar to the laser absorption spectrum but relative intensities of spectral features may be very different. The method is particularly suitable for detecting unstable (radical) species.

### 3.3. Thermochemical Cycles

The relationships between the different quantities measured in the above experimental techniques can be exploited to derive additional thermochemical information. In Table 2, such derivations have been made wherever possible. In the table, the quantities which have been *derived* from the experimentally-determined value are indicated by superscripted letters, which correspond to the various types of derivation described here, while the quantity actually determined in the reported experiment is given without any superscripted letter. A list of the various approaches to derivation and their corresponding superscript letters is given in the Table in Sec. 5.2.

The *heat of formation of an anion* can be derived from the heat of formation of the acid, its gas phase acidity, the heat of formation of the proton:

$$\Delta_f H(A^-) = \Delta_{acid}H(AH) - \Delta_f H(H^+) + \Delta_f H^\circ(AH) \quad (58)$$

The quantity $\Delta_f H^\circ(AH)$ is lacking in many cases where acidities are now available; various group additivity estimation schemes (see below, and Sec. 4.) have been employed to fill in this information.

As discussed in Sec. 1.6.3., the calculation of the anion heat of formation as the heat of formation of the neutral species less the electron affinity:

$$\Delta_f H(A^-) = \Delta_f H^\circ(A) - EA(A) \quad (59)$$

is not, strictly speaking, correct, since for most of the species given here the heat of formation of the neutral species is a 298 K value, while the electron affinity is a threshold 0 K value. The preference is for anion heats of formation calculated by Eq. 58.

In an inversion of the bond strength/electron affinity Eq. 32 for calculating acidities, a known acidity and bond strength can yield an *electron affinity*.

$$EA(A) = BDE(A\text{–}H) + IP(H\cdot) - \Delta_{acid}H(AH) \quad (60)$$

Based on the temperature cancellation effect, this should correspond to the 0 K value. This is also an adiabatic value, which can be less than the vertical electron affinity obtained from the optical techniques if the geometries of the neutral and anion differ appreciably.

The difference between the anion and neutral heats of formation (at 298 K) give a 298 K electron affinity:

$$EA(A) = \Delta_f H^\circ(A) - \Delta_f H(A^-) \quad (61)$$

If the geometry change is small, this should be a reasonable approximation to the 0 K value.

*Gas phase acidities*, taken as the enthalpy of acidity, can be calculated from the homolytic bond strength of the acidity site, the electron affinity of the resulting radical, and the ionization energy of the hydrogen atom:

$$\Delta_{acid}H(AH) = BDE(A\text{–}H) - EA(A) + IP(H) \quad (62)$$

The last is common to all acids, and is very accurately known (1311.98 kJ/mol), and does not present a limitation in determining the values. A more valid concern is the temperature of definition for these terms. The acidity and bond strength are commonly taken as 298 K values, while the electron affinity and ionization potential are threshold values defined at 0 K. The cancellation necessary for this equation to be considered valid is discussed in Sec. 1.6.3.

Sometimes a heat of formation of an anion or an electron affinity value may be known without a value for the bond strength being available. The *acidity of the conjugate acid* can be derived in those cases from the acid heat of formation:

$$\Delta_{acid}H(AH) = \Delta_f H(A^-) + \Delta_f H(H^+) - \Delta_f H^\circ(AH) \quad (63)$$

While the primary goal of this work is not to obtain values for *homolytic bond strengths*, such values can be derived from gas phase acidities and electron affinities in cases where they are not known from more conventional sources.

$$BDE(A\text{–}H) = \Delta_{acid}H(AH) + EA(A) - IP(H\cdot) \quad (64)$$

$$BDE(A\text{–}H) = \Delta_f H^\circ(AH) - \Delta_f H^\circ(A) - \Delta_f H^\circ(H) \quad (65)$$

### 3.4. Priority of Data

At the present time, the heat of formation of an anion in the gas phase is not directly measurable, since gas phase plasma calorimetry is not a known technique. Likewise, direct measurement of an electron affinity, in the sense of exothermic electron attachment to a neutral, is not feasible in a calorimetric sense, although the combination of attachment and detachment rate constants can be used. The electron affinity and anionic heat of formation are available from either thermochemical cycles, based on other known and measurable quantities, or by reasonable assumptions about the reversibility of processes such as electron detachment from anions.

For electron affinities, we adopt the following order of priority for the evaluation of "best" values. There are exceptions in many cases to this order, where a given method is known not to be suitable. The user should be aware of the difference between adiabatic and vertical values that these techniques yield.

Laser photoelectron spectroscopy
Laser photodetachment
Photodetachment
From bond strengths and gas phase acidities
Neutral beam ionization/appearance potentials
Electron impact appearance potentials
Ion/molecule bracketing reactions
Electron swarm

For gas phase acidities, the following priorities are assigned to data sources:

Direct gas phase equilibrium constant determinations
Kinetic methods for gas phase acidities:branching ratios in collisional dissociation and ion/molecule complex breakup.
From bond strengths and electron affinities
Ion/molecule bracketing reactions (using either the heat of formation of the anion or of the acid as the unknown quantity).

## 4. Thermochemistry of Neutral Species

Tables 1 and 2 display values for heats of formation of the neutral gas phase molecules which are "related" to the archived ions. In Table 1, which is concerned with cation thermochemistry, the "related" neutral species is either (a) the neutral molecule which corresponds to the ion plus an electron (for ionization potential data) or (b) the molecule which has one less proton than the ion of interest (for proton affinity data). In Table 2, concerned with anion thermochemistry, the term "related" means that the neutral is formed from the ion either by loss of an electron (electron affinity) or gaining of a proton (gas phase acidity). For every case, the identity of the neutral molecule corresponding to the displayed heat of formation is made unambiguous.

### 4.1. Literature Sources

Values for the heats of formation of neutral molecules were taken from the experimental literature whenever possible. If a value for a particular compound was available from an evaluated data compilation, this value was generally selected for inclusion here. The primary compilations which were used were as follows.

#### 4.1.1. Organic Compounds

J. B. Pedley and J. Rylance, "Sussex-N. P. L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds," University of Sussex (1977). The numerous data from this evaluated compilation[91] of 298 K heats of formation of gas phase organic compounds are identified by the squib 77PED/RYL. A second edition of this work (86PED/NAY) has appeared[92], but regrettably, was available to the authors of the current compilation too late to obviate an extensive literature search for heats of formation from the primary literature to cover the period 1976-mid-1986. Since the updated compilation of Pedley, Naylor and Kirby[92] (which is complete only through 1982) became available only as this work was nearing completion, references to 77PED/RYL or to recent primary literature have been retained even in cases where the data are given in 86PED/NAY.

#### 4.1.2. Inorganic Compounds

(1) D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, "The NBS Tables of Chemical Thermodynamic Properties: Selected Values for Inorganic and $C_1$ and $C_2$ Organic Substances in SI Units," J. Phys. Chem. Ref. Data, Vol. 11, Suppl. 2 (1982), hereafter referred to as 82TN270, from the original publication of this compilation[14] as a series of NBS Technical Notes called the 270-series. (It should be noted that when this source is used in Table 2, both the value and an associated error limit are given, while only the former is given in Table 1.)

(2) (a) D. R. Stull and H. Prophet, "JANAF Thermochemical Tables," NSRDS-NBS 37 (1971); (b) M. W. Chase, J. C. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, "JANAF Thermochemical Tables," 1975 Supplement, J. Phys. Chem. Ref. Data 2, 1 (1975); (c) M. W. Chase, Jr., J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela, J. Phys. Chem. Ref. Data, 11, 695 (1982). Information from these sources[13] is referenced as 71JANAF, 75JANAF, or 82JANAF. An updated composite edition[13c] of this compilation was in press at the time this work was being prepared, but was not actually available until these tables were near completion. A few values for heats of formation from the updated version have been inserted here where warranted by changes in recommended values, but an exhaustive check of the new publication was not made.

(3) L. V. Gurvich, I. V. Veits, V. A. Medvedev, G. A. Khachkuruzov, V. S. Yungman, G. A. Bergman, et al, "Termodinamicheskie Svoistva Individual'nykh Veshchestv" (Thermodynamic Properties of Individual Substances); V. P. Glushko, Gen. Ed., Vols. 1 through 4 (in 8 parts), (1978–1982), Izdatel'stvo "Nauka" Moscow. These volumes[15] are collectively cited as 82TPIS.

#### 4.1.3. Specialized Classes of Compounds and Radicals

In addition, various literature compilations which cover well-defined, but restricted, classes of compounds such as nitriles, organometallic compounds, free radicals, or strained hydrocarbons were utilized. The preferential use of data compilations as sources of experimental data recognizes that these data have been evaluated for internal consistency insofar as possible.

Many values for heats of formation of free radicals were taken from the review of McMillen and Golden[93]. With respect to the alkyl radicals, however, a recent re-evaluation of data from the literature has led to the suggestion that C–H bond energies in alkanes should be revised upwards[94]. The heats of formation of these radicals are still a matter of controversy at this writing. Values cited in the tables are based on the following revised[94] C–H bond strengths: Primary C–H bond (101 kcal/mol, 422 kJ/mol); Secondary C–H bond (99 kcal/mol, 415 kJ/mol); Tertiary C–H bond (95 kcal/mol, 398 kJ/mol).

The corresponding values for the heats of formation of the alkyl radicals are in some cases (e.g. t-butyl radical) entirely consistent with the differences between well-established heats of formation of the corresponding alkyl cations and experimental ionization energy values, but there are also cases for which the relevant values show inconsistencies. These are pointed out in Table 1 by a specific comment.

#### 4.1.4. Other Literature Sources

Experimental information about heats of formation of species not included in evaluated compilations was generally obtained from primary literature sources. When more than one value for a heat of formation was available from such unevaluated primary sources, and no supplementary information was available which would allow an educated choice, the most recent value was usually arbitrarily chosen in the possibly naive expectation that "improved instrumentation" as well as a greater (historical) awareness of the problems inherent in an analysis of the thermochemistry of the particular species would lead to a more reliable value.

Care was taken in utilizing these data from unrelated literature sources to be aware of ambiguities in thermochemical reference states. Values for heats of formation derived from heats of reaction (e.g. hydrolysis, bromination) were used in preference to directly-determined heats of combustion because of the inherent problems associated with numbers derived from relatively small differences between two large numbers. In many cases, heats of formation of neutral species were derived using well-established ionization energies or proton affinity values in combination with well-established heats of formation of relevant ions; these values are identified by an explanatory sentence in the comment field.

### 4.2. Conventions Used and Assumptions Made

Implicitly, in assigning gas phase heats of formation to the neutral species, the compounds are assumed to be ideal gases at S. T. P. Whenever sufficient information is readily available, values for heats of formation at both 0 and 298 K are given. In some cases, the 0 K value has been obtained by combining the 298 K values from a preferred literature source (i.e., an evaluated compilation) with the 298—0 K difference taken from another reference. In other cases, this difference was calculated from experimental or estimated extrathermodynamic quantities such as vibrational frequencies and the appropriate elemental thermochemical functions. Another approach was to use isoelectronic or isostructural analogies (e.g., data for $O_3$ may be compared with that on $NO_2^-$ and neutral $NO_2$).

### 4.3. Use of Condensed Phase Heats of Formation

Numerous methods exist for measuring and interpreting experimental heats of sublimation and heats of vaporization. Where available, such measurements were used to translate condensed phase data into gas phase values for heats of formation. In such cases, the cited reference is the source of the condensed phase heat of formation data, although the bibliography includes the references from which the information about heats of sublimation or vaporization were obtained.

In most cases, data on heats of sublimation (and the associated methodologies for translating condensed phase heats of formation to gas phase values at 298 K) are from the recent publication[95], 87CHI, for organic compounds.

Regrettably, while work on this publication was in progress no such single literature source for heats of vaporization was available, although such a compilation has since appeared[96]. In fact, however, experimental data on heats of vaporization do not exist for numerous species of interest here, either because of experimental difficulties associated with such determinations (i.e. lack of adequate volatility, purity, or thermal stability) or perhaps because of a lack interest in, or availability of, the compound.

Estimation methods for heats of vaporization and sublimation have been described in the literature[95,97]. Some require auxiliary experimental data (e.g. critical constants). Other such estimation methods can be applied only to well-defined classes of compounds. For heats of vaporization, these estimates are usually reliable to approximately 4 kJ/mol (1 kcal/mol). In presenting data on heats of formation incorporating the use of such estimated heats of vaporization, a choice had to be made of whether to cite the source of the experimental heat of formation of the liquid or the paper from which the method for estimating the heat of vaporization was obtained; the experimental work is given as the primary citation. For heats of sublimation, no generally accurate estimation approaches exist. Thermochemical values obtained using estimated heats of sublimation are clearly labelled as estimates in the tables.

### 4.4. Estimated Heats of Formation

Estimates were also made for heats of formation of neutral molecules and radicals for which no experimental data were available. Several estimation approaches were utilized and are now briefly described. The relationships between the various estimation approaches have been described in a recent review[98].

#### 4.4.1. Estimates from Data on Isomeric Species

One approach utilizes experimental information about isoenergetic processes for the formation of two or more isomeric species in a particular reaction. That is, given a pair of isomers for which information about the heat of formation is available for only one of the pair, an estimate of the thermochemistry of the second compound can be based on the casual and generally rather reliable assumption that if two isomers are formed in comparable yield in a particular process then their Gibbs energies and enthalpies of formation are generally comparable. Likewise, though less reliable, one may assert if one isomer is formed in higher yield, then this is the more stable product. Estimates made in this way often include the assumption that heats of vaporization and of solution are also comparable for the relevant pair of isomers; this will be a valid approximation except when there are great differences in the extent of hydrogen bonding (such as might exist for isomeric alcohols and ethers), and even in these cases, approximate corrections (such as assuming constant H-bond strengths) can be made.

In estimating thermochemical data from known information about an isomeric species, a common assumption made is that $\Delta(\Delta_f H) = \Delta(\Delta_f G)$ for the pair of isomers (i.e. $\Delta(\Delta_f S)$ is negligible). A related approach examines experimentally-determined reaction rates and/or kinetic activation energies. The thermochemical estimate is based on the assumption that the structural effects on rates and equilibria will vary in a parallel manner, and that thermodynamic and kinetic control of arbitrary reactions result in the same products. While not in fact absolutely true, experience has shown this to be a useful assumption for predicting substituent effects for numerous homologous series.

Another approach to estimating heats of formation is based on the assumption that $\Delta(\Delta_f H)$ can be equated with $\Delta E_{tot}$ for two isomers, where $\Delta E_{tot}$ is the difference in total energies of the two species calculated by quantum mechanics. For this assumption, as well as all other estimation approaches in this study employing results from quantum mechanics, ab initio calculations were given preference over results from any of the plethora of semi-empirical methods in the literature. (The reader should note that heats of formation from MNDO and from molecular mechanical calculations were occasionally used, however). Care was explicitly taken to contrast only species studied with the same basis set and degree of geometry optimization. Implicit, however, are the requirements that both the zero-point energy and 0 K - 298 K corrections are essentially identical for a pair of isomers. These last assumptions are surprisingly valid where sufficient experimental data are available to test them.

All values for heats of formation based on these approaches are labelled as estimates (EST) in the Tables.

#### 4.4.2. Summing of Increments

There remain three related approaches which were employed to estimate heats of formation of molecules here. The best characterized is Benson's "group increment" approach[99] in which the molecule of interest is defined as a collection of groups, and a "group" is then defined as a polyvalent atom (ligancy $>$ 2) with all of its associated ligands in the molecule. The heat of formation of the molecule is obtained by summing the contributions of the heats of formation of the various groups, correcting for various higher order interactions and "correction" terms. These corrections include the presence of gauche configurations in substituted alkanes, gem-substitution of large and/or polar groups, and the presence of rings that are strained because of heteroatoms and/or are not six-membered. These group energies and the various corrections have been obtained using both statistical analysis and by chemical intuition, and for "reasonable" molecules generally give reasonable results. Estimates using this approach are better defined, though not necessarily of better quality, than the others.

Because this approach is now very common in the chemical literature, many of the papers included here which are primarily concerned with aspects of ion chemistry (e.g. ionization energy, gas phase basicity or acidity determinations) include estimates of heats of formation of relevant neutral species based on this approach; rather than cite the work of the authors who made the (rather standard) estimate, these values, when they were used, have been labelled as estimates. In Table 2 estimates utilizing this approach are labelled "Est", but are accompanied by error bars.

A related approach takes advantage of regularities in trends in heats of formation of different homologous series of compounds. As an example of how this approach works, if it is observed that the heats of formation of several RXR compounds differ from those of RYR compounds by some approximately constant increment, then this difference is defined as a "correction term" for deriving heats of formation of any -Y- compound from the heat of formation of the corresponding -X- compound (or vice versa)[100]. The unknown heat of formation is taken to the be the sum of the known heat of formation and the suitable correction term associated with the exchange of the substituent and parent components. One may also derive correction terms from suitable bond energies, e.g., assume that the O-H bond energy in all carboxylic acids is the same. This approach is more commonly used in anion chemistry and is designated as Est2 in Table 2 (but as EST without a special designator in Table 1).

The final estimation approach used here is commonly called "macroincrementation"[101,102], and, as the name implies, involves building up the molecule of interest by adding increments (as in the Benson approach), but with the difference that the incremental heats of formation are specifically derived from thermochemical data for molecules or large ("macro") molecular fragments which incorporate factors which need to be considered, such as resonance, strain energy, steric effects, etc. This approach assumes that "if for each of two sets of molecules the total number of bonds, atoms and structural types is the same, then the total heat of formation of each set of molecules is the same. Then, if all but one of the heats of formation are available, the remaining one can be estimated by simple arithmetic." Macroincrementation maximizes the direct use of chemical intuition with regard to electronic and/or steric effects, as well as the direct use of available experimental data. The majority of estimates for organic compounds in Table 1 were made using this approach.

The heats of formation of only a few inorganic or organometallic compounds were estimated. Where estimates were made, it generally was assumed that the heat of ligand exchange was negligible, i.e. the heats of reaction of the following generic reactions for suitably similar ligands ($L_1$ and $L_2$) could be taken to be zero:

$$M\text{-}L_1 + L_2 \rightleftharpoons M\text{-}L_2 + L_1 \tag{66}$$

$$L_1\text{-}M\text{-}L_1 + L_2\text{-}M\text{-}L_2 \rightleftharpoons 2(L_1\text{-}M\text{-}L_2) \tag{67}$$

Likewise, simple additive assumptions were made as to heats of vaporization and sublimation and the 0 K - 298 K energy differences.

## 5. Summary of Conventions Used in Tables

In an attempt to present as much information as possible in Tables 1 and 2, while keeping the pages uncluttered, it was sometimes necessary to resort to the use of bold face, italic typefaces, asterisks, etc. to convey additional information. The various conventions are summarized below. The user is particularly cautioned that these conventions are different for Table 1 and Table 2. In particular, italicized numbers have different meanings in Table 1 (zero Kelvin heats of formation) and Table 2 (a hydride or halide affinity, and information relating to thermochemistry of neutral species).

### 5.1. Positive Ion Table (Table 1)

*Value underscored*: A well-established value of an ionization energy or ion heat of formation.

*Value enclosed in parentheses*: A value of an ionization energy or heat of formation which is not well established, or not evaluated, for one of the following reasons: (1) Only one determination of the ionization energy has been reported, and there are no auxiliary data which would permit one to judge its accuracy; (2) The heat of formation of relevant neutral species is/are not well established; (3) Two or more contradictory values for the ionization energy or appearance energy have been reported, and while one value has been selected, there is sufficient doubt that one can not regard the selected value as well-established. (For data falling under category (3), an explanatory comment is always included.)

*Value given in italics*: Thermochemical data corresponding to a temperature of absolute zero.

*Literature citations*: In Table 1, there is no column giving references to the source of ionization energy/appearance energy data. Such data are always taken from the earlier compilations[1,2,3,4] unless specifically noted in a comment. When data are from the 1981–1986 primary literature, the reference is always specifically mentioned in the comment, and is specifically given in the bibliography. Heats of formation derived from proton affinity data (and the proton affinity data themselves) are taken from the evaluated compilation[4] or from more recent literature, which will always be specifically cited in the comment and listed in the bibliography.

*Sort scheme*: Data are sorted by empirical formula ordered according to the so-called Hill scheme, which is the same sort scheme used by Chemical Abstracts. Formulas are written as $C_nH_mX_xY_y$... , where the primary sort is ordered by n, the number of carbon atoms, and the first sub-sort is ordered according to m, the number of H atoms. All other atoms in the molecule (X, Y, etc) are ordered alphabetically, and the various sub-subsorts follow accordingly. Any molecules which do not contain carbon appear according to a strictly alphabetical sort.

*Proton affinity data*: To locate the proton affinity of a molecule, look under the empirical formula of the protonated molecule, i.e. the proton affinity of $CH_4$ appears under $CH_5$.

*Estimated heats of formation of neutral molecules*: The literature citation column contains the acronym EST for estimated values.

### 5.2 Negative Ion Table (Table 2)

*Chemical species*: Each entry is headed by an empirical formula of the relevant anion, with the atoms ordered according to the Hill formulation. Below this there appears a structural representation of the anion where this can be conveniently represented on one line; the last-listed atom is usually the atom judged to carry the negative charge (insofar as this can be ascertained). These formulas may contain simplifying abbreviations in common use by organic chemists, for example "Me" for $CH_3$, "Et" for $C_2H_5$, "Pr" for $C_3H_7$, "COT" for cyclooctatetraene, or "Ph" for phenyl. For chemical species which have structures which are too complex to be represented by a semi-structural formulation, a name is given. The names chosen for inclusion are easily recognizable by most chemists, or at least can be readily located in standard texts.

*Units*: In Table 2, all data are presented in kJ/mol, except the values for electron affinities, which (as specifically indicated) are given in electron volts.

*Presentation of Data*: Each line presents data from a different reference, which is cited at the end of the line. The value (or values) which results (or result) from a primary experimental measurement will appear without an affiliated superscript alphabetic letter. These letters point out data which have been derived from the experimental result; the derivations are described in Sec. 3.3., and summarized (along with their alphabetic identifiers) in Table 5.2. The data in the Table are divided into columns as follows:

| Ion | $\Delta_fH$(A); or [X··Y⁻] | EA(A) eV | $\Delta_{acid}H$(AH); or $\Delta_{aff}H$(X··Y⁻) | $\Delta_{acid}G$(AH); or $\Delta_{aff}G$(X·Y⁻) | Method, Comment; | Reference |
|---|---|---|---|---|---|---|

*Ion*: The chemical formula of the anion of interest.

*$\Delta_fH(A^-)$ or $[X\cdot\cdot Y^-]$*: The second column presents the heat of formation of the listed anion in kJ/mol. The column heading specifies that the data correspond to anion $A^-$ which may also be represented as $[X\cdot\cdot Y^-]$. The second designation is included for the cases where the heat of formation of the anion has been derived from data on the clustering of anion $Y^-$ to neutral molecule X (see reaction 52). For example, data on the heat of formation of $AlF_4^-$ $(X\cdot\cdot Y^-)$ is derived from information on the fluoride affinity of $AlF_3$ (that is, $AlF_3$ is X and $F^-$ is $Y^-$).

*EA(A)*: The electron affinity of neutral species A is listed in this column in electron volts.

*$\Delta_{acid}H(AH)$ or $\Delta_{aff}H(X \cdot\cdot Y^-)$ and $\Delta_{acid}G(AH)$ or $\Delta_{aff}G(X \cdot\cdot Y^-)$*: The fourth and fifth columns serve double purposes, with normal typefaced data representing the enthalpy change (fourth column) or Gibbs energy-change (fifth column), respectively, of reaction 10 for the species AH leading to a value for the heat of formation of anion $A^-$. Data given in italics represent enthalpy changes for reaction 52, that is the *affinity* of molecule X for anion $Y^-$. These have been derived either from direct determinations of equilibrium constants for reaction 52, or from equilibrium constants for $Y^-$ transfer reaction 51 which yield scales of relative $Y^-$-affinities.

*Method*: This column gives an acronym to indicate the experimental technique used in determining a particular piece of data. These are discussed in detail in Sec. 3.2. For quick reference, an alphabetized summary of the acronyms with their definitions, and the locations of the relevant discussions, is given in Table 5.2. This table also includes other acronyms, abbreviations, and symbols used in Table 2 for ready reference.

*Comment*: Where necessary for clarity, details of a particular experiment are given as a comment. In this column, there also appears information about auxiliary thermochemistry concerning neutral species. All data pertaining to neutral species appear in a different italicized typeface.

*Reference*: The squib given in this column refers to the article in which the primary datum reported on a particular line was reported. The complete reference can be found in the bibliography for Tables 1 and 2.

*Thermochemistry of neutral species*: The relevant heats of formation of neutral species and accompanying references are given in the top line of the "Comment" column. All data and the references pertaining to neutral molecules are presented in a different italicized typeface, so that they will not be mistaken for data concerning the anion.

*Sort scheme*: Data are sorted by empirical formula using the same sort scheme as that used for the Positive Ion Table. This is the Hill (or Chemical Abstracts) scheme.

*Acidity data*: Data on the acidity of a given neutral species is given under the empirical formula of the conjugate base, i.e. the acidity of $CH_3OH$ is found under $CH_3O^-$.

*Asterisk in left hand margin*: Due to the comprehensive nature of the Negative Ion compilation, there can be numerous entries in Table 2 for a given quantity associated with a particular negative ion, unlike the convention adopted for the cation table, where only one value of an ionization energy/heat of formation is given. A special indication must be given, therefore, to denote the preferred value. Any line with an asterisk in the left margin contains the selected "best" value for a given piece of data pertaining to that ion. There may be more than one line thus marked for a given anion, since the best values for an acidity value and an electron affinity value may be from different sources. (The quantity without a superscripted letter is the primary piece of information for any given line.)

*Absence of asterisk in margin*: If no line is marked as preferred in the data collected for an ion, then no definitive evaluation could be made. Some preference should be given to the first reference cited in such cases, but this is a qualitative judgement on the part of the compiler, and should not be given undue weight.

*Superscript "o" after method acronym [IMRE]*: Original data which were re-evaluated to take into account new results which expanded a portion of the acidity[81,82] scale; corrected values are shown above "original" data, with original reference cited for both values.

*Primary data originating from cited experimental reference*: In Table 2, on any given line (which presents information derived from a single paper) items which were *derived* from the primary experimental data using the relationships listed in Sec. 3.3. and summarized in Table 5.2., have a superscripted letter indicating the relationship used to derive the value (see Table 5.2.). The primary data do not display a superscript.

TABLE 5.2. Acronyms, abbreviations and symbols used in Negative Ion Table

| | |
|---|---|
| **BDE(A-H):** | Bond dissociation energy of A-H bond |
| **Bran:** | Branching ratio in an exothermic reaction (see Sec. Sec. 3.2.14.) |
| **Calc:** | Calculation |
| **CIDC:** | Collision-induced dissociation of cluster ion-branching ratio (see Sec. 3.2.7.) |
| **CIDT:** | Collision induced dissociation threshold (see Sec. 3.2.10.) |
| **Def:** | Defined |
| **EA(A):** | Electron affinity of A. |
| **ECD:** | Electron capture detector (see Sec. 3.2.16.) |
| **EIAP:** | Electron impact appearance potentials (see Sec. 3.2.7.) |
| **EnCT:** | Endothermic charge transfer threshold (see Sec. 3.2.10.) |
| **Endo:** | Endothermic reaction threshold energy (see Sec. 3.2.10.) |
| **ES:** | Electron swarm (see Sec. 3.2.12.) |
| **Est:** | Estimate, based on addition of increments |
| **Est2:** | Estimate, based on thermochemistry of analogous compounds |
| **ETS:** | Electron transmission spectroscopy (see Sec. 3.2.15.) |
| **IMRB:** | Ion/molecule reaction—bracketing (see Sec. 3.2.6.) |
| **IMRE:** | Ion/molecule reaction equilibrium constant determination (see Sec. 3.2.5.) |
| **Kine:** | Attachment/detachment rate ratio (see Sec. 3.2.5.) |
| **Latt:** | Lattice energy calculation (see Sec. 3.2.13.) |
| **LOG:** | Laser optogalvanic spectroscopy |
| **LPD:** | Laser photodetachment (see Sec. 3.2.2.) |
| **LPES:** | Laser photoelectron spectroscopy (see Sec. 3.2.1.) |
| **Mobl:** | Mobility of ion in gas (see Sec. 3.2.17.) |
| **NBAP:** | Neutral beam appearance potential (see Sec. 3.2.8.) |
| **NBIP:** | Neutral beam ionization potential (see Sec. 3.2.8.) |
| **PD:** | Photodetachment (see Sec. 3 2.3.) |
| **PDis:** | Photodissociation (see Sec. 3.2.4.) |

TABLE 5.2. Acronyms, abbreviations and symbols used in Negative Ion Table — Continued

| | |
|---|---|
| PI: | Photoionization (see Sec. 3.2.9.) |
| PLA: | Plasma absorption |
| SI: | Surface ionization (Magnetron) (see Sec. 3.2.11.) |
| TDAs: | Temperature dependent association equilibrium constant determination (see Sec. 3.2.5.) |
| TDEq: | Temperature dependent equilibrium constant determination (see Sec. 3.2.5.) |
| $\Delta_f H(A^-)$: | Heat of formation of $A^-$ |
| $\Delta_{aff} H(X \cdot\cdot Y^-)$: | Enthalpy of association of neutral X to anion $Y^-$, the affinity of X for $Y^-$ |
| $\Delta_{aff} G(X \cdot\cdot Y^-)$: | Gibbs energy of association of neutral X to anion $Y^-$ |
| $\Delta_{acid} H(AH)$: | Acidity of molecule AH; see definition below under f |

Single letter codes which define chemical reaction types (superscripts)

a: $\Delta_f H(A^-) = \Delta_{acid} H(AH) - \Delta_f H^\circ(AH) + \Delta_f H(H^+)$
b: $\Delta_f H(A^-) = \Delta_f H^\circ(A) - EA(A)$
c: $\Delta_f H(X \cdot\cdot Y^-) = -\Delta_{aff} H(X \cdot\cdot Y^-) + \Delta_f H^\circ(X) + \Delta_f H(Y^-)$
d: $EA(A) = \Delta_{acid} H(AH) - IP(H^+) - BDE(A\text{–}H)$
e: $BDE(A\text{–}H) = \Delta_{acid} H(AH) - IP(H^+) + EA(A)$
f: $\Delta_{acid} H(AH) = \Delta_f H(A^-) + \Delta_f H(H^+) - \Delta_f H^\circ(AH)$
g: $\Delta_{Rxn} H = \Delta_{Rxn} G + T\Delta_{Rxn} S$
h: $\Delta_{Rxn} G = \Delta_{Rxn} H - T\Delta_{Rxn} S$
i: $EA(A) = \Delta_f H^\circ(A) - \Delta_f H(A^-)$
j: $\Delta_{aff} H(X \cdot\cdot Y^-) = \Delta_f H^\circ(X) + \Delta_f H(Y^-) - \Delta_f H(X \cdot\cdot Y^-)$

### 5.3. References to Tables 1 and 2

The bibliography given at the back of the volume includes (a) references to the sources data having a bearing on the thermochemistry of the positive ions given in Table 1 (including ionization potentials, appearance potentials, proton affinities, and other related information) *except when those references appeared in the bibliographies of references 1 through 4*; (b) references to the sources of *all* data on the thermochemistry of negative ions from Table 2; and (c) references to the sources of the data on the thermochemistry of neutral molecules.

The references are identified in the tables, and in the bibliography, by a squib, made up of the year of the publication, the first three letters of the surname of the first author, followed by a slash and the first three letters of the surname of the second author. Example: A publication by J. B. Pedley and J. Rylance which appeared in 1977 would be designated by 77PED/RYL.

The references given in the bibliography are sorted according to these squibs, that is, first according to year, and then alphabetically according to the first three letters of the names of the first two authors. Example: Within the papers which appeared during a given year, reference to a paper by "Beauchamp and Armentrout" (BEA/ARM) would precede a reference to a paper by "Beach and Jackson" (BEA/JAC), which in turn would appear above a reference to "Beauchamp and Schwarz" (BEA/SCH). Note that papers of a given first author do not necessarily follow one another in the listing.

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**Table 1. Positive Ion Table**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $Ac^+$ | | | | | | | |
| Ac | 5.17±0.12 | 216 | 905 | 97 | 406 | 82TN270 | 7440-34-8 |
| $Ag^+$ | | | | | | | |
| Ag | 7.576 | 242.7 | 1015.6 | 68.0 | 284.6 | 82TN270 | 7440-22-4 |
| | | *242.6* | *1015.1* | *67.9* | *284.1* | | |
| | See also: 80KRA. | | | | | | |
| $AgAl^+$ | | | | | | | |
| AgAl | (7.8±0.5) | *(287)* | *(1200)* | *107* | *448* | 79HUB/HER | 12379-67-8 |
| | 0 K values. | | | | | | |
| $AgBr^+$ | | | | | | | |
| AgBr | ≤9.59 | *≤246* | *≤1028* | *25* | *103* | 79HUB/HER | 7785-23-1 |
| | 0 K values. | | | | | | |
| $AgCl^+$ | | | | | | | |
| AgCl | (≤10.08) | *(≤255)* | *(≤1065)* | *22* | *93* | 79HUB/HER | 7783-90-6 |
| | 0 K values. | | | | | | |
| $AgF^+$ | | | | | | | |
| AgF | (11.0±0.3) | *(256)* | *(1071)* | *2* | *10* | 79HUB/HER | 7775-41-9 |
| | 0 K values. | | | | | | |
| $AgH^+$ | | | | | | | |
| AgH | (9.2) | *(280)* | *(1170)* | *67* | *282* | 79HUB/HER | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). 0 K value. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $Ag_2^+$ | | | | | | | |
| $Ag_2$ | (7.35) | (267) | (1119) | 98.0 | 410.0 | 82TN270 | 12187-06-3 |
| | | *(268)* | *(1120)* | *98* | *411* | | |
| $Al^+$ | | | | | | | |
| Al | 5.986 | 216.3 | 904.9 | 78.2 | 327.3 | 85JANAF | 7429-90-5 |
| | | *216.8* | *907.3* | *78.8* | *329.7* | | |
| $AlAu^+$ | | | | | | | |
| AuAl | (7.6±0.3) | *(263)* | *(1101)* | *88* | *368* | 79HUB/HER | 12250-38-3 |
| | 0 K values. | | | | | | |
| $AlBO_2^+$ | | | | | | | |
| $AlBO_2$ | (9.5±0.5) | (90) | (376) | −129±4 | −541±17 | 71JANAF | |
| $AlBr^+$ | | | | | | | |
| AlBr | (9.3) | (218.3) | (913.2) | 3.8±3.0 | 15.9±12.6 | 85JANAF | 22359-97-3 |
| | | *(220.0)* | *(920.4)* | *5.5±3.0* | *23.1±12.5* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $AlBr_3^+$ | | | | | | | |
| $AlBr_3$ | (10.4) | (142) | (593) | −98.1 | −410.4 | 85JANAF | 7727-15-3 |
| | | *(147)* | *(616)* | *−92.5* | *−387.2* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $AlCl^+$ | | | | | | | |
| AlCl | 9.4 | 204 | 855 | −12.3 | −51.5 | 85JANAF | 13595-81-8 |
| | | *204* | *855* | *−12.3* | *−51.7* | | |
| $AlClF^+$ | | | | | | | |
| AlClF | (7.9±1.0) | (66) | (276) | −117 | −489 | 85JANAF | |
| | | *(65)* | *(271)* | *−117* | *−488* | | |
| $AlCl_3^+$ | | | | | | | |
| $AlCl_3$ | (12.01) | (137) | (574) | −140 | −585 | 85JANAF | 7446-70-0 |
| | | *(138)* | *(576)* | *−139* | *−583* | | |
| $AlF^+$ | | | | | | | |
| AlF | 9.73±0.01 | 160.9 | 673.1 | −63.5±0.8 | −265.7±3.4 | 79HUB/HER | 13595-82-9 |
| | | *160.9* | *673.9* | *−63.5±0.8* | *−265.6±3.4* | | |
| | IP from 84DYK/KIR. | | | | | | |
| $AlF_2^+$ | | | | | | | |
| $AlF_2$ | (8.1) | (8) | (33) | −179 | −749 | 81WOO | 13569-23-8 |
| | IP from 85JANAF. | | | | | | |
| $AlF_3^+$ | | | | | | | |
| $AlF_3$ | ≤15.45 | ≤67 | ≤282 | −289 | −1209 | 85JANAF | 7784-18-1 |
| | | *≤68* | *≤285* | *−288* | *−1206* | | |
| | IP from 84DYK/KIR. | | | | | | |
| $AlI^+$ | | | | | | | |
| AlI | (9.3±0.3) | (230.7) | (965.3) | 16.3±1 | 68.0±4.2 | 85JANAF | 29977-41-1 |
| | | *(231.0)* | *(966.6)* | *16.6±1* | *69.3±4.2* | | |
| $AlI_3^+$ | | | | | | | |
| $AlI_3$ | (9.1) | (160) | (670) | −49 | −208 | 82TN270 | 7784-23-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $AlO^+$ | | | | | | | |
| AlO | 9.46±0.06 | 234.1 | 979.6 | 16.0±2 | 66.9±8 | 85JANAF | 14457-64-8 |
| | | *234.2* | *979.7* | *16.0±2* | *67.0±8* | | |
| | IP from 82ARM/HAL. See also: 80MUR/HIL, 81KAP/STA. | | | | | | |
| $AlO_2^+$ | | | | | | | |
| $AlO_2$ | (10.0±1.0) | (200) | (835) | −31 | −130 | 82KAS/CHE | 11092-32-3 |
| $AlP^+$ | | | | | | | |
| AlP | (8.4±0.4) | *(295)* | *(1232)* | *101* | *422* | 79HUB/HER | 20859-73-8 |
| | 0 K values. | | | | | | |

Table 1. Positive Ion Table - Continued

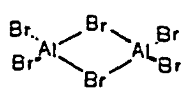
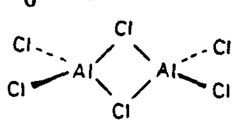
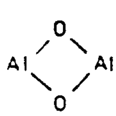
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | • CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$AlSe^+$** | | | | | | | |
| AlSe | (8.3±0.5) | *(243)* | *(1016)* | *52* | *215* | 79HUB/HER | 23330-87-2 |
| | 0 K values. | | | | | | |
| **$Al_2^+$** | | | | | | | |
| $Al_2$ | (5.4±1.0) | (240.9) | (1008.0) | 116.4±0.8 | 487.0±3.5 | 85JANAF | 32752-94-6 |
| | | *(240.8)* | *(1007.3)* | *116.2±0.8* | *486.3±3.5* | | |
| **$Al_2Br_6^+$** | | | | | | | |
|  | (10.97) | (21) | (87) | −232 | −971 | 82TN270 | 18898-34-5 |
| **$Al_2Cl_6^+$** | | | | | | | |
|  | (12.18) | (−28) | (−116) | −309 | −1291 | 82TN270 | 13845-12-0 |
| **$Al_2O^+$** | | | | | | | |
| $Al_2O$ | (7.7±0.2) | (144) | (603) | −33±5 | −140±22 | 82KAS/CHE | 12004-36-3 |
| | | *(145)* | *(605)* | *−33* | *−138* | | |
| **$Al_2O_2^+$** | | | | | | | |
|  | (9.9±0.5) | (131) | (551) | −97±12 | −404±48 | 82KAS/CHE | 12252-63-0 |
| **$Am^+$** | | | | | | | |
| Am | 5.99 | 206 | 862 | 68 | 284 | 85KLE/WAR | 7440-35-9 |
| | See also: 81CHE/GAB. | | | | | | |
| **$Ar^+$** | | | | | | | |
| Ar | 15.75973±0.00001 | 363.42 | 1520.57 | 0 | 0 | *DEF | 7440-37-1 |
| | | *363.42* | *1520.57* | | | | |
| | See also: 81KIM/KAT. | | | | | | |
| **$ArH^+$** | | | | | | | |
| ArH | | 277 | 1159 | | | | |
| | From proton affinity of Ar (RN 7440-37-1). PA = 88.6 kcal/mol, 371. kJ/mol. | | | | | | |
| **$ArHe^+$** | | | | | | | |
| ArHe | 15.735 | *362.8* | *1518.0* | *−0.055* | *−0.23* | 79HUB/HER | 12254-69-2 |
| | $\Delta_f H$(Ion) from 81DAB/HER. 0 K values. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $ArHg^+$ | | | | | | | |
| ArHg | (10.217±0.012) | *(250.6)* | *(1048.6)* | *15.0* | *62.8* | 84BOU/BRA | 87193-95-1 |
| | IP from 85LIN/BRO. | | | | | | |
| $ArKr^+$ | | | | | | | |
| ArKr | 13.484±0.015 | *310.6* | *1299.7* | *−0.3* | *−1.3* | 79HUB/HER | 51184-77-1 |
| | IP from 82DEH/PRA. 0 K values. | | | | | | |
| $ArNe^+$ | | | | | | | |
| ArNe | 15.685±0.004 | *361.6* | *1512.9* | *−0.10* | *−0.43* | 76BOB/BAR | 12301-65-4 |
| | IP from 82PRA/DEH2. 0 K values. | | | | | | |
| $ArXe^+$ | | | | | | | |
| ArXe | 11.968±0.012 | *275.7* | *1153.4* | *−0.32* | *−1.35* | 76BOB/BAR | 58206-67-0 |
| | IP from 82DEH/PRA. See also: 85PRA/DEH, 85PRA/DEH2. 0 K values. | | | | | | |
| $Ar_2^+$ | | | | | | | |
| $Ar_2$ | 14.501±0.025 | *334.2* | *1398.1* | *−0.24* | *−1.01* | 79HUB/HER | 12595-59-4 |
| | IP from 82DEH/PRA2. See also: 81DEH/POL, 82LEV/LIA. 0 K values. | | | | | | |
| $As^+$ | | | | | | | |
| As | 9.7883±0.0002 | 298.0 | 1246.9 | 72.3 | 302.5 | 82TN270 | 7440-38-2 |
| | | *297.7* | *1245.8* | *72.0* | *301.4* | | |
| $AsBr_3^+$ | | | | | | | |
| $AsBr_3$ | (10.0) | (200) | (835) | −31 | −130 | 82TN270 | 7784-33-0 |
| | | *(205)* | *(858)* | *−25.5* | *−106.9* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $AsClO^+$ | | | | | | | |
| AsOCl | (11.1) | (249) | (1040) | −7 | −31 | 83BIN | 14525-25-8 |
| | IP from 83BIN. | | | | | | |
| $AsCl_3^+$ | | | | | | | |
| $AsCl_3$ | (10.55±0.025) | (181) | (756) | −63 | −262 | 82TN270 | 7784-34-1 |
| | | *(181)* | *(758)* | *−62* | *−260* | | |
| | See also: 83OZG. | | | | | | |
| $AsF_3^+$ | | | | | | | |
| $AsF_3$ | (12.84±0.05) | (108) | (453) | −188 | −786 | 82TN270 | 7784-35-2 |
| | | *(109)* | *(457)* | *−187* | *−782* | | |
| $AsF_3H^+$ | | | | | | | |
| $F_3AsH$ | | 23 | 96 | | | | |
| | From proton affinity of $AsF_3$ (RN 7784-35-2). PA = 155 kcal/mol, 648 kJ/mol. | | | | | | |
| $AsH_3^+$ | | | | | | | |
| $AsH_3$ | 9.89 | 244 | 1020 | 16 | 66 | 82TN270 | 7784-42-1 |
| | | *246* | *1028* | *18* | *74* | | |
| | See also: 82ELB/DIE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $AsH_4^+$ | | | | | | | |
| $AsH_4$ | | 202 | 846 | | | | |
| | From proton affinity of $AsH_3$ (RN 7784-42-1). PA = 179.2 kcal/mol, 750 kJ/mol. | | | | | | |
| $As_2^+$ | | | | | | | |
| $As_2$ | (10.1±0.2) | (278) | (1165) | 45.5±0.7 | 190.4±2.9 | 73BEN/MAR | 23878-46-8 |
| | | *(278)* | *(1164)* | *45.5±0.7* | *190.4±2.9* | | |
| | See also: 85HIR/STR. | | | | | | |
| $As_4^+$ | | | | | | | |
|  | (9.07±0.07) | (244) | (1019) | 34 | 144 | 82TN270 | 12187-08-5 |
| | See also: 85HIR/STR. | | | | | | |
| $As_4O_6^+$ | | | | | | | |
|  | (9.6) | (-68) | (-283) | -289 | -1209 | 82TN270 | 12505-67-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $Au^+$ | | | | | | | |
| Au | 9.225 | 300 | 1256 | 87 | 366 | 82TN270 | 7440-57-5 |
| | | *300.2* | *1256.0* | *87.5* | *365.9* | | |
| $AuB^+$ | | | | | | | |
| AuB | (8.7±0.5) | *(337)* | *(1411)* | *137* | *572* | 79HUB/HER | 12408-81-0 |
| | 0 K values. | | | | | | |
| $AuCe^+$ | | | | | | | |
| AuCe | (6.0±0.3) | (248) | (1036) | 109 | 457 | 82TN270 | 12408-82-1 |
| | | *(248)* | *(1039)* | *110* | *460* | | |
| $AuHo^+$ | | | | | | | |
| AuHo | (6.2±0.5) | (242) | (1013) | 99.1 | 414.5 | 82TN270 | 12044-80-3 |
| | | *(243)* | *(1016)* | *100* | *418* | | |
| $AuLa^+$ | | | | | | | |
| AuLa | (5.9±0.5) | (247) | (1033) | 111 | 464 | 82TN270 | 12429-32-2 |
| | | *(247)* | *(1035)* | *111* | *466* | | |
| $AuNd^+$ | | | | | | | |
| AuNd | (5.8±0.8) | (228) | (955) | 94 | 395 | 82TN270 | 12429-33-3 |
| | | *(229)* | *(957)* | *95* | *397* | | |
| $AuPr^+$ | | | | | | | |
| AuPr | (5.4±0.8) | (224) | (937) | 99 | 416 | 82TN270 | 12429-34-4 |
| | | *(224)* | *(939)* | *100* | *418* | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $AuSi^+$ | | | | | | | |
| AuSi | (9.5±0.5) | *(340)* | *(1422)* | *(121)* | *(505)* | 79HUB/HER | 12256-53-0 |
| | 0 K values. | | | | | | |
| $Au_2^+$ | | | | | | | |
| $Au_2$ | (9.5±0.3) | (343) | (1433) | 123.5 | 516.7 | 79HUB/HER | 12187-09-6 |
| | | *(341)* | *(1427)* | *122.0* | *510.4* | | |
| $B^+$ | | | | | | | |
| B | 8.29808±0.00002 | 325.9 | 1363.3 | 134.5 | 562.7 | 82TN270 | 7440-42-8 |
| | | *324.7* | *1358.2* | *133.3* | *557.6* | | |
| $BBr_2H^+$ | | | | | | | |
| $BHBr_2$ | (10.92±0.02) | (227) | (949) | −25±5 | −105±21 | 71JANAF | 13709-65-4 |
| | | *(231)* | *(966)* | *−21±5* | *−88±21* | | |
| | IP from 81FRO/KIR. | | | | | | |
| $BBr_3^+$ | | | | | | | |
| $BBr_3$ | (10.51±0.02) | (194) | (810) | −49±0.2 | −204±1 | 71JANAF | 10294-33-4 |
| $BCl^+$ | | | | | | | |
| BCl | (10.2) | (269.0) | (1125.5) | 33.8 | 141.4 | 85JANAF | 20583-55-5 |
| | | *(268.3)* | *(1122.5)* | *33.1* | *138.4* | | |
| | $\Delta_f H$(Ion) from appearance potential (18.37±0.02 eV) in $BCl_3$. Cited ionization potential is difference between heats of formation of ion and neutral. | | | | | | |
| $BClF_2^+$ | | | | | | | |
| $BClF_2$ | (13.06±0.11) | (88) | (370) | −213 | −890 | 82TN270 | 14720-30-0 |
| $BCl_2^+$ | | | | | | | |
| $BCl_2$ | (7.8) | (159) | (664) | −20±15 | −83±63 | 71JANAF | 13842-52-9 |
| | $\Delta_f H$(Ion) from appearance potential (12.30±0.02 eV) in $BCl_3$. Cited ionization potential is difference between heats of formation of ion and neutral. | | | | | | |
| $BCl_2F^+$ | | | | | | | |
| $BCl_2F$ | (12.18±0.10) | (130) | (544) | −151 | −631 | 82TN270 | 14720-31-1 |
| $BCl_2H^+$ | | | | | | | |
| $HBCl_2$ | (11.91±0.02) | (215) | (901) | −59.3±1 | −248.1±4 | 71JANAF | 10325-39-0 |
| | | *(216)* | *(904)* | *−58.6±1* | *−245.2±4* | | |
| | IP from 81FRO/KIR. | | | | | | |
| $BCl_3^+$ | | | | | | | |
| $BCl_3$ | 11.60±0.02 | 171 | 715 | −96 | −404 | 82TN270 | 10294-34-5 |
| | | *171* | *716* | *−96* | *−403* | | |
| $BF^+$ | | | | | | | |
| BF | 11.12±0.01 | 229 | 957 | −27.7 | −115.8 | 79HUB/HER | 13768-60-0 |
| | | *228* | *954* | *−28.4* | *−118.8* | | |
| | IP from 83DYK/KIR. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $BFS^+$ | | | | | | | |
| FBS | (10.90±0.01) | (165) | (690) | −86 | −362 | *EST | 83995-89-5 |
| | IP from 84COO/KRO. | | | | | | |
| $BF_2^+$ | | | | | | | |
| $BF_2$ | (9.4) | (75) | (314) | −141.0±3 | −589.9±12 | 71JANAF | |
| | From appearance potential of 15.81±0.04 eV in $BF_3$. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $BF_2H^+$ | | | | | | | |
| $HBF_2$ | (13.60±0.05) | (138) | (578) | −175.4±0.8 | −733.8±3.3 | 71JANAF | 13709-83-6 |
| | | *(139)* | *(582)* | *−174.5±0.8* | *−730.1±3.3* | | |
| | IP from 81CHO/KIR. | | | | | | |
| $BF_3^+$ | | | | | | | |
| $BF_3$ | 15.56±0.03 | 87.1 | 364.3 | −271.7 | −1137.0 | 82TN270 | 7637-07-2 |
| | | *87.8* | *367.3* | *−271.0* | *−1134.0* | | |
| | See also: 84FAR/SRI, 84DEH/PAR, 81ASB/SVE, 81KIM/KAT. | | | | | | |
| $BH^+$ | | | | | | | |
| BH | 9.77±0.05 | 331.1 | 1385.4 | 105.8±2.0 | 442.7±8.4 | 85JANAF | 13766-26-2 |
| | | *330.3* | *1382.2* | *105.0±2.0* | *439.5±8.4* | | |
| $BHO_2^+$ | | | | | | | |
| $BHO_2$ | (12.6±0.2) | (156) | (654) | −134 | −562 | 82TN270 | 13460-50-9 |
| $BHS^+$ | | | | | | | |
| HBS | 11.11±0.03 | (268) | (1122) | 12±10 | 50±42 | 78JANAF | 14457-85-3 |
| $BH_2^+$ | | | | | | | |
| $BH_2$ | (9.8±0.2) | (274) | (1146) | 48±15 | 201±63 | 71JANAF | 14452-64-3 |
| $BH_3^+$ | | | | | | | |
| $BH_3$ | 12.3±0.1 | (308) | (1287) | 24 | 100 | 82TN270 | 13283-31-3 |
| $BI_3^+$ | | | | | | | |
| $BI_3$ | (9.25±0.03) | (230) | (964) | 17.0 | 71.1 | 82TN270 | 13517-10-7 |
| | | *(231)* | *(967)* | *18* | *75* | | |
| $BKO_2^+$ | | | | | | | |
| $KBO_2$ | (8.62±0.14) | (38) | (160) | −161±2 | −672±10 | 85FAR/SRI | |
| | See also: 85FAR/SRI. | | | | | | |
| $BLiO^+$ | | | | | | | |
| LiBO | 7.7±0.5 | (136) | (568) | −42 | −175 | *EST | 77965-53-8 |
| | IP from 85NEU. | | | | | | |
| $BLiO_2^+$ | | | | | | | |
| $LiBO_2$ | (9.8±0.5) | (66) | (274) | −160 | −671 | 71JANAF | |
| | IP from 85NEU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

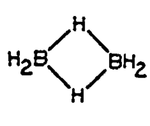
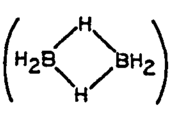
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $BNaO_2^+$ | | | | | | | |
| $NaBO_2$ | (9.18±0.10) | (58) | (242) | −154 | −644 | 82TN270 | |
| | | *(59)* | *(244)* | *−153* | *−642* | | |
| $BO^+$ | | | | | | | |
| BO | 13.0±0.3 | (300) | (1254) | 0 | 0 | 83PED/MAR | 12505-77-0 |
| | | *(299)* | *(1251)* | *−1* | *−3* | | |
| | See also: 79BAG/NIK, 85NEU. | | | | | | |
| $BO_2^+$ | | | | | | | |
| $BO_2$ | (13.5±0.3) | (240) | (1003) | −72 | −300 | 82TN270 | 13840-88-5 |
| | IP from 79BAG/NIK. | | | | | | |
| $BSe^+$ | | | | | | | |
| BSe | (10.3) | *(315)* | *(1320)* | *78* | *326* | 79HUB/HER | 29750-36-5 |
| | 0 K values. | | | | | | |
| $B_2Cl_2^+$ | | | | | | | |
| $B_2Cl_2$ | | (223) | (934) | | | | |
| | From appearance potential (17.24±0.03 eV) in $B_2Cl_4$ assumed to give $B_2Cl_2^+$ + 2Cl. | | | | | | |
| $B_2Cl_3^+$ | | | | | | | |
| $B_2Cl_3$ | | 120 | 502 | | | | |
| | From appearance potential of 11.52±0.02 eV in $B_2Cl_4$. 0 K values. | | | | | | |
| $B_2Cl_4^+$ | | | | | | | |
| $B_2Cl_4$ | 10.32±0.02 | 121 | 506 | −117 | −490 | 82TN270 | 13701-67-2 |
| | | *121* | *506* | *−117* | *−490* | | |
| $B_2F_3^+$ | | | | | | | |
| $B_2F_3$ | | *−7* | *−28* | | | | |
| | From appearance potential of 15.40±0.01 eV in $B_2F_4$. 0 K values. | | | | | | |
| $B_2F_4^+$ | | | | | | | |
| $B_2F_4$ | 12.07±0.01 | −66 | −275 | −344 | −1440 | 82TN270 | 13965-73-6 |
| | | *−65* | *−272* | *−343* | *−1437* | | |
| $B_2H_6^+$ | | | | | | | |
|  | 11.38±0.03 | 271 | 1134 | 8.5 | 35.6 | 82TN270 | 19287-45-7 |
| | | *275* | *1149* | *12.3* | *51.4* | | |
| | See also: 81ASB/SVE, 81KIM/KAT. | | | | | | |
| $B_2H_7^+$ | | | | | | | |
|  $H^+$ | | 228 | 955 | | | | |
| | From proton affinity of Diborane(6). (RN 19287-45-7). PA = −146 kcal/mol, −611 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

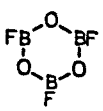
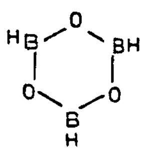
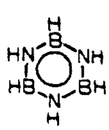
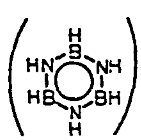
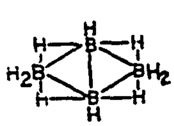
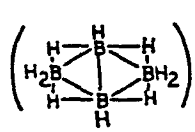
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $B_2O_2^+$ | | | | | | | |
| O=BB=O | 13.58 | 204 | 854 | −109±2 | −456±8 | 71JANAF | 13766-28-4 |
| | IP from 84RUS/CUR. See also: 79BAG/NIK. | | | | | | |
| $B_2O_3^+$ | | | | | | | |
| $B_2O_3$ | 13.5±0.15 | 110 | 460 | −201.3 | −842.1 | 79BAG/NIK | 1303-86-2 |
| | | *110* | *462* | *−201* | *−841* | | |
| | IP from 79BAG/NIK. | | | | | | |
| $B_3F_3O_3^+$ | | | | | | | |
|  | (13.9±0.1) | (−244) | (−1024) | −565±1 | −2365±4 | 71JANAF | 13703-95-2 |
| $B_3H_3O_3^+$ | | | | | | | |
|  | (13.5±0.5) | (20) | (85) | −291 | −1218 | 71JANAF | 289-56-5 |
| $B_3H_6N_3^+$ | | | | | | | |
|  | 9.88±0.02 | 106 | 441 | −122.3 | −511.8 | 82TN270 | 6569-51-3 |
| | | *112* | *467* | *−116.2* | *−486.2* | | |
| $B_3H_7N_3^+$ | | | | | | | |
|  $H^+$ | | 49 | 206 | | | | |
| | From proton affinity of borazine (RN 6569-51-3). PA = 194.1 kcal/mol, 812 kJ/mol. | | | | | | |
| $B_4H_{10}^+$ | | | | | | | |
|  | 10.76±0.04 | 264 | 1104 | 16 | 66 | 82TN270 | 18283-93-7 |
| $B_4H_{11}^+$ | | | | | | | |
|  $H^+$ | | 237 | 993 | | | | |
| | From proton affinity of $B_4H_{10}$ (RN 18283-93-7). PA = -144 kcal/mol, -602 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

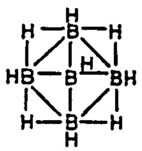
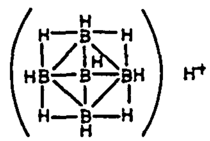
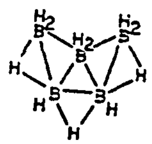
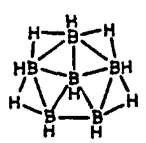
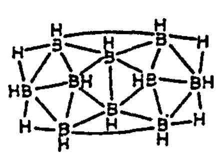
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $B_5H_9^+$ | | | | | | | |
|  | 9.90±0.04 | 246 | 1028 | 17.5 | 73.2 | 82TN270 | 19624-22-7 |
| | | *253* | *1057* | *24.4* | *102.1* | | |
| $B_5H_{10}^+$ | | | | | | | |
|  | | 214 | 896 | | | | |
| | From proton affinity of $B_5H_9$ (RN 19624-22-7). PA = 169 kcal/mol, 707 kJ/mol. | | | | | | |
| $B_5H_{11}^+$ | | | | | | | |
|  | (10.1) | (257) | (1078) | 24.6 | 103.3 | 82TN270 | 18433-84-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $B_6H_{10}^+$ | | | | | | | |
|  | (9.0) | (230) | (963) | 23 | 95 | 82TN270 | 2377-80-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $B_{10}H_{14}^+$ | | | | | | | |
|  | 9.88±0.03 | 235 | 985 | 7.6 | 31.6 | 82TN270 | 17702-41-9 |
| | | *247* | *1031* | *18.7* | *78.1* | | |
| $Ba^+$ | | | | | | | |
| Ba | 5.212 | 163 | 683 | 43 | 180 | 82TN270 | 7440-39-3 |
| | | *163* | *684* | *43* | *181* | | |
| $BaBr^+$ | | | | | | | |
| BaBr | (5.0) | (88.9) | (371.8) | −26.4±10.0 | −111±41 | 85JANAF | 14832-97-4 |
| | | *(91.0)* | *(380.8)* | *−24.3±10.0* | *−102±41* | | |
| $BaBr_2^+$ | | | | | | | |
| $BaBr_2$ | (8.5) | (90) | (377) | −106 | −443 | 82EMO/KIE | 10553-31-8 |
| | | *(93)* | *(391)* | *−102* | *−429* | | |
| | IP is onset of photoelectron band (79LEE/POT). See also: 82EMO/KIE, 79LEE/POT2. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $BaCl^+$ | | | | | | | |
| BaCl | 5.01±0.010 | 81 | 340 | −34 | −143 | 85JANAF | 14832-99-6 |
| | | *82* | *341* | *−34* | *−142* | | |
| $BaCl_2^+$ | | | | | | | |
| $BaCl_2$ | (9.4) | *(97)* | *(405)* | *−120* | *−502* | 82EMO/KIE | 10361-37-2 |
| | IP is onset of photoelectron band (79LEE/POT, 79LEE/POT2). See also: 82EMO/KIE. | | | | | | |
| | 0 K values. | | | | | | |
| $BaF^+$ | | | | | | | |
| BaF | (4.8±0.3) | (34) | (144) | −77 | −324 | 82TN270 | 13966-70-6 |
| | | *(34)* | *(142)* | *−77* | *−326* | | |
| $BaHO^+$ | | | | | | | |
| BaOH | 4.35±0.3 | 45 | 189 | −55±4 | −230±17 | 81MUR | 12009-08-4 |
| | IP from 81MUR. See also: 81FAR/SRI. | | | | | | |
| $BaH_2O_2^+$ | | | | | | | |
| $Ba(OH)_2$ | (8) | (44) | (186) | −140 | −586 | 82TN270 | 17194-00-2 |
| | IP from 81FAR/SRI. | | | | | | |
| $BaI^+$ | | | | | | | |
| BaI | (5.0±0.3) | (105.2) | (440.0) | −10.1±20.1 | −42.4±84 | 85JANAF | 12524-20-8 |
| | | *(105.9)* | *(443.1)* | *−9.4±20.1* | *−39.3±84* | | |
| $BaI_2^+$ | | | | | | | |
| $BaI_2$ | (8.24) | (116) | (487) | −74 | −308 | 82EMO/KIE | 13718-50-8 |
| | | *(117)* | *(490)* | *−73* | *−305* | | |
| | IP is onset of photoelectron band (79LEE/POT, 79LEE/POT2). See also: 82EMO/KIE. | | | | | | |
| $BaO^+$ | | | | | | | |
| BaO | 6.91±0.06 | 129.8 | 542.9 | −29.6±2 | −123.8±8 | 85JANAF | 1304-28-5 |
| | | *130.3* | *545.1* | *−29.1±2* | *−121.6±8* | | |
| | See also: 81MUR. | | | | | | |
| $BaO_4W^+$ | | | | | | | |
| $BaWO_4$ | (9.8±0.5) | (−181) | (−757) | −407 | −1703 | 76DEL/HAL | |
| $Be^+$ | | | | | | | |
| Be | 9.322 | 292.5 | 1223.7 | *77.5* | 324.3 | 82TN270 | 7440-41-7 |
| | | *291.5* | *1219.4* | *76.5* | *320.0* | | |
| $BeCl_2^+$ | | | | | | | |
| $BeCl_2$ | (11.15) | (171) | (717) | −86 | −359 | 82TN270 | 7787-47-5 |
| | IP is onset of photoelectron band (79LEE/POT2). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $BeF^+$ | | | | | | | |
| BeF | | | | −40.6±2 | −169.9±8 | 85JANAF | 13597-96-1 |
| | | | | *−41.2±2* | *−172.2±8* | | |
| | A value of 168 kcal/mol, 703 kJ/mol is obtained for the enthalpy of formation of $BeF^+$ based on experimental ionization potential values of 9.1±0.5 or 9.3±1.0 eV; the enthalpy of formation based on an appearance potential of 15.4±0.4 eV in $BeF_2$ is 147 kcal/mol, 615 kJ/mol. | | | | | | |
| $BeF_2^+$ | | | | | | | |
| $BeF_2$ | (14.6±0.5) | (147) | (615) | −190 | −794 | 82TN270 | 7787-49-7 |
| $BeH^+$ | | | | | | | |
| BeH | 8.21±0.04 | 272 | 1136 | 82 | 344 | 79HUB/HER | 13597-97-2 |
| | | *271* | *1132* | *81.2* | *339.8* | | |
| $BeO^+$ | | | | | | | |
| BeO | (10.1±0.4) | (265.5) | (1110.9) | 32.6±3 | 136.4±13 | 85JANAF | 1304-56-9 |
| | | *(264.9)* | *(1108.5)* | *32.0±3* | *134.0±13* | | |
| $Be_2O^+$ | | | | | | | |
| $Be_2O$ | (10.5±0.5) | (227) | (950) | −15±10 | −63±42 | 71JANAF | 12009-99-3 |
| $Be_2O_2^+$ | | | | | | | |
| $(BeO)_2$ | (10.8±0.7) | (151) | (632) | −98±12 | −410±50 | 71JANAF | 70478-90-9 |
| $Be_3O_3^+$ | | | | | | | |
| $(BeO)_3$ | (10.9±0.6) | (−1) | (−2) | −252±9 | −1054±38 | 71JANAF | 61279-73-0 |
| $Be_4O_4^+$ | | | | | | | |
| $(BeO)_4$ | (11.0) | (−126) | (−529) | −380±12 | −1590±50 | 71JANAF | 61279-74-1 |
| $Be_5O_5^+$ | | | | | | | |
| $(BeO)_5$ | (~11) | (~−251) | (~−1052) | −505±23 | −2113±95 | 71JANAF | 61279-75-2 |
| $Be_6O_6^+$ | | | | | | | |
| $(BeO)_6$ | (~11) | (~−239) | (~−1000) | −492±22 | −2061±92 | 71JANAF | 61279-76-3 |
| $Bi^+$ | | | | | | | |
| Bi | 7.289 | 218 | 910 | 49 | 207 | 82TN270 | 7440-69-9 |
| | | *217.7* | *910.7* | *49.6* | *207.4* | | |
| $BiCl_3^+$ | | | | | | | |
| $BiCl_3$ | (10.4) | (176) | (738) | −64 | −266 | 82TN270 | 7787-60-2 |
| | | *(177)* | *(739)* | *−63* | *−264* | | |
| | IP is onset of photoelectron band (83NOV/POT). See also: 83OZG. | | | | | | |
| $BiH_3^+$ | | | | | | | |
| $BiH_3$ | (10.1) | (288) | (1204) | 55 | 230 | 64GUN | 18288-22-7 |

**Table 1. Positive Ion Table - Continued**

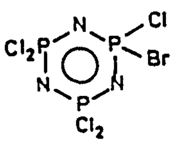
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $BiO^+$ | | | | | | | |
| BiO | (9.0±0.5) | (236) | (989) | 29±3 | 121±13 | 83PED/MAR | 1332-64-5 |
| | | *(236)* | *(988)* | *29* | *120* | | |
| $BiS^+$ | | | | | | | |
| BiS | (8.7±0.5) | *(243)* | *(1017)* | *42* | *178* | 79HUB/HER | 12048-34-9 |
| | 0 K values. | | | | | | |
| $BiTe^+$ | | | | | | | |
| BiTe | (8.4±0.5) | *(235)* | *(983)* | *41* | *173* | 79HUB/HER | 12010-57-0 |
| | 0 K values. | | | | | | |
| $Bi_2^+$ | | | | | | | |
| $Bi_2$ | (7.3±0.5) | (221) | (924) | 53 | 220 | 82TN270 | 12187-12-1 |
| | | *(221)* | *(926)* | *53.1* | *222.2* | | |
| $Bk^+$ | | | | | | | |
| Bk | 6.30±0.09 | 219 | 918 | 74 | 310 | 85KLE/WAR | 7440-40-6 |
| $Br^+$ | | | | | | | |
| Br | 11.814 | 299.2 | 1251.7 | 26.7 | 111.9 | 82BAU/COX | 10097-32-2 |
| | | *300.6* | *1257.8* | *28.2* | *117.9* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $BrCa^+$ | | | | | | | |
| CaBr | 5.54 | *123* | *513* | *-5* | *-21* | 79HUB/HER | 10024-43-8 |
| | IP from 84MEY/SCH. 0 K values. | | | | | | |
| $BrCl^+$ | | | | | | | |
| BrCl | 11.01 | 257 | 1077 | 4 | 15 | 82TN270 | 13863-41-7 |
| | | *259* | *1084* | *5* | *22* | | |
| | IP from 84DYK/JOS. | | | | | | |
| $BrCl_5N_3P_3^+$ | | | | | | | |
|  | (9.83±0.1) | (52) | (218) | -174 | -730 | *EST | 14740-93-3 |
| $BrCs^+$ | | | | | | | |
| CsBr | 7.72±0.05 | 130 | 545 | -48 | -200 | 84PAR/WEX | 7787-69-1 |
| | | *133* | *554* | *-45.5±1.8* | *-190.4±7.5* | | |
| $BrF^+$ | | | | | | | |
| BrF | 11.77±0.01 | 257.4 | 1077.1 | -14.0±0.4 | -58.5±1.7 | 85JANAF | 13863-59-7 |
| | | *259.3* | *1084.8* | *-12.1±0.4* | *-50.8±1.7* | | |
| | See also: 84DYK/JOS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$BrF_3^+$** | | | | | | | |
| $BrF_3$ | (12.15±0.04) | (219) | (917) | −61.1 | −255.6 | 82TN270 | 7787-71-5 |
| | | *(222)* | *(928)* | *−58.4* | *−244.4* | | |
| **$BrF_5^+$** | | | | | | | |
| $BrF_5$ | (13.17±0.01) | (201) | (842) | −103 | −429 | 82TN270 | 7789-30-2 |
| | | *(205)* | *(858)* | *−99* | *−413* | | |
| **$BrH^+$** | | | | | | | |
| HBr | 11.66±0.03 | 260 | 1089 | −9 | −36 | 82TN270 | 10035-10-6 |
| | | *262* | *1096* | *−7* | *−29* | | |
| | IP from 79HUB/HER, 77ROS/DRA, 82LEV/LIA. See also: 81KIM/KAT. | | | | | | |
| **$BrH_2^+$** | | | | | | | |
| $H_2Br$ | | 218 | 911 | | | | |
| | From proton affinity of HBr (RN 10035-10-6) (84POL/MUN, 85MCM/KEB). PA = 139 kcal/mol, 582 kJ/mol. | | | | | | |
| **$BrH_3Si^+$** | | | | | | | |
| $SiH_3Br$ | 10.6 | (226) | (945) | −19±4 | −78±17 | 82JANAF | 13465-73-1 |
| | IP is onset of photoelectron band. | | | | | | |
| **$BrI^+$** | | | | | | | |
| IBr | 9.790±0.004 | 235.5 | 985.4 | 9.8 | 40.8 | 82TN270 | 7789-33-5 |
| | | *237.7* | *994.4* | *11.9* | *49.8* | | |
| | See also: 84DYK/JOS, 71POT/PRI. | | | | | | |
| **$BrIn^+$** | | | | | | | |
| InBr | (9.09) | (202) | (845) | −8 | −32 | 79HUB/HER | 14280-53-6 |
| | | *(204)* | *(854)* | *−6* | *−23* | | |
| **$BrK^+$** | | | | | | | |
| KBr | 7.85±0.1 | 138 | 577 | −43 | −180 | 82TN270 | 7758-02-3 |
| | | *140* | *586* | *−41* | *−171* | | |
| **$BrLi^+$** | | | | | | | |
| LiBr | (8.7) | (164) | (685) | −37±3 | −154±13 | 71JANAF | 7550-35-8 |
| | | *(166)* | *(693)* | *−35±3* | *−146±13* | | |
| | IP is onset of photoelectron band. | | | | | | |
| **$BrNO^+$** | | | | | | | |
| NOBr | 10.17±0.03 | 254 | 1063 | 20 | 82 | 82BAU/COX | 13444-87-6 |
| **$BrNa^+$** | | | | | | | |
| NaBr | 8.31±0.1 | 157 | 659 | −34 | −143 | 82TN270 | 7647-15-6 |
| | | *160* | *668* | *−32* | *−134* | | |
| **$BrO^+$** | | | | | | | 15656-19-6 |
| BrO | (10.2) | (265) | (1110) | 30.1 | 125.8 | 82TN270 | ~~14380-62-2~~ |
| | | *(267)* | *(1118)* | *31.9* | *133.5* | | |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

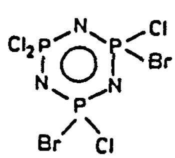
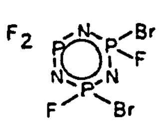
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $BrRb^+$ | | | | | | | |
| RbBr | 7.94±0.03 | 139 | 583 | −43.7 | −182.8 | 82TN270 | 7789-39-1 |
| | | *142* | *592* | *−41.4* | *−173.4* | | |
| $BrSi^+$ | | | | | | | |
| SiBr | (7.3) | (224.6) | (939.6) | 56.3±11.0 | 235.3±46.0 | 85JANAF | 14791-57-2 |
| | | *(225.9)* | *(945.1)* | *57.6±11.0* | *240.8±46.0* | | |
| $BrSr^+$ | | | | | | | |
| SrBr | (5.5) | (106) | (442) | −21±10 | −89±42 | 85JANAF | 14519-13-2 |
| | | *(108)* | *(450)* | *−19.2±10* | *−80.4±42* | | |
| $BrTl^+$ | | | | | | | |
| TlBr | 9.14±0.02 | 202 | 844 | −9 | −38 | 82TN270 | 7789-40-4 |
| | | *204* | *853* | *−7* | *−29* | | |
| | See also: 83BAN/BRI. | | | | | | |
| $Br_2^+$ | | | | | | | |
| $Br_2$ | 10.515±0.005 | 250 | 1046 | 7.4 | 31.0 | 82BAU/COX | 7726-95-6 |
| | | *253* | *1061* | *11* | *46* | | |
| | Cited IP leads to $Br_2^+$ ($^2\Pi_{3/2\ g}$); formation of $Br_2^+$ ($^2\Pi_{1/2\ g}$) requires 10.865±0.005 eV. IP from 84VAN/DEL2, 84DYK/JOS, 77ROS/DRA. See also: 81KIM/KAT. | | | | | | |
| $Br_2Ca^+$ | | | | | | | |
| $CaBr_2$ | ≤9.68 | ≤130 | ≤545 | −93 | −389 | 82TPIS | 7789-41-5 |
| | | *≤134* | *≤560* | *−89±2* | *−374±9* | | |
| | IP is onset of photoelectron band (79LEE/POT2). | | | | | | |
| $Br_2Cl_4N_3P_3^+$ | | | | | | | |
|  | (9.80±0.1) | (63) | (265) | −163 | −681 | *EST | 15964-99-5 |
| $Br_2F_4N_3P_3^+$ | | | | | | | |
|  | (10.63±0.03) | (−135) | (−563) | −380 | −1589 | *EST | 29871-63-4 |
| | IP from 81CLA/SOW. | | | | | | |
| $Br_2Fe^+$ | | | | | | | |
| $FeBr_2$ | (10.7±0.5) | (237) | (991) | −10±0.5 | −41±2 | 71JANAF | 7789-46-0 |
| $Br_2Ge^+$ | | | | | | | |
| $GeBr_2$ | (9.60±0.05) | (206) | (863) | −15 | −63 | 82TN270 | 24415-00-7 |
| | IP from 82JON/VAN. | | | | | | |

**Table 1. Positive Ion Table - Continued**

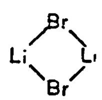
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Br_2H_2Si^+$ | | | | | | | |
| $SiH_2Br_2$ | (10.7) | (201) | (842) | −45±4 | −190±17 | 82JANAF | 13768-94-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $Br_2Hg^+$ | | | | | | | |
| $HgBr_2$ | 10.560±0.003 | 223 | 934 | −20±2 | −85±8 | 71JANAF | 7789-47-1 |
| | Cited ionization potential (83LIN/TZE) refers to formation of $HgBr_2^+(^2\Pi_{3/2\,g})$. IP for formation of $HgBr_2^+(^2\Pi_{1/2\,g})$ is 10.8846±0.0012 eV. See also: 81LEE/POT. | | | | | | |
| $Br_2Li_2^+$ | | | | | | | |
|  | (≤10.05±0.08) | (≤112) | (≤469) | −120 | −501 | 81LIN/BES | 12380-84-6 |
| $Br_2Mg^+$ | | | | | | | |
| $MgBr_2$ | 10.47 | 169 | 708 | −72 | −302 | 82TPIS | 7789-48-2 |
| | | *173* | *723* | *−69±4* | *−287±15* | | |
| | IP is onset of photoelectron band (79LEE/POT2). | | | | | | |
| $Br_2OS^+$ | | | | | | | |
| $SOBr_2$ | (10.1) | (204) | (851) | −29 | −123 | 82TN270 | 507-16-4 |
| | | *(209)* | *(872)* | *−24* | *−102* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Br_2Pb^+$ | | | | | | | |
| $PbBr_2$ | 9.6 | (196) | (822) | −25±1 | −104±6 | 75JANAF | 10031-22-8 |
| | IP is onset of photoelectron band (84NOV/POT2, 82LEV/LIA). | | | | | | |
| $Br_2S_2^+$ | | | | | | | |
| $S_2Br_2$ | (9.23±0.03) | (221) | (923) | 8 | 33 | 82TN270 | 13172-31-1 |
| | IP from 81KAU/VAH. | | | | | | |
| $Br_2Se^+$ | | | | | | | |
| $SeBr_2$ | 9.07 | 204 | 854 | −5 | −21 | 82TN270 | 22987-45-7 |
| $Br_2Sn^+$ | | | | | | | |
| $SnBr_2$ | 9.0 | 201 | 839 | −7 | −29 | 82TPIS | 10031-24-0 |
| | IP is onset of photoelectron band (84NOV/POT2, 82LEV/LIA). | | | | | | |
| $Br_2Sr^+$ | | | | | | | |
| $SrBr_2$ | (9.11) | (114) | (477) | −96 | −402 | 82TPIS | 10476-81-0 |
| | | *(118)* | *(492)* | *−92±3* | *−387±11* | | |
| | IP is onset of photoelectron band (79LEE/POT2). See also: 82EMO/KIE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

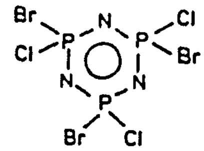
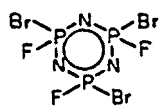
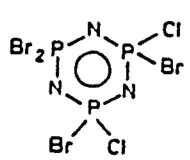
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $Br_3Cl_3N_3P_3^+$ | | | | | | | |
|  | (9.72±0.1) | (73) | (306) | −151 | −632 | *EST | 16032-52-3 |
| $Br_3F_3N_3P_3^+$ | | | | | | | |
|  | (10.37±0.03) | (−74) | (−311) | −314 | −1312 | *EST | 67336-18-9 |
| | IP from 81CLA/SOW. | | | | | | |
| $Br_3Ga^+$ | | | | | | | |
| $GaBr_3$ | 10.40 | 170 | 710 | −70 | −293 | 82TN270 | 13450-88-9 |
| $Br_3In^+$ | | | | | | | |
| $InBr_3$ | (10.0) | (163) | (683) | −67 | −282 | 82TN270 | 13465-09-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $Br_3La^+$ | | | | | | | |
| $LaBr_3$ | (9.85) | (87) | (364) | −140±2 | −586±7 | 78TPIS | 13536-79-3 |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| $Br_3OP^+$ | | | | | | | |
| $POBr_3$ | 10.75±0.02 | 151 | 632 | −97 | −405 | 71JANAF | 7789-59-5 |
| | | *161* | *673* | *−87* | *−364* | | |
| $Br_3P^+$ | | | | | | | |
| $PBr_3$ | 9.7 | (190) | (797) | −33 | −139 | 82TN270 | 7789-60-8 |
| | | *(196)* | *(821)* | *−27* | *−115* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Br_4Cl_2N_3P_3^+$ | | | | | | | |
|  | (9.60±0.1) | (82) | (343) | −139 | −583 | *EST | 15965-00-1 |
| $Br_4Hf^+$ | | | | | | | |
| $HfBr_4$ | (10.9) | (87) | (365) | −164 | −687 | 81SPE | 13777-22-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $Br_4Sn^+$ | | | | | | | |
| $SnBr_4$ | 10.6 | 169 | 708 | −75 | −315 | 82TN270 | 7789-67-5 |
| | | *177* | *739* | *−68* | *−284* | | |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

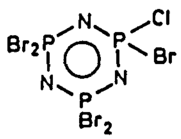
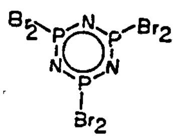
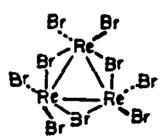
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$Br_4Ti^+$** | | | | | | | |
| $TiBr_4$ | 10.3 | (90) | (376) | −148±1 | −618±5 | 71JANAF | 7789-68-6 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Br_4Zr^+$** | | | | | | | |
| $ZrBr_4$ | (10.7) | (93) | (387) | −154±2 | −645±8 | 78JANAF | 13777-25-8 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Br_5ClN_3P_3^+$** | | | | | | | |
|  | (9.47±0.1) | (91) | (380) | −128 | −534 | *EST | 15608-37-4 |
| **$Br_5W^+$** | | | | | | | |
| $WBr_5$ | (8.3±0.2) | (144) | (602) | −48±5 | −199±21 | 71JANAF | 13470-11-6 |
| | | *(153)* | *(638)* | *−39* | *−163* | | |
| **$Br_6N_3P_3^+$** | | | | | | | |
|  | 9.62±0.03 | (82) | (343) | −140 | −585 | *EST | 13701-85-4 |
| | IP from 81CLA/SOW. | | | | | | |
| **$Br_9Re_3^+$** | | | | | | | |
|  | (8.4) | (125) | (521) | −69 | −289 | 82TN270 | 33517-16-7 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C^+$** | | | | | | | |
| C | 11.260 | 431.0 | 1803.2 | 171.3 | 716.7 | 82TN270 | 7440-44-0 |
| | | *429.7* | *1797.6* | *170.0* | *711.2* | | |
| **$CBr^+$** | | | | | | | |
| CBr | (10.43±0.02) | (362.5) | (1516.7) | 122.0±15 | 510.4±63 | 85JANAF | |
| | | *(363.4)* | *(1520.6)* | *122.9±15* | *514.3±63* | | |
| **$CBrClF_2^+$** | | | | | | | |
| $CF_2BrCl$ | (≤11.83) | (≤168) | (≤703) | −105±2 | −438±8 | 78KUD/KUD | 353-59-3 |
| **$CBrCl_3^+$** | | | | | | | |
| $CCl_3Br$ | (10.6) | (234) | (980) | −10.2±0.6 | −42.7±2.4 | 77PED/RYL | 75-62-7 |
| | IP is onset of photoelectron band (81NOV/CVI3). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CBrF_3^+$ | | | | | | | |
| $CF_3Br$ | 11.4 | 108 | 450 | −155 | −650 | 78KUD/KUD | 75-63-8 |
| | | *111* | *463* | *−152* | *−637* | | |
| | IP is onset of photoelectron band. See also: 82BOC/WIT. | | | | | | |
| $CBrN^+$ | | | | | | | |
| BrCN | 11.84±0.01 | 316 | 1323 | 43±1 | 181±4 | 77PED/RYL | 506-68-3 |
| $CBr_2Cl_2^+$ | | | | | | | |
| $CCl_2Br_2$ | (10.4) | (242) | (1012) | 2±2 | 9±8 | 78KUD/KUD | 594-18-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $CBr_2F_2^+$ | | | | | | | |
| $CF_2Br_2$ | 11.07±0.03 | 165 | 689 | −91±2 | −379±8 | 78KUD/KUD | 75-61-6 |
| $CBr_2O^+$ | | | | | | | |
| $COBr_2$ | (10.8) | (222) | (929) | −27±0.5 | −113±2 | 77PED/RYL | 593-95-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $CBr_3^+$ | | | | | | | |
| $CBr_3$ | (8.2) | (239) | (1000) | 49.6 | 207.5 | *EST | |
| | From appearance potential (10.47±0.02 eV) in $CBr_4$; IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CBr_3F^+$ | | | | | | | |
| $CFBr_3$ | 10.67±0.01 | 190 | 793 | −56±2 | −236±8 | 78KUD/KUD | 353-54-8 |
| $CBr_4^+$ | | | | | | | |
| $CBr_4$ | (10.31±0.02) | (258) | (1079) | 20.1±0.8 | 83.9±3.4 | 84BIC/MIN | 558-13-4 |
| | | *(265)* | *(1109)* | *27.2* | *113.8* | | |
| $CCe^+$ | | | | | | | |
| CCe | (7.5±1.0) | (336) | (1406) | 163 | 682 | 82TN270 | 12011-58-4 |
| $CCl^+$ | | | | | | | |
| CCl | (8.9±0.2) | (297) | (1243) | (92) | (384) | | |
| | $\Delta_f H$(Ion) from appearance potential determination. $\Delta_f H$(Neutral) is $\Delta_f H$(Ion) - IP. IP from 82HEP/TRE. | | | | | | |
| $CClF^+$ | | | | | | | |
| CClF | (10.7) | (243) | (1017) | −5±7 | −20±29 | 85LIA/KAR | 1691-88-9 |
| | $\Delta_f H$(Ion) from appearance potential determinations. IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). See: 85LIA/KAR (re-evaluated here). | | | | | | |
| $CClF_2^+$ | | | | | | | |
| $CClF_2$ | (8.3) | 126 | 528 | −66 | −275 | *EST | 1691-89-0 |
| | Cited heat of formation based on observation of near-thermoneutral reaction: ($C_2H_5^+$ + $CF_2Cl_2 \rightarrow CF_2Cl^+$ + $C_2H_5Cl$). Value based on appearance potential of ion (11.99 eV) in $CF_2Cl_2$ is 133 kcal/mol, 556 kJ/mol. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CClF_3{}^+$ | | | | | | | |
| $CF_3Cl$ | 12.39 | 116 | 485 | −169.7±0.6 | −710.0±2.3 | 77PED/RYL | 75-72-9 |
| | | *117* | *491* | *−168* | *−704* | | |
| | See also: 85KIS/MOR. | | | | | | |
| $CClN^+$ | | | | | | | |
| ClCN | 12.34±0.01 | 318 | 1329 | 33.0 | 138.0 | 77PED/RYL | 506-77-4 |
| | | *317* | *1328* | *32.8* | *137.3* | | |
| | Cited ionization potential corresponds to the formation of $CNCl^+(^2\Pi_{3/2})$. Formation of $CNCl^+(^2\Pi_{1/2})$ requires 12.37 eV. | | | | | | |
| $CClNO^+$ | | | | | | | |
| ClNCO | (10.72±0.01) | (253) | (1057) | 5.5 | 23.0 | 83DEW/RZE | 13858-09-8 |
| $CCl_2{}^+$ | | | | | | | |
| $CCl_2$ | 10.36 | 278 | 1163 | 39 | 163 | 85LIA/KAR | 1605-72-7 |
| | $\Delta_f H$(Ion) from appearance potential determinations. Cited IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). See 85LIA/KAR. | | | | | | |
| $CCl_2F^+$ | | | | | | | |
| $CCl_2F$ | (8.0) | (168) | (703) | −17.5 | −73 | *EST | 1691-90-3 |
| | From observation of near-thermoneutral reaction: ($C_2H_5{}^+ + CF_2Cl_2 \rightarrow CCl_2F^+ + C_2H_5F$) (77LIA/AUS). Appearance potential determinations lead to values of 175 kcal/mol, 732 kJ/mol, for the heat of formation of this ion. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CCl_2F_2{}^+$ | | | | | | | |
| $CF_2Cl_2$ | 11.75±0.04 | 157 | 656 | −114.1±1.3 | −477.5±5.6 | 77PED/RYL | 75-71-8 |
| | | *158* | *661* | *−113* | *−473* | | |
| | See also: 85KIS/MOR. | | | | | | |
| $CCl_2O^+$ | | | | | | | |
| $COCl_2$ | (11.4) | (210) | (880) | −53 | −220 | 82BAU/COX | 75-44-5 |
| | | *(211)* | *(882)* | *−52* | *−218* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $CCl_2S^+$ | | | | | | | |
| $CSCl_2$ | 9.61±0.02 | 215 | 900 | −6 | −27 | 79JOS | 463-71-8 |
| $CCl_3{}^+$ | | | | | | | |
| $CCl_3$ | (7.8) | (199) | (831) | 19 | 79 | 82MCM/GOL | 3170-80-7 |
| | $\Delta_f H$(Ion) is based on the observation of the reaction ($H_3O^+ + CFCl_3 \rightarrow CCl_3{}^+ + HF + H_2O$) and lack of occurrence of (sec-$C_3H_7{}^+ + CFCl_3 \rightarrow CCl_3{}^+ + C_3H_7F$) which brackets the heat of formation between 197 and 200 kcal/mol, 824 and 837 kJ/mol (77LIA/AUS). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). Experimental value: 8.28 eV. | | | | | | |
| $CCl_3F^+$ | | | | | | | |
| $CFCl_3$ | 11.77±0.02 | 207 | 868 | −64±2 | −268±8 | 77PED/RYL | 75-69-4 |
| | | *208* | *871* | *−63* | *−265* | | |
| | See also: 85KIS/MOR. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CCl_4^+$ | | | | | | | |
| $CCl_4$ | 11.47±0.01 | 241 | 1010 | −23.2±0.7 | −97.1±3 | 77PED/RYL | 56-23-5 |
| | | *242* | *1012* | *−22.7* | *−95.0* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| $CCo^+$ | | | | | | | |
| CCo | | (364) | (1524) | | | | |
| | $\Delta_fH$(Ion) from photodissociation onset to give $Co^+$ (86HET/FRE). | | | | | | |
| $CF^+$ | | | | | | | |
| CF | 9.11±0.01 | 271.1 | 1134.2 | 61.0±2 | 255.2±8 | 85JANAF | 3889-75-6 |
| | | *270.2* | *1130.6* | *60.1±2* | *231.6±8* | | |
| | IP from 84DYK/LEW. See also: 82HEP/TRE. | | | | | | |
| $CFN^+$ | | | | | | | |
| FCN | 13.32±0.01 | 316 | 1321 | 9±4 | 36±17 | 71JANAF | 1495-50-7 |
| $CFO^+$ | | | | | | | |
| FCO | 8.76±0.32 | (160) | (669) | −42±4 | −175±16 | 81DYK/JON2 | |
| | IP from 81DYK/JON2. | | | | | | |
| $CF_2^+$ | | | | | | | |
| $CF_2$ | 11.42±0.01 | 214 | 897 | −49±3 | −205±12 | 85LIA/KAR | 2154-59-8 |
| $CF_2O^+$ | | | | | | | |
| $COF_2$ | 13.03 | 147 | 617 | −153 | −640 | 77PED/RYL | 353-50-4 |
| | | *148* | *620* | *−152* | *−637* | | |
| $CF_2S^+$ | | | | | | | |
| $CSF_2$ | (10.45±0.01) | (157) | (658) | −84 | −350 | 79JOS | 420-32-6 |
| | See also: 85BIN/GRO. | | | | | | |
| $CF_2Se^+$ | | | | | | | |
| $CSeF_2$ | (9.6±0.2) | (154) | (646) | −67 | −280 | *EST | 54393-39-4 |
| | IP from 85BIN/GRO, 84BOC/AYG. | | | | | | |
| $CF_3^+$ | | | | | | | |
| $CF_3$ | (≤8.9) | (95.4) | (399.0) | −110 | −460 | 86TSA | 2264-21-3 |
| | | *(96.1)* | *(402.0)* | *−109* | *−457* | | |
| | $\Delta_fH$(Ion) from appearance potential determinations (82BOM/DAN). See also: 81BER/BEA, 83WAN/LER. IP estimated in 81LOG/TAK. | | | | | | |
| $CF_3I^+$ | | | | | | | |
| $CF_3I$ | 10.23 | 95 | 397 | −141±5 | −590±21 | 78KUD/KUD | 2314-97-8 |
| | See also: 81BER/BEA, 84BAN/YAT. | | | | | | |
| $CF_3NO^+$ | | | | | | | |
| $CF_3NO$ | (10.5±0.1) | (116) | (484) | −126 | −529 | *EST | 334-99-6 |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CF_4^+$ | | | | | | | |
| $CF_4$ | | | | −223.4±0.1 | −934.5±0.4 | 77PED/RYL | 75-73-0 |
| | | | | *−221.6* | *−927* | | |
| | The stable region of the $CF_4^+$ ground state is not accessible by a vertical transition from the $CF_4$ molecule; no $CF_4^+$ ions have been experimentally observed. The onset of the photoelectron spectrum is at ~15.3 eV(81BIE/ASB, 84CAR/FAH, 85NOV/POT). A value of < 14.7 eV was suggested in 77ROS/DRA. See also: 75LLO/ROB, 85KIS/MOR. | | | | | | |
| $CF_4O^+$ | | | | | | | |
| $CF_3OF$ | (13.0) | (112) | (469) | −188 | −785 | 69STU/WES | 373-91-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $CF_5N^+$ | | | | | | | |
| $CF_3NF_2$ | (11.9) | (105) | (440) | −169±0.5 | −708±2 | 77PED/RYL | 335-01-3 |
| | IP from 82BUR/PAW. | | | | | | |
| $CFe^+$ | | | | | | | |
| FeC | | (358) | (1499) | | | | |
| | $\Delta_f H$(Ion) from photodissociation onset to give $Fe^+$ (86HET/FRE). | | | | | | |
| $CGe^+$ | | | | | | | |
| GeC | (10.3±0.3) | *(388)* | *(1622)* | *150* | *628* | 79HUB/HER | 12334-26-8 |
| | 0 K values. | | | | | | |
| $CH^+$ | | | | | | | |
| CH | 10.64±0.01 | 387.8 | 1622.4 | 142.4 | 595.8 | 79HUB/HER | 3315-37-5 |
| | | *387.0* | *1619.1* | *141.6* | *592.5* | | |
| | See also: 83PLE/MAR. | | | | | | |
| $CHBrCl_2^+$ | | | | | | | |
| $CHBrCl_2$ | 10.6 | 233 | 974 | −12 | −49 | 78KUD/KUD | 75-27-4 |
| | IP is onset of photoelectron band (81NOV/CVI3). | | | | | | |
| $CHBrF_3^+$ | | | | | | | |
| $CF_3BrH$ | | 73 | 305 | | | | |
| | From proton affinity of $CBrF_3$(RN 75-63-8) (85MCM/KEB) re-evaluated relative to CO standard (84LIA/LIE). PA = 137.5 kcal/mol, 575.3 kJ/mol. | | | | | | |
| $CHBrN^+$ | | | | | | | |
| BrCNH | | 231 | 965 | | | | |
| | From proton affinity of BrCN (RN 506-68-3). PA = 178.3 kcal/mol, 746 kJ/mol. | | | | | | |
| $CHBr_2^+$ | | | | | | | |
| $CHBr_2$ | (7.4) | (224) | (936) | 54 | 227 | 82MCM/GOL✓ | 14362-13-1 |
| | Ion heat of formation from appearance potential (10.70±0.02 eV) in $CHBr_3$. Cited ionization potential is difference between this heat of formation and that of neutral. Experimental determinations of this ionization potential gave values of 8.13±0.16 eV (77ROS/DRA), 8.41±0.03 eV (V) (84AND/DYK3). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CHBr_2Cl^+$ | | | | | | | |
| $CHClBr_2$ | 10.59±0.01 | 246 | 1031 | 2±2 | 9±8 | 78KUD/KUD | 124-48-1 |
| | IP (77ROS/DRA) in good agreement with onset of photoelectron band (81NOV/CVI3). | | | | | | |
| $CHBr_3^+$ | | | | | | | |
| $CHBr_3$ | 10.48±0.02 | 247.4 | 1035.0 | 5.7±1.1 | 23.8±4.5 | 84BIC/MIN | 75-25-2 |
| | See also: 82VON/ASB. | | | | | | |
| $CHCl^+$ | | | | | | | |
| CHCl | 9.84 | 298 | 1247 | 71 | 297 | 85LIA/KAR | 2108-20-5 |
| | $\Delta_f H$(Ion) derived from hydrogen affinity considerations. IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). | | | | | | |
| $CHClF^+$ | | | | | | | |
| CClFH | (8.81±0.02) | (178) | (743) | (−25) | (−105) | | 33272-71-8 |
| | $\Delta_f H$(Ion) from observation of: ($CF_2Cl^+$ + $CHFCl_2$ → $CHFCl^+$ + $CF_2Cl_2$) and non-observation of: ($C_2H_5^+$ + $CHFCl_2$ → $CHFCl^+$ + $C_2H_5Cl$)(77LIA/AUS). Appearance potential determinations lead to a value of 205 kcal/mol, 858 kJ/mol. IP from 84AND/DYK. | | | | | | |
| $CHClF_2^+$ | | | | | | | |
| $CHF_2Cl$ | (12.2) | (166) | (694) | −115.6±0.5 | −483.5±2.2 | 77PED/RYL | 75-45-6 |
| | See also: 81NOV/CVI3. | | | | | | |
| $CHClF_3^+$ | | | | | | | |
| $CF_3ClH$ | | 60 | 251 | | | | |
| | From proton affinity of $CF_3Cl$(RN 75-72-9) (85MCM/KEB) re-evaluated relative to CO standard(84LIA/LIE). PA = 136 kcal/mol, 569 kJ/mol. | | | | | | |
| $CHClN^+$ | | | | | | | |
| ClCNH | | 224 | 937 | | | | |
| | From proton affinity of ClCN (RN 506-77-4). PA = 174.8 kcal/mol, 731 kJ/mol (86MAR/TOP). | | | | | | |
| $CHCl_2^+$ | | | | | | | |
| $CHCl_2$ | (8.1) | (212) | (887) | 26±1 | 108±4 | 83WEI/BEN | 3474-12-2 |
| | $\Delta_f H$(Ion) from appearance potential (11.49±0.02 eV) in $CCl_3H$. Cited IP is difference between heats of formation of ion and neutral. An experimental determination of the IP gave a value of 8.32 eV(84AND/DYK) which would correspond to a $\Delta_f H$(Radical) of 20 kcal/mol, 84 kJ/mol. | | | | | | |
| $CHCl_2F^+$ | | | | | | | |
| $CHFCl_2$ | (11.5) | (198) | (829) | −67±2 | −281±8 | 78KUD/KUD | 75-43-4 |
| | IP is onset of photoelectron band (82LEV/LIA, 81NOV/CVI3). | | | | | | |
| $CHCl_3^+$ | | | | | | | |
| $CHCl_3$ | 11.37±0.02 | 237 | 992 | −25.0±0.5 | −104.8±2 | 77PED/RYL | 67-66-3 |
| | | *238* | *997* | *−23.8* | *−99.7* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CHCo^+$ | | | | | | | |
| CHCo | | (325) | (1361) | | | | |
| | $\Delta_f H$(Ion) from photodissociation onset to give $Co^+$ (86HET/FRE). | | | | | | |
| $CHF^+$ | | | | | | | |
| CHF | (10.49) | (268) | (1121) | 26±3 | 109±12 | 85LIA/KAR | 13453-52-6 |
| | $\Delta_f H$(Ion) from hydrogen affinity considerations. IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral)(85LIA/KAR). | | | | | | |
| $CHFN^+$ | | | | | | | |
| FCNH | | (224) | (934) | | | | |
| | $\Delta_f H$(Ion) from core binding energies of isoelectronic neutral HNCO (84BEA/EYE). | | | | | | |
| $CHFO^+$ | | | | | | | |
| HFCO | (12.37±0.02) | (195) | (817) | −90 | −377 | 71JANAF | 1493-02-3 |
| $CHF_2^+$ | | | | | | | |
| $CHF_2$ | (8.78) | (146) | (611) | −57±1 | −237±5 | 83PIC/ROD | 2670-13-5 |
| | Heat of formation of ion derived from observed ion-molecule reactions (74BLI/MCM, 77LIA/AUS); cited ionization potential is the difference between the heats of formation of the ion and the radical. | | | | | | |
| $CHF_2O^+$ | | | | | | | |
| $F_2COH$ | | 52 | 219 | | | | |
| | From proton affinity of $CF_2O$ (RN 353-50-4). PA = 160.5 kcal/mol, 671.5 kJ/mol. | | | | | | |
| $CHF_3^+$ | | | | | | | |
| $CHF_3$ | 13.86 | 154 | 642 | −166±2 | −695±8 | 78KUD/KUD | 75-46-7 |
| | | *156* | *649* | *−164* | *−688* | | |
| | See also: 81BIE/ASB, 85NOV/POT, 82BOC/WIT. | | | | | | |
| $CHF_3I^+$ | | | | | | | |
| $CF_3IH$ | | (78) | (326) | | | | |
| | From proton affinity of $CF_3I$ (RN 2314-97-8) (85MCM/KEB) re-evaluated relative to CO standard (84LIA/LIE). PA = 146.7 kcal/mol, 614 kJ/mol. | | | | | | |
| $CHF_3NO^+$ | | | | | | | |
| $CF_3NHO$ | | (70) | (294) | | | | |
| | From the proton affinity of $CF_3NO$ (RN 334-99-6). PA = 70. kcal/mol, 294. kJ/mol. | | | | | | |
| $CHF_4^+$ | | | | | | | |
| $F_3CFH$ | | 17 | 70 | | | | |
| | From proton affinity of $CF_4$ (RN 75-73-0). PA = -126 kcal/mol, -527 kJ/mol. | | | | | | |
| $CHF_4N^+$ | | | | | | | |
| $CHF_2NF_2$ | (11.5) | (156) | (655) | −109 | −455 | *EST | 24708-53-0 |
| | IP from 82BUR/PAW. | | | | | | |
| $CHFe^+$ | | | | | | | |
| CHFe | | (322) | (1349) | | | | |
| | $\Delta_f H$(Ion) from photodissociation onset to give $Fe^+$ (86HET/FRE). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CHI_3^+$ | | | | | | | |
| $CHI_3$ | 9.25±0.02 | 241 | 1010 | 28±5 | 118±21 | 78KUD/KUD | 75-47-8 |
| | | *244* | *1019* | *30* | *127* | | |
| $CHN^+$ | | | | | | | |
| HCN | 13.60±0.01 | 346 | 1447 | 32.3 | 135.1 | 82TN270 | 74-90-8 |
| | | *346* | *1448* | *32.4* | *135.5* | | |
| | See also: 82KRE/SCH, 81KIM/KAT. | | | | | | |
| HNC | (12.5±0.1) | (336) | (1407) | 48±2 | 201±8 | 82PAU/HEH | 6914-07-4 |
| | IP by charge exchange bracketing of $HNC^+$ ions generated in $CH_3NC$(78BIE/JON). See also: 80MCL/MCG. | | | | | | |
| $CHNO^+$ | | | | | | | |
| HNCO | 11.61±0.03 | 243 | 1015 | −25±3 | −105±13 | 86SPI/PER | 75-13-8 |
| HCNO | (10.83) | (302) | (1263) | 52 | 218 | *EST | 506-85-4 |
| $CHNS^+$ | | | | | | | |
| HNCS | 9.94±0.02 | 260 | 1087 | 31 | 128 | 82TN270 | 3129-90-6 |
| $CHO^+$ | | | | | | | |
| HCO | 8.10±0.05 | 197.3 | 825.6 | 10.7 | 44.8 | 77BEC/LIP | 17030-74-9 |
| | $\Delta_f H$(Ion) from appearance potential measurements (85TRA2). See also: 76GUY/CHU, 84WAN/CAP, 80DYK/JON. | | | | | | |
| COH | | (230) | (963) | | | | |
| | $\Delta_f H$(Ion) from correlation with oxygen 1s binding energy (85MCM/KEB2). See also: 85WAG/KEM, 83BUR/MOM. | | | | | | |
| $CHOS^+$ | | | | | | | |
| COSH | | 181 | 757 | | | | |
| | From proton affinity of COS (RN 463-58-1) (85MCM/KEB, 85MCM/KEB2) re-evaluated relative to CO standard (84LIA/LIE). PA = 150.7 kcal/mol, 631 kJ/mol. | | | | | | |
| $CHOSe^+$ | | | | | | | |
| COSeH | | 230 | 962 | | | | |
| | From proton affinity of COSe (RN 1603-84-5) (85KAR). PA = 152. kcal/mol, 637. kJ/mol. | | | | | | |
| $CHO_2^+$ | | | | | | | |
| COOH | | 141 | 589 | | | | 2564-86-5 |
| | $\Delta_f H$(Ion) from appearance potential in HCOOH. | | | | | | |
| $CHP^+$ | | | | | | | |
| HCP | (10.79±0.01) | (289) | (1208) | 40±15 | 167±63 | 71JANAF | 6829-52-3 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CHS^+$ | | | | | | | |
| HCS | > (7.3) | 243 | 1018 | ≤73 | ≤305 | 83BUT/BAE | |
| | | *243* | *1018* | *≤74* | *≤310* | | |
| | $\Delta_f H$(Ion) from appearance potential determinations in thiirane (RN 420-12-2) (82BUT/BAE) in good agreement with value derived from proton affinity of CS (RN 2944-05-0) (85SMI/ADA). PA = 188.2 kcal/mol, 787 kJ/mol. IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). See also: 82KUT/EDW, 82KUT/EDW. | | | | | | |
| $CHS_2{}^+$ | | | | | | | |
| HSCS | | 229 | 959 | | | | |
| | From proton affinity of $CS_2$(RN 75-15-0), re-evaluated. PA = 164.4 kcal/mol, 688. kJ/mol. See also: 85MCM/KEB, 85WEI/PLA. | | | | | | |
| $CHTi^+$ | | | | | | | |
| TiCH | | *(289)* | *(1209)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). 0 K value. | | | | | | |
| $CHV^+$ | | | | | | | |
| VCH | | *(307)* | *(1283)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM, 86ARI/ARM). 0 K value. | | | | | | |
| $CH_2{}^+$ | | | | | | | |
| $CH_2$ | 10.396±.003 | 331 | 1386 | 93 | 390 | 82TN270 | 60528-76-9 |
| | | *331* | *1386* | *93* | *390* | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83PLE/MAR). | | | | | | |
| $CH_2Br^+$ | | | | | | | |
| $CH_2Br$ | (7.9) | (224) | (937) | 42 | 174 | 82MCM/GOL | 16519-97-4 |
| | Heat of formation of ion from appearance potential (11.35±0.02) in $CH_2Br_2$. Cited ionization potential is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). An experimental value of 8.61±0.01 eV has been reported for the ionization potential (84AND/DYK3). | | | | | | |
| $CH_2BrCl^+$ | | | | | | | |
| $CH_2ClBr$ | 10.77±0.01 | 259 | 1084 | 11±2 | 45±8 | 78KUD/KUD | 74-97-5 |
| | IP from 77ROS/DRA, 81NOV/CVI3. | | | | | | |
| $CH_2Br_2{}^+$ | | | | | | | |
| $CH_2Br_2$ | 10.50±0.02 | 242 | 1013 | 0±1 | 0±4 | EST | 74-95-3 |
| | See also: 82VON/ASB. | | | | | | |
| $CH_2Cl^+$ | | | | | | | |
| $CH_2Cl$ | (8.6) | (229.2) | (959.0) | 31 | 130 | 83WEI/BEN | 6806-86-6 |
| | | *(229.9)* | *(962.1)* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations. Cited ionization potential is difference in heats of formation of ion and radical; an experimental determination of the ionization potential gives 8.75±0.01 eV(84AND/DYK) which would correspond to a radical heat of formation of 27 kcal/mol, 115 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CH_2ClF^+$ | | | | | | | |
| $CH_2FCl$ | 11.71±0.01 | 208 | 869 | −62±2 | −261±8 | 78KUD/KUD2 | 593-70-4 |
| | IP from 84AND/DYK. | | | | | | |
| $CH_2Cl_2^+$ | | | | | | | |
| $CH_2Cl_2$ | 11.32±0.01 | 238 | 997 | −22.9±0.2 | −95.7±0.8 | 77PED/RYL | 75-09-2 |
| | | *240* | *1003* | *−21.2* | *−88.8* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| $CH_2Cl_4Si^+$ | | | | | | | |
| $Cl_3SiCH_2Cl$ | (10.7) | (116) | (486) | −130 | −546 | *EST | 1558-25-4 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| $CH_2Co^+$ | | | | | | | |
| $CH_2=Co$ | | *(290)* | *(1213)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction and photodissociation (81ARM/HAL, 81ARM/BEA2, 86HET/FRE). 0 K values. | | | | | | |
| $CH_2Cr^+$ | | | | | | | |
| $CH_2=Cr$ | | *(292)* | *(1223)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARI). See also: 81ARM/HAL, 81HAL/ARM. 0 K values. | | | | | | |
| $CH_2F^+$ | | | | | | | |
| $CH_2F$ | 9.05±0.01 | 199 | 833 | −8±2 | −33±8 | 82MCM/GOL | 3744-29-4 |
| | IP from 84AND/DYK. $\Delta_f H$(Ion) evaluated from observed ion-molecule reactions (77LIA/AUS). | | | | | | |
| $CH_2F_2^+$ | | | | | | | |
| $CH_2F_2$ | 12.71 | 185 | 773 | −108±2 | −453±8 | 78KUD/KUD | 75-10-5 |
| | See also: 81BIE/ASB. | | | | | | |
| $CH_2F_3^+$ | | | | | | | |
| $F_2CHFH$ | | 53 | 220 | | | | |
| | From proton affinity of $CF_3H$ (RN 75-46-7). PA = 147 kcal/mol, 615 kJ/mol. | | | | | | |
| $CH_2F_3O_3S^+$ | | | | | | | |
| $CF_3SO_3H_2$ | | (−85) | (−356) | | | | |
| | From proton affinity of $CF_3SO_3H$ (RN 1493-13-6). PA = (169) kcal/mol, (707) kJ/mol. | | | | | | |
| $CH_2Fe^+$ | | | | | | | |
| $CH_2=Fe$ | | *(292)* | *(1222)* | | | | |
| | $\Delta_f H$(Ion) from photodissociation onset to give $Fe^+$ (86HET/FRE). See also: 81ARM/HAL, 84JAC/JAC. | | | | | | |
| $CH_2I_2^+$ | | | | | | | |
| $CH_2I_2$ | 9.46±0.02 | 246 | 1031 | 28±5 | 118±21 | 78KUD/KUD | 75-11-6 |
| | | *249* | *1040* | *30* | *127* | | |
| $CH_2Mn^+$ | | | | | | | |
| $CH_2=Mn$ | | *(237)* | *(992)* | | | | 65127-77-7 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (81ARM/HAL). 0 K values. | | | | | | |

Table 1. Positive Ion Table - Continued

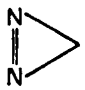
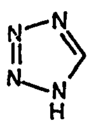
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CH_2N^+$ | | | | | | | |
| HCNH | | 226 | 947 | | | | |
| | From proton affinity of HCN (RN 74-90-8) (PA = 171 kcal/mol, 717 kJ/mol) and HNC (RN 6914-07-4) (PA = 190 kcal/mol, 796 kJ/mol). | | | | | | |
| $CNH_2$ | | (265) | (1109) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (84BUR/HOL). | | | | | | |
| $CH_2NO^+$ | | | | | | | |
| $H_2NCO$ | | 167 | 700 | | | | |
| | From proton affinity of HNCO (RN 75-13-8) (PA = 173 kcal/mol, 725 kJ/mol). | | | | | | |
| $CH_2N_2^+$ | | | | | | | |
| $CH_2N_2$ | 8.999±0.001 | 263 | 1098 | 55±4 | 230±17 | 78VOG/WIL | 334-88-3 |
| $H_2NCN$ | (10.4) | (272) | (1137) | 32 | 134 | 77PED/RYL | 420-04-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (10.3) | (301) | (1259) | 63.3±2.7 | 264.8±11 | 72LAU/OKA | 157-22-2 |
| $CH_2N_4^+$ | | | | | | | |
|  | (10.95) | (333) | (1392) | 80±1 | 335±4 | 77PED/RYL | 288-94-8 |
| | IP is onset of photoelectron band (82LEV/LIA, 81PAL/SIM). | | | | | | |
| $CH_2Ni^+$ | | | | | | | |
| $CH_2$=Ni | | *(285)* | *(1193)* | | | | 60187-22-6 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (81ARM/HAL). 0 K values. | | | | | | |
| $CH_2O^+$ | | | | | | | |
| $CH_2O$ | 10.874±0.002 | 224.8 | 940.5 | -26.0±0.2 | -108.7±0.7 | 77PED/RYL | 50-00-0 |
| | | *225.8* | *944.5* | *-25.0* | *-104.7* | | |
| | See also: 81BOM/DAN, 76GUY/CHU, 80VON/BIE, 84WAN/CAP, 81KIM/KAT. | | | | | | |
| HCOH | | 230 | 962 | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurement (83BUR/MOM). | | | | | | |
| $CH_2O_2^+$ | | | | | | | |
| HCOOH | 11.33±0.01 | 170.7 | 714.3 | -90.5±0.1 | -378.8±0.5 | 78CHA/ZWO | 64-18-6 |
| | See also: 80VON/BIE, 81KIM/KAT. | | | | | | |
| $C(OH)_2$ | - | 175 | 732 | | | | 71946-83-3 |
| | $\Delta_f H$(Ion) from appearance potential determinations (82BUR/HOL, 83BUR/MOM). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$CH_2S^+$** | | | | | | | |
| $CH_2S$ | 9.34±0.01 | 240 | 1006 | 25 | 105 | 82ROY/MCM | 865-36-1 |
| | See also: 83ERM/AKO, 82KUT/EDW. | | | | | | |
| HCSH | | *(270)* | *(1130)* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (82KUT/EDW). 0 K values. | | | | | | |
| **$CH_2Se^+$** | | | | | | | |
| $CH_2Se$ | (8.95) | (245) | (1024) | 38 | 160 | *EST | 6596-50-5 |
| | IP from 84BOC/AYG. | | | | | | |
| **$CH_2Ti^+$** | | | | | | | |
| $CH_2=Ti$ | | *(277)* | *(1158)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). 0 K value. | | | | | | |
| **$CH_2V^+$** | | | | | | | |
| $CH_2=V$ | | *(295)* | *(1234)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM, 86ARI/ARM). 0 K value. | | | | | | |
| **$CH_3^+$** | | | | | | | |
| $CH_3$ | 9.84±0.01 | 261.3±0.4 | 1093.3±1.7 | 34.8±0.3 | 145.8±1 | 81HEN/KNO | 2229-07-4 |
| | | *262* | *1098* | *35.6* | *149.0* | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (81TRA/MCL). See also: 83PLE/MAR. | | | | | | |
| **$CH_3BBr_2^+$** | | | | | | | |
| $CH_3BBr_2$ | 10.60 | 197 | 824 | −48 | −199 | 82HOL/SMI | 17933-16-3 |
| **$CH_3BCl_2^+$** | | | | | | | |
| $CH_3BCl_2$ | (11.51) | (185) | (774) | −81 | −337 | 82HOL/SMI | 7318-78-7 |
| **$CH_3BF_2^+$** | | | | | | | |
| $CH_3BF_2$ | (12.54±0.03) | (90) | (377) | −199 | −833 | 82HOL/SMI | 373-64-8 |
| **$CH_3BO^+$** | | | | | | | |
| $BH_3CO$ | 11.14±0.02 | 230 | 964 | −27 | −111 | 82TN270 | 13205-44-2 |
| | | *232* | *970* | *−25.0* | *−104.8* | | |
| **$CH_3Br^+$** | | | | | | | |
| $CH_3Br$ | 10.541±0.003 | 234 | 979 | −9.1±0.3 | −38.1±1.3 | 84BIC/MIN | 74-83-9 |
| | | *238* | *994* | *−5.5* | *−23.0* | | |
| | Cited IP leads to $CH_3Br^+$ ($^2E_{3/2}$); formation of $CH_3Br^+$ ($^2E_{1/2}$) requires 10.857 eV. IPs from 82BAI/CON,82LEV/LIA,77ROS/DRA,82VON/ASB,81HOL/FIN,84AND/DYK3,81KIM/KAT,77KAR/JAD. | | | | | | |
| $CH_2BrH$ | | (237) | (990) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83HOL/LOS2). | | | | | | |
| **$CH_3BrHg^+$** | | | | | | | |
| $CH_3HgBr$ | (9.9) | (224) | (937) | −4±0.7 | −18±3 | 77PED/RYL | 506-83-2 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CH_3Cd^+$ | | | | | | | |
| $CH_3Cd$ | | (213) | (891) | | | | |
| | From appearance potential (9.69 eV) in $(CH_3)_2Cd$. | | | | | | |
| $CH_3Cl^+$ | | | | | | | |
| $CH_3Cl$ | 11.22±0.01 | 239 | 1000 | −19.6±0.1 | −82.0±0.5 | 79KUD/KUD | 74-87-3 |
| | | *241* | *1009* | *−17.5* | *−73.4* | | |
| | See also: 81KIM/KAT, 77KAR/JAD. | | | | | | |
| $CH_2ClH$ | | (246) | (1029) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83HOL/LOS2). | | | | | | |
| $CH_3ClHg^+$ | | | | | | | |
| $CH_3HgCl$ | (10.5) | (230) | (962) | −12±0.7 | −51±3 | 77PED/RYL | 115-09-3 |
| | IP is onset of photoelectron band (77ROS/DRA, 81BAI/CHI2). | | | | | | |
| $CH_3ClO^+$ | | | | | | | |
| $CH_3OCl$ | (10.39±0.02) | (226) | (944) | −14 | −58 | *EST | 593-78-2 |
| | IP from 81COL/FRO. | | | | | | |
| $CH_3ClO_2S^+$ | | | | | | | |
| $CH_3SO_2Cl$ | 11.3 | (173) | (722) | −88 | −368 | *EST | 124-63-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3Cl_2N^+$ | | | | | | | |
| $CH_3NCl_2$ | 9.52 | (264) | (1104) | 44 | 185 | *EST | 7651-91-4 |
| $CH_3Cl_2OP^+$ | | | | | | | |
| $CH_3POCl_2$ | 10.91 | 119 | 497 | −133±6 | −556±25 | 77PED/RYL | 676-97-1 |
| | IP from 80ZVE/VIL, 82LEV/LIA. | | | | | | |
| $CH_3Cl_2P^+$ | | | | | | | |
| $CH_3PCl_2$ | (9.5) | (168) | (703) | −51 | −214 | *EST | 676-83-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3Cl_3Si^+$ | | | | | | | |
| $CH_3SiCl_3$ | (11.36±0.03) | (131) | (547) | −131 | −549 | 81BEL/PER | 75-79-6 |
| $CH_3Co^+$ | | | | | | | |
| $CH_3Co$ | (7.0±0.3) | *(257)* | *(1075)* | *(96)* | *(400)* | 81ARM/BEA | 76826-90-9 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (81ARM/HAL). IP from 81ARM/BEA. 0 K values. | | | | | | |
| $CH_3Cr^+$ | | | | | | | |
| $CH_3Cr$ | (7.2) | *(257)* | *(1074)* | *90* | *375* | 86ELK/ARI | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARI).<br>See also: 81ARM/HAL. 0 K values. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CH_3F^+$ | | | | | | | |
| $CH_3F$ | 12.47±0.02 | 228 | 956 | −59 | −247 | 85LIA/KAR | 593-53-3 |
| | See also: 81BIE/ASB, 81KIM/KAT, 77KAR/JAD. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$CH_3F^+$** | | | | | | | |
| $CH_2FH$ | | 217 | 908 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83HOL/LOS2). | | | | | | |
| **$CH_3F_2^+$** | | | | | | | |
| $FCH_2FH$ | | 110 | 462 | | | | |
| | From proton affinity of $CH_2F_2$ (RN 75-10-5). PA = 147 kcal/mol, 615 kJ/mol. | | | | | | |
| **$CH_3F_2P^+$** | | | | | | | |
| $CH_3PF_2$ | (9.8) | (68) | (285) | −158 | −661 | *EST | 753-59-3 |
| | IP is onset of photoelectron band. | | | | | | |
| **$CH_3F_2Si^+$** | | | | | | | |
| $CH_3SiF_2$ | | 23 | 95 | | | | |
| | From appearance potential (11.70±0.03) of ion in $(CH_3)_2SiF_2$. | | | | | | |
| **$CH_3F_3Si^+$** | | | | | | | |
| $CH_3SiF_3$ | 12.48±0.04 | −8 | −33 | −296 | −1237 | 71JANAF | 373-74-0 |
| **$CH_3Fe^+$** | | | | | | | |
| $CH_3Fe$ | (8.1) | *(257)* | *(1075)* | *71* | *298* | 86ELK/ARI | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARI). See also: 81ARM/HAL, 84JAC/JAC. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |
| **$CH_3Hg^+$** | | | | | | | |
| $CH_3Hg$ | | 221 | 926 | | | | |
| | | *225* | *942* | | | | |
| | From appearance potential (10.10±0.02 eV) in $(CH_3)_2Hg$. | | | | | | |
| **$CH_3HgI^+$** | | | | | | | |
| $CH_3HgI$ | (9.0) | (213) | (891) | 5.3±0.4 | 22.4±1.9 | 77PED/RYL | 143-36-2 |
| | IP is onset of photoelectron band. | | | | | | |
| **$CH_3I^+$** | | | | | | | |
| $CH_3I$ | 9.538 | 223.6 | 935.7 | 3.7±0.2 | 15.4±0.9 | 77PED/RYL | 74-88-4 |
| | | *226* | *945* | *6* | *25* | | |
| | See: 78LIA/AUS, 83POW, 81KIM/KAT, 77KAR/JAD. | | | | | | |
| **$CH_3Mn^+$** | | | | | | | |
| $CH_3Mn$ | | *(223)* | *(934)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ARM). See also: 81ARM/HAL. 0 K values. | | | | | | |
| **$CH_3Mn_2^+$** | | | | | | | |
| $CH_3Mn_2$ | | *(261)* | *(1090)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ARM). 0 K values. | | | | | | |
| **$CH_3N^+$** | | | | | | | |
| $CH_2=NH$ | (9.9) | (260) | (1090) | 32 | 135 | 78DEF/HEH | 2053-29-4 |
| | IP is onset of photoelectron band (82SCH/SCH, 86WER). | | | | | | |
| $HCNH_2$ | | 258 | 1079 | | | | 35430-17-2 |
| | $\Delta_f H$(Ion) from appearance potential determinations(84BUR/HOL). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$CH_3NO^+$** | | | | | | | |
| $HCONH_2$ | 10.16±0.06 | 190 | 794 | −44 | −186 | 69BEN/CRU | 75-12-7 |
| | See also: 81KIM/KAT, 81ASB/SVE, 81HEN/ISA. | | | | | | |
| $CH_2=NOH$ | 10.11 | (240) | (1004) | 7 | 29 | *EST | 75-17-2 |
| | IP is onset of photoelectron band (82FRO/LAU, 84DOG/POU). | | | | | | |
| $CH_3NO$ | 9.3 | 231 | 967 | 17±0.7 | 70±3 | 73BAT/MIL | 865-40-7 |
| | IP is onset of photoelectron band (82CHO/FRO, 82FRO/LAU). | | | | | | |
| **$CH_3NO_2^+$** | | | | | | | |
| $CH_3NO_2$ | 11.02±0.04 | 236 | 987 | −17.9±0.2 | −74.8±1.0 | 77PED/RYL | 75-52-5 |
| | See also: 83GIL/HSI, 83OGD/SHA, 81ALL/MIG, 81ASB/SVE, 81KIM/KAT. | | | | | | |
| $CH_3ONO$ | 10.38±0.03 | 223 | 935 | −15.9±0.2 | −66.5±0.9 | 74BAT/CHR | 624-91-9 |
| | IP from 83GIL/HSI, 83GIL/HSI2, 80MEI/HSI, 83OGD/SHA. | | | | | | |
| **$CH_3NO_3^+$** | | | | | | | |
| $CH_3ONO_2$ | (11.53±0.01) | (237) | (990) | −29±1 | −122±4 | 77PED/RYL | 598-58-3 |
| **$CH_3NS^+$** | | | | | | | |
| $HCSNH_2$ | 8.69 | (210) | (877) | 9 | 39 | *EST | 115-08-2 |
| | See also: 81HEN/ISA. | | | | | | |
| **$CH_3N_2^+$** | | | | | | | |
| $CH_3N_2$ | | 216 | 902 | | | | |
| | From appearance energy and from proton affinity of $CH_2N_2$ (RN 334-88-3)(PA = 205 kcal/mol, 858 kJ/mol). | | | | | | |
| $H_2NCNH$ | | (234) | (978) | | | | |
| | From core binding energy of isoelectronic $CH_3CN$ (84BEA/EYE). PA of $H_2NCN$ = (164) kcal/mol, (686) kJ/mol. | | | | | | |
| **$CH_3N_3^+$** | | | | | | | |
| $CH_3N_3$ | 9.81±0.02 | 293 | 1227 | 67 | 280 | 69BEN/CRU | 624-90-8 |
| | See also: 81BOC/DAM. | | | | | | |
| **$CH_3Ni^+$** | | | | | | | |
| $CH_3Ni$ | | *(265)* | *(1109)* | | | | 63583-16-4 |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (81ARM/HAL, 86ELK/ARI). 0 K values. | | | | | | |
| **$CH_3O^+$** | | | | | | | |
| $CH_2OH$ | 7.56±0.01 | 168 | 703 | −6.2±1.5 | −25.9±6 | 82MCM/GOL | 17691-31-5 |
| | $\Delta_fH$(Ion) from proton affinity of formaldehyde. PA = 171.7 kcal/mol, 718 kJ/mol. $\Delta_fH$(Ion) from appearance potential measurements is 169 kcal/mol, 709 kJ/mol. (82MAC, 83HOL/LOS2, 84LOS/HOL). IP from 84DYK/ELL2. | | | | | | |
| $CH_3O$ | (8.6) | (201) | (842) | 3.7±0.7 | 15.5±2.9 | 74BAT/CHR | 2143-68-2 |
| | The reaction: $HCO^+ + H_2 \rightarrow CH_3O^+$ is 3.9 kcal/mol, 16.3 kJ/mol, exothermic (77HIR/KEB). A value of 247 kcal/mol, 1034 kJ/mol, has been reported for $^3CH_3O^+$ (84BUR/HOL2) in agreement with 87FER/RON. IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CH_3O_2^+$ | | | | | | | |
| $HC(OH)_2$ | | 96 | 403 | | | | |
| | From proton affinity of HCOOH (RN 64-18-6) and appearance potential determinations (84HOL/LOS). PA = 178.8 kcal/mol, 748 kJ/mol. | | | | | | |
| $CH_2OOH$ | | (185) | (774) | | | | |
| | $\Delta_f H$(Ion) from 87FER/RON. | | | | | | |
| $CH_3O_3^+$ | | | | | | | |
| $C(OH)_3$ | | 37 | 155 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations(82HOL/LOS2). | | | | | | |
| $CH_3S^+$ | | | | | | | |
| $CH_2SH$ | | 206 | 862 | | | | 20879-50-9 |
| | | *208* | *870* | | | | |
| | Heat of formation of ion from appearance potential determinations (83BUT/BAE, 82LEV/LIA). See also: 83ERM/AKO, 83HOL/LOS2. | | | | | | |
| $CH_3S$ | (8.06±0.1) | (215) | (901) | 29.4±2.1 | 123.0±8.8 | 82MCM/GOL | 7175-75-9 |
| | Collisional activation results (79DIL/MCL) indicate that this structure is a stable triplet; ab initio calculations predict its heat of formation to be ~10 kcal/mol above that of $CH_2SH^+$, in agreement with the experimentally obtained value given here. | | | | | | |
| $CH_3S_2^+$ | | | | | | | |
| $CH_3SS$ | (8.0) | 200 | 835 | 16 | 69 | 86HAW/GRI | |
| | | *201* | *839* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83BUT/BAE). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CH_3Sc^+$ | | | | | | | |
| $CH_3Sc$ | (5.1) | *(212)* | *(887)* | *93* | *391* | 86SUN/ARI | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 87SUN/ARI. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |
| $CH_3Se^+$ | | | | | | | |
| $CH_2SeH$ | | 219 | 916 | | | | |
| | From proton affinity of $CH_2Se$ (RN 6596-50-5)(85KAR). PA = 185 kcal/mol, 774 kJ/mol. | | | | | | |
| $CH_3Ti^+$ | | | | | | | |
| $CH_3Ti$ | (6.3) | *(248)* | *(1039)* | *(102)* | *(426)* | 86ELK/ARI | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |
| $CH_3V^+$ | | | | | | | |
| $CH_3V$ | (6.6) | *(263)* | *(1102)* | *111* | *463* | 86ARI/ARM | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM, 86ARI/ARM). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CH_3Xe^+$ | | | | | | | |
| $CH_3Xe$ | | (210) | (877) | | | | |
| | $\Delta_f H$(Ion) derived from results of 86HOV/MCM. | | | | | | |
| $CH_3Zn^+$ | | | | | | | |
| $CH_3Zn$ | (7.2) | *(213)* | *(890)* | *(47)* | *(197)* | | |
| | From appearance potential (10.22±0.02 eV) in $(CH_3)_2Zn$.<br>Value from onset of endothermic reaction (86GEO/ARM) is in agreement.<br>IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |
| $CH_4^+$ | | | | | | | |
| $CH_4$ | 12.51 | 271 | 1132 | −17.8±0.1 | −74.5±0.4 | 77PED/RYL | 74-82-8 |
| | | *272* | *1140* | *−16.0* | *−66.8* | | |
| | See also: 83PLE/MAR, 81KIM/KAT, 84CHA/HIL. | | | | | | |
| $CH_4Br^+$ | | | | | | | |
| $CH_3BrH$ | | 191 | 800 | | | | |
| | From proton affinity of $CH_3Br$ (RN 74-83-9). PA = 165.7 kcal/mol, 693 kJ/mol. | | | | | | |
| $CH_4Cl^+$ | | | | | | | |
| $CH_3ClH$ | | 183 | 767 | | | | |
| | From proton affinity of $CH_3Cl$ (RN 74-87-3). PA = ~163 kcal/mol, ~682 kJ/mol. | | | | | | |
| $CH_4ClN^+$ | | | | | | | |
| $CH_3NHCl$ | (9.19±0.02) | (230) | (964) | 18 | 77 | *EST | 6154-14-9 |
| $CH_4Cl_2Si^+$ | | | | | | | |
| $CH_3SiHCl_2$ | (11.47) | (168) | (705) | −96±2 | −402±8 | 81BEL/PER | 20156-50-7 |
| $CH_4F^+$ | | | | | | | |
| $CH_3FH$ | | (162) | (678) | | | | |
| | From proton affinity of $CH_3F$ (RN 593-53-3). PA = 145 kcal/mol, 605 kJ/mol<br>(86MCM/KEB, 85MCM/KEB3). | | | | | | |
| $CH_4I^+$ | | | | | | | |
| $CH_3IH$ | | (198) | (830) | | | | |
| | From proton affinity of $CH_3I$ (RN 74-88-4). PA = ~171 kcal/mol, ~715 kJ/mol. | | | | | | |
| $CH_4N^+$ | | | | | | | |
| $CH_2NH_2$ | 6.1 | (178) | (745) | 38±2 | 159±8 | 81GRI/LOS | 54088-53-8 |
| | $\Delta_f H$(Ion) from appearance potential determinations (81LOS/LAM).<br>See also: 81GRI/LOS, 84LOS/HOL, 82MAC, 83BUR/CAS. | | | | | | |
| $CH_3NH$ | (6.7) | (199) | (833) | 43.6±3.0 | 182.4±12.5 | 78SEN/FRA | 49784-84-1 |
| | $\Delta_f H$(Ion) from appearance potential determinations (84LOS/HOL). IP is<br>$\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CH_4NO^+$ | | | | | | | |
| $HC(OH)NH_2$ | | 123 | 514 | | | | |
| | From proton affinity of $HCONH_2$ (RN 75-12-7). PA = 198.4 kcal/mol, 830 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CH_4NO_2^+$ | | | | | | | |
| $CH_3NOOH$ | | 169 | 705 | | | | |
| | From proton affinity of $CH_3NO_2$ (RN 75-52-5). PA = 179.2 kcal/mol, 750 kJ/mol. | | | | | | |
| $CH_3ONHO$ | | 157 | 658 | | | | |
| | From proton affinity of $CH_3ONO$ (RN 624-91-9). PA = 192.5 kcal/mol, 805 kJ/mol. | | | | | | |
| $CH_4N_2^+$ | | | | | | | |
| (E)-$CH_3N=NH$ | 8.8±0.1 | (248) | (1037) | 45±2 | 188±8 | *EST | 26981-93-1 |
| $CH_4N_2O^+$ | | | | | | | |
| $(NH_2)_2CO$ | 9.7 | 165 | 690 | -58.8±0.5 | -245.9±2.1 | 77PED/RYL | 57-13-6 |
| | See also: 82BIE/ASB. | | | | | | |
| $CH_4N_2S^+$ | | | | | | | |
| $(NH_2)_2CS$ | 7.9 | 188 | 785 | 5±0.5 | 23±2 | 82TOR/SAB | 62-56-6 |
| $CH_4O^+$ | | | | | | | |
| $CH_3OH$ | 10.85±0.01 | 202.0 | 845.3 | -48.2±0.1 | -201.6±0.2 | 77PED/RYL | 67-56-1 |
| | | *204.6* | *856.2* | *-45.6* | *-190.7* | | |
| | See also: 82MIS/POK, 80VON/BIE, 82ALL/MIG, 84BOW/MAC, 81KIM/KAT, 80BAC/MOU, 77KAR/JAD. | | | | | | |
| $CH_2OH_2$ | | 195±2 | 815±8 | | | | 25765-84-8 |
| | $\Delta_f H$(Ion) from appearance potential measurements (82HOL/LOS). | | | | | | |
| $CH_4S^+$ | | | | | | | |
| $CH_3SH$ | 9.44±0.005 | 212.3 | 888.2 | -5.5±0.1 | -22.9±0.6 | 77PED/RYL | 74-93-1 |
| | | *214.8* | *899.0* | *-2.9* | *-12.1* | | |
| | IP from 83BUT/BAE, 81KIM/KAT, 82KUT/EDW. | | | | | | |
| $CH_2SH_2$ | | 219 | 916 | | | | 63933-47-1 |
| | | *221* | *925* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83HOL/LOS2). | | | | | | |
| $CH_4S_2^+$ | | | | | | | |
| $CH_2(SH)_2$ | (9.42) | (225) | (942) | 8±2 | 33±8 | 78BEN | 6725-64-0 |
| $CH_4Sc^+$ | | | | | | | |
| $CH_3ScH$ | | (214) | (895) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 86ELK/ARI. | | | | | | |
| $CH_5^+$ | | | | | | | |
| $CH_5$ | | 216 | 905 | | | | |
| | From proton affinity of $CH_4$. (RN 74-82-8) See also: 85MCM/KEB.<br>PA = 131.6 kcal/mol, 551. kJ/mol. | | | | | | |
| $CH_5As^+$ | | | | | | | |
| $CH_3AsH_2$ | (8.5) | (207) | (868) | 11 | 48 | *EST | 593-52-2 |
| | IP is onset of photoelectron band (82ELB/DIE). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$CH_5N^+$** | | | | | | | |
| $CH_2NH_3$ | | (≤201) | (≤841) | | | | |
| | The reaction c-$C_3H_6^+$ + $NH_3$ → $CH_2NH_3^+$ + $C_2H_4$ is at least 15 kcal/mol exothermic (84LIA/BUC). See also: 83HOL/LOS2, 72GRO. | | | | | | |
| $CH_3NH_2$ | 8.97±0.02 | 201 | 842 | −5.5±0.1 | −23.0±0.4 | 77PED/RYL | 74-89-5 |
| | See also: 81KIM/KAT, 82BIE/ASB, 82ELB/DIE. | | | | | | |
| **$CH_5NO^+$** | | | | | | | |
| $CH_3ONH_2$ | 9.55 | (214) | (895) | −6±2 | −26±8 | 69BEN/CRU | 67-62-9 |
| | IP from 83MOL/PIK. See also: 81KIM/KAT. | | | | | | |
| $CH_3NHOH$ | (9.0) | (196) | (818) | −12±2 | −50±8 | 69BEN/CRU | 593-77-1 |
| | IP is onset of photoelectron band. | | | | | | |
| **$CH_5N_3^+$** | | | | | | | |
| $(NH_2)_2C{=}NH$ | (9.10±0.05) | (218) | (910) | 8 | 32 | 82JOS | 113-00-8 |
| **$CH_5O^+$** | | | | | | | |
| $CH_3OH_2$ | | 136 | 567 | | | | |
| | From proton affinity of $CH_3OH$ (RN 67-56-1). PA = 181.9 kcal/mol, 761 kJ/mol. | | | | | | |
| **$CH_5P^+$** | | | | | | | |
| $CH_3PH_2$ | 9.12±0.07 | (206) | (862) | −4 | −18 | *EST | 593-54-4 |
| | See also: 82COW/KEM, 82ELB/DIE. | | | | | | |
| **$CH_5S^+$** | | | | | | | |
| $CH_3SH_2$ | | 173 | 723 | | | | |
| | From proton affinity of $CH_3SH$ (RN 74-93-1). PA = 187.4 kcal/mol, 784 kJ/mol. | | | | | | |
| **$CH_6N^+$** | | | | | | | |
| $CH_3NH_3$ | (4.3±0.1) | (146) | (611) | | | | |
| | $\Delta_f H$(Ion) from proton affinity of $CH_3NH_2$ (RN 74-89-5). PA = 214.1 kcal/mol, 896 kJ/mol. IP estimated from neutralized ion-beam spectroscopy data (85JEO/RAK). | | | | | | |
| **$CH_6N_2^+$** | | | | | | | |
| $CH_3NHNH_2$ | 7.67±0.02 | 199 | 835 | 22.6±0.1 | 94.6±0.6 | 77PED/RYL | 60-34-4 |
| | IP from charge transfer equilibrium constant determinations (84MAU/NEL) is in agreement. See also: 81KIM/KAT. | | | | | | |
| **$CH_6P^+$** | | | | | | | |
| $CH_3PH_3$ | | 158 | 658 | | | | |
| | From proton affinity of $CH_3PH_2$ (RN 593-54-4). PA = 204.1 kcal/mol, 854 kJ/mol. | | | | | | |
| **$CH_6Si^+$** | | | | | | | |
| $CH_3SiH_3$ | 10.7 | 240 | 1003 | −7±1 | −29±4 | 86DON/WAL | 992-94-9 |
| **$CH_7N_2^+$** | | | | | | | |
| $CH_3NH_2NH_2$ | | (174) | (729) | | | | |
| | From proton affinity of $CH_3NHNH_2$ (RN 60-34-4). PA = (214.1) kcal/mol, (896) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CH_8BN^+$ | | | | | | | |
| $CH_3NH_2BH_3$ | (9.66±0.01) | (210) | (878) | −13±1 | −54±4 | 80TEL/RAB | 1722-33-4 |
| $CIN^+$ | | | | | | | |
| ICN | 10.87±0.02 | 305 | 1274 | 53.9 | 225.5 | 82TN270 | 506-78-5 |
| | | *305* | *1275* | *54.0* | *226.1* | | |
| $CI_4^+$ | | | | | | | |
| $CI_4$ | 8.95 | 142 | 596 | −64 | −268 | 78KUD/KUD | 507-25-5 |
| | IP is onset of photoelectron band (82JON/DEL). | | | | | | |
| $CIr^+$ | | | | | | | |
| IrC | (9.5±1) | *(400)* | *(1670)* | *180* | *753* | 79HUB/HER | 12385-37-4 |
| | 0 K values. | | | | | | |
| $CKN^+$ | | | | | | | |
| KCN | (9.3±0.3) | (236) | (988) | 22 | 91 | 82TN270 | 151-50-8 |
| | | *(236)* | *(987)* | *21* | *90* | | |
| $CN^+$ | | | | | | | |
| CN | (14.09) | (428.9) | (1794.6) | 104.0±2 | 435.1±10 | 85JANAF | 57-12-5 |
| | | *(429.3)* | *(1796.3)* | *104.4±2* | *436.8±10* | | |
| | $\Delta_f H$(Ion) from appearance potential measurements. IP cited is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). | | | | | | |
| $CNO^+$ | | | | | | | |
| NCO | (11.76±0.01) | (308) | (1289) | 37±3 | 154±14 | 70OKA | |
| | IP from 83DYK/JON. | | | | | | |
| $CN_2O^+$ | | | | | | | |
| ONCN | 10.93 | 300.9 | 1259.0 | 48.85±0.03 | 204.4±0.1 | 84NAD/REI | 4343-68-4 |
| | IP from 81JON/MOO. See also: 81KIM/KAT. | | | | | | |
| $CN_4^+$ | | | | | | | |
| $N{\equiv}CN_3$ | (≤10.98±0.02) | (≤361) | (≤1512) | 108±5 | 453±20 | 69OKA/MEL | 764-05-6 |
| $CO^+$ | | | | | | | |
| CO | 14.0139 | <u>296.74</u> | <u>1241.59</u> | −26.42 | −110.53 | 82TN270 | 630-08-0 |
| | | <u>*295.97*</u> | <u>*1238.32*</u> | *−27.20* | *−113.80* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $COS^+$ | | | | | | | |
| COS | 11.1736±0.0015 | 224 | 936 | −34 | −142 | 77PED/RYL | 463-58-1 |
| | | *224* | *936* | *−34* | *−142* | | |
| | Cited ionization potential corresponds to formation of $COS^+(^2\Pi_{3/2})$. Formation of $COS^+(^2\Pi_{1/2})$ requires 11.2204±0.0015 eV. IP from 81ONO/OSU,80DEL/HUB. | | | | | | |
| $COSe^+$ | | | | | | | |
| COSe | 10.36±0.01 | (222) | (928) | −17 | −72 | *EST | 1603-84-5 |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $CO_2^+$ | | | | | | | |
| $CO_2$ | 13.773±0.002 | 223.6 | 935.4 | −94.05 | −393.51 | 82TN270 | 124-38-9 |
| | | *223.7* | *935.7* | *−93.96* | *−393.14* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $CP^+$ | | | | | | | |
| CP | (10.5±0.5) | (365) | (1529) | 123 | 516 | 79HUB/HER | 12326-85-1 |
| $CRh^+$ | | | | | | | |
| CRh | (8.9±0.5) | *(370)* | *(1550)* | *165±1* | *692±4* | 84SHI/GIN | 12127-42-3 |
| | 0 K values. See also: 81HAQ/GIN. | | | | | | |
| $CS^+$ | | | | | | | |
| CS | 11.33±0.01 | 327 | 1368 | 64 | 267 | | 2944-05-0 |
| | | *324* | *1356* | *63* | *262* | | |
| | Heat of formation of ion from appearance potentials in $CS_2$ of 13.64±0.02 eV (to give $CS^+ + S^-$) and 15.75±0.02 eV (to give $CS^+ + S$). $\Delta_f H$(Neutral) = $\Delta_f H$(Ion) - IP, in good agreement with 79HUB/HER. | | | | | | |
| $CS_2^+$ | | | | | | | |
| $CS_2$ | 10.0685±0.0020 | 260 | 1088 | 28±0.2 | 117±1 | 77PED/RYL | 75-15-0 |
| | | *260* | *1088* | *28* | *117* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $CSe_2^+$ | | | | | | | |
| $CSe_2$ | 9.258±0.0002 | 275 | 1149 | 61±5 | 256±20 | 82PIL/SKI | 506-80-9 |
| $CSi_2^+$ | | | | | | | |
| $Si_2C$ | (9.2±0.4) | (344) | (1440) | 132 | 552 | 82TN270 | 12070-04-1 |
| | | *(343)* | *(1437)* | *131* | *549* | | |
| $CV^+$ | | | | | | | |
| CV | | *(360)* | *(1506)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). 0 K value. | | | | | | |
| $C_2^+$ | | | | | | | |
| $C_2$ | 12.11 | 478 | 1998 | 198.8 | 831.9 | 79HUB/HER | 12070-15-4 |
| | | *476* | *1992* | *196.8* | *823.4* | | |
| | IP from 79HUB/HER. | | | | | | |
| $C_2BrI^+$ | | | | | | | |
| BrC≡CI | (9.34) | (276.56) | (1157.15) | 61.18 | 255.98 | 84DEW/HEA | 26395-29-9 |
| $C_2Br_2^+$ | | | | | | | |
| BrC≡CBr | 9.67 | 285 | 1192 | 61.8 | 258.6 | 83DEW/HEA | 624-61-3 |
| $C_2Br_2F_4^+$ | | | | | | | |
| $(CF_2Br)_2$ | (11.1) | (67) | (282) | −189±1 | −789±4 | 83KOL/PAP | 124-73-2 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_2Br_2O_2^+$ | | | | | | | |
| BrCOCOBr | (10.49±0.1) | (180) | (752) | −62 | −260 | *EST | 15219-34-8 |
| $C_2Ce^+$ | | | | | | | |
| $C_2Ce$ | (5.6±0.5) | (265) | (1110) | 136 | 570 | 82TN270 | 12012-32-7 |
| | | *(265)* | *(1109)* | *136* | *569* | | |
| $C_2ClF_3^+$ | | | | | | | |
| $C_2F_3Cl$ | 9.81±0.03 | (89) | (374) | −137±2 | −573±8 | 77PED/RYL | 79-38-9 |
| | | *(90)* | *(377)* | *−136* | *−570* | | |
| $C_2ClF_5^+$ | | | | | | | |
| $CF_3CF_2Cl$ | (12.6) | (23) | (98) | −267±1 | −1118±4 | 81BUC/FOR | 76-15-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2ClI^+$ | | | | | | | |
| ClC≡CI | (9.44) | (271.94) | (1137.79) | 54.25 | 226.98 | 84DEW/HEA | 25604-71-1 |
| $C_2Cl_2^+$ | | | | | | | |
| ClC≡CCl | 10.09 | 283 | 1183 | 50±10 | 209±42 | 71JANAF | 7572-29-4 |
| | | *282* | *1180* | *49±10* | *205±42* | | |
| | See: 81BOC/RIE, 82MAI/THO, 83KLA/MAI. | | | | | | |
| $C_2Cl_2F_2^+$ | | | | | | | |
| $CF_2=CCl_2$ | 9.65±0.03 | 142 | 593 | −81±3 | −338±11 | 83KOL/PAP | 79-35-6 |
| CFCl=CFCl | (10.2±0.1) | (157) | (657) | −78 | −327 | 82TN270 | 598-88-9 |
| $C_2Cl_2F_4^+$ | | | | | | | |
| $(CF_2Cl)_2$ | 12.2 | 60 | 252 | −221±1 | −925±4 | 83KOL/PAP | 76-14-2 |
| $C_2Cl_2O^+$ | | | | | | | |
| $Cl_2C=C=O$ | 9.0 | (191) | (799) | −16 | −69 | *EST | 4591-28-0 |
| | IP is onset of photoelectron band (81BOC/HIR, 82LEV/LIA). | | | | | | |
| $C_2Cl_2O_2^+$ | | | | | | | |
| $(COCl)_2$ | 10.91±0.05 | 173 | 724 | −79±1 | −329±5 | 77PED/RYL | 79-37-8 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2Cl_3F_3^+$ | | | | | | | |
| $CF_3CCl_3$ | 11.5 | 92 | 385 | −173±2 | −725±10 | 83KOL/PAP | 354-58-5 |
| | IP is onset of photoelectron band (81DUM/DUP). See also: 77ROS/DRA. | | | | | | |
| $CFCl_2CF_2Cl$ | 11.99±0.02 | 103 | 430 | −174±0.7 | −727±3 | 83KOL/PAP | 76-13-1 |
| $C_2Cl_3N^+$ | | | | | | | |
| $CCl_3CN$ | 11.89 | (294) | (1229) | 20 | 82 | *EST | 545-06-2 |
| | IP from 83MOL/PIK2. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2Cl_4^+$ | | | | | | | |
| $C_2Cl_4$ | 9.32 | 212 | 888 | −3±0.5 | −11±2 | 83KOL/PAP | 127-18-4 |
| | | *212* | *889* | *−2* | *−10* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| $C_2Cl_4F_2^+$ | | | | | | | |
| $CFCl_2CFCl_2$ | 11.3 | 135 | 563 | −126±2 | −527±10 | 83KOL/PAP | 76-12-0 |
| | IP is onset of photoelectron band (81DUM/DUP). | | | | | | |
| $C_2Cl_4O^+$ | | | | | | | |
| $CCl_3COCl$ | (11.0) | (198) | (828) | −56±2 | −236±9 | 77PED/RYL | 76-02-8 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_2Cl_6^+$ | | | | | | | |
| $CCl_3CCl_3$ | 11.1 | 220 | 921 | −36±1 | −150±5 | 83KOL/PAP | 67-72-1 |
| | IP is onset of photoelectron band (81KIM/KAT). See also: 82LEV/LIA. | | | | | | |
| $C_2F_2^+$ | | | | | | | |
| FC≡CF | 11.18 | (263) | (1100) | 5±5 | 21±21 | 71JANAF | 689-99-6 |
| | See also: 81BIE/ASB. | | | | | | |
| $C_2F_2O_2^+$ | | | | | | | |
| FCOCOF | (12.20±0.02) | (107) | (449) | −174 | −728 | *EST | 359-40-0 |
| $C_2F_3^+$ | | | | | | | |
| $C_2F_3$ | (10.2) | (189) | (791) | −45.9±2.0 | −192.0±8.4 | 83SPY/SAU | |
| | From appearance potentials of 15.84±0.02 eV in $C_2F_4$ and 15.4±0.1 eV in $C_2F_3Cl$. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_2F_3N^+$ | | | | | | | |
| $CF_3CN$ | 13.86 | 200 | 837 | −119.4±0.3 | −499.8±1.2 | 77PED/RYL | 353-85-5 |
| | IP from 81ASB/SVE. See also: 83MOL/PIK2. | | | | | | |
| $C_2F_4^+$ | | | | | | | |
| $C_2F_4$ | 10.12±0.02 | 75 | 316 | −158±0.7 | −659±3 | 83KOL/PAP | 116-14-3 |
| | | *76* | *319* | *−157* | *−657* | | |
| | See also: 81BIE/VON, 81BIE/ASB. | | | | | | |
| $C_2F_5^+$ | | | | | | | |
| $C_2F_5$ | | (0) | (0) | −213±1 | −893±4 | 82MCM/GOL | 3369-48-0 |
| | Appearance potentials of this ion in $C_2F_6$ (15.46 eV), $C_2F_5I$ (11.71 eV); $C_3F_8$ (13.32 eV), and n-$C_4F_{10}$ (13.05 eV) lead to estimated values for the heat of formation of 15 kcal/mol, 5 kcal/mol, -5 kcal/mol and -14 kcal/mol, respectively. See: 80ING/HAN. | | | | | | |
| $C_2F_5I^+$ | | | | | | | |
| $C_2F_5I$ | (10.66±0.1) | (6) | (25) | −240±1 | −1004±4 | 81BUC/FOR | 354-64-3 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2F_6^+$ | | | | | | | |
| $C_2F_6$ | (13.4) | (−12) | (−50) | −321 | −1343 | 75CHE/ROD | 76-16-4 |
| | | *(−10)* | *(−41)* | *−319* | *−1334* | | |
| | IP is onset of photoelectron band. (80ING/HAN). | | | | | | |
| $C_2F_7N^+$ | | | | | | | |
| $(CF_3)_2NF$ | (11.6) | (−10) | (−44) | −278 | −1163 | *EST | 359-62-6 |
| | IP from 82BUR/PAW. | | | | | | |
| $C_2H^+$ | | | | | | | |
| $C_2H$ | (11.7) | (405) | (1693) | 135±1 | 565±4 | 82MCM/GOL | 2122-48-7 |
| | | *(404)* | *(1689)* | *134* | *560* | | |
| | Heat of formation of ion from appearance potential measurement; IP given is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_2HBr^+$ | | | | | | | |
| HC≡CBr | 10.31±0.02 | 297.0 | 1242.4 | 59.2 | 247.7 | 75OKA | 593-61-3 |
| | IP from 77ALL/KLO. See also: 82LEV/LIA. | | | | | | |
| $C_2HBrClF_3^+$ | | | | | | | |
| $CF_3CHClBr$ | 11.0 | 86 | 361 | −167±1 | −700±4 | 83KOL/PAP | 151-67-7 |
| | IP is onset of photoelectron band (81DUM/DUP). | | | | | | |
| $C_2HBrO^+$ | | | | | | | |
| CHBr=C=O | (≤9.10) | (≤207) | (≤868) | −2 | −10 | *EST | 78957-22-9 |
| | IP from 81BOC/HIR. | | | | | | |
| $C_2HCl^+$ | | | | | | | |
| HC≡CCl | 10.58±0.02 | 305 | 1276 | 61 | 255 | 70KLO/PAS | 593-63-5 |
| | IP from 77ALL/KLO. See also: 84MAI/THO. | | | | | | |
| $C_2HClF_2^+$ | | | | | | | |
| $CF_2$=CHCl | 9.80±0.04 | 150 | 629 | −76 | −316 | 82TN270 | 359-10-4 |
| $C_2HClF_3O^+$ | | | | | | | |
| $CF_3C(OH)Cl$ | | 4 | 14 | | | | |
| | From proton affinity of $CF_3COCl$ (RN 354-32-5)(85MCM/KEB, 85MCM/KEB2). PA = 161.2 kcal/mol, 674 kJ/mol. | | | | | | |
| $C_2HClO^+$ | | | | | | | |
| CHCl=C=O | (≤9.3) | (≤201) | (≤840) | −14 | −57 | *EST | 29804-89-5 |
| | See also: 81BOC/HIR. | | | | | | |
| $C_2HCl_2F_3^+$ | | | | | | | |
| $CF_3CHCl_2$ | 11.5 | 88 | 370 | −177±2 | −740±10 | 83KOL/PAP | 306-83-2 |
| | IP is onset of photoelectron band (81DUM/DUP). | | | | | | |
| $CF_2ClCHFCl$ | ≤12.00 | ≤104 | ≤434 | −173±2 | −724±10 | 83KOL/PAP | 354-23-4 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2HCl_3{}^+$ | | | | | | | |
| $C_2HCl_3$ | 9.47±0.01 | 214 | 895 | −4.5±0.7 | −19±3 | 85PAP/KOL | 79-01-6 |
| | | *215* | *898* | *−4* | *−16* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| $C_2HCl_3N^+$ | | | | | | | |
| $CCl_3CNH$ | | 209 | 876 | | | | |
| | From proton affinity of $CCl_3CN$ (RN 545-06-2). PA = 175.8 kcal/mol, 735.5 kJ/mol. | | | | | | |
| $C_2HCl_3O^+$ | | | | | | | |
| $CCl_3CHO$ | (10.5) | (195) | (816) | −47 | −197 | 82TN270 | 75-87-6 |
| | IP is onset of photoelectron band (81KIM/KAT). See also: 85GUI/PFI2. | | | | | | |
| $CHCl_2COCl$ | (11.0) | (196) | (820) | −58±2 | −241±9 | 77PED/RYL | 79-36-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2HCl_5{}^+$ | | | | | | | |
| $CHCl_2CCl_3$ | (11.0) | (220) | (919) | −34±2 | −143±7 | 78GUN/HEA | 76-01-7 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_2HF^+$ | | | | | | | |
| HC≡CF | 11.26 | 285 | 1193 | 26 | 107 | 80STA/VOG | 2713-09-9 |
| | See also: 81BIE/ASB. | | | | | | |
| $C_2HF_3{}^+$ | | | | | | | |
| $C_2HF_3$ | 10.14 | 117 | 487 | −117±2 | −491±8 | 77PED/RYL | 359-11-5 |
| | See also: 81BIE/VON, 81BIE/ASB. | | | | | | |
| $C_2HF_3N^+$ | | | | | | | |
| $CF_3CNH$ | | 82 | 343 | | | | |
| | From proton affinity of $CF_3CN$ (RN 353-85-5) (85MCM/KEB, 85MCM/KEB2).<br>PA = 164.3 kcal/mol, 687. kJ/mol. | | | | | | |
| $C_2HF_3O_2{}^+$ | | | | | | | |
| $CF_3COOH$ | 11.46 | 18 | 75 | −246.3±0.3 | −1030.7±1 | 77PED/RYL | 76-05-1 |
| | See also: 81ASB/SVE. | | | | | | |
| $C_2HF_4O^+$ | | | | | | | |
| $CF_3C(OH)F$ | | −44 | −182 | | | | |
| | From proton affinity of $CF_3COF$ (RN 354-34-7). PA = 160.2 kcal/mol, 670 kJ/mol. | | | | | | |
| $C_2HN^+$ | | | | | | | |
| HCCN | | *(366)* | *(1531)* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations. See also: 85HAR/MCI. 0 K values. | | | | | | |
| $C_2HN_2{}^+$ | | | | | | | |
| NCCNH | | 277 | 1161 | | | | |
| | From proton affinity of NCCN (RN 460-19-5) (87DEA/MAU).<br>PA = 162 kcal/mol, 678 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2HO^+$ | | | | | | | |
| HCCO | (9.5) | (262) | (1096) | 42.4±2.1 | 177.4±8.8 | *EST | 51095-15-9 |
| | Heat of formation from appearance potential determination (84LOS/HOL). | | | | | | |
| | IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_2HV^+$ | | | | | | | |
| $VC_2H$ | | *(303)* | *(1268)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). 0 K value. | | | | | | |
| $C_2H_2^+$ | | | | | | | |
| $C_2H_2$ | 11.400±0.002 | 317.4 | 1327.9 | 54.5±0.25 | 228.0±1 | 77PED/RYL | 74-86-2 |
| | | *317.5* | *1328.5* | *54.7* | *228.6* | | |
| | See also: 81KIM/KAT, 82HAY/IWA. | | | | | | |
| $C_2H_2Br_2^+$ | | | | | | | |
| (E)-CHBr=CHBr | 9.51±0.04 | (245) | (1024) | 25 | 106 | *EST | 590-12-5 |
| | An IP of 9.30±0.02 has also been reported (72CHA/FRO). | | | | | | |
| (Z)-BrCH=CHBr | 9.63±0.01 | 247 | 1035 | 25 | 106 | *EST | 590-11-4 |
| | An IP of 9.32±0.02 eV has also been reported (72CHA/FRO). | | | | | | |
| $CBr_2=CH_2$ | 9.78±0.01 | (247) | (1034) | 21 | 90 | *EST | 593-92-0 |
| | See also: 82VON/ASB. | | | | | | |
| $C_2H_2Br_2F_2^+$ | | | | | | | |
| $CF_2BrCH_2Br$ | 10.83±0.01 | 147 | 614 | −103±5 | −431±20 | 83KOL/PAP | 75-82-1 |
| $C_2H_2ClN^+$ | | | | | | | |
| $CH_2ClCN$ | 11.95±0.01 | (296) | (1239) | 21 | 86 | *EST | 107-14-2 |
| $C_2H_2Cl_2^+$ | | | | | | | |
| $CH_2=CCl_2$ | 9.79±0.04 | 226 | 947 | 0.5±0.2 | 2.3±0.7 | 77PED/RYL | 75-35-4 |
| | | *228* | *953* | *2.0* | *8.4* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| (Z)-CHCl=CHCl | 9.66±0.01 | 224 | 936 | 1±0.2 | 4±1 | 83KOL/PAP | 156-59-2 |
| | | *225* | *942* | *2* | *10* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| (E)-CHCl=CHCl | 9.65±0.02 | 224 | 937 | 1±0.2 | 6±1 | 83KOL/PAP | 156-60-5 |
| | | *225* | *942* | *3* | *11* | | |
| | See also: 82VON/ASB, 81KIM/KAT. | | | | | | |
| $C_2H_2Cl_2F_2^+$ | | | | | | | |
| $CF_2ClCH_2Cl$ | ≤11.8 | ≤142 | ≤596 | −130±2 | −543±10 | 83KOL/PAP | 1649-08-7 |
| | IP from 81DUM/DUP. | | | | | | |
| $C_2H_2Cl_2O^+$ | | | | | | | |
| $CHCl_2CHO$ | 10.5 | (199) | (833) | −43±5 | −180±20 | *EST | 79-02-7 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_2H_2Cl_2O^+$ | | | | | | | |
| $CH_2ClCOCl$ | (11.0) | (195) | (815) | −59±2 | −246±9 | 77PED/RYL | 79-04-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_2Cl_3O_2^+$ | | | | | | | |
| $CCl_3C(OH)_2$ | | 76 | 318 | | | | |
| | From proton affinity of $CCl_3COOH$ (RN 76-03-9)(PA = 183.5 kcal/mol, 768 kJ/mol). | | | | | | |
| $C_2H_2Cl_4^+$ | | | | | | | |
| $CH_2ClCCl_3$ | (11.1) | (220) | (919) | −36±0.2 | −152±1 | 83KOL/PAP | 630-20-6 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $(CHCl_2)_2$ | (≤11.62) | (≤232) | (≤971) | −36±1 | −150±5 | 77PED/RYL | 79-34-5 |
| | IP from 81KIM/KAT. | | | | | | |
| $C_2H_2F^+$ | | | | | | | |
| $CH_2CF$ | | 227 | 951 | | | | |
| | From appearance potential of 13.56 eV in $C_2H_3F$ in agreement with value from proton affinity of HCCF (PA = 165 kcal/mol, 689 kJ/mol). See also: 85HEI/BAR, 84BEA/EYE. | | | | | | |
| $C_2H_2F_2^+$ | | | | | | | |
| $CH_2=CF_2$ | 10.29±0.01 | 155 | 648 | −82±2 | −345±10 | 76WIL/LEB | 75-38-7 |
| | | *157* | *655* | *−81* | *−338* | | |
| | See also: 81BIE/VON, 81BIE/ASB. | | | | | | |
| (Z)-CHF=CHF | 10.23 | 165 | 690 | −71 | −297 | 80STA/VOG | 1630-77-9 |
| | See also: 81BIE/VON, 81BIE/ASB, 79JOC/LOH, 81MAI/THO2. | | | | | | |
| (E)-CHF=CHF | 10.21 | 165 | 692 | −70 | −293 | 80STA/VOG | 1630-78-0 |
| | See also: 81BIE/VON, 81BIE/ASB, 79JOC/LOH. | | | | | | |
| $C_2H_2F_3^+$ | | | | | | | |
| $CHF_2CHF$ | | (79) | (332) | | | | |
| | From proton affinity of $CF_2=CHF$ (RN 359-11-5). PA = ~169 kcal/mol, ~707 kJ/mol. | | | | | | |
| $CF_3CH_2$ | (10.6±0.1) | (120) | (506) | −124±2 | −517±8 | 82MCM/GOL | 3248-58-6 |
| $C_2H_2F_3I^+$ | | | | | | | |
| $CF_3CH_2I$ | 9.998 | 75 | 316 | −155±1 | −649±4 | 83KOL/PAP | 353-83-3 |
| $C_2H_2F_3NO^+$ | | | | | | | |
| $CF_3CONH_2$ | (10.8) | (49) | (206) | −200 | −836 | *EST | 354-38-1 |
| | IP from 81ASB/SVE. | | | | | | |
| $C_2H_2F_3O^+$ | | | | | | | |
| $CF_3CHOH$ | | 12 | 49 | | | | |
| | From proton affinity of $CF_3CHO$ (RN 75-90-1). PA = 165.1 kcal/mol, 691 kJ/mol. | | | | | | |
| $C_2H_2F_3O_2^+$ | | | | | | | |
| $CF_3C(OH)_2$ | | −50 | −208 | | | | |
| | From proton affinity of $CF_3COOH$ (RN 76-05-1). PA = 169.0 kcal/mol, 707 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

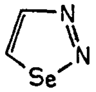
| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_2H_2I_2^+$ | | | | | | | |
| (Z)-CHI=CHI | (8.6) | (248) | (1037) | 49.5±0.3 | 207.2±1.1 | 77PED/RYL | 590-26-1 |
| | IP is onset of photoelectron band. | | | | | | |
| (E)-CHI=CHI | (8.6) | (248) | (1037) | 49.5±0.3 | 207.2±1.1 | 77PED/RYL | 590-27-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_2N^+$ | | | | | | | |
| $CH_2CN$ | (10.0) | (290) | (1214) | 59±2 | 245±10 | 82MCM/GOL | 2932-82-3 |
| | $\Delta_fH$(Ion) from appearance potential measurements (77ROS/DRA, 85HAR/MCI) IP cited is $\Delta_fH$(Ion)-$\Delta_fH$(Neutral). See also: 82ALL/MIG. | | | | | | |
| $C_2H_2N_2Se^+$ | | | | | | | |
|  | (8.9) | (290) | (1212) | 84 | 353 | *EST | 26223-16-5 |
| | IP from 80BOC/AYG, 82LEV/LIA. | | | | | | |
| $C_2H_2N_4^+$ | | | | | | | |
|  | (9.14) | (322) | (1346) | 111 | 464 | 82JOS | 290-96-0 |
| $C_2H_2O^+$ | | | | | | | |
| HC≡COH | | 247 | 1033 | | | | |
| | $\Delta_fH$(Ion) from appearance potential determination (86BAA/WEI). | | | | | | |
| $CH_2CO$ | 9.61±0.02 | 210.2 | 879.6 | −11.4±0.6 | −47.7±2.5 | 71NUT/LAU | 463-51-4 |
| | | *210.9* | *882.7* | *−10.7* | *−44.6* | | |
| | See also: 81BOC/HIR. | | | | | | |
| $C_2H_2O_2^+$ | | | | | | | |
| $(CHO)_2$ | 10.1 | 182 | 763 | −50.6±0.2 | −211.9±0.8 | 77PED/RYL | 107-22-2 |
| | IP is onset of photoelectron band (80VON/BIE, 81KIM/KAT). | | | | | | |
| $C_2H_2O_4^+$ | | | | | | | |
| HOOCCOOH | (10.8) | (74) | (310) | −175±0.7 | −732±3 | 77PED/RYL | 144-62-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_2S^+$ | | | | | | | |
| $CH_2$=C=S | (8.77) | (242) | (1011) | 39 | 165 | *EST | 18282-77-4 |
| | | *(234)* | *(979)* | | | | |
| | Cited IP is onset of photoelectron band (77ROS/SOL). Heat of formation of ion from appearance potential in $CH_3SSCH_3$ (83BUT/BAE). $\Delta_fH$(Neutral) is ($\Delta_fH$(Ion) - IP). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_2S_2^+$ | | | | | | | |
|  | (8.5) | (258) | (1080) | 62 | 260 | *EST | 7092-01-5 |
| | IP is onset of photoelectron band (83SCH/SCH). | | | | | | |
| $C_2H_2Se^+$ | | | | | | | |
| $CH_2=C=Se$ | 8.7 | (256) | (1071) | 55 | 232 | *EST | 61134-37-0 |
| | IP is onset of photoelectron band (80BOC/AYG). | | | | | | |
| $C_2H_3^+$ | | | | | | | |
| $C_2H_3$ | 8.9 | 265.9 | 1112 | 63.4±1 | 265.3±4 | 85KIE/WEI | 2669-89-8 |
| | | *267.9* | *1120.9* | *62.7* | *262.2* | | |
| | Heat of formation of ion from appearance potential measurement; IP from J.L. Beauchamp, personal communication. | | | | | | |
| $C_2H_3Br^+$ | | | | | | | |
| $C_2H_3Br$ | 9.80±0.02 | 244.9 | 1024.8 | 18.9±0.5 | 79.3±1.9 | 77PED/RYL | 593-60-2 |
| | | *248.5* | *1039.7* | *22.5* | *94.2* | | |
| | See also: 82VON/ASB, 83CAM/CIU, 84MIL/BAE. | | | | | | |
| $C_2H_3BrHg^+$ | | | | | | | |
| $CH_2=CHHgBr$ | (9.8) | (256) | (1072) | 30 | 126 | *EST | 16188-37-7 |
| | IP is onset of photoelectron band (81BAI/CHI). | | | | | | |
| $C_2H_3BrO^+$ | | | | | | | |
| $CH_3COBr$ | 10.4±0.1 | 194 | 813 | −45.5±0.1 | −190.4±0.5 | 77PED/RYL | 506-96-7 |
| | IP is onset of photoelectron band (82LEV/LIA, 81KIM/KAT). | | | | | | |
| $C_2H_3BrO_2^+$ | | | | | | | |
| $CH_2BrCOOH$ | (10.4) | (145) | (608) | −94.4±1.5 | −395±6 | *EST | 79-08-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_3Cl^+$ | | | | | | | |
| $C_2H_3Cl$ | 9.99±0.02 | 236 | 987 | 5±0.5 | 23±2 | 83KOL/PAP | 75-01-4 |
| | | *238* | *995* | *7* | *31* | | |
| | See also: 83CAM/CIU, 82VON/ASB, 81KIM/KAT. | | | | | | |
| $C_2H_3ClF_2^+$ | | | | | | | |
| $CH_3CF_2Cl$ | 11.98±0.01 | 149.7 | 626.2 | −126.6±1.2 | −529.7±5.0 | 78PAP/KOL | 75-68-3 |
| $C_2H_3ClN^+$ | | | | | | | |
| $ClCH_2CNH$ | | 207 | 865 | | | | |
| | From proton affinity of $ClCH_2CN$ (RN 107-14-2). PA = 179.5 kcal/mol, 751 kJ/mol. | | | | | | |
| $C_2H_3ClO^+$ | | | | | | | |
| $CH_3COCl$ | 10.85±0.05 | 192 | 804 | −58±0.2 | −243±1 | 77PED/RYL | 75-36-5 |
| | | *194* | *813* | *−56* | *−234* | | |
| | See: 81KIM/KAT | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_3ClO^+$ | | | | | | | |
| $CH_2ClCHO$ | 10.48±0.03 | (195) | (816) | −47±4 | −195±15 | *EST | 107-20-0 |
| | See: 81KIM/KAT. | | | | | | |
| $C_2H_3ClO_2^+$ | | | | | | | |
| $CH_2ClCOOH$ | (10.7) | (143) | (597) | −104±2 | −435±9 | 77PED/RYL | 79-11-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_3Cl_3^+$ | | | | | | | |
| $CHCl_2CH_2Cl$ | 11.0 | 218 | 912 | −36±0.5 | −149±2 | 77PED/RYL | 79-00-5 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $CH_3CCl_3$ | (11.0) | (219) | (916) | −34.6±0.1 | −144.9±0.6 | 83KOL/PAP | 71-55-6 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_2H_3Cl_3O^+$ | | | | | | | |
| $CCl_3CH_2OH$ | (10.94) | (182) | (763) | (−70) | (−293) | *EST | 115-20-8 |
| | IP from 83KOP/MOL. | | | | | | |
| $C_2H_3Cl_3Si^+$ | | | | | | | |
| $CH_2=CHSiCl_3$ | (≤11.0) | (≤144) | (≤603) | −109 | −458 | *EST | 75-94-5 |
| | IP from 81KHV/ZYK. | | | | | | |
| $C_2H_3F^+$ | | | | | | | |
| $C_2H_3F$ | 10.363±0.015 | 205.8 | 861.1 | −33.2±0.4 | −138.8±1.7 | 76WIL/LEB | 75-02-5 |
| | See also: 81BIE/VON, 81BIE/ASB. | | | | | | |
| $C_2H_3FO^+$ | | | | | | | |
| $CH_3COF$ | 11.51±0.02 | 159 | 667 | −106±0.7 | −444±3 | 77PED/RYL | 557-99-3 |
| | See: 81KIM/KAT. | | | | | | |
| $C_2H_3F_2^+$ | | | | | | | |
| $CH_2FCHF$ | | 130 | 543 | | | | |
| | From proton affinity of (E)-CHF=CHF (RN 1630-78-0). PA = 166 kcal/mol, 694 kJ/mol. | | | | | | |
| $CH_3CF_2$ | (7.92) | (109) | (458) | −72±2 | −303±8 | 82MCM/GOL | 40640-67-3 |
| | Value of $\Delta_f H$(Ion) from appearance potential determination (84HEI/BAR, 85HEI/BAR); value from proton affinity of $CH_2=CF_2$ (RN 75-38-7) = 108 kcal/mol, 451 kJ/mol. PA = 176 kcal/mol, 736 kJ/mol. | | | | | | |
| $C_2H_3F_3^+$ | | | | | | | |
| $CH_3CF_3$ | 12.9±0.1 | 118 | 496 | −179±0.7 | −749±3 | 83KOL/PAP | 420-46-2 |
| | | *122* | *509* | *−176* | *−736* | | |
| | IP from 73GOL/KOR. | | | | | | |
| $C_2H_3F_3O^+$ | | | | | | | |
| $CF_3CH_2OH$ | 11.49 | 53 | 221 | −212±1 | −888±5 | 77PED/RYL | 75-89-8 |
| | IP from 83KOP/MOL. | | | | | | |
| $C_2H_3I^+$ | | | | | | | |
| $CH_2=CHI$ | 9.30 | (246) | (1027) | 31 | 130 | *EST | 593-66-8 |

**Table 1. Positive Ion Table - Continued**

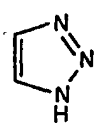
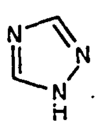
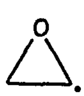
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_3N^+$ | | | | | | | |
| $CH_3CN$ | 12.194±0.005 | 299 | 1251 | 18±0.2 | 74±1 | 83AN/MAN | 75-05-8 |
| | | *300* | *1258* | *19* | *81* | | |
| | IP from 81RID/RAY. See also: 82CHE/LAP, 84OHN/MAT,82ALL/MIG, 81KIM/KAT, 85HAR/MCI. | | | | | | |
| $CH_2CNH$ | | (240) | (1004) | | | | |
| | | *(242)* | *(1011)* | | | | |
| | From appearance potential determinations. | | | | | | |
| $CH_3NC$ | 11.24 | 300 | 1257 | 41±0.2 | 173±1 | 83AN/MAN | 593-75-9 |
| | | *302* | *1262* | *43* | *178* | | |
| | See also: 82CHE/LAP, 81BEV/SAN, 85HAR/MCI. | | | | | | |
| $C_2H_3NO^+$ | | | | | | | |
| $CH_3NCO$ | (10.67±0.02) | (215) | (899) | −31 | −130 | 75COM/DES | 624-83-9 |
| $C_2H_3NS^+$ | | | | | | | |
| $CH_3SCN$ | (9.96±0.05) | (268) | (1121) | 38 | 160 | 82TN270 | 556-64-9 |
| $CH_3NCS$ | (9.25±0.03) | (245) | (1023) | 31 | 131 | 82TN270 | 556-61-6 |
| | | *(247)* | *(1032)* | *33* | *140* | | |
| $C_2H_3N_3^+$ | | | | | | | |
|  | 10.06 | 291 | 1218 | 59 | 247 | 82JOS | 288-36-8 |
| | See: 81PAL/SIM. | | | | | | |
|  | (9.8) | (272) | (1140) | 46±0.5 | 194±2 | 85FAO/AKA | 288-88-0 |
| | IP is onset of photoelectron band (81PAL/SIM). | | | | | | |
| $C_2H_3O^+$ | | | | | | | |
| $CH_3CO$ | 7.0 | 156 | 653 | −6±0.5 | −24±2 | 82MCM/GOL | 15762-07-9 |
| | $\Delta_f H$(Ion) at 298 K from 82TRA/MCL, 84LIA/LIE, and 81LIF/TZI. See also: 84LOS/HOL, 83LIF/BER. Value derived from proton affinity of ketene is 157 kcal/mol, 657 kJ/mol. PA = 198.0 kcal/mol, 828 kJ/mol. IP cited is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). Experimentally determined IP of this radical is 8.05±0.17 eV. See also: 82BUR/HOL2. | | | | | | |
| $CH_2{=}COH$ | | (192) | (803) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (82HOL/LOS, 82HOL/LOS2, 83BUR/HOL2). | | | | | | |
|  | | (201) | (841) | | | | 31586-84-2 |
| | $\Delta_f H$(Ion) from appearance potential measurements. See also: 83BUR/HOL2. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_3O_2I^+$ | | | | | | | |
| $CH_2ICOOH$ | (9.6) | (327) | (1367) | 105 | 441 | *EST | 64-69-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_3S^+$ | | | | | | | |
| $CH_3CS$ | | 204 | 853 | | | | |
| | From proton affinity of $CH_2=C=S$ (RN 18282-77-4) (83CAS/KIM). PA = 201.2 kcal/mol, 842 kJ/mol. Original authors recommend value of 210 kcal/mol, 879 kJ/mol, using $\Delta_f H(CH_2=C=S)$ = 46 kcal/mol, 196 kJ/mol, from MNDO calculation. | | | | | | |
| $C_2H_3V^+$ | | | | | | | |
| $VC_2H_3$ | | *(266)* | *(1115)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). 0 K value. | | | | | | |
| $C_2H_4^+$ | | | | | | | |
| $C_2H_4$ | 10.507±0.004 | 254.8 | 1066 | 12.5±0.2 | 52.2±1 | 77PED/RYL | 74-85-1 |
| | | *256.8* | *1074* | *14.5* | *60.7* | | |
| | See also: 81KIM/KAT, 84POL/TRE. | | | | | | |
| $C_2H_4BrCl^+$ | | | | | | | |
| $CH_2BrCH_2Cl$ | 10.67±0.03 | 225 | 942 | −21±1 | −87±5 | 83KOL/PAP | 107-04-0 |
| | See: 81KIM/KAT. | | | | | | |
| $CH_3CHClBr$ | 10.37 | 219±1 | 918±5 | −20±1 | −83±5 | 83KOL/PAP | 593-96-4 |
| $C_2H_4BrF^+$ | | | | | | | |
| $CH_2FCH_2Br$ | ≤10.57 | (≤184) | (≤769) | −60±5 | −251±20 | 83KOL/PAP | 762-49-2 |
| $C_2H_4Br_2^+$ | | | | | | | |
| $CH_2BrCH_2Br$ | 10.37 | 230 | 962 | −9±0.2 | −38.3 ± 1.2 ~~−39±1~~ | 83KOL/PAP | 106-93-4 |
| | See: 78GAN/PEE, 81KIM/KAT, 77STA/WIE. | | | | | | |
| $CH_3CHBr_2$ | 10.17 | 226 | 944 | −9±1 | −26.7 ± 1.9 ~~−37±6~~ | 83KOL/PAP | 557-91-5 |
| $C_2H_4Cl^+$ | | | | | | | |
| $CH_3CHCl$ | | (199) | (832) | | | | |
| | From appearance potential (11.20 eV) in $CH_3CHCl_2$. | | | | | | |
| $CH_2ClCH_2$ | | (204) | (855) | | | | |
| | From appearance potential (11.47 eV) in $CH_2ClCH_2Cl$. | | | | | | |
| $C_2H_4ClO_2^+$ | | | | | | | |
| $CH_2ClC(OH)_2$ | | 79 | 332 | | | | |
| | From proton affinity of $CH_2ClCOOH$ (RN 79-11-8). PA = 182.4 kcal/mol, 763 kJ/mol. | | | | | | |
| $C_2H_4Cl_2^+$ | | | | | | | |
| $CH_3CHCl_2$ | 11.06 | 224 | 936 | −31±0.7 | −131±3 | 83KOL/PAP | 75-34-3 |
| | | *229* | *959* | *−26* | *−108* | | |
| | See also: 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

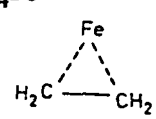
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_4Cl_2^+$ | | | | | | | |
| $CH_2ClCH_2Cl$ | 11.04 | 222 | 931 | −32±0.2 | −134±1 | 83KOL/PAP | 107-06-2 |
| | | *225* | *942* | *−29* | *−123* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2H_4Cl_2O^+$ | | | | | | | |
| $CH_3OCHCl_2$ | (10.6) | (191) | (800) | −53 | −222 | *EST | 4885-02-3 |
| | IP is onset of photoelectron band (80VER/SAL). | | | | | | |
| $C_2H_4Cl_3O^+$ | | | | | | | |
| $CCl_3CH_2OH_2$ | | 118 | 495 | | | | |
| | From proton affinity of $CCl_3CH_2OH$ (RN 115-20-8). PA = 177.4 kcal/mol, 742 kJ/mol. | | | | | | |
| $C_2H_4F^+$ | | | | | | | |
| $CH_3CHF$ | 7.93 | 157 | 659 | −26 | −106 | ? | |
| | $\Delta_f H$(Ion) from proton affinity of $C_2H_3F$ (RN 75-02-5). PA = 175 kcal/mol, 732 kJ/mol.<br>$\Delta_f H$(Neutral) = IP - $\Delta_f H$(Ion). | | | | | | |
| $C_2H_4FO_2^+$ | | | | | | | |
| $CH_2FC(OH)_2$ | | 42 | 176 | | | | |
| | From proton affinity of $CH_2FCOOH$ (RN 144-49-0). PA = 183.5 kcal/mol, 768. kJ/mol. | | | | | | |
| $C_2H_4F_2^+$ | | | | | | | |
| $CH_3CHF_2$ | 11.87±0.03 | 154 | 644 | −120±1 | −501±6 | 75CHE/ROD | 75-37-6 |
| | IP from 84HEI/BAR, 85HEI/BAR. | | | | | | |
| $C_2H_4F_3N^+$ | | | | | | | |
| $CF_3CH_2NH_2$ | (9.8±0.1) | (58) | (244) | (−167) | (−701) | *EST | 753-90-2 |
| | IP is average of values from 83MOL/PIK3, 79AUE/BOW. | | | | | | |
| $C_2H_4F_3O^+$ | | | | | | | |
| $CF_3CH_2OH_2$ | | −16 | −65 | | | | |
| | From proton affinity of $CF_3CH_2OH$ (RN 75-89-8). See also: 85MCM/KEB.<br>PA = 169.0 kcal/mol, 707 kJ/mol. | | | | | | |
| $C_2H_4Fe^+$ | | | | | | | |
|  | | (256) | (1071) | | | | |
| | $\Delta_f H$(Ion) from 84JAC/JAC. | | | | | | |
| $C_2H_4I_2^+$ | | | | | | | |
| $CH_2ICH_2I$ | (9.4) | (233) | (973) | 15.8±0.3 | 66.3±1.4 | 77PED/RYL | 624-73-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_4N^+$ | | | | | | | |
| $CH_3CNH$ | | 195 | 817 | | | | |
| | From proton affinity of $CH_3CN$ (RN 75-05-8). PA = 188.2 kcal/mol, 787 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

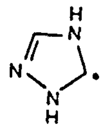
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_4N^+$ | | | | | | | |
| $CH_3NCH$ | | 205 | 860 | | | | |
| | From proton affinity of $CH_3NC$ (RN 593-75-9) (86KNI/FRE, 86MAU/KAR). PA = 201.4 kcal/mol, 843 kJ/mol. | | | | | | |
| $C_2H_4NO^+$ | | | | | | | |
| $CH_3NHCO$ | | 150 | 628 | | | | |
| | From proton affinity of $CH_3NCO$ (RN 624-83-9)(85KAR/STE). PA = 184.5 kcal/mol, 772. kJ/mol. | | | | | | |
| $C_2H_4NS^+$ | | | | | | | |
| $CH_3SCNH$ | | 212 | 886 | | | | |
| | From proton affinity of $CH_3SCN$ (RN 556-64-9) (85KAR/STE). PA = 192. kcal/mol, 804. kJ/mol. | | | | | | |
| $CH_3NCS\dot{H}$ | | 204 | 853 | | | | |
| | From proton affinity of $CH_3NCS$ (RN 556-61-6) (85KAR/STE). PA = 193.0 kcal/mol, 807.5 kJ/mol. | | | | | | |
| $C_2H_4N_2^+$ | | | | | | | |
| $CH_2=NN=CH_2$ | (8.95) | (264) | (1104) | 58 | 241 | 82JOS | 503-27-5 |
| | See also: 84KIR/POP. | | | | | | |
| $C_2H_4N_2O_2^+$ | | | | | | | |
| $NH_2COCONH_2$ | (9.41) | (121) | (505) | −96±1 | −403±5 | 77PED/RYL | 471-46-5 |
| $C_2H_4N_3^+$ | | | | | | | |
|  | | 199 | 835 | | | | |
| | From proton affinity of 1H-1,2,4-Triazole (RN 288-88-0) (86MAU/LIE). PA = 212.4 kcal/mol, 889. kJ/mol. | | | | | | |
| $C_2H_4N_4^+$ | | | | | | | |
| $NCN=C(NH_2)_2$ | (8.4) | (230) | (963) | 36 | 153 | 77PED/RYL | 10191-60-3 |
| | IP is onset of photoelectron band (80KLA/BUT). | | | | | | |
| $C_2H_4O^+$ | | | | | | | |
| $CH_3CHO$ | 10.229±0.0007 | 196.3 | 821.1 | −39.6±0.1 | −165.8±0.4 | 77PED/RYL | 75-07-0 |
| | | *198.9* | *831.9* | *−37.0* | *−155.0* | | |
| | See also: 82JOH/POW, 72POT/SOR, 81ELS/ALL, 81KIM/KAT, 77STA/WIE. | | | | | | |
| $CH_2=CHOH$ | 9.14 | 181 | 757 | −30 | −125 | 82HOL/LOS3 | 557-75-5 |
| | From 82HOL/LOS3, 84ALB/ALL. | | | | | | |
| $CH_3COH$ | | (207) | (865) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (83TER/WEZ). | | | | | | |

**Table 1. Positive Ion Table - Continued**

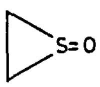
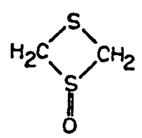
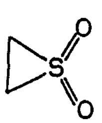
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_4O^+$ | | | | | | | |
|  | 10.566±0.01 | 231.0 | 966.8 | −12.6±0.1 | −52.6±0.6 | 77PED/RYL | 75-21-8 |
| | | *234.1* | *979.4* | *−9.6* | *−40.1* | | |
| | See also: 82JOH/POW, 81KIM/KAT, 82BIE/ASB. | | | | | | |
| $C_2H_4OS^+$ | | | | | | | |
| $CH_3COSH$ | 10.00±0.02 | 189 | 790 | −42±2 | −175±8 | 77PED/RYL | 507-09-5 |
|  | 9.2 | (205) | (858) | −7 | −30 | *EST | 7117-41-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_4OS_2^+$ | | | | | | | |
|  | (8.8) | (199) | (831) | −4 | −18 | *EST | 58816-63-0 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |
| $C_2H_4O_2^+$ | | | | | | | |
| $HCOOCH_3$ | 10.815±0.005 | 164.4 | 688.0 | −85.0±0.2 | −355.5±0.7 | 77PED/RYL | 107-31-3 |
| | See also: 81KIM/KAT, 85CAN/HAM. | | | | | | |
| $CH_3COOH$ | 10.66±0.02 | 142.5 | 596.4 | −103.3±0.1 | −432.1±0.4 | 78CHA/ZWO | 64-19-7 |
| | | *145.9* | *610.4* | *−99.9±0.1* | *−418.1±0.4* | | |
| | See also: 81HOL/FIN, 80VON/BIE, 81KIM/KAT. | | | | | | |
| $CH_2C(OH)_2$ | | 120 | 503 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations. | | | | | | |
| HOCH = CHOH | (9.62±0.10) | (146) | (612) | −76 | −316 | *EST | |
| | IP from 86TUR/HAV3. | | | | | | |
| $CH_3OCOH$ | | 158 | 661 | | | | |
| | $\Delta_f H$(Ion) from appearance potential of metastable ion (83TER/WEZ). | | | | | | |
| $CH_2CO(H_2O)$ | | (138) | (579) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (86POS/RUT). | | | | | | |
| $C_2H_4O_2S^+$ | | | | | | | |
|  | (10.3) | (177) | (741) | −60 | −253 | *EST | 1782-89-4 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

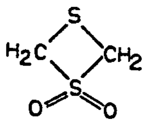
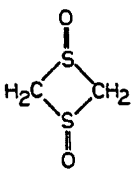
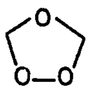
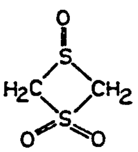
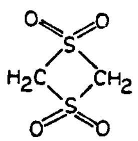
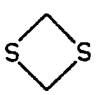
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_4O_2S_2^+$ | | | | | | | |
|  | (9.4) | (159) | (666) | –58 | –241 | *EST | 60743-07-9 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |
|  | (8.6) | (167) | (700) | –31 | –130 | *EST | 60743-08-0 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |
| $C_2H_4O_3^+$ | | | | | | | |
|  | (10.1) | (183) | (765) | –50 | –209 | 82CRE | 289-14-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_4O_3S_2^+$ | | | | | | | |
|  | (9.6) | (137) | (573) | –84 | –353 | *EST | 60743-10-4 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |
| $C_2H_4O_4S_2^+$ | | | | | | | |
|  | (10.6) | (107) | (447) | –138 | –576 | *EST | 21511-46-6 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |
| $C_2H_4S^+$ | | | | | | | |
| $CH_3CHS$ | 8.98±0.02 | 218 | 910 | 11 | 44 | 79JOS | 6851-93-0 |
| | See also: 83BUT/BAE2. | | | | | | |
|  | 9.051±0.006 | 228 | 955 | 19.6±0.3 | 82.1±1.2 | 77PED/RYL | 420-12-2 |
| | | *231* | *967* | *22.4* | *93.7* | | |
| | See also: 82BUT/BAE, 83BUT/BAE2. | | | | | | |
| $C_2H_4S_2^+$ | | | | | | | |
|  | (8.5) | (218) | (914) | 22 | 94 | *EST | 287-53-6 |
| | IP is onset of photoelectron band (82BLO/COR). | | | | | | |

**Table 1. Positive Ion Table - Continued**

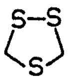
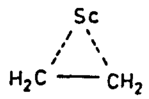
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_4S_3^+$ | | | | | | | |
|  | (≤8.72) | (≤196) | (≤818) | −5 | −23 | *EST | 289-16-7 |
| $C_2H_4Sc^+$ | | | | | | | |
|  | | (215) | (899) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 86ELK/ARI. | | | | | | |
| $C_2H_4Se^+$ | | | | | | | |
| $CH_3CH=Se$ | (8.3) | (219) | (915) | 27 | 114 | *EST | 67281-48-5 |
| | IP is onset of photoelectron band (84BOC/AYG). | | | | | | |
| $C_2H_5^+$ | | | | | | | |
| $C_2H_5$ | 8.13 | 215.6±1.0 | 902±4 | 28 | 118 | 84CAO/BAC | ~~14936-94-8~~ |
| | | *<u>218.5±1.0</u>* | *<u>914±4</u>* | *31* | *130* | | 2025-56-1 |
| | Heat of formation of ion from appearance potential measurements (See: 81TRA/MCL, 80BAE, 82DYK/JON2, 82ROS/BUF). IP given is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. Experimental IP of radical ≤8.26±0.02 eV.(84DYK/ELL). | | | | | | |
| $C_2H_5Br^+$ | | | | | | | |
| $C_2H_5Br$ | 10.28 | 222.2 | 929.6 | −14.9±0.2 | −62.3±1.0 | 77PED/RYL | 74-96-4 |
| | | *227.4* | *951.5* | *−9.6±0.2* | *−40.4±1.0* | | |
| | See also: 81KIM/KAT, 85OHN/IMA. | | | | | | |
| $C_2H_5BrO^+$ | | | | | | | |
| $CH_2BrCH_2OH$(gauche) | (≤10.75) | (≤196) | (≤820) | (−52) | (−217) | *EST | 540-51-2 |
| | See also: 84KOB, 81KIM/KAT, 85OHN/IMA. | | | | | | |
| $CH_2BrCH_2OH$(trans) | (≤10.65) | (≤194) | (≤811) | (−52) | (−217) | *EST | 540-51-2 |
| | See also: 84KOB, 81KIM/KAT, 85OHN/IMA. | | | | | | |
| $C_2H_5Cl^+$ | | | | | | | |
| $C_2H_5Cl$ | 10.97±0.02 | 226 | 946 | −26.8±0.1 | −112.1±0.5 | 77PED/RYL | 75-00-3 |
| | | *230* | *961* | *−23.3* | *−97.6* | | |
| | See also: 83OHN/IMA, 81KIM/KAT. | | | | | | |
| $CH_3CHClH$ | | 227 | 951 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83HOL/BUR). | | | | | | |
| $C_2H_5ClHg^+$ | | | | | | | |
| $C_2H_5HgCl$ | 9.9 | 212 | 888 | −16±1 | −67±4 | 80TEL/RAB | 107-27-7 |
| | IP is onset of photoelectron band (81BAI/CHI2). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_5ClO^+$ | | | | | | | |
| $C_2H_5OCl$ | (10.13±0.02) | (212) | (886) | −22 | −91 | *EST | 624-85-1 |
| | IP from 81COL/FRO. | | | | | | |
| $CH_2ClCH_2OH$ | (10.52) | (181) | (756) | −62 | −259 | *EST | 107-07-3 |
| | IP is onset of photoelectron band (81KIM/KAT, 85OHN/IMA). See also: 84KOB. | | | | | | |
| $CH_3OCH_2Cl$ | (10.2) | (184) | (769) | −51 | −215 | *EST | 107-30-2 |
| | IP is onset of photoelectron band (80VER/SAL). | | | | | | |
| $C_2H_5ClS^+$ | | | | | | | |
| $CH_3SCH_2Cl$ | (≤7.74) | (≤157) | (≤657) | −22 | −90 | *EST | 2373-51-5 |
| $C_2H_5Cl_2P^+$ | | | | | | | |
| $C_2H_5PCl_2$ | 9.3 | 153 | 638 | −62±4 | −259±18 | 80TEL/RAB | 1498-40-4 |
| | IP is onset of photoelectron band (83ZVE/BAZ, 82LEV/LIA). | | | | | | |
| $C_2H_5Cl_3Si^+$ | | | | | | | |
| $C_2H_5SiCl_3$ | (10.74±0.04) | (122) | (509) | −126±6 | −527±25 | 80TEL/RAB | 115-21-9 |
| $CH_3SiCl_2(CH_2Cl)$ | (10.4) | (129) | (538) | −111 | −465 | *EST | 1558-33-4 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| $C_2H_5F^+$ | | | | | | | |
| $C_2H_5F$ | (11.6) | (205) | (856) | −63±0.5 | −263±2 | 75CHE/ROD | 353-36-6 |
| | IP is onset of photoelectron band (81BIE/ASB). See also: 81KIM/KAT. | | | | | | |
| $C_2H_5FO^+$ | | | | | | | |
| $CH_2FCH_2OH$ | (10.66) | (146) | (612) | −100 | −417 | *EST | 371-62-0 |
| | IP from 83KOP/MOL. | | | | | | |
| $C_2H_5F_2N^+$ | | | | | | | |
| $CF_2HCH_2NH_2$ | (9.4) | (326) | (1366) | 110 | 462 | *EST | 430-67-1 |
| | IP from 79AUE/BOW. | | | | | | |
| $C_2H_5F_2O^+$ | | | | | | | |
| $CF_2HCH_2OH_2$ | | 34 | 144 | | | | |
| | From proton affinity of $CF_2HCH_2OH$ (RN 359-13-7). PA = 176.2 kcal/mol, 737 kJ/mol. | | | | | | |
| $C_2H_5F_3N^+$ | | | | | | | |
| $CF_3CH_2NH_3$ | | −4 | −18 | | | | |
| | From proton affinity of $CF_3CH_2NH_2$ (RN 753-90-2). PA = 202.5 kcal/mol, 847 kJ/mol. | | | | | | |
| $C_2H_5I^+$ | | | | | | | |
| $C_2H_5I$ | 9.346 | 213.3 | 891.9 | −2.2±0.2 | −9.0±0.9 | 77PED/RYL | 75-03-6 |
| | | *216.9* | *907.8* | *1.6* | *6.9* | | |
| | See: 78LIA/AUS, 83OHN/IMA, 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_5IO^+$ | | | | | | | |
| gauche-$ICH_2CH_2OH$ | 9.73 | (186) | (778) | −38 | −161 | *EST | 624-76-0 |
| trans-$ICH_2CH_2OH$ | 9.60 | (183) | (765) | −38 | −161 | *EST | 624-76-0 |
| $C_2H_5N^+$ | | | | | | | |
| $CH_2=NCH_3$ | (9.4) | (234) | (979) | 17 | 72 | 69BEN/CRU | 1761-67-7 |
| | IP is onset of photoelectron band. See also: 86WER. | | | | | | |
| $CH_3CH=NH$ | (9.6) | (222) | (930) | 2±4 | 8±17 | 79ELL/EAD | 20729-41-3 |
| | IP is onset of photoelectron band (86LAF/GON). | | | | | | |
| $CH_2=CHNH_2$ | (8.20) | (196) | (820) | 7 | 29 | 81ELL/DIX | 593-67-9 |
| | IP from 84ALB/ALL2. | | | | | | |
|  | 9.2±0.1 | 242 | 1014 | 30.2±0.2 | 126.5±0.9 | 77PED/RYL | 151-56-4 |
| | See also: 82BIE/ASB. | | | | | | |
| $C_2H_5NO^+$ | | | | | | | |
| $CH_3CONH_2$ | 9.65±0.03 | 165 | 693 | −57.0±0.2 | −238.3±0.8 | 77PED/RYL | 60-35-5 |
| | See also: 81ASB/SVE. | | | | | | |
| (E)-$CH_3CH=NOH$ | (10.0) | (226) | (945) | −4.7±2 | −20±8 | 69BEN/CRU | 107-29-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $HCONHCH_3$ | 9.79 | (181) | (758) | −45±0.7 | −187±3 | *EST | 123-39-7 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2H_5NO_2^+$ | | | | | | | |
| $NH_2CH_2COOH$ | 8.8 | 109 | 458 | −93±1 | −391±5 | 77NGA/SAB | 56-40-6 |
| | See also: 83CAN/HAM. | | | | | | |
| $C_2H_5NO_2$ | 10.88±0.05 | 226.5 | 947.5 | −24.4±0.1 | −102.2±0.6 | 77PED/RYL | 79-24-3 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2H_5ONO$ | (10.53±0.01) | (218) | (913) | −25 | −103 | 74BAT/CHR | 109-95-5 |
| $C_2H_5NO_3^+$ | | | | | | | |
| $C_2H_5ONO_2$ | (11.22) | (222) | (928) | −36.8±0.2 | −154.1±1.0 | 77PED/RYL | 625-58-1 |
| $C_2H_5NS^+$ | | | | | | | |
| $CH_3CSNH_2$ | 8.33 | 194 | 814 | 2±0.2 | 10±1 | 82TOR/SAB2 | 62-55-5 |
| $C_2H_5N_2^+$ | | | | | | | |
| $NCCH_2NH_3$ | | 194 | 812 | | | | |
| | From proton affinity of $NCCH_2NH_2$ (RN 540-61-4). PA = 197.4 kcal/mol, 826 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

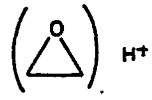
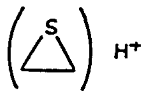
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_5O^+$ | | | | | | | |
| $CH_3CHOH$ | 6.7 | 139 | 583 | −16±1 | −66±4 | 82MCM/GOL | 17104-36-8 |
| | $\Delta_fH$(Ion) from proton affinity of acetaldehyde (RN 75-07-0). PA = 186.6 kcal/mol, 781 kJ/mol. The IP given is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). See also: 82MAC, 84LOS/HOL. | | | | | | |
| $CH_3OCH_2$ | 6.94 | (157)<br>*(165)* | (657)<br>*(690)* | −3±1 | −13±4 | 82MCM/GOL | 16520-04-0 |
| | $\Delta_fH$(Ion) at 0 K from appearance potential determination (82MAC, 84BUT/HOL). See also: 84BOW/MAC. | | | | | | |
| $CH_2{=}CHOH_2$ | | 148 | 619 | | | | |
| | $\Delta_fH$(Ion) from appearance potential determination (82BUR/TER2). | | | | | | |
|  | | 165 | 691 | | | | |
| | From proton affinity of oxirane (RN 75-21-8). PA = 187.9 kcal/mol, 786 kJ/mol. | | | | | | |
| $C_2H_5O_2^+$ | | | | | | | |
| $CH_3C(OH)_2$ | | 72 | 302 | | | | |
| | From proton affinity of $CH_3COOH$ (RN 64-19-7). See also: 84HOL/LOS. 85AUD/MIL. PA = 190.2 kcal/mol, 796. kJ/mol. | | | | | | |
| $HC(OH)OCH_3$ | | 92 | 386 | | | | |
| | From proton affinity of $HCOOCH_3$ (RN 107-31-3). PA = 188.4 kcal/mol, 788. kJ/mol. (86KNI/FRE, 84LIA/LIE). | | | | | | |
| $C_2H_5P^+$ | | | | | | | |
|  | (9.4±0.1) | (200) | (838) | −16±0.5 | −69±2 | *EST | 6569-82-0 |
| $C_2H_5S^+$ | | | | | | | |
| $CH_3CHSH$ | | 197<br>*200* | 823<br>*836* | | | | 58794-14-2 |
| | $\Delta_fH$(Ion) from appearance potential determinations (83BUT/BAE). | | | | | | |
| $CH_3SCH_2$ | | *(194)* | *(812)* | | | | 31533-72-9 |
| | $\Delta_fH$(Ion) from appearance potential determinations. See also: 83ERM/AKO. 0 K values. | | | | | | |
|  | | 191 | 798 | | | | |
| | From proton affinity of thiirane (RN 420-12-2). PA = 194.6 kcal/mol, 814 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

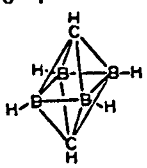
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_2H_6^+$** | | | | | | | |
| $C_2H_6$ | 11.52±0.01 | 245.6 | 1028 | −20.1±0.05 | −84.0±0.2 | 77PED/RYL | 74-84-0 |
| | | *249.3* | *1043* | *−16.4* | *−68.4* | | |
| | See also: 81KIM/KAT, 84CHA/HIL. | | | | | | |
| **$C_2H_6BBr^+$** | | | | | | | |
| $(CH_3)_2BBr$ | 10.25 | 192 | 804 | −44 | −185 | 82HOL/SMI | 5158-50-9 |
| **$C_2H_6BCl^+$** | | | | | | | |
| $(CH_3)_2BCl$ | (10.2) | (173) | (725) | −62 | −259 | 82HOL/SMI | 1803-36-7 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_2H_6BCl_2N^+$** | | | | | | | |
| $(CH_3)_2NBCl_2$ | 9.56 | 125 | 521 | −96±1 | −401±4 | 77PED/RYL | 1113-31-1 |
| **$C_2H_6B_4^+$** | | | | | | | |
|  | (9.77) | (236.3) | (988.6) | 11.0±2.9 | 45.9±12.1 | 85GAL/TAM | 20693-67-8 |
| **$C_2H_6Br^+$** | | | | | | | |
| $C_2H_5BrH$ | | (180) | (753) | | | | |
| | From proton affinity of $C_2H_5Br$ (RN 74-96-4). PA = ~171 kcal/mol, ~715 kJ/mol. | | | | | | |
| **$C_2H_6BrSi^+$** | | | | | | | |
| $(CH_3)_2SiBr$ | | 146 | 612 | | | | |
| | | *151* | *633* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (84SZE/BAE). | | | | | | |
| **$C_2H_6Cd^+$** | | | | | | | |
| $(CH_3)_2Cd$ | (8.56±0.02) | (223) | (932) | 25.3±0.3 | 105.8±1.3 | 77PED/RYL | 506-82-1 |
| **$C_2H_6Cl^+$** | | | | | | | |
| $C_2H_5ClH$ | | 170 | 711 | | | | |
| | From proton affinity of $C_2H_5Cl$ (RN 75-00-3). PA = 169 kcal/mol, 707 kJ/mol. | | | | | | |
| $CH_3ClCH_3$ | | (177) | (743) | | | | 24400-15-5 |
| | Derived (85SHA/HOJ). | | | | | | |
| **$C_2H_6ClN^+$** | | | | | | | |
| $(CH_3)_2NCl$ | 8.75 | (221) | (925) | 19 | 81 | *EST | 1585-74-6 |
| **$C_2H_6ClP^+$** | | | | | | | |
| $(CH_3)_2PCl$ | (8.7) | (163) | (681) | −38 | −158 | *EST | 811-62-1 |
| | IP is onset of photoelectron band (82LEV/LIA, 86BOC/BAN). | | | | | | |
| **$C_2H_6Cl_2NOP^+$** | | | | | | | |
| $(CH_3)_2NPOCl_2$ | (9.5) | (86) | (361) | −133 | −556 | *EST | 677-43-0 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_2H_6Cl_2NP^+$** | | | | | | | |
| $(CH_3)_2NPCl_2$ | (8.9) | (171) | (716) | −34 | −143 | *EST | 683-85-2 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_2H_6Cl_2Si^+$** | | | | | | | |
| $(CH_3)_2SiCl_2$ | (10.7) | (137) | (574) | −109 | −458 | 81BEL/PER | 75-78-5 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_2H_6Cl_2Sn^+$** | | | | | | | |
| $(CH_3)_2SnCl_2$ | (10.43) | (174) | (727) | −67 | −279 | *EST | 753-73-1 |
| **$C_2H_6F^+$** | | | | | | | |
| $CH_3FCH_3$ | | (147) | (614) | | | | |
| | $\Delta_fH$(Ion) derived from results of 86HOV/MCM. | | | | | | |
| $C_2H_5FH$ | | 138 | 577 | | | | |
| | From proton affinity of $C_2H_5F$ (RN 75-02-5). PA = 165 kcal/mol, 690 kJ/mol. | | | | | | |
| **$C_2H_6FN^+$** | | | | | | | |
| $CH_2FCH_2NH_2$ | (9.1) | (155) | (650) | −55 | −229 | *EST | 406-34-8 |
| | IP from 79AUE/BOW. | | | | | | |
| **$C_2H_6FP^+$** | | | | | | | |
| $(CH_3)_2PF$ | (8.8) | (112) | (468) | −91 | −381 | *EST | 507-15-3 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_2H_6FSi^+$** | | | | | | | |
| $(CH_3)_2SiF$ | | 86 | 359 | | | | |
| | From appearance potential (10.70±0.04 eV) of ion in $(CH_3)_3SiF$. | | | | | | |
| **$C_2H_6F_2N^+$** | | | | | | | |
| $CF_2HCH_2NH_3$ | | 269 | 1124 | | | | |
| | From proton affinity of $CF_2HCH_2NH_2$ (RN 430-67-1). PA = 207.5 kcal/mol, 868 kJ/mol. | | | | | | |
| **$C_2H_6F_2Si^+$** | | | | | | | |
| $(CH_3)_2SiF_2$ | 11.03±0.03 | 42 | 177 | −212 | −887 | 77MUR/BEA | 353-66-2 |
| **$C_2H_6Hg^+$** | | | | | | | |
| $(CH_3)_2Hg$ | (9.10±0.05) | (232) | (972) | 22.5±0.2 | 94.0±1.0 | 77PED/RYL | 593-74-8 |
| | | *(237)* | *(991)* | *27.0* | *113.3* | | |
| **$C_2H_6I^+$** | | | | | | | |
| $C_2H_5IH$ | | (188) | (785) | | | | |
| | From proton affinity of $C_2H_5I$ (RN 75-03-6). PA = ~176 kcal/mol, ~736 kJ/mol. | | | | | | |
| **$C_2H_6N^+$** | | | | | | | |
| $CH_2NHCH_3$ | 5.9 | 166 | 695 | 30 | 126 | 83BUR/CAS | 31277-24-4 |
| | $\Delta_fH$(Ion) from appearance potential determination(81LOS/LAM); IP derived (81GRI/LOS, 83BUR/CAS). | | | | | | |
| $CH_3CHNH_2$ | 5.7 | 157 | 657 | 26 | 109 | 83BUR/CAS | 30208-36-7 |
| | $\Delta_fH$(Ion) from appearance potential determination(81LOS/LAM); IP derived(83BUR/CAS). | | | | | | |

**Table 1. Positive Ion Table - Continued**

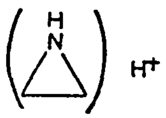
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_6N^+$ | | | | | | | |
| $(CH_3)_2N$ | (5.17) | (154) | (644) | 35±2 | 145±8 | 82MCM/GOL | 15337-44-7 |
| | $\Delta_f H$(Ion) from appearance potential measurement. IP cited is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
|  | | 180 | 755 | | | | |
| | From proton affinity of aziridine (RN 151-56-4). PA = 215.7 kcal/mol, 902 kJ/mol. | | | | | | |
| $C_2H_6NO^+$ | | | | | | | |
| $CH_3C(OH)NH_2$ | | 103 | 429 | | | | |
| | From proton affinity of $CH_3CONH_2$ (RN 60-35-5). PA = 206.2 kcal/mol, 863 kJ/mol. | | | | | | |
| $HC(OH)NHCH_3$ | | 115 | 481 | | | | |
| | From proton affinity of $HCONHCH_3$ (RN 123-39-7). PA = 205.8 kcal/mol, 861 kJ/mol. | | | | | | |
| $C_2H_6NO_2^+$ | | | | | | | |
| $NH_3CH_2COOH$ | | 61 | 254 | | | | |
| | From proton affinity of $NH_2CH_2COOH$ (RN 56-40-6). PA = 211.6 kcal/mol, 885 kJ/mol. | | | | | | |
| $C_2H_5ONHO$ | | 144 | 602 | | | | |
| | From proton affinity of $C_2H_5ONO$ (RN 109-95-5). PA = 197.3 kcal/mol, 825.5 kJ/mol. | | | | | | |
| $C_2H_5NOOH$ | | 157 | 655 | | | | |
| | From proton affinity of $C_2H_5NO_2$ (RN 79-24-3). PA = 184.8 kcal/mol, 773 kJ/mol. | | | | | | |
| $C_2H_6N_2^+$ | | | | | | | |
| (E)-$CH_3N=NCH_3$ | 8.45±0.05 | 231 | 964 | 36 | 149 | 82PAM/ROG | 4143-41-3 |
| $C_2H_6N_2O^+$ | | | | | | | |
| (E)-$CH_3NN(O)CH_3$ | | | | | | | |
| | (9.7) | (238) | (997) | 15 | 61 | *EST | 54168-20-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3NHCONH_2$ | (≤9.66) | (≤164) | (≤688) | −58 | −244 | *EST | 598-50-5 |
| $(CH_3)_2NNO$ | 8.69 | 200 | 835 | −0.7±2 | −3±8 | 67KOR/PEP | 62-75-9 |
| $C_2H_6N_2O_2^+$ | | | | | | | |
| $(CH_3)_2NNO_2$ | (9.53) | (219) | (914) | −1±0.8 | −5±3 | 77PED/RYL | 4164-28-7 |
| (E)-$(CH_3NO)_2$ | (≤8.68) | (≤217) | (≤908) | 17±0.2 | 71±1 | 73BAT/MIL | 37765-15-4 |
| $C_2H_6O^+$ | | | | | | | |
| $C_2H_5OH$ | 10.47±0.02 | 185.3 | 775.4 | −56.1±0.1 | −234.8±0.2 | 77PED/RYL | 64-17-5 |
| | | *189.5* | *793.1* | *−51.9* | *−217.1* | | |
| | See also: 82MIS/POK, 72POT/SOR, 80VON/BIE, 84BOW/MAC, 83OHN/IMA, 81KIM/KAT, 80BAC/MOU, 74BET/BAK. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_6O^+$ | | | | | | | |
| $(CH_3)_2O$ | 10.025±0.025 | 187.2 | 783.3 | −44.0±0.1 | −184.0±0.5 | 77PED/RYL | 115-10-6 |
| | | *191.5* | *801.0* | *−39.7* | *−166.3* | | |
| | IP from 84BUT/HOL. See also: 84BOW/MAC, 81KIM/KAT, 80BAC/MOU, 82BIE/ASB. | | | | | | |
| $C_2H_4OH_2$ | | 175 | 732 | | | | 60786-90-5 |
| | $\Delta_f H$(Ion) from appearance potential measurements (85BUR/HOL). See also: 82HOL/LOS, 82BUR/HOL). The authors propose the structure $C_2H_3..H^+..OH_2$ for the ion. See also: 81TER/HEE. | | | | | | |
| $C_2H_6OS^+$ | | | | | | | |
| $(CH_3)_2SO$ | (9.01) | (172) | (718) | −36.2±0.2 | −151.3±0.8 | 77PED/RYL | 67-68-5 |
| | | *(176)* | *(738)* | *−31.4* | *−131.5* | | |
| | See: 81KIM/KAT. | | | | | | |
| $C_2H_6O_2^+$ | | | | | | | |
| $HOCH_2CH_2OH$ | 10.16 | 142 | 593 | −92.6±0.4 | −387.6±1.7 | 77PED/RYL | 107-21-1 |
| | IP from 82HOL/LOS2. See also: 80VON/BIE, 81KIM/KAT. | | | | | | |
| $(CH_3O)_2$ | 9.1 | 180 | 752 | −30.0±0.3 | −125.7±1.3 | 77PED/RYL | 690-02-8 |
| | IP is onset of photoelectron band (81KIM/KAT, 82LEV/LIA). | | | | | | |
| $C_2H_6O_2S^+$ | | | | | | | |
| $(CH_3)_2SO_2$ | (10.3) | (148) | (621) | −89±0.7 | −373±3 | 77PED/RYL | 67-71-0 |
| | | *(154)* | *(644)* | *−84* | *−350* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_6O_3S^+$ | | | | | | | |
| $(CH_3O)_2SO$ | (9.9) | (113) | (472) | −115±0.5 | −483±2 | 77PED/RYL | 616-42-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_6P^+$ | | | | | | | |
|  | | 158 | 660 | | | | |
| | From proton affinity of phosphirane (RN 6569-82-0). PA = 191.4 kcal/mol, 801 kJ/mol. | | | | | | |
| $C_2H_6S^+$ | | | | | | | |
| $C_2H_5SH$ | 9.285±0.005 | 203 | 850 | −11.1±0.1 | −46.3±0.6 | 77PED/RYL | 75-08-1 |
| | | *207* | *867* | *−7.0* | *−29.5* | | |
| | See also: 83OHN/IMA, 81KIM/KAT. | | | | | | |
| $(CH_3)_2S$ | 8.69±0.01 | 191 | 801 | −9.0±0.1 | −37.5±0.5 | 77PED/RYL | 75-18-3 |
| | | *195* | *817* | *−5.1* | *−21.3* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2H_6SSi^+$ | | | | | | | |
| $(CH_3)_2Si{=}S$ | | (203) | (848) | | | | 1111-83-7 |
| | $\Delta_f H$(Ion) from appearance potential determination (81GUS/VOL). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_2H_6S_2^+$ | | | | | | | |
| $(CH_3S)_2$ | (7.4±0.3) | (165±4) | (690±15) | −5.8±0.2 | −24.2±1.0 | 77PED/RYL | 624-92-0 |
| | | *(169)* | *(707)* | *−1.6* | *−6.8* | | |
| | Adiabatic ionization potential determined from consideration of dissociation rates; experimentally observed onset of ionization, 8.33 eV, is much higher because of change in the CSSC bond angle upon ionization from 90° to 180°. (83BUT/BAE). See also: 81KIM/KAT. | | | | | | |
| $C_2H_6S_3^+$ | | | | | | | |
| $CH_3SSSCH_3$ | (8.73±0.03) | (199) | (831) | −3 | −11 | *EST | 3658-80-8 |
| $C_2H_6Sc^+$ | | | | | | | |
| $C_2H_5ScH$ | | (205) | (858) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $(CH_3)_2Sc$ | | 189 | 791 | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 86ELK/ARI. | | | | | | |
| $C_2H_4ScH_2$ | | (218) | (912) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $C_2H_6Se^+$ | | | | | | | |
| $(CH_3)_2Se$ | 8.40±0.01 | (198) | (827) | 4 | 17 | *EST | 593-79-3 |
| | IP from 84BOC/AYG, 82LEV/LIA. | | | | | | |
| $C_2H_6Se_2^+$ | | | | | | | |
| $(CH_3Se)_2$ | (8.1) | (197) | (826) | 11 | 44 | *EST | 7101-31-7 |
| | IP is onset of photoelectron band (84BOC/AYG). | | | | | | |
| $C_2H_6Si^+$ | | | | | | | |
| $CH_2=CHSiH_3$ | 10.1 | 234 | 978 | 1±3 | 4±13 | 80TEL/RAB | 7291-09-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_6Zn^+$ | | | | | | | |
| $(CH_3)_2Zn$ | (9.00±0.02) | (220) | (919) | 12.1±0.3 | 50.6±1.3 | 77PED/RYL | 544-97-8 |
| $C_2H_7^+$ | | | | | | | |
| $C_2H_7$ | | 202 | 845 | | | | |
| | From proton affinity of $C_2H_6$ (RN 74-84-0). See also: 85MCM/KEB. PA = 143.6 kcal/mol, 601 kJ/mol. | | | | | | |
| $C_2H_7As^+$ | | | | | | | |
| $(CH_3)_2AsH$ | (8.1) | (194) | (813) | 7 | 31 | *EST | 593-57-7 |
| | IP is onset of photoelectron band (82ELB/DIE). | | | | | | |
| $C_2H_7BO_2^+$ | | | | | | | |
| $(CH_3O)_2BH$ | (9.7±1.0) | (85) | (355) | −138.8±0.4 | −580.7±1.7 | 77PED/RYL | 4542-61-4 |

**Table 1. Positive Ion Table - Continued**

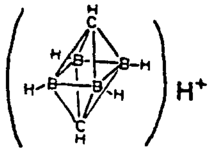
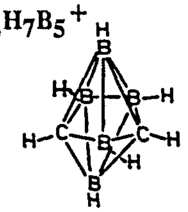
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_7B_4{}^+$ | | | | | | | |
|  | | (170) | (710) | | | | |
| | From proton affinity of 1,6-dicarbahexaborane(6) (RN 20693-67-8).<br>PA = 207. kcal/mol, 866. kJ/mol. | | | | | | |
| $C_2H_7B_5{}^+$ | | | | | | | |
|  | 10.54 | 240.5 | 1006.3 | −2.5±2.6 | −10.6±10.9 | 85GAL/TAM | 20693-69-0 |
| $C_2H_7ClO^+$ | | | | | | | |
| $(CH_3)_2OHCl$ | (10.4) | (167) | (698) | −73 | −305 | 82TN270 | 24521-77-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2H_7FN^+$ | | | | | | | |
| $CH_2FCH_2NH_3$ | | 99 | 413 | | | | |
| | From proton affinity of $CH_2FCH_2NH_2$ (RN 406-34-8). PA = 212.3 kcal/mol, 888 kJ/mol. | | | | | | |
| $C_2H_7Hg^+$ | | | | | | | |
| $(CH_3)_2HgH$ | | (202) | (846) | | | | |
| | From proton affinity of $CH_3HgCH_3$ (RN 593-74-8). PA = ~186 kcal/mol, ~778 kJ/mol. | | | | | | |
| $C_2H_7N^+$ | | | | | | | |
| $C_2H_5NH_2$ | 8.86±0.02 | 193 | 807 | −11.3±0.2 | −47.5±0.7 | 77PED/RYL | 75-04-7 |
| | See also: 83OHN/IMA, 81KIM/KAT. | | | | | | |
| $(CH_3)_2NH$ | 8.23±0.08 | 185 | 776 | −4.4±0.1 | −18.5±0.4 | 77PED/RYL | 124-40-3 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_2H_7NO^+$ | | | | | | | |
| $NH_2CH_2CH_2OH$ | 8.96 | 158 | 662 | −48 | −202 | 77REI/PRA | 141-43-5 |
| | IP from 83KOP/MOL, 83MOL/PIK3, in agreement with onset of photoelectron band (81KIM/KAT). | | | | | | |
| $CH_3NHOCH_3$ | 8.92 | (197) | (824) | −9 | −37 | *EST | 1117-97-1 |
| | IP from 83MOL/PIK. | | | | | | |
| $C_2H_7N_2{}^+$ | | | | | | | |
| $CH_3NNHCH_3$ | | 194 | 813 | | | | |
| | From proton affinity of (E)-$CH_3N{=}NCH_3$ (RN 4143-41-3). PA = 206.9 kcal/mol, 866 kJ/mol. | | | | | | |
| $C_2H_7O^+$ | | | | | | | |
| $C_2H_5OH_2$ | | 121 | 507 | | | | |
| | From proton affinity of $C_2H_5OH$ (RN 64-17-5). PA = 188.3 kcal/mol, 788 kJ/mol. | | | | | | |
| $(CH_3)_2OH$ | | 130 | 542 | | | | |
| | From proton affinity of $(CH_3)_2O$ (RN 115-10-6). PA = 192.1 kcal/mol, 804 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

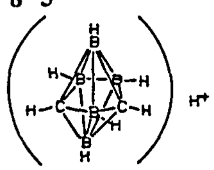
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_7OS^+$ | | | | | | | |
| $(CH_3)_2SOH$ | | 118 | 495 | | | | |
| | From proton affinity of $(CH_3)_2SO$ (RN 67-68-5). PA = 211.3 kcal/mol, 834 kJ/mol. | | | | | | |
| $C_2H_7O_3P^+$ | | | | | | | |
| $(CH_3O)_2PHO$ | (10.53) | (43) | (179) | (−200) | (−837) | *EST | 868-85-9 |
| | IP from 80ZVE/VIL. | | | | | | |
| $C_2H_7P^+$ | | | | | | | |
| $(CH_3)_2PH$ | 8.47±0.07 | (181) | (757) | −14 | −60 | *EST | 676-59-5 |
| | See also: 82COW/KEM. | | | | | | |
| $C_2H_7S^+$ | | | | | | | |
| $C_2H_5SH_2$ | | 164 | 686 | | | | |
| | From proton affinity of $C_2H_5SH$ (RN 75-08-1). PA = 190.8 kcal/mol, 798 kJ/mol. | | | | | | |
| $(CH_3)_2SH$ | | 156 | 653 | | | | |
| | From proton affinity of $(CH_3)_2S$ (RN 75-18-3). PA = 200.6 kcal/mol, 839 kJ/mol. | | | | | | |
| $C_2H_7S_2^+$ | | | | | | | |
| $CH_3SSHCH_3$ | | (164) | (686) | | | | |
| | From proton affinity of $CH_3SSCH_3$ (RN 624-92-0). PA = ~196 kcal/mol, ~820 kJ/mol. | | | | | | |
| $C_2H_8B_5^+$ | | | | | | | |
|  | | (195) | (816) | | | | |
| | From proton affinity of 2,4-dicarbaheptabornane(7) (RN 20693-69-0). PA = 168. kcal/mol, 703. kJ/mol. | | | | | | |
| $C_2H_8N^+$ | | | | | | | |
| $C_2H_5NH_3$ | | 137 | 574 | | | | |
| | From proton affinity of $C_2H_5NH_2$ (RN 75-04-7). PA = 217.0 kcal/mol, 908. kJ/mol. | | | | | | |
| $(CH_3)_2NH_2$ | | 141 | 588 | | | | |
| | From proton affinity of $(CH_3)_2NH$ (RN 124-40-3). PA = 220.6 kcal/mol, 923. kJ/mol. | | | | | | |
| $C_2H_8NO^+$ | | | | | | | |
| $H_3N(CH_2)_2OH$ | | 96 | 402 | | | | |
| | From proton affinity of $NH_2(CH_2)_2OH$ (RN 141-43-5). PA = 221.3 kcal/mol, 926. kJ/mol. | | | | | | |
| $C_2H_8N_2^+$ | | | | | | | |
| $H_2NCH_2CH_2NH_2$ | (8.6) | (194) | (812) | −4.3±0.5 | −17.8±2.1 | 77PED/RYL | 107-15-3 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $(CH_3)_2NNH_2$ | 7.28±0.04 | 188 | 786 | 20±0.5 | 84±2 | 77PED/RYL | 57-14-7 |
| | IP from charge transfer equilibrium constant determination. Reference standard: IP ($C_6H_5N(CH_3)_2$) = 7.12 eV (84MAU/NEL). See also: 81KIM/KAT. | | | | | | |

Table 1. Positive Ion Table - Continued

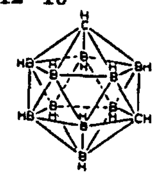
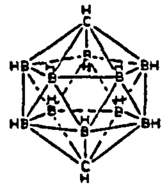
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_2H_8N_2^+$ | | | | | | | |
| $C_2H_5NHNH_2$ | | | | 16±0.2 | 69±1 | *EST | 624-80-6 |
| | A value of 8.12 eV has been reported for the adiabatic IP of this compound. Values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. | | | | | | |
| $(CH_3NH)_2$ | | | | 22±1 | 92±4 | 77PED/RYL | 540-73-8 |
| | Values of 7.75 and 8.22 eV have been reported for the adiabatic IP of this compound. Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 81KIM/KAT. | | | | | | |
| $C_2H_8P^+$ | | | | | | | |
| $(CH_3)_2PH_2$ | | 134 | 559 | | | | |
| | From proton affinity of $(CH_3)_2PH$ (RN 676-59-5). PA = 216.3 kcal/mol, 905 kJ/mol. | | | | | | |
| $C_2H_8Si^+$ | | | | | | | |
| $C_2H_5SiH_3$ | (10.18±0.05) | (262) | (1095) | 27±3 | 113±13 | 80TEL/RAB | 2814-79-1 |
| $(CH_3)_2SiH_2$ | 10.3 | 215 | 899 | −23±1 | −95±4 | 86DON/WAL | 1111-74-6 |
| $C_2H_9N_2^+$ | | | | | | | |
| $H_2NCH_2CH_2NH_3$ | | 135 | 567 | | | | |
| | From proton affinity of $H_2NCH_2CH_2NH_2$ (RN 107-15-3). PA = 225.9 kcal/mol, 945 kJ/mol. | | | | | | |
| $(CH_3)_2NHNH_2$ | | 166 | 694 | | | | |
| | From proton affinity of $(CH_3)_2NNH_2$ (RN 57-14-7). PA = 219.9 kcal/mol, 920 kJ/mol (84MAU/NEL). | | | | | | |
| $C_2H_{10}BN^+$ | | | | | | | |
| $((CH_3)_2NH)(BH_3)$ | (9.39±0.01) | (202) | (847) | −14±1 | −59±4 | 80TEL/RAB | 74-94-2 |
| $C_2H_{12}B_{10}^+$ | | | | | | | |
|  | (10.19) | (191) | (800) | −44±2 | −183±8 | 82PIL/SKI | 16986-24-6 |
|  | (10.2) | (175) | (733) | −60±2 | −251±8 | 82PIL/SKI | 20644-12-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2I_2^+$ | | | | | | | |
| IC≡CI | (9.03) | (269.57) | (1127.90) | 61.34 | 256.64 | 84DEW/HEA | 624-74-8 |

**Table 1. Positive Ion Table - Continued**

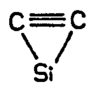
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_2La^+$ | | | | | | | |
| $LaC_2$ | (5.4±0.3) | (266) | (1113) | 141±2 | 592±6 | 81GIN/PEL | 12071-15-7 |
| | | *(266)* | *(1112)* | *141* | *591* | | |
| $C_2N^+$ | | | | | | | |
| CCN | 12.0 | (410) | (1715) | 133 | 556 | 85JANAF | 12327-12-7 |
| | $\Delta_f H$(Ion) from appearance potential measurements (83SMI, 85HAR/MCI). | | | | | | |
| | IP cited is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| CNC | | (387) | (1620) | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurements (85HAR/MCI). | | | | | | |
| $C_2N_2^+$ | | | | | | | |
| NCCN | 13.37±0.01 | 381.6 | 1596.7 | 73.3±0.2 | 306.7±0.7 | 77PED/RYL | 460-19-5 |
| | | *381.1* | *1594.8* | *72.8* | *304.8* | | |
| | See also: 83SMI. | | | | | | |
| $C_2N_2O^+$ | | | | | | | |
| NCNCO | (11.49±0.02) | (296) | (1238) | 31 | 129 | *EST | 22430-66-6 |
| $C_2N_2S_2^+$ | | | | | | | |
| $(SCN)_2$ | (10.5) | (326) | (1363) | 84±1 | 350±6 | 77PED/RYL | 505-14-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_2Sc^+$ | | | | | | | |
| $C_2Sc$ | 7.7±0.2 | 325 | 1360 | 147±3 | 617±12 | 81HAQ/GIN | 12175-91-6 |
| | | *324* | *1357* | *147* | *614* | | |
| | See also: 81HAQ/GIN. | | | | | | |
| $C_2Si^+$ | | | | | | | |
|  | (10.2±0.5) | (382) | (1599) | 147 | 615 | 82TN270 | 12071-27-1 |
| | | *(381)* | *(1594)* | *146* | *610* | | |
| $C_2Th^+$ | | | | | | | |
| $C_2Th$ | (6.4±0.5) | (321) | (1341) | 173 | 724 | 82TN270 | 12071-31-7 |
| $C_2V^+$ | | | | | | | |
| $C_2V$ | | *(335)* | *(1401)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). 0 K value. | | | | | | |
| $C_2Y^+$ | | | | | | | |
| $C_2Y$ | 6.7±0.3 | 297 | 1243 | 143 | 597 | 82TN270 | 12071-35-1 |
| | | *296* | *1240* | *142* | *594* | | |
| $C_3^+$ | | | | | | | |
| $C_3$ | (12.1±0.3) | (479) | (2004) | 200±4 | 837±17 | 83RAK/BOH | 12075-35-3 |

Table 1. Positive Ion Table - Continued

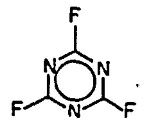
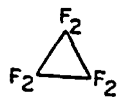
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3BrN^+$ | | | | | | | |
| BrC≡CCN | (10.71±0.02) | (350) | (1466) | 103±5 | 433±20 | 79BUC/VOG | 3114-46-3 |
| | See also: 84KUH/MAI. | | | | | | |
| $C_3ClN^+$ | | | | | | | |
| ClC≡CCN | 10.95±0.02 | 334 | 1396 | 81±5 | 339±20 | 79BUC/VOG | 2003-31-8 |
| $C_3FN^+$ | | | | | | | |
| CF≡CCN | (11.51±0.02) | (305) | (1278) | 40±12 | 167±50 | 79BUC/VOG | 32038-83-8 |
| $C_3F_3N^+$ | | | | | | | |
| $CF_2$=CFCN | (10.6±0.1) | (139) | (584) | −105±0.7 | −439±3 | 71JANAF | 433-43-2 |
| $C_3F_3N_3^+$ | | | | | | | |
|  | (11.3) | (131) | (548) | −129 | −542 | *EST | 675-14-9 |
| | IP is onset of photoelectron band (81ASB/SVE). | | | | | | |
| $C_3F_4^+$ | | | | | | | |
| $CF_2$=C=$CF_2$ | (10.88) | (109) | (456) | −142 | −594 | 86SMA | 461-68-7 |
| $C_3F_6^+$ | | | | | | | |
| $CF_3CF$=$CF_2$ | 10.60±0.03 | −24 | −102 | −269 | −1125 | 75CHE/ROD | 116-15-4 |
| | IP from 81BER/BOM. | | | | | | |
|  | 11.18±0.03 | 24 | 101 | −234 | −978 | 81BOM/BER | 931-91-9 |
| | IP from 81BER/BOM. | | | | | | |
| $C_3F_6O^+$ | | | | | | | |
| $(CF_3)_2CO$ | (11.44) | (−70) | (−293) | −334 | −1397 | 72GOR | 684-16-2 |
| $C_3F_8^+$ | | | | | | | |
| $C_3F_8$ | 13.38 | −118 | −492 | −426±2 | −1783±7 | 77PED/RYL | 76-19-7 |
| $C_3F_9N^+$ | | | | | | | |
| $(CF_3)_3N$ | 11.7 | (−168) | (−703) | −438 | −1832 | *EST | 432-03-1 |
| | IP is onset of photoelectron band (82ELB/DIE, 82BUR/PAW). | | | | | | |
| $C_3H^+$ | | | | | | | |
| HCCC | | (381) | (1593) | | | | |
| | From proton affinity of $C_3$ (RN 12075-35-3). PA = ~185 kcal/mol, ~774 kJ/mol. | | | | | | |
| $C_3HF_3^+$ | | | | | | | |
| $CF_3C$≡CH | (11.96±0.02) | (177) | (741) | −99 | −413 | 86SMA | 661-54-1 |
| | See also: 81BIE/ASB. | | | | | | |

**Table 1. Positive Ion Table - Continued**

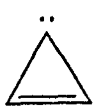
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3HF_5N^+$ | | | | | | | |
| $C_2F_5CNH$ | | −21 | −86 | | | | |
| | From proton affinity of $C_2F_5CN$ (RN 422-04-8). PA = 167.1 kcal/mol, 699 kJ/mol. | | | | | | |
| $C_3HF_6O^+$ | | | | | | | |
| $(CF_3)_2COH$ | | −118 | −495 | | | | |
| | From proton affinity of $(CF_3)_2CO$ (RN 684-16-2) (85MCM/KEB, 85MCM/KEB2) re-evaluated relative to CO standard (84LIA/LIE). PA = 150.0 kcal/mol, 628. kJ/mol. | | | | | | |
| $C_3HF_8N^+$ | | | | | | | |
| $(CF_3)_2NCHF_2$ | (11.7) | (−110) | (−461) | −380 | −1590 | *EST | 73563-15-2 |
| | IP from 82BUR/PAW. | | | | | | |
| $C_3HN^+$ | | | | | | | |
| HC≡CCN | 11.64±0.01 | 352 | 1474 | 84 | 351 | 85HAR | 1070-71-9 |
| $C_3HNO^+$ | | | | | | | |
| NCCH=C=O | (≤10.07) | (≤256) | (≤1073) | 24 | 101 | *EST | |
| | IP from 81BOC/HIR. | | | | | | |
| $C_3HO^+$ | | | | | | | |
| HC≡C-C=O | | 232 | 971 | | | | |
| | From appearance potential determinations (83TER/HOL). | | | | | | |
| $C_3H_2^+$ | | | | | | | |
| HC≡CCH | | (330±3) | (1381±12) | | | | 2008-19-7 |
| | $C_3H^+ + H_2 \rightarrow C_3H_2^+ + H$ is ~1 kcal/mol endothermic. (84SMI/ADA). | | | | | | |
|  | | 281±3 | 1176±12 | | | | 75123-91-0 |
| | From appearance potentials in $CH_3CCX$ compounds. (84HOL/SZU). | | | | | | |
| $C_3H_2F_2^+$ | | | | | | | |
| $CF_2=C=CH_2$ | (9.79±0.03) | (178) | (743) | −48 | −202 | 86SMA | 430-64-8 |
| $C_3H_2F_4O^+$ | | | | | | | |
| $(CHF_2)_2CO$ | (10.7) | (15) | (61) | −232±4 | −971±16 | *EST | 360-52-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_2F_6O^+$ | | | | | | | |
| $CF_3CH(OH)CF_3$ | 11.94 | (−92) | (−384) | −367±2 | −1536±8 | *EST | 920-66-1 |
| | IP from 83KOP/MOL. | | | | | | |
| $C_3H_2F_7N^+$ | | | | | | | |
| $(CF_2H)_2NCF_3$ | (11.4) | (−60) | (−250) | −323 | −1350 | *EST | 73551-02-7 |
| | IP from 82BUR/PAW. | | | | | | |
| $C_3H_2N^+$ | | | | | | | |
| HCCCNH | | 269 | 1127.5 | | | | |
| | From proton affinity of HC≡CCN (RN 1070-71-9) (87DEA/MAU, 85KNI/FRE). PA = 180. kcal/mol, 753.5 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

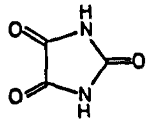
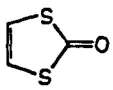
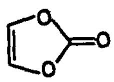
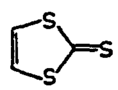
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_2N_2^+$ | | | | | | | |
| $CH_2(CN)_2$ | (12.70) | (356) | (1491) | 63.5±0.4 | 265.5±1.5 | 77PED/RYL | 109-77-3 |
| | IP from 83MOL/PIK2. | | | | | | |
| $C_3H_2N_2O_3^+$ | | | | | | | |
|  | (10.67) | (134) | (559) | −112 | −470 | *EST | 120-89-8 |
| $C_3H_2O^+$ | | | | | | | |
| HC≡CCHO | (10.8) | (276) | (1157) | 27 | 115 | *EST | 624-67-9 |
| | IP from 80VON/BIE. See also: 79CAR/MOU. | | | | | | |
| $CH_2=C=C=O$ | 9.12±0.05 | (233) | (975) | 23 | 95 | *EST | 61244-93-7 |
| | IP from 83TER/HOL. See also: 85MCN/SUF. | | | | | | |
|  | (9.47) | (251) | (1052) | 33±2 | 138±8 | *EST | 2961-80-0 |
| $C_3H_2OS_2^+$ | | | | | | | |
|  | (8.6) | (195) | (815) | −3.6±1.2 | −15.0±5.1 | 77PED/RYL | 2314-40-1 |
| | IP is onset of photoelectron band (83SCH/SCH). | | | | | | |
| $C_3H_2O_2^+$ | | | | | | | |
| HC≡CCOOH | (10.45) | (213) | (891) | −28 | −117 | *EST | 471-25-0 |
| | IP is onset of photoelectron band (80VON/BIE). | | | | | | |
| $C_3H_2O_3^+$ | | | | | | | |
|  | (9.8) | (126) | (527) | −100±5 | −419±21 | 77PED/RYL | 872-36-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_2S_3^+$ | | | | | | | |
|  | 8.26 | 251 | 1050 | 60.5±2 | 253±7 | 77PED/RYL | 930-35-8 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_3^+$ | | | | | | | |
| $CH_2C{\equiv}CH$ | 8.68 | 282 | 1179 | 82 | 343 | | 2932-78-7 |
| | $HCCCH^+ + H_2 \rightarrow CH_2C{\equiv}CH^+ + H$ is 4 kcal/mol endothermic (84SMI/ADA); value derived from appearance potential measurements is 281±3 kcal/mol; 1176 kJ/mol. $\Delta_f H$(Neutral) = $\Delta_f H$(Ion) - IP. | | | | | | |
|  | 6.6 | 257 | 1075 | 105±4 | 440±17 | 82MCM/GOL | 28933-84-8 |
| | Heat of formation of ion from appearance potential measurements; IP given is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_3H_3Cl^+$ | | | | | | | |
| $CH_2{=}C{=}CHCl$ | (9.57) | (263) | (1102) | 43 | 179 | *EST | 3223-70-9 |
| $CH_3C{\equiv}CCl$ | 9.82 | (276) | (1153) | 49±4 | 206±15 | *EST | 7747-84-4 |
| $CH_2ClC{\equiv}CH$ | 10.68 | (285) | (1192) | 39 | 162 | *EST | 624-65-7 |
| | See also: 81ZVE/ERM, 82BIE/ASB. | | | | | | |
| $C_3H_3F_3^+$ $CF_3CH=CH_2$ | (put in double bond) | | | | | | 677-21-4 |
| $CH_2CHCF_3$ | (10.9) | (104) | (438) | −147±2 | −614±7 | 77PED/RYL | ~~32718-30-2~~ |
| $C_3H_3F_3O^+$ | | | | | | | |
| $CH_3COCF_3$ | 10.67 | (52) | (217) | −194 | −812 | *EST | 421-50-1 |
| $C_3H_3F_3O_2^+$ | | | | | | | |
| $HCOOCH_2CF_3$ | (11.31) | (5) | (18) | −256 | −1073 | *EST | 32042-38-9 |
| $C_3H_3F_4O^+$ | | | | | | | |
| $(CF_2H)_2COH$ | | −32 | −134 | | | | |
| | From proton affinity of $CF_2HCOCF_2H$ (RN 360-52-1). PA = 170 kcal/mol, 711 kJ/mol. | | | | | | |
| $C_3H_3F_5O^+$ | | | | | | | |
| $C_2F_5CH_2OH$ | (11.2) | (−55) | (−229) | −313±0.7 | −1310±3 | 77PED/RYL | 422-05-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_3F_6N^+$ | | | | | | | |
| $(CF_2H)_3N$ | (11.2) | (−7) | (−29) | −265 | −1110 | *EST | 73551-03-8 |
| | IP from 82BUR/PAW. | | | | | | |
| $C_3H_3F_6O^+$ | | | | | | | |
| $(CF_3)_2CHOH_2$ | | −180 | −755 | | | | |
| | From proton affinity of $(CF_3)_2CHOH$ (RN 920-66-1). PA = 165.0 kcal/mol, 690 kJ/mol. | | | | | | |
| $C_3H_3N^+$ | | | | | | | |
| $CH_2CHCN$ | 10.91±0.01 | 296 | 1237 | 44 | 184 | 82CHU/NGU | 107-13-1 |
| | See also: 84OHN/MAT, 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

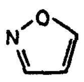
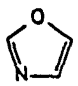
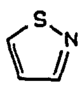
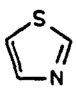
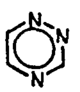
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_3NO^+$ | | | | | | | |
| $CH_2=CHNCO$ | (9.3) | (208) | (872) | −6 | −25 | *EST | 3555-94-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $HC\equiv CCONH_2$ | (9.85) | (244) | (1023) | 17 | 73 | *EST | 7341-96-0 |
| | IP is onset of photoelectron band (81ASB/SVE). | | | | | | |
|  | 9.93±0.05 | 248 | 1037 | 19 | 79 | 78MCC/HAM | 288-14-2 |
| | IP from 81BOU/HOP. | | | | | | |
|  | (9.6) | (217) | (910) | −4±0.2 | −16±1 | 78MCC/HAM | 288-42-6 |
| $C_3H_3NS^+$ | | | | | | | |
|  | (9.55) | (261) | (1090) | 40 | 169 | *EST | 288-16-4 |
|  | (≤9.50) | (≤256) | (≤1070) | 37±2 | 153±10 | *EST | 288-47-1 |
| $C_3H_3N_2^+$ | | | | | | | |
| $NCCH_2CNH$ | | 254 | 1061 | | | | |
| | From proton affinity of $CH_2(CN)_2$ (RN 109-77-3). PA = 175.6 kcal/mol, 735 kJ/mol. | | | | | | |
| $C_3H_3N_3^+$ | | | | | | | |
|  | (9.3) | (314) | (1313) | 99 | 416 | *EST | 289-96-3 |
| | IP is onset of photoelectron band (83GLE/SPA). | | | | | | |
|  | (9.2) | (292) | (1222) | 80 | 334 | *EST | 290-38-0 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

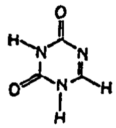
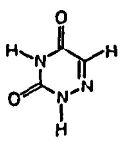
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_3N_3{}^+$ | | | | | | | |
|  | 10.03±0.05 | 285 | 1194 | 54±0.2 | 226±1 | 82BYS | 290-87-9 |
| | See also: 84SHA/URA. | | | | | | |
| $C_3H_3N_3O_2{}^+$ | | | | | | | |
|  | (10.59) | (181) | (756) | −64 | −266 | *EST | |
| | IP from 81AJO/CAS2. | | | | | | |
|  | 10.18 | (181) | (756) | −54 | −226 | *EST | |
| | IP from 81AJO/CAS2, 77ROS/DRA. | | | | | | |
| $C_3H_3O^+$ | | | | | | | |
| $CH_2=CHCO$ | (7.0) | (179) | (751) | 17 | 72 | 82MCM/GOL | 72241-20-4 |
| | IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). $\Delta_f H$(Ion) from appearance potential determination. | | | | | | |
| $HC\equiv CCH_2O$ | | 227 | 950 | | | | 92056-62-7 |
| | $\Delta_f H$(Ion) from appearance potential determination (84LOS/HOL). | | | | | | |
| $C_3H_4{}^+$ | | | | | | | |
| $CH_2=C=CH_2$ | 9.69±0.01 | 269 | 1126 | 45.6±.2 | 190.6±1 | 77PED/RYL | 463-49-0 |
| | | *271* | *1134* | *47.7* | *199.5* | | |
| | See also: 81KIM/KAT, 84MOM/BUR. | | | | | | |
| $CH_3C\equiv CH$ | 10.36±0.01 | 283.5 | 1186.2 | 44.6±.5 | 186.6±2 | 77PED/RYL | 74-99-7 |
| | | *285.5* | *1194.5* | *46.6* | *195.1* | | |
| | See also: 81KIM/KAT, 84MOM/BUR. | | | | | | |
|  | 9.67±0.01 | 289 | 1210 | 66±0.7 | 277±3 | 77PED/RYL | 2781-85-3 |
| $C_3H_4F_3O^+$ | | | | | | | |
| $CH_3C(OH)CF_3$ | | −3 | −11 | | | | |
| | From proton affinity of $CH_3COCF_3$ (RN 421-50-1). PA = 174.2 kcal/mol, 729 kJ/mol. | | | | | | |
| $C_3H_4F_3O_2{}^+$ | | | | | | | |
| $HC(OH)CH_2CF_3$ | | −70 | −294 | | | | |
| | From proton affinity of $HCOOCH_2CF_3$ (RN 32042-38-9). PA = 179.4 kcal/mol, 751 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

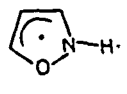
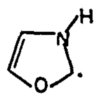
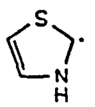
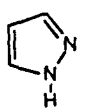
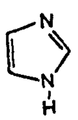
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_4F_3O_2^+$ | | | | | | | |
| $CF_3C(OH)CH_3$ | | −55 | −231 | | | | |
| | From proton affinity of $CF_3COOCH_3$ (RN 431-47-0). PA = 178.8 kcal/mol, 748 kJ/mol. | | | | | | |
| $C_3H_4N^+$ | | | | | | | |
| $CH_2CHCNH$ | (7.37) | 220 | 920 | 50±2 | 209±10 | 82MCM/GOL | 74738-52-6 |
| | From proton affinity of $CH_2=CHCN$ (RN 107-13-1). PA = 189.7 kcal/mol, 794. kJ/mol. IP cited is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_3H_4NO^+$ | | | | | | | |
| $CH_3COCNH$ | | 181 | 759 | | | | |
| | From proton affinity of $CH_3COCN$ (RN 631-57-2). PA = 179.5 kcal/mol, 751. kJ/mol (86MAR/TOP). | | | | | | |
|  | | 182 | 761 | | | | |
| | From proton affinity of isooxazole (RN 288-14-2). PA = 202.7 kcal/mol, 848 kJ/mol. | | | | | | |
|  | | 154 | 643 | | | | |
| | From proton affinity of oxazole (RN 288-42-6). PA = 208.2 kcal/mol, 871 kJ/mol. | | | | | | |
| $C_3H_4NO_2^+$ | | | | | | | |
| $CH_3COOCNH$ | | 138 | 576 | | | | |
| | From proton affinity of $CH_3OOCCN$ (86MAR/TOP). PA = 179.5 kcal/mol, 751. kJ/mol. | | | | | | |
| $C_3H_4NS^+$ | | | | | | | |
|  | | 189 | 791 | | | | |
| | From proton affinity of thiazole (RN 288-47-1). PA = 213.2 kcal/mol, 892 kJ/mol. | | | | | | |
| $C_3H_4N_2^+$ | | | | | | | |
|  | 9.25±0.01 | 258 | 1077 | 44±0.5 | 185±2 | 80SAB | 288-13-1 |
| | | *261* | *1093* | *48* | *201* | | |
| | IP from 86MAI/OLE. | | | | | | |
|  | 8.81±0.01 | 238 | 995 | 35±0.5 | 145±2 | 80SAB | 288-32-4 |
| | | *242* | *1011* | *38* | *161* | | |
| | IP from 86MAI/OLE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

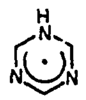
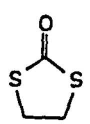
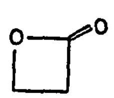
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_4N_3^+$ | | | | | | | |
|  | | 219 | 915 | | | | |
| | From proton affinity of 1,3,5-triazine (RN 290-87-9). PA = 201.1 kcal/mol, 841 kJ/mol. | | | | | | |
| $C_3H_4O^+$ | | | | | | | |
| $CH_3CH=C=O$ | 8.95 | 181 | 759 | −25 | −105 | 80DEM/WUL | 6004-44-0 |
| | IP from 81BOC/HIR. | | | | | | |
| $CH_2=CHCHO$ | 10.103±0.006 | 215 | 898 | −18 | −77 | 79VAJ/HAR | 107-02-8 |
| | See also: 80VON/BIE, 81KIM/KAT, 78VAN/OSK. | | | | | | |
| $HC{\equiv}CCH_2OH$ | 10.51 | (253) | (1060) | 11 | 46 | *EST | 107-19-7 |
| | IP from 83KOP/MOL, 80VON/BIE. | | | | | | |
| $HC{\equiv}COCH_3$ | 9.48 | (236) | (989) | 18 | 74 | *EST | 6443-91-0 |
| | IP from 86HOL/LOS. | | | | | | |
|  | (9.1±0.1) | (214) | (894) | 4 | 16 | 76ROD/CHA | 5009-27-8 |
| $C_3H_4OS_2^+$ | | | | | | | |
|  | (9.2) | (182) | (762) | −30±1 | −126±5 | 77PED/RYL | 2080-58-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_4O_2^+$ | | | | | | | |
| $CH_2=CHCOOH$ | 10.60 | 167 | 699 | −77 | −324 | 80VIL/PER | 79-10-7 |
| | See also: 78VAN/OSK. | | | | | | |
| $CH_3COCHO$ | 9.60±0.06 | 156 | 655 | −65±1 | −271±5 | 77PED/RYL | 78-98-8 |
| | See also: 81KIM/KAT. | | | | | | |
|  | (9.70±0.01) | (156) | (653) | −67.6±0.2 | −282.9±0.8 | 77PED/RYL | 57-57-8 |

**Table 1. Positive Ion Table - Continued**

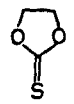
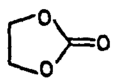
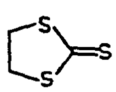
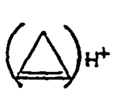
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_4O_2S^+$ | | | | | | | |
|  | (8.6) | (129) | (538) | −70 | −292 | *EST | 20628-59-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_4O_3^+$ | | | | | | | |
|  | (10.4) | (117) | (491) | −122±1 | −512±4 | 83CAL | 96-49-1 |
| $CH_3COCOOH$ | 9.9 | 97 | 407 | −131 | −548 | 83TER/WEZ | 127-17-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_4S^+$ | | | | | | | |
| $CH_2{=}CHCH{=}S$ | (8.3) | (223) | (934) | 32 | 133 | *EST | 53439-64-8 |
| | IP from 82BOC/MOH. | | | | | | |
| $CH_3SC{\equiv}CH$ | (8.3) | (247) | (1036) | 56 | 235 | *EST | 10152-75-7 |
| | IP is onset of photoelectron band (81BOC/RIE). | | | | | | |
| $C_3H_4S_3^+$ | | | | | | | |
|  | (8.40) | (216) | (904) | 22.4±0.5 | 93.8±2.2 | 77PED/RYL | 822-38-8 |
| $C_3H_5^+$ | | | | | | | |
| $CH_2CH{=}CH_2$ | 8.13 | 226.0 | 945.6 | 39 | 161 | 84HOL/LOS | 1981-80-2 |
| | | *228.9* | *957.7* | *41* | *173* | | |
| | $\Delta H_f$(Ion) from appearance potential measurements. (See also: 84TRA, 82MAC). For IP determination, see also 83KAG/UJS. For $\Delta_f H$(Neutral), 81TSA recommends 43 kcal/mol, 179 kJ/mol and 82MCM/GOL recommends 40 kcal/mol, 167 kJ/mol. | | | | | | |
| $CH_3CCH_2$ | | 231 | 969 | | | | ? |
| | $\Delta_f H$(Ion) from appearance potential determinations (83BUR/HOL). | | | | | | |
|  | 8.18±0.03 | 255 | 1069 | 66.9 | 279.9 | 82MCM/GOL | 2417-82-5 |
| | IP from 85DYK/ELL. | | | | | | |
| $C_3H_5Br^+$ | | | | | | | |
| $CH_3CH{=}CHBr$ | (9.30±0.05) | (224) | (938) | 10±1 | 41±4 | 77PED/RYL | 41407-21-0 |
| $CH_2{=}CHCH_2Br$ | 10.06 | 243 | 1018 | 11.4±0.6 | 47.7±2.4 | 84TRA | 106-95-6 |
| | See also: 82BIE/ASB. | | | | | | |

**Table 1. Positive Ion Table - Continued**

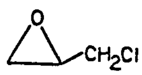
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_5BrO^+$ | | | | | | | |
| $CH_3COCH_2Br$ | (9.73) | (181) | (758) | −43±2 | −181±8 | 77PED/RYL | 598-31-2 |
| | IP from 84OLI/GUE. | | | | | | |
| $C_3H_5Cl^+$ | | | | | | | |
| $CH_2=CHCH_2Cl$ | 9.9 | 227 | 949 | −1.3±0.6 | −5.6±2.4 | 84TRA | 107-05-1 |
| | IP is onset of photoelectron band (82BIE/ASB). See also: 82LEV/LIA, 81ZVE/ERM. | | | | | | |
| $C_3H_5ClN^+$ | | | | | | | |
| $ClCH_2CH_2CNH$ | | 188 | 787 | | | | |
| | From proton affinity of $ClCH_2CH_2CN$ (RN 542-76-7). PA = 187.5 kcal/mol, 784.5 kJ/mol. | | | | | | |
| $C_3H_5ClO^+$ | | | | | | | |
| $CH_3COCH_2Cl$ | 9.91±0.03 | (175) | (731) | −54 | −225 | *EST | 78-95-5 |
| | See also: 84OLI/GUE. | | | | | | |
|  | (10.2) | (209) | (876) | −26±1 | −108±4 | 77PED/RYL | 106-89-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_5ClO_2^+$ | | | | | | | |
| $ClH_2CCOOCH_3$ | (10.3) | (138) | (577) | −100 | −417 | *EST | 96-34-4 |
| | IP is onset of photoelectron band (85CAN/HAM). | | | | | | |
| $C_3H_5F^+$ | | | | | | | |
| $CH_2=CHCH_2F$ | 10.11 | 196 | 819 | −37 | −156 | 82DOL/MED | 818-92-8 |
| $C_3H_5FO^+$ | | | | | | | |
| $CH_3COCH_2F$ | (9.9) | (136) | (572) | −92 | −383 | *EST | 430-51-3 |
| | See also: 84OLI/GUE. | | | | | | |
| $C_3H_5F_2O^+$ | | | | | | | |
| $(CFH_2)_2COH$ | | 52 | 219 | | | | |
| | From proton affinity of $CFH_2COCFH_2$ (RN 453-14-5). PA = 187 kcal/mol, 782 kJ/mol. | | | | | | |
| $C_3H_5F_3O^+$ | | | | | | | |
| $CF_3CH_2OCH_3$ | 10.53 | (35) | (147) | −208 | −869 | *EST | 460-43-5 |
| | IP from 83MOL/PIK. | | | | | | |
| $C_3H_5I^+$ | | | | | | | |
| $CH_2CHCH_2I$ | 9.298 | 238.2 | 996.6 | 23.8 | 99.5 | 84TRA | 556-56-9 |
| $C_3H_5IO^+$ | | | | | | | |
| $CH_3COCH_2I$ | (9.3) | (183) | (767) | −31±1 | −130±5 | 77PED/RYL | 3019-04-3 |
| | IP is onset of photoelectron band (84OLI/GUE). | | | | | | |

**Table 1. Positive Ion Table - Continued**

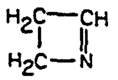
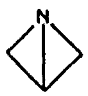
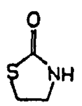
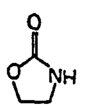
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_5N^+$ | | | | | | | |
| $C_2H_5CN$ | 11.84±0.02 | 285 | 1194 | 12.3±0.1 | 51.5±0.5 | 82CHU/NGU | 107-12-0 |
| | See also: 82CHE/LAP, 81KIM/KAT. | | | | | | |
| $C_2H_5NC$ | 11.2±0.1 | 292 | 1222 | 33.8±1 | 141.4±4.2 | 77BAG/COL | 624-79-3 |
| | IP from 82CHE/LAP, 77ROS/DRA. | | | | | | |
| (E)-$CH_2$=CHCH=NH | (9.65) | (249) | (1043) | 27 | 112 | *EST | 73311-40-7 |
| | IP is onset of photoelectron band (82SCH/SCH). | | | | | | |
|  | (9.30) | (265) | (1108) | 50 | 211 | *EST | 6788-85-8 |
| | IP from 83DAM/BOC. | | | | | | |
|  | (≤9.76±0.22) | (≤300) | (≤1256) | 75 | 314 | *EST | 19540-05-7 |
| $C_3H_5NO^+$ | | | | | | | |
| $C_2H_5NCO$ | (10.1) | (196) | (819) | −37 | −155 | *EST | 109-90-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $NCCH_2OCH_3$ | 10.75 | (240) | (1002) | −8 | −35 | *EST | 1738-36-9 |
| | IP from 83MOL/PIK. | | | | | | |
| $CH_2CHCONH_2$ | 9.5 | (172) | (722) | −47 | −195 | *EST | 79-06-1 |
| | IP is onset of photoelectron band (78VAN/OSK). | | | | | | |
| $C_3H_5NOS^+$ | | | | | | | |
|  | (9.2) | (177) | (743) | −35 | −145 | *EST | 2682-49-7 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_3H_5NO_2^+$ | | | | | | | |
|  | (9.6) | (139) | (582) | −82 | −344 | *EST | 497-25-6 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |

Table 1. Positive Ion Table - Continued

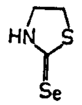
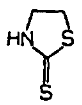
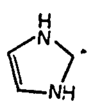
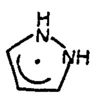
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_5NSSe^+$ | | | | | | | |
|  | 7.3 | (155) | (650) | −13 | −54 | *EST | 63369-86-8 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_3H_5NS_2^+$ | | | | | | | |
|  | ≤8.25 | (≤161) | (≤672) | −30 | −124 | *EST | 96-53-7 |
| | IP from 80AND/DEV, 82LEV/LIA. | | | | | | |
| $C_3H_5N_2^+$ | | | | | | | |
|  | | 177 | 740 | | | | |
| | From proton affinity of imidazole (RN 288-32-4) (86MAU/LIE, 84FLA/MAQ, 86TAF/ANV). PA = 223.4 kcal/mol, 935. kJ/mol. | | | | | | |
|  | | 197 | 825 | | | | |
| | From proton affinity of pyrazole (RN 288-13-1) (86MAU/LIE, 84FLA/MAQ). PA = 212.8 kcal/mol, 890. kJ/mol. | | | | | | |
| $C_3H_5O^+$ | | | | | | | |
| $C_2H_5CO$ | (5.7) | 141 | 591 | 10±1 | 43±4 | 82MCM/GOL | 15843-24-0 |
| | $\Delta_f H$(Ion) from appearance potential measurements (85TRA) and from proton affinity of $CH_3CH=CO$ (RN 6004-44-0). PA = 199.4 kcal/mol, 834 kJ/mol. IP given is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $CH_2CHCHOH$ | | 153 | 642 | | | | |
| | From proton affinity of $CH_2=CHCHO$ (RN 107-02-8). PA = 193.9 kcal/mol, 811 kJ/mol. | | | | | | |
| $C_3H_6^+$ | | | | | | | |
| $CH_3CH=CH_2$ | 9.73±0.02 | 229 | 959 | 4.8±0.2 | 20.2±0.4 | 77PED/RYL | 115-07-1 |
| | See also: 81KIM/KAT. | | | | | | |
|  | 9.86 | 240 | 1004 | 12.7±.2 | 53.3±0.5 | 77PED/RYL | 75-19-4 |
| | | *244* | *1022* | *16.9* | *70.9* | | |
| | IP from 84LIA/BUC. See also: 81KIM/KAT. | | | | | | |
| $C_3H_6Br_2^+$ | | | | | | | |
| $CH_2BrCHBrCH_3$ | 10.1 | 216 | 903 | −17±0.2 | −71±1 | 77PED/RYL | 78-75-1 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $CH_2BrCH_2CH_2Br$ | ≤10.26 | (≤220) | (≤919) | −17 | −71 | *EST | 109-64-8 |

**Table 1. Positive Ion Table - Continued**

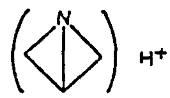
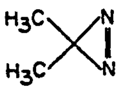
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_6Cl_2^+$ | | | | | | | |
| $CH_3CHClCH_2Cl$ | (10.87±0.05) | (212) | (886) | −38.9±0.3 | −162.6±0.3 | 77PED/RYL | 78-87-5 |
| $CH_2ClCH_2CH_2Cl$ | 10.85±0.05 | 212 | 887 | −38±2 | −160±8 | 77PED/RYL | 142-28-9 |
| $C_3H_6FO^+$ | | | | | | | |
| $CH_3C(OH)CH_2F$ | | 82 | 344 | | | | |
| | From proton affinity of $CH_3COCH_2F$ (RN 430-51-3). PA = 192.0 kcal/mol, 803. kJ/mol. | | | | | | |
| $C_3H_6F_2^+$ | | | | | | | |
| $(CH_3)_2CF_2$ | (11.42±0.02) | (138) | (578) | −125±3 | −524±13 | 82DOL/MED | 420-45-1 |
| $C_3H_6F_3N^+$ | | | | | | | |
| $CF_3CH_2CH_2NH_2$ | (9.3) | (40) | (166) | −175 | −731 | *EST | 460-39-9 |
| | IP from 79AUE/BOW | | | | | | |
| $CF_3N(CH_3)_2$ | (9.2) | (25) | (104) | −187 | −784 | *EST | 677-41-8 |
| | IP from 79AUE/BOW. | | | | | | |
| $C_3H_6N^+$ | | | | | | | |
| $C_2H_5CNH$ | | 185 | 775 | | | | |
| | From proton affinity of $C_2H_5CN$ (RN 107-12-0). PA = 192.6 kcal/mol, 806 kJ/mol. | | | | | | |
| $C_2H_5NCH$ | | 196 | 819 | | | | |
| | From proton affinity of $C_2H_5NC$ (RN 624-79-3) (86MAU/KAR). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | |
| $HCCCH_2NH_3$ | | 208 | 870 | | | | |
| | From proton affinity of $HC{\equiv}CCH_2NH_2$ (RN 2450-71-7). PA = 210.8 kcal/mol, 882 kJ/mol. | | | | | | |
|  | | (229) | (957) | | | | |
| | From proton affinity of 1-azabicyclo[1.1.0]butane (RN 19540-05-7). PA = (212) kcal/mol, (887) kJ/mol. | | | | | | |
| $C_3H_6N_2^+$ | | | | | | | |
| $(CH_3)_2NC{\equiv}N$ | (9.0) | (241) | (1007) | 33 | 139 | *EST | 1467-79-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.76) | (≤267) | (≤1118) | 42 | 176 | *EST | 5161-49-9 |

**Table 1. Positive Ion Table – Continued**

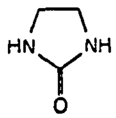
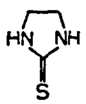
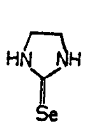
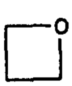
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_6N_2O^+$ | | | | | | | |
|  | (8.9) | (163) | (683) | –42 | –176 | *EST | 120-93-4 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_3H_6N_2S^+$ | | | | | | | |
|  | 8.15 | 210 | 880 | 22 | 94 | *EST | 96-45-7 |
| $C_3H_6N_2Se^+$ | | | | | | | |
|  | (7.0) | (192) | (803) | 31 | 128 | *EST | 33251-51-3 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_3H_6O^+$ | | | | | | | |
| $C_2H_5CHO$ | 9.953±0.005 | 184.7 | 772.9 | –44.8±0.4 | –187.4±1.5 | 77PED/RYL | 123-38-6 |
| | See also: 81ELS/ALL, 85STRA, 81KIM/KAT, 77STA/WIE. | | | | | | |
| $(CH_3)_2CO$ | 9.705 | 171.9 | 719.2 | –51.9±0.1 | –217.2±0.4 | 76CHA/ZWO | 67-64-1 |
| | See also: 72POT/SOR, 81KIM/KAT, 77STA/WIE. | | | | | | |
| $CH_2=CHCH_2OH$ | 9.67±0.05 | 193 | 809 | –30±0.5 | –124±2 | 77PED/RYL | 107-18-6 |
| | See also: 83BOM/DAN, 82HOL/BUR. | | | | | | |
| (E)-$CH_3CH=CHOH$ | 8.64±0.02 | 159 | 665 | –40 | –169 | 84TUR2 | 57642-95-2 |
| | $\Delta_f H$(Ion) from appearance potential determinations. (82HOL/LOS3, 82HOL/BUR). IP from 84TUR2. $\Delta_f H$(Neutral) is $\Delta_f H$(Ion) - IP. (See 84TUR2). | | | | | | |
| (Z)-$CH_3CH=CHOH$ | 8.70±0.03 | 159 | 665 | –42 | –174 | 84TUR2 | 57642-96-3 |
| | $\Delta_f H$(Ion) from appearance potential determinations. (82HOL/LOS3, 82HOL/BUR) IP from 84TUR2. $\Delta_f H$(Neutral) is $\Delta_f H$(Ion) - IP. (See 84TUR2). | | | | | | |
| $CH_2=C(OH)CH_3$ | 8.67±0.05 | 158 | 661 | –42 | –176 | 84TUR/HAN | 29456-04-0 ~~74324-85-9~~ |
| | $\Delta_f H$(Ion) from appearance potential determinations 82HOL/LOS3. (See also: 82LIF2). IP from 84TUR/HAN. | | | | | | |
| $CH_2=CHOCH_3$ | (8.93±0.02) | (182) | (762) | –24±2 | –100±7 | *EST | 107-25-5 |
|  | 9.668±0.005 | 203.7 | 852.3 | –19.2±0.1 | –80.5±0.6 | 77PED/RYL | 503-30-0 |
| | See also: 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

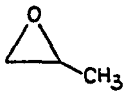
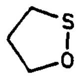
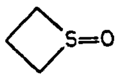
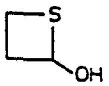
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_6O^+$ | | | | | | | |
|  | 10.22±0.02 | 213 | 891 | −22.6±0.1 | −94.7±0.6 | 77PED/RYL | 75-56-9 |
| | See also: 81KIM/KAT, 79AUE/BOW. | | | | | | |
|  | (9.10) | (188) | (785) | −22 | −93 | *EST | 16545-68-9 |
| | IP from 83BOM/DAN. See also: 82HOL/BUR. | | | | | | |
| $C_3H_6OS^+$ | | | | | | | |
| $CH_3C(=O)SCH_3$ | (9.5) | (182) | (761) | −37 | −156 | *EST | 1534-08-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.1) | (231) | (966) | 44 | 184 | *EST | 5684-29-7 |
| | IP is onset of photoelectron band (83JOR/CAR). | | | | | | |
|  | (8.5) | (184) | (769) | −12 | −51 | *EST | 13153-11-2 |
| | IP is onset of photoelectron band (83JOR/CAR). | | | | | | |
|  | (8.3) | (137) | (572) | −55 | −229 | *EST | 50879-06-6 |
| | IP is onset of photoelectron band (83JOR/CAR). | | | | | | |
| $C_3H_6O_2^+$ | | | | | | | |
| $C_2H_5COOH$ | 10.525±0.003 | 136 | 567 | −107±0.5 | −448±2 | 77PED/RYL | 79-09-4 |
| | See also: 81HOL/FIN, 81KIM/KAT. | | | | | | |
| $HCOOC_2H_5$ | 10.61±0.01 | (153) | (637) | −92 | −387 | *EST | 109-94-4 |
| $CH_3COOCH_3$ | 10.27±0.02 | 139 | 581 | −98.0±0.2 | −410.0±0.8 | 77PED/RYL | 79-20-9 |
| | See also: 85CAN/HAM. | | | | | | |
| $CH_2=C(OH)OCH_3$ | | 114 | 477 | | | | 4453-91-2 |
| | From appearance potential determination. | | | | | | |
| $CH_3CH=C(OH)_2$ | | 104 | 437 | | | | |
| | From appearance potential determinations. | | | | | | |
| $CH_3C(OH)OCH_2$ | | (127) | (533) | | | | |
| | Estimated in 86BUR/HOL. | | | | | | |

**Table 1. Positive Ion Table - Continued**

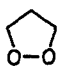
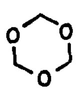
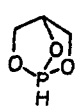
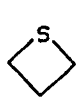
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_6O_2^+$ | | | | | | | |
|  | (≤9.86) | (≤203) | (≤847) | −25 | −104 | *EST | 4362-13-4 |
|  | (9.9) | (157) | (658) | −71.1±0.1 | −297.5±0.6 | 77PED/RYL | 646-06-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_6O_2S^+$ | | | | | | | |
| $(CH_3O)_2CS$ | (8.7) | (121) | (504) | −80 | −335 | *EST | 1115-13-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_6O_3^+$ | | | | | | | |
| $CH_3OCOOCH_3$ | (10.5) | (103) | (432) | −139 | −581 | *EST | 616-38-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (10.3) | (126) | (528) | −111.4±0.1 | −465.9±0.3 | 77PED/RYL | 110-88-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_6O_3P^+$ | | | | | | | |
|  | | 25 | 105 | | | | |
| | From proton affinity of 2,6,7-trioxa-1-phosphabicyclo[2.2.1]heptane (RN 279-53-8).<br>PA = 194.0 kcal/mol, 812. kJ/mol. | | | | | | |
| $C_3H_6S^+$ | | | | | | | |
| $(CH_3)_2CS$ | ≤8.60±0.05 | ≤196 | ≤821 | −2 | −9 | 79JOS | 4756-05-2 |
| $CH_2=CHCH_2SH$ | 9.25 | (228) | (956) | 15±2 | 64±9 | *EST | 870-23-5 |
| $CH_2=CHSCH_3$ | 8.2 | (207) | (865) | 18±0.2 | 74±1 | *EST | 1822-74-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.69 | 214.9 | 899.1 | 14.5 | 60.7 | 77PED/RYL | 287-27-4 |
| | | *219.5* | *918.4* | *19.1* | *79.9* | | |
| | Results from 83BUT/BAE2. See also: 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

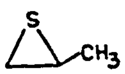
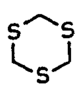
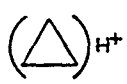
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_6S^+$ | | | | | | | |
|  | 8.7 | 212 | 885 | 11±0.5 | 46±2 | 77PED/RYL | 1072-43-1 |
| | IP is onset of photoelectron band. See also: 79AUE/BOW. | | | | | | |
| $C_3H_6S_2^+$ | | | | | | | |
| $CH_3CSSCH_3$ | (8.1) | (211) | (882) | 24±3 | 100±13 | *EST | 2168-84-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.6) | (170) | (712) | −5 | −21 | *EST | 557-22-2 |
| | IP is onset of photoelectron band (80BOC/STE). | | | | | | |
|  | 8.6 | (201) | (840) | 2 | 10 | *EST | 4829-04-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_6S_3^+$ | | | | | | | |
| $(CH_3S)_2CS$ | (7.9) | (203) | (851) | 21 | 89 | *EST | 2314-48-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.7) | (190) | (797) | 13 | 54 | *EST | 291-21-4 |
| | IP is onset of photoelectron band. (81BOC/SCH). | | | | | | |
| $C_3H_7^+$ | | | | | | | |
| n-$C_3H_7$ | 8.09±0.01 | 211 | 881 | 24.0±0.5 | 100.5±2.1 | 85TSA | 2143-61-5 |
| | | *214* | *896* | *27* | *115* | | |
| | IP from 85DYK/ELL. See also: 84SCH/HOU. $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | | | | | | |
| iso-$C_3H_7$ | 7.36±0.02 | 190.9 | 798.9 | 22.3±0.6 | 93.3±2.5 | 85TSA | 19252-53-0 |
| | | *195.3* | *817.1* | *25.6* | *107.0* | | |
| | Heat of formation of ion from appearance potential measurements (80BAE, 82ROS/BUF, 81TRA/MCL). IP from 85DYK/ELL. See also: 83BRA/BAE2. $\Delta_f H$(Neutral) based on D[C-H] = 99 kcal/mol. PA ($CH_3CH=CH_2$) = 179.5 kcal/mol, 751. kJ/mol. | | | | | | |
|  | | 198.5 | 831 | | | | |
| | From proton affinity of c-$C_3H_6$. (RN 75-19-4). PA = 179.8 kcal/mol, 752 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_3H_7Br^+$** | | | | | | | |
| n-$C_3H_7Br$ | 10.18±0.01 | 214 | 898 | −20.2±0.1 | −84.5±0.5 | 77PED/RYL | 106-94-5 |
| | | *221* | *926* | *−13* | *−56* | | |
| | See also: 81KIM/KAT. | | | | | | |
| iso-$C_3H_7Br$ | 10.07±0.01 | 209 | 873 | −23.4±0.2 | −98.3±0.9 | 80TRA | 75-26-3 |
| | | *215* | *901* | *−17* | *−70* | | |
| | See also: 81KIM/KAT. | | | | | | |
| **$C_3H_7Cl^+$** | | | | | | | |
| n-$C_3H_7Cl$ | 10.82±0.03 | 218 | 911 | −31.6±0.1 | −132.4±0.6 | 77PED/RYL | 540-54-5 |
| | See also: 81KIM/KAT. | | | | | | |
| iso-$C_3H_7Cl$ | 10.78±0.02 | 214 | 895 | −34.6±0.1 | −145.0±0.6 | 80TRA | 75-29-6 |
| | See also: 81KIM/KAT. | | | | | | |
| **$C_3H_7ClHg^+$** | | | | | | | |
| n-$C_3H_7HgCl$ | ≤10.15 | ≤213 | ≤891 | −21±2 | −88±8 | 80TEL/RAB | 2440-40-6 |
| | IP from 81BAI/CHI2. | | | | | | |
| iso-$C_3H_7HgCl$ | ≤9.80 | ≤206 | ≤863 | −20±2 | −83±8 | 80TEL/RAB | 30615-19-1 |
| | IP from 81BAI/CHI2. | | | | | | |
| **$C_3H_7ClO^+$** | | | | | | | |
| $ClCH_2OC_2H_5$ | 10.30 | (184) | (771) | −53 | −223 | *EST | 3188-13-4 |
| | IP from 83MOL/PIK. | | | | | | |
| **$C_3H_7F^+$** | | | | | | | |
| n-$C_3H_7F$ | (11.3) | (192) | (804) | −68±0.5 | −286±2 | 77PED/RYL | 460-13-9 |
| | IP is onset of photoelectron band. | | | | | | |
| iso-$C_3H_7F$ | (11.08±0.02) | (185) | (776) | −70±0.5 | −293±2 | 77PED/RYL | 420-26-8 |
| **$C_3H_7F_3N^+$** | | | | | | | |
| $CF_3NH(CH_3)_2$ | | −15 | −65 | | | | |
| | From proton affinity of $CF_3N(CH_3)_2$ (RN 677-41-8). PA = 193.8 kcal/mol, 811 kJ/mol. | | | | | | |
| $CF_3CH_2CH_2NH_3$ | | −20 | −82 | | | | |
| | From proton affinity of $CF_3CH_2CH_2NH_2$ (RN 460-39-9). PA = 210.6 kcal/mol, 881 kJ/mol. | | | | | | |
| $CF_3CH_2NH_2CH_3$ | | −11 | −47 | | | | |
| | From proton affinity of $CF_3CH_2NHCH_3$ (RN 2730-67-8). PA = 209.8 kcal/mol, 878 kJ/mol. | | | | | | |
| **$C_3H_7I^+$** | | | | | | | |
| n-$C_3H_7I$ | 9.269 | 206 | 862 | −7.8±0.4 | −32.5±1.7 | 77PED/RYL | 107-08-4 |
| | | *211* | *884* | *−2.4±0.5* | *−10.2±2* | | |
| | See: 82ROS/BUF, 83BRA/BAE2, 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

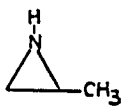
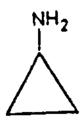
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_7I^+$ | | | | | | | |
| iso-$C_3H_7I$ | 9.175 | 202 | 844 | −9.9±0.4 | −41.6±1.7 | 77PED/RYL | 75-30-9 |
| | | *207* | *865* | *−4.8±0.5* | *−20.1±2* | | |
| | See: 82ROS/BUF, 83BRA/BAE2, 81KIM/KAT. | | | | | | |
| $C_3H_7N^+$ | | | | | | | |
| $CH_2=CHCH_2NH_2$ | 8.76 | (213) | (893) | 11 | 48 | *EST | 107-11-9 |
| | See also: 79AUE/BOW. | | | | | | |
|  | (8.3) | (215) | (898) | 24±1 | 99±4 | *EST | 503-29-7 |
| | IP from 79AUE/BOW. | | | | | | |
|  | (8.7) | (230) | (964) | 30±0.5 | 127±2 | *EST | 1072-44-2 |
| | IP from 79AUE/BOW. See also: 86CAU/DIV. | | | | | | |
|  | (9.0) | (230) | (961) | 22±1 | 91±6 | *EST | 75-55-8 |
| | IP from 79AUE/BOW. | | | | | | |
|  | (8.7) | (219) | (916) | 18.4±0.1 | 77.0±0.6 | 77PED/RYL | 765-30-0 |
| | IP is onset of photoelectron band (81KIM/KAT). See also: 79AUE/BOW. | | | | | | |
| $C_3H_7NO^+$ | | | | | | | |
| $HCON(CH_3)_2$ | 9.13±0.02 | 165 | 689 | −45.8±0.4 | −191.7±1.7 | 77PED/RYL | 68-12-2 |
| | See also: 82BIE/ASB, 81HEN/ISA. | | | | | | |
| $(CH_3)_2C=NOH$ | (9.1) | (195) | (815) | −15±3 | −63±12 | *EST | 127-06-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3CONHCH_3$ | 9.3 | 158 | 661 | −56 | −236 | *EST | 79-16-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_7NO_2^+$ | | | | | | | |
| n-$C_3H_7NO_2$ | 10.81±0.03 | 220 | 919 | −29.7±0.1 | −124.0±0.6 | 77PED/RYL | 108-03-2 |
| | See also: 81KIM/KAT. | | | | | | |
| i-$C_3H_7NO_2$ | 10.71±0.05 | 214 | 894 | −33.2±0.2 | −139.0±0.9 | 77PED/RYL | 79-46-9 |
| | See also: 81KIM/KAT. | | | | | | |
| n-$C_3H_7ONO$ | (10.34±0.01) | (210) | (879) | −28±1 | −119±4 | 74BAT/CHR | 543-67-9 |

**Table 1. Positive Ion Table - Continued**

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3H_7NO_2^+$ | | | | | | | |
| $i$-$C_3H_7ONO$ | (10.23±0.01) | (204) | (854) | −32±1 | −133±4 | 74BAT/CHR | 541-42-4 |
| $H_2NCH_2CH_2COOH$ | (8.8) | (101) | (425) | −101±0.5 | −424±2 | 83SKO/SAB | 28854-76-4 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $CH_3NHCH_2COOH$ | (8.4) | (106) | (443) | −88±0.2 | −367±1 | 78SAB/LAF | 107-97-1 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| L-$CH_3CH(NH_2)COOH$ | | | | | | | |
| | 8.88 | 106 | 442 | −99±1 | −415±4 | 77NGA/SAB | 56-41-7 |
| | See also: 83CAN/HAM. | | | | | | |
| $NH_2COOC_2H_5$ | (10.15) | (127) | (533) | −107 | −446 | 75BER/BOU | 51-79-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $NH_2CH_2COOCH_3$ | (9.1) | (121) | (505) | −89 | −373 | *EST | 616-34-2 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $C_3H_7NO_2S^+$ | | | | | | | |
| L-$HSCH_2CH(NH_2)COOH$ | | | | | | | |
| | (9.5) | (128) | (534) | −92 | −383 | *EST | 3374-22-9 |
| | IP from 83CAN/HAM. | | | | | | |
| $C_3H_7NO_3^+$ | | | | | | | |
| $n$-$C_3H_7ONO_2$ | (11.07±0.02) | (214) | (894) | −41.6±0.3 | −173.9±1.3 | 77PED/RYL | 627-13-4 |
| L-$HOCH_2CH(NH_2)COOH$ | | | | | | | |
| | (8.7) | (67) | (278) | −134 | −561 | *EST | 302-84-1 |
| | IP is onset of photoelectron band(83CAN/HAM). | | | | | | |
| $C_3H_7NS^+$ | | | | | | | |
| $HCSN(CH_3)_2$ | (≤8.2) | (≤201) | (≤840) | 12 | 49 | *EST | 758-16-7 |
| | IP from 81HEN/ISA. | | | | | | |
| $C_3H_7N_2^+$ | | | | | | | |
| $H_3N(CH_2)_2CN$ | | 180 | 755 | | | | |
| | From proton affinity of $H_2N(CH_2)_2CN$ (RN 151-18-8). PA = 207.0 kcal/mol, 866. kJ/mol. | | | | | | |
| $CH_3NH_2CH_2CN$ | | 185 | 775 | | | | |
| | From proton affinity of $CH_3NHCH_2CN$ (RN 5616-32-0). PA = 206.0 kcal/mol, 862. kJ/mol. | | | | | | |
| $(CH_3)_2NCNH$ | | 194 | 811 | | | | |
| | From proton affinity of $(CH_3)_2NCN$ (RN 1467-79-4) (86MAR/TOP). PA = 205.0 kcal/mol, 858 kJ/mol. | | | | | | |
| $C_3H_7O^+$ | | | | | | | |
| $n$-$C_3H_7O$ | (9.20±0.05) | (202) | (847) | −10 | −41 | 82MCM/GOL | 16499-18-6 |
| $i$-$C_3H_7O$ | (9.20±0.05) | (197) | (825) | −15 | −63 | 82MCM/GOL | 3958-66-5 |

**Table 1. Positive Ion Table - Continued**

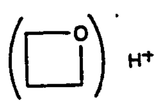
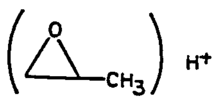
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_3H_7O^+$** | | | | | | | |
| $C_2H_5CHOH$ | | 131 | 550 | | | | |
| | From proton affinity of $C_2H_5CHO$ (RN 123-38-6). PA = 189.6 kcal/mol, 793. kJ/mol. $C_3H_7O^+$ formed in n-$C_3H_7OH$ with appearance potential of 10.71 eV is probably the same species. See also: 82MAC. | | | | | | |
| $(CH_3)_2COH$ | | 117 | 490 | | | | |
| | From proton affinity of $(CH_3)_2CO$ (RN 67-64-1). PA = 196.7 kcal/mol, 823 kJ/mol. See also: 84LOS/HOL. | | | | | | |
| $C_2H_5OCH_2$ | | (142) | (593) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination. See also: 82MAC. | | | | | | |
| $CH_3CHOCH_3$ | | 134 | 562 | | | | |
| | From proton affinity of $CH_2{=}CHOCH_3$ (RN 107-25-5). PA = 207.4 kcal/mol, 868 kJ/mol. See also: 82MAC. | | | | | | |
|  | | 149 | 625 | | | | |
| | From proton affinity of oxetane (RN 503-30-0). PA = 196.9 kcal/mol, 824 kJ/mol. | | | | | | |
|  | | 148 | 620 | | | | |
| | From proton affinity of methyloxirane (RN 75-56-9). PA = 194.7 kcal/mol, 815 kJ/mol. | | | | | | |
| **$C_3H_7OS^+$** | | | | | | | |
| $CH_3C(SH)OCH_3$ | | 125 | 522 | | | | |
| | From proton affinity of $CH_3C({=}S)OCH_3$ (RN 21119-13-1) (83CAS/KIM). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | |
| $CH_3C(OH)SCH_3$ | | 106 | 443 | | | | |
| | From proton affinity of $CH_3C({=}O)SCH_3$ (RN 1534-08-3) (83CAS/KIM). PA = 199.7 kcal/mol, 836. kJ/mol. | | | | | | |
| **$C_3H_7O_2^+$** | | | | | | | |
| $C_2H_5C(OH)_2$ | | 67 | 280 | | | | |
| | From proton affinity of $C_2H_5COOH$ (RN 79-09-4). PA = 191.8 kcal/mol, 802 kJ/mol. | | | | | | |
| $HC(OH)OC_2H_5$ | | 80 | 335 | | | | |
| | From proton affinity of $HCOOC_2H_5$ (RN 109-94-4). PA = 193.1 kcal/mol, 808 kJ/mol. | | | | | | |
| $CH_3C(OH)OCH_3$ | | 69 | 288 | | | | |
| | From proton affinity of $CH_3COOCH_3$ (RN 79-20-9). PA = 197.8 kcal/mol, 828. kJ/mol. | | | | | | |
| $CH(OCH_3)_2$ | | 97 | 406 | | | | 4483-45-8 |
| | From appearance potential determination (82HOL/LOS2). | | | | | | |

**Table 1. Positive Ion Table - Continued**

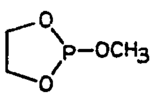
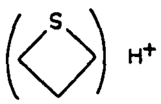
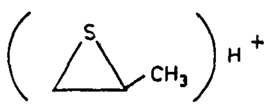
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_3H_7O_3^+$** | | | | | | | |
| $CH_3OC(OH)OCH_3$ | | 27 | 111 | | | | |
| | From proton affinity of $CH_3OCOOCH_3$ (RN 616-38-6). PA = 200.2 kcal/mol, 838. kJ/mol. | | | | | | |
| **$C_3H_7O_3P^+$** | | | | | | | |
|  | (9.06±0.1) | (45) | (186) | −164 | −688 | *EST | 3741-36-4 |
| | See also: 82WOR/HAR. | | | | | | |
| **$C_3H_7S^+$** | | | | | | | |
|  | | (179) | (749) | | | | |
| | From proton affinity of thietane (RN 287-27-4). PA = (201.3) kcal/mol, (842) kJ/mol. | | | | | | |
|  | | (176) | (737) | | | | |
| | From proton affinity of 2-methylthiirane (RN 1072-43-1). PA = (200.6) kcal/mol, (839) kJ/mol. | | | | | | |
| **$C_3H_7S_2^+$** | | | | | | | |
| $CH_3C(SH)SCH_3$ | | 182 | 763 | | | | |
| | From proton affinity of $CH_3C(=S)SCH_3$ (RN 2168-84-5). PA = 207.3 kcal/mol, 867. kJ/mol. | | | | | | |
| **$C_3H_8^+$** | | | | | | | |
| $C_3H_8$ | 10.95±0.05 | 227.5 | 951.5 | −25.0±0.1 | −104.5±0.3 | 77PED/RYL | 74-98-6 |
| | See also: 81KIM/KAT. | | | | | | |
| **$C_3H_8Cl^+$** | | | | | | | |
| $CH_3ClC_2H_5$ | | (164) | (688) | | | | |
| | $\Delta_f H$(Ion) from equilibrium constant determination (85SHA/HOJ). | | | | | | |
| **$C_3H_8Cl_2Si^+$** | | | | | | | |
| $(CH_3)_2SiCl(CH_2Cl)$ | (9.2) | (126) | (527) | −86 | −361 | *EST | 1719-57-9 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| **$C_3H_8N^+$** | | | | | | | |
| $CH_3CH_2CHNH_2$ | | 152 | 636 | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurements (81LOS/LAM). | | | | | | |
| $CH_3CHCH_2NH_2$ | | (161) | (673) | | | | |
| | From proton affinity of $CH_2=CHCH_2NH_2$ (RN 107-11-9). PA = 215.6 kcal/mol, 903 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

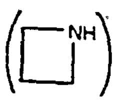
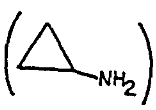
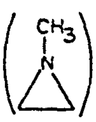
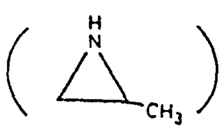
| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_3H_8N^+$** | | | | | | | |
| $(CH_3)_2CNH_2$ | (5.4) | (141) | (590) | (17) | (69) | 81LOS/LAM | 26374-12-9 |
| | $\Delta_f H$(Ion) from appearance potential measurements (81LOS/LAM). IP derived (83BUR/CAS). Value derived from proton affinity of $CH_2=C(CH_3)NH_2$ (PA = 226.3 kcal/mol, 947 kJ/mol) and $(CH_3)_2C=NH_2$ (PA = 221 kcal/mol, 925 kJ/mol) is 147 kcal/mol, 615 kJ/mol. (84LIA/LIE). | | | | | | |
| $CH_3CH_2NHCH_2$ | | 156 | 653 | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurements (81LOS/LAM). | | | | | | |
| $CH_3CHNHCH_3$ | | (147) | (615) | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurements (81LOS/LAM). | | | | | | |
| $CH_2N(CH_3)_2$ | 5.7 | (158) | (661) | (26) | (109) | 81GRI/LOS | 30208-47-0 |
| | $\Delta_f H$(Ion) from appearance potential measurements (81LOS/LAM), IP derived (81GRI/LOS, 83BUR/CAS, 81LOG/TAK). | | | | | | |
|  $H^+$ | | (167) | (698) | | | | |
| | From proton affinity of azetidine. (RN 503-29-7). PA = 222.8 kcal/mol, 932. kJ/mol. | | | | | | |
|  $H^+$ | | 169 | 707 | | | | |
| | From proton affinity of c-$C_3H_5NH_2$ (RN 765-30-0). PA = 215.2 kcal/mol, 900 kJ/mol. | | | | | | |
|  $H^+$ | | 174 | 730 | | | | |
| | From proton affinity of N-methylaziridine (RN 1072-44-2). PA = 221.6 kcal/mol, 927. kJ/mol. | | | | | | |
|  $H^+$ | | (168) | (704) | | | | |
| | From proton affinity of 2-methylaziridine (RN 75-55-8). PA = (219.2) kcal/mol, (917) kJ/mol. | | | | | | |
| **$C_3H_8NO^+$** | | | | | | | |
| $HC(OH)N(CH_3)_2$ | | 108 | 454 | | | | |
| | From proton affinity of $HCON(CH_3)_2$ (RN 68-12-2). PA = 211.4 kcal/mol, 884 kJ/mol. | | | | | | |
| **$C_3H_8NO_2^+$** | | | | | | | |
| i-$C_3H_7ONHO$ | | 132 | 552 | | | | |
| | From proton affinity of i-$C_3H_7ONO$ (RN 541-42-4). PA = 201.9 kcal/mol, 845 kJ/mol. | | | | | | |
| $CH_3CH(NH_3)COOH$ | | 52 | 216 | | | | |
| | From proton affinity of L-alanine (RN 56-41-7). PA = 214.8 kcal/mol, 899. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

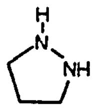
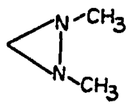
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_3H_8NO_2^+$** | | | | | | | |
| $CH_3NH_2CH_2COOH$ | | 59 | 248 | | | | |
| | From proton affinity of sarcosine (RN 107-97-1). PA = 218.7 kcal/mol, 915. kJ/mol. | | | | | | |
| **$C_3H_8NO_3^+$** | | | | | | | |
| $HOCH_2CH(NH_3)COOH$ | | 15 | 62 | | | | |
| | From proton affinity of L-serine (RN 302-84-1). PA = 216.8 kcal/mol, 907. kJ/mol. | | | | | | |
| **$C_3H_8N_2^+$** | | | | | | | |
|  | (≤7.90) | (≤216) | (≤903) | 34 | 141 | *EST | 504-70-1 |
|  | (8.7) | (259) | (1082) | 58 | 243 | *EST | 6794-95-2 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_3H_8N_2O^+$** | | | | | | | |
| $(CH_3NH)_2CO$ | (≤9.23) | (≤155) | (≤649) | −58 | −242 | *EST | 96-31-1 |
| $(CH_3)_2NCONH_2$ | (≤8.96) | (≤149) | (≤622) | −58 | −242 | *EST | 598-94-7 |
| **$C_3H_8N_2S^+$** | | | | | | | |
| $(CH_3NH)_2CS$ | (≤8.08±0.03) | (≤194) | (≤814) | 8 | 34 | *EST | 534-13-4 |
| **$C_3H_8O^+$** | | | | | | | |
| n-$C_3H_7OH$ | 10.22±0.03 | 175 | 731 | −60.9±0.2 | −254.8±1. | 77PED/RYL | 71-23-8 |
| | | *181* | *756* | *−55.1* | *−230.4* | | |
| | See also: 84BOW/MAC, 81KIM/KAT, 80BAC/MOU. | | | | | | |
| iso-$C_3H_7OH$ | 10.12±0.08 | 168 | 704 | −65.1±0.1 | −272.5±0.4 | 77PED/RYL | 67-63-0 |
| | | *174* | *729* | *−59.2* | *−247.7* | | |
| | See also: 72POT/SOR, 81KIM/KAT, 80BAC/MOU, 84BOW/MAC. | | | | | | |
| $C_2H_5OCH_3$ | 9.72 | 172 | 721 | −51.7±0.1 | −216.4±0.6 | 77PED/RYL | 540-67-0 |
| | IP from 81HOL/FIN, 84BOW/MAC, 81KIM/KAT, 80BAC/MOU, 82LEV/LIA, 79AUE/BOW. | | | | | | |
| $CH_2CH_2CH_2OH_2$ | | 171 | 714 | | | | |
| | From appearance potential determinations (84HOL/MOM). | | | | | | |
| $CH_2CHCH_2HOH_2$ | | 172 | 721 | | | | |
| | From appearance potential determinations (84HOL/MOM). Authors propose that ion is proton-bound dimer of water and allyl radical. | | | | | | |

Table 1. Positive Ion Table - Continued

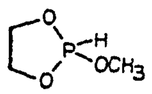
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_8O_2^+$ | | | | | | | |
| $(CH_3O)_2CH_2$ | 9.5 | 136 | 568 | −83.2±0.2 | −348.2±0.7 | 77PED/RYL | 109-87-5 |
| | IP from 82HOL/LOS2. See also: 81JOR, 82ZVE/VIL, 81KIM/KAT. | | | | | | |
| $HOCH_2CH_2OCH_3$ | 9.6 | 134 | 562 | −87 | −364 | *EST | 109-86-4 |
| | IP is onset of photoelectron band (83BIE/MOR, 81KIM/KAT). | | | | | | |
| $C_3H_8O_3P^+$ | | | | | | | |
|  | | −11 | −48 | | | | |
| | From proton affinity of 2-methoxy-1,3,2-dioxaphospholane (RN 3741-36-4). PA = 212.7 kcal/mol, 890 kJ/mol. | | | | | | |
| $C_3H_8S^+$ | | | | | | | |
| n-$C_3H_7SH$ | 9.195±0.005 | 195.8 | 819.2 | −16.2±0.1 | −67.9±0.6 | 77PED/RYL | 107-03-9 |
| | See also: 81KIM/KAT. | | | | | | |
| iso-$C_3H_7SH$ | 9.14 | 193 | 806 | −18.2±0.1 | −76.2±0.6 | 77PED/RYL | 75-33-2 |
| | See: 81KIM/KAT. | | | | | | |
| $C_2H_5SCH_3$ | 8.54±0.1 | 183 | 764 | −14.2±0.3 | −59.6±1.1 | 77PED/RYL | 624-89-5 |
| | See also: 79AUE/BOW. | | | | | | |
| $C_3H_8S_2^+$ | | | | | | | |
| $CH_3SCH_2SCH_3$ | (8.4) | (195) | (815) | 1±2 | 5±8 | *EST | 1618-26-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_8Sc^+$ | | | | | | | |
| $C_2H_4ScH(CH_3)$ | | (197) | (824) | | | | |
| | $\Delta_fH$(Ion) from 84TOL/BEA. | | | | | | |
| $C_3H_8Si^+$ | | | | | | | |
| $(CH_3)_2Si=CH_2$ | 7.71±0.03 | 183 | 765 | 5 | 21 | 86WAL | 4112-23-6 |
| | IP from 82DYK/JOS. See also: 81KOE/MCK. | | | | | | |
| $C_3H_9^+$ | | | | | | | |
| $C_3H_9$ | | 191 | 797 | | | | |
| | From proton affinity of $C_3H_8$. (RN 74-98-6). PA = 150 kcal/mol, 628 kJ/mol. | | | | | | |
| $C_3H_9Al^+$ | | | | | | | |
| $(CH_3)_3Al$ | (≤9.76) | (≤206) | (≤861) | −19±3 | −81±11 | 77PED/RYL | 75-24-1 |
| $C_3H_9As^+$ | | | | | | | |
| $(CH_3)_3As$ | (8.2) | (192) | (804) | 3±2 | 13±10 | 77PED/RYL | 593-88-4 |
| | IP is onset of photoelectron band (82ELB/DIE). | | | | | | |
| $C_3H_9AsO_3^+$ | | | | | | | |
| $As(OCH_3)_3$ | (7.93) | (51) | (215) | −131±0.5 | −550±2 | 77PED/RYL | 6596-95-8 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3H_9B^+$ | | | | | | | |
| $(CH_3)_3B$ | (9.5) | (190) | (794) | −29±2 | −123±10 | 77PED/RYL | 593-90-8 |
| | | *(196)* | *(820)* | *−23* | *−97* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_9BO_3^+$ | | | | | | | |
| $B(OCH_3)_3$ | (10.0) | (15) | (65) | −215±0.5 | −900±2 | 77PED/RYL | 121-43-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_9BS_3^+$ | | | | | | | |
| $B(SCH_3)_3$ | (8.74) | (164) | (687) | −37±0.7 | −156±3 | 77PED/RYL | 997-49-9 |
| $C_3H_9BrPb^+$ | | | | | | | |
| $(CH_3)_3PbBr$ | (≤9.30) | (≤229) | (≤956) | 14 | 59 | 85DEW/HOL | 6148-48-7 |
| $C_3H_9BrSi^+$ | | | | | | | |
| $(CH_3)_3SiBr$ | 10.0 | (161) | (672) | −70±1 | −293±4 | 77PED/RYL | 2857-97-8 |
| | | *(169)* | *(707)* | *−61±0.8* | *−258±4* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_9BrSn^+$ | | | | | | | |
| $(CH_3)_3SnBr$ | (9.4) | (184) | (769) | −33±1 | −138±6 | 77PED/RYL | 1066-44-0 |
| $C_3H_9ClGe^+$ | | | | | | | |
| $(CH_3)_3GeCl$ | (9.2) | (148) | (620) | −64±3 | −268±13 | 80TEL/RAB | 1529-47-1 |
| | IP is onset of photoelectron band. See also: 79DRA/GLA2. | | | | | | |
| $C_3H_9ClSi^+$ | | | | | | | |
| $(CH_3)_3SiCl$ | (10.15) | (149) | (625) | −85 | −354 | 81BEL/PER | 75-77-4 |
| | | *(156)* | *(654)* | *−78* | *−325* | | |
| | IP is onset of photoelectron band. See also: 84SZE/BAE, 81ZYK/KHV. | | | | | | |
| $C_3H_9ClSn^+$ | | | | | | | |
| $(CH_3)_3SnCl$ | (9.90) | (185) | (773) | −43 | −182 | *EST | 1066-45-1 |
| | IP from 82LEV/LIA. | | | | | | |
| $C_3H_9FN^+$ | | | | | | | |
| $CH_2FCH_2CH_2NH_3$ | | 87 | 365 | | | | |
| | From proton affinity of $CH_2FCH_2CH_2NH_2$ (RN 462-41-9). PA = 217.8 kcal/mol, 911. kJ/mol. | | | | | | |
| $C_3H_9FSi^+$ | | | | | | | |
| $(CH_3)_3SiF$ | 10.31±0.04 | 112 | 468 | −126 | −527 | 77MUR/BEA | 420-56-4 |
| $C_3H_9Ga^+$ | | | | | | | |
| $(CH_3)_3Ga$ | (8.9) | (195) | (817) | −10±1 | −42±6 | 77PED/RYL | 1445-79-0 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | kJ/mol | $\Delta_fH$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3H_9Ge^+$ | | | | | | | |
| $(CH_3)_3Ge$ | | 180 | 754 | | | | |
| | $\Delta_fH$(Ion) from appearance potential determinations. Proton affinity of $(CH_3)_2Ge=CH_2$ (RN 82064-99-1) = 204.9 kcal, 857. kJ/mol. | | | | | | |
| $C_3H_9N^+$ | | | | | | | |
| $n\text{-}C_3H_7NH_2$ | 8.78±0.02 | 186 | 777 | −16.8±0.1 | −70.2±0.4 | 77PED/RYL | 107-10-8 |
| | See also: 81KIM/KAT. | | | | | | |
| $iso\text{-}C_3H_7NH_2$ | 8.72±0.03 | 181 | 758 | −20.0±0.1 | −83.8±0.5 | 77PED/RYL | 75-31-0 |
| | See also: 81KIM/KAT. | | | | | | |
| $(CH_3)(C_2H_5)NH$ | (8.15) | (177) | (740) | −11±0.5 | −46±2 | *EST | 624-78-2 |
| | IP from 79AUE/BOW. | | | | | | |
| $(CH_3)_3N$ | 7.82±0.06 | 175 | 731 | −5.7±0.1 | −23.7±0.6 | 77PED/RYL | 75-50-3 |
| | See also: 81KIM/KAT, 82ELB/DIE. | | | | | | |
| $C_3H_9NO^+$ | | | | | | | |
| $NH_2(CH_2)_3OH$ | (9.0) | (156) | (650) | −52 | −218 | *EST | 156-87-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3OCH_2CH_2NH_2$ | (8.9) | (161) | (675) | −44±0.7 | −184±3 | *EST | 109-85-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3ON(CH_3)_2$ | ≤8.78 | (≤194) | (≤810) | −9 | −37 | *EST | 5669-39-6 |
| | IP from 83MOL/PIK. See also: 82LEV/LIA. | | | | | | |
| $C_3H_9N_3Si^+$ | | | | | | | |
| $(CH_3)_3SiN_3$ | (≤9.7±0.1) | (≤241) | (≤1007) | 17±2 | 71±8 | 80TEL/RAB | 4648-54-8 |
| $C_3H_9O^+$ | | | | | | | |
| $n\text{-}C_3H_7OH_2$ | | 114 | 476 | | | | |
| | From proton affinity of $n\text{-}C_3H_7OH$ (RN 71-23-8). PA = 190.8 kcal/mol, 798. kJ/mol. | | | | | | |
| $i\text{-}C_3H_7OH_2$ | | 109 | 457 | | | | |
| | From proton affinity of $i\text{-}C_3H_7OH$ (RN 67-63-0). PA = 191.2 kcal/mol, 800. kJ/mol. | | | | | | |
| $C_2H_5OHCH_3$ | | 118 | 492 | | | | |
| | From proton affinity of $C_2H_5OCH_3$ (RN 540-67-0). PA = 196.4 kcal/mol, 822. kJ/mol. | | | | | | |
| $C_3H_9OP^+$ | | | | | | | |
| $(CH_3)_3PO$ | (9.5) | (115) | (482) | −104±2 | −434±8 | 77PED/RYL | 676-96-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_3H_9O_2^+$ | | | | | | | |
| $HOCH_2CH_2OHCH_3$ | | 96 | 402 | | | | |
| | From proton affinity of $HOCH_2CH_2OCH_3$ (RN 109-86-4) (78TAF/TAA). PA = 182.6 kcal/mol, 764. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3H_9O_3P^+$ | | | | | | | |
| $P(OCH_3)_3$ | (8.50) | (29) | (123) | −167±5 | −697±20 | 77PED/RYL | 121-45-9 |
| | See also: 81CHA/FIN, 82WOR/HAR, 77COW/GOO. | | | | | | |
| $C_3H_9O_3PS^+$ | | | | | | | |
| $(CH_3O)_3PS$ | (≤9.16) | (≤28) | (≤117) | −183 | −767 | *EST | 152-18-1 |
| $C_3H_9O_4P^+$ | | | | | | | |
| $(CH_3O)_3PO$ | 9.99 | (−34) | (−143) | −265 | −1107 | *EST | 512-56-1 |
| | See also: 81CHA/FIN. | | | | | | |
| $C_3H_9P^+$ | | | | | | | |
| $(CH_3)_3P$ | 8.06±0.05 | 162 | 677 | −24±1 | −101±5 | 77PED/RYL | 594-09-2 |
| | See also: 82IKU/KEB, 82COW/KEM, 82ELB/DIE, 82BAN/CHA2. | | | | | | |
| $C_3H_9Pb^+$ | | | | | | | |
| $(CH_3)_3Pb$ | | 200 | 840 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations. Proton affinity of $(CH_3)_2Pb=CH_2$ (RN 82065-01-8) = 223.9 kcal/mol, 937. kJ/mol. | | | | | | |
| $C_3H_9S^+$ | | | | | | | |
| $n\text{-}C_3H_7SH_2$ | | 158 | 660 | | | | |
| | From proton affinity of $n\text{-}C_3H_7SH$ (RN 107-03-9). PA = 191.6 kcal/mol, 802 kJ/mol. | | | | | | |
| $i\text{-}C_3H_7SH_2$ | | 153 | 642 | | | | |
| | From proton affinity of $i\text{-}C_3H_7SH$ (RN 75-33-2). PA = 194.1 kcal/mol, 812 kJ/mol. | | | | | | |
| $CH_3SHC_2H_5$ | | 148 | 619 | | | | |
| | From proton affinity of $CH_3SC_2H_5$ (RN 624-89-5). PA = 203.5 kcal/mol, 851 kJ/mol. | | | | | | |
| $C_3H_9Sb^+$ | | | | | | | |
| $(CH_3)_3Sb$ | (7.7) | (185) | (775) | 8±6 | 32±25 | 77PED/RYL | 594-10-5 |
| | IP is onset of photoelectron band(82ELB/DIE). | | | | | | |
| $C_3H_9Si^+$ | | | | | | | |
| $(CH_3)_3Si$ | (6.5) | (150) | (630) | −0.8±2 | −3±8 | 86DON/WAL | 16571-41-8 |
| | | *(157)* | *(656)* | *6* | *26* | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (84SZE/BAE, 84SZE/BAE2). IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). | | | | | | |
| $C_3H_9Sn^+$ | | | | | | | |
| $(CH_3)_3Sn$ | (7.10±0.05) | (181) | (759) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations. Proton affinity of $(CH_3)_2Sn=CH_2$ (RN 82065-00-7) = 215.8 kcal/mol, 903. kJ/mol. | | | | | | |
| $C_3H_{10}As^+$ | | | | | | | |
| $(CH_3)_3AsH$ | | 155 | 650 | | | | |
| | From proton affinity of $(CH_3)_3As$ (RN 593-88-4). PA = 213.4 kcal/mol, 893 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_3H_{10}N^+$ | | | | | | | |
| n-$C_3H_7NH_3$ | | 131 | 548 | | | | |
| | From proton affinity of n-$C_3H_7NH_2$ (RN 107-10-8). PA = 217.9 kcal/mol, 912. kJ/mol. | | | | | | |
| i-$C_3H_7NH_3$ | | 127 | 531 | | | | |
| | From proton affinity of i-$C_3H_7NH_2$ (RN 75-31-0). PA = 218.6 kcal/mol, 915. kJ/mol. | | | | | | |
| $(CH_3)(C_2H_5)NH_2$ | | 132 | 552 | | | | |
| | From proton affinity of $(CH_3)(C_2H_5)NH$ (RN 624-78-2). PA = 222.8 kcal/mol, 932. kJ/mol. | | | | | | |
| $(CH_3)_3NH$ | | 135 | 564 | | | | |
| | From proton affinity of $(CH_3)_3N$ (RN 75-50-3). PA = 225.1 kcal/mol, 942. kJ/mol. | | | | | | |
| $C_3H_{10}NO^+$ | | | | | | | |
| $NH_3(CH_2)_3OH$ | | 85 | 356 | | | | |
| | From proton affinity of $NH_2(CH_2)_3OH$ (RN 156-87-6). PA = 228.6 kcal/mol, 956.5 kJ/mol. | | | | | | |
| $CH_3OCH_2CH_2NH_3$ | | 98 | 412 | | | | |
| | From proton affinity of $CH_3OCH_2CH_2NH_2$ (RN 109-85-3). PA = 223.3 kcal/mol, 934 kJ/mol. | | | | | | |
| $C_3H_{10}N_2{}^+$ | | | | | | | |
| $(CH_3)_2NNH(CH_3)$ | | | | 21 | 87 | 69BEN/CRU | 1741-01-1 |
| | A value of 7.93 eV has been reported for the adiabatic IP of this compound. Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. | | | | | | |
| $C_3H_{10}OP^+$ | | | | | | | |
| $(CH_3)_3POH$ | | 124 | 518 | | | | |
| | From proton affinity of $(CH_3)_3PO$ (RN 676-96-0) (84BOL/HOU). PA = 217.1 kcal/mol, 908. kJ/mol. | | | | | | |
| $C_3H_{10}O_3P^+$ | | | | | | | |
| $HP(OCH_3)_3$ | | −22 | −92 | | | | |
| | From proton affinity of $P(OCH_3)_3$ (RN 121-45-9). PA = 220.6 kcal/mol, 923. kJ/mol. | | | | | | |
| $C_3H_{10}O_3PS^+$ | | | | | | | |
| $(CH_3O)_3PSH$ | | −32 | −134 | | | | |
| | From proton affinity of $(CH_3O)_3PS$ (RN 152-18-1). PA = 214.5 kcal/mol, 897. kJ/mol. | | | | | | |
| $C_3H_{10}O_4P^+$ | | | | | | | |
| $(CH_3O)_3POH$ | | −111 | −464 | | | | |
| | From proton affinity of $(CH_3O)_3PO$ (RN 512-56-1). PA = 212.0 kcal/mol, 887. kJ/mol. | | | | | | |
| $C_3H_{10}P^+$ | | | | | | | |
| $(CH_3)_3PH$ | | 114 | 479 | | | | |
| | From proton affinity of $(CH_3)_3P$ (RN 594-09-2). PA = 227.1 kcal/mol, 950. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

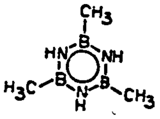
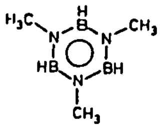
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_3H_{10}Si^+$ | | | | | | | |
| $(CH_3)_3SiH$ | 9.9 | 189 | 792 | −39±1 | −163±4 | 86DON/WAL | 993-07-7 |
| | IP from 81HOT. | | | | | | |
| $C_3H_{10}Sn^+$ | | | | | | | |
| $(CH_3)_3SnH$ | (≤9.9) | (≤228) | (≤955) | 0±2 | 0±8 | 80TEL/RAB | 1631-73-8 |
| $C_3H_{11}N_2^+$ | | | | | | | |
| $NH_2(CH_2)_3NH_3$ | | 124 | 518 | | | | |
| | From proton affinity of $NH_2(CH_2)_3NH_2$ (RN 109-76-2). PA = 234.1 kcal/mol, 979. kJ/mol. | | | | | | |
| $C_3H_{12}BN^+$ | | | | | | | |
| $(CH_3)_3NBH_3$ | (9.28±0.2) | (194) | (810) | −20 | −85 | 82TN270 | 75-22-9 |
| | | *(203)* | *(848)* | *−11* | *−47* | | |
| $C_3H_{12}B_3N_3^+$ | | | | | | | |
|  | (9.1±0.15) | (−13) | (−55) | −223 | −933 | 70FIN/GAR | 1004-35-9 |
|  | (9.07) | (−8) | (−33) | −217±1 | −908±4 | 80TEL/RAB | 5314-85-2 |
| $C_3IN^+$ | | | | | | | |
| IC≡CCN | (10.18±0.02) | (347) | (1451) | 112±10 | 469±40 | 79BUC/VOG | 2003-32-9 |
| | See also: 84KUH/MAI. | | | | | | |
| $C_3La^+$ | | | | | | | |
| $LaC_3$ | (6.8±0.5) | (336) | (1404) | 179±1 | 748±1 | 81GIN/PEL | 12602-63-0 |
| $C_3N_2O^+$ | | | | | | | |
| $(CN)_2CO$ | (≤12.56) | (≤349) | (≤1459) | 59±1 | 247±6 | 77PED/RYL | 1115-12-4 |
| $C_3O_2^+$ | | | | | | | |
| $C_3O_2$ | 10.60 | 222 | 929 | −22±0.5 | −94±2 | 71JANAF | 504-64-3 |
| $C_4^+$ | | | | | | | |
| $C_4$ | (12.6) | (522) | (2187) | 232±8 | 971±33 | 71JANAF | 12184-80-4 |
| $C_4Cl_2Hg^+$ | | | | | | | |
| $(ClC≡C)_2Hg$ | 9.58±0.02 | (373) | (1559) | 152 | 635 | *EST | 64771-59-1 |
| | IP is onset of photoelectron band (81FUR/PIA). | | | | | | |

Table 1. Positive Ion Table - Continued

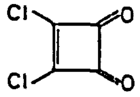
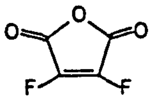
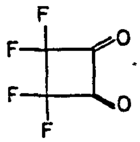
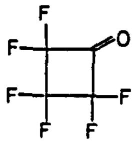
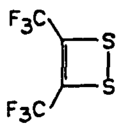
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4Cl_2O_2^+$ | | | | | | | |
|  | (9.5) | (204) | (856) | −14 | −61 | *EST | 2892-63-9 |
| | IP is onset of photoelectron band (81BOC/RIE). | | | | | | |
| $C_4F_2O_3^+$ | | | | | | | |
|  | (11.45) | (79) | (330) | −185 | −775 | *EST | 669-78-3 |
| | IP from 81ASB/SVE. | | | | | | |
| $C_4F_4O_2^+$ | | | | | | | |
|  | 10.05±0.1 | (47) | (199) | −184 | −771 | *EST | 663-45-6 |
| | IP is onset of photoelectron band (85GLE/SCH, 85ALB/HEL). | | | | | | |
| $C_4F_6^+$ | | | | | | | |
| $CF_2=CFCF=CF_2$ | (9.5) | (−5) | (−21) | −224 | −938 | 68LAC/SKI | 685-63-2 |
| $C_4F_6O^+$ | | | | | | | |
| $(CF_3)_2C=C=O$ | (10.67) | (−95) | (−398) | −341 | −1427 | *EST | |
| | IP is onset of photoelectron band (83GLE/SAA). | | | | | | |
|  | (10.7) | (−30) | (−124) | −276 | −1157 | *EST | 699-35-4 |
| | IP is onset of photoelectron band (85GLE/SCH). | | | | | | |
| $C_4F_6S^+$ | | | | | | | |
| $(CF_3)_2C=C=S$ | (9.4) | (−71) | (−295) | −287 | −1202 | *EST | 7445-60-5 |
| | IP is onset of photoelectron band (83GLE/SAA). | | | | | | |
| $C_4F_6S_2^+$ | | | | | | | |
|  | 9.6 | (37) | (154) | −185 | −772 | *EST | 360-91-8 |
| | IP is onset of photoelectron band (83SCH/SCH, 83JIA/MOH). | | | | | | |
| $C_4F_8^+$ | | | | | | | |
| (Z)-2-$C_4F_8$ | (11.1) | (−126) | (−526) | −382 | −1597 | 70BEN/O'N | 1516-65-0 |
| | IP is onset of photoelectron band. | | | | | | |
| (E)-2-$C_4F_8$ | (11.0) | (−129) | (−540) | −383 | −1601 | 70BEN/O'N | 1516-64-9 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

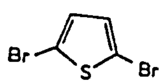
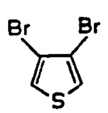
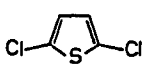
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4FeI_2O_4^+$ | | | | | | | |
| $Fe(CO)_4I_2$ | (8.4) | (42) | (174) | −152±2 | −636±9 | 82PIL/SKI | 14911-55-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4HCl^+$ | | | | | | | |
| CH≡CC≡CCl | (9.72±0.02) | (345) | (1443) | 121±0.5 | 505±2 | *EST | 6089-44-7 |
| $C_4HCoO_4^+$ | | | | | | | |
| $HCo(CO)_4$ | (8.2) | (53) | (222) | −136±0.5 | −569±2 | 77PED/RYL | 16842-03-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4HF_7N^+$ | | | | | | | |
| $n\text{-}C_3F_7CNH$ | | −110 | −460 | | | | |
| | From proton affinity of $n\text{-}C_3F_7CN$ (RN 375-00-8). PA = 167.4 kcal/mol, 700. kJ/mol. | | | | | | |
| $C_4HF_9O^+$ | | | | | | | |
| $(CF_3)_3COH$ | 12.25 | (−266) | (−1115) | (−549) | (−2297) | *EST | 2378-02-1 |
| | IP from 83KOP/MOL. | | | | | | |
| $C_4HNiO_4^+$ | | | | | | | |
| $HNi(CO)_4$ | | (43) | (179) | | | | |
| | From proton affinity of $Ni(CO)_4$ (RN 13463-39-3). PA = (180) kcal/mol, (753) kJ/mol. | | | | | | |
| $C_4H_2^+$ | | | | | | | |
| HC≡CC≡CH | 10.180±0.003 | 340 | 1422 | 105 | 440 | 85STE/FAH | 460-12-8 |
| | See also: 80MAI/THO. | | | | | | |
| $C_4H_2Br_2S^+$ | | | | | | | |
|  | (≤8.49) | (≤233) | (≤976) | 38 | 157 | *EST | 3141-27-3 |
|  | (≤8.94) | (≤246) | (≤1028) | 39 | 165 | *EST | 3141-26-2 |
| $C_4H_2Cl_2S^+$ | | | | | | | |
|  | (8.60±0.05) | (213) | (890) | 14 | 60 | *EST | 3172-52-9 |
| $C_4H_2F_4^+$ | | | | | | | |
| $CF_2CHCHCF_2$ | (10.6±0.1) | (82) | (343) | −163 | −680 | *EST | 407-70-5 |

**Table 1. Positive Ion Table - Continued**

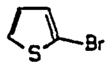
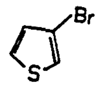
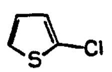
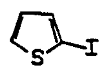
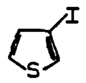
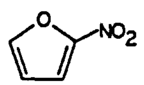
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_3BrS^+$ | | | | | | | |
|  | 8.6 | (231) | (966) | 33 | 136 | *EST | 1003-09-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.812±0.005 | (236) | (986) | 33 | 136 | *EST | 872-31-1 |
| $C_4H_3ClS^+$ | | | | | | | |
|  | 8.89±0.05 | (225) | (941) | 20 | 83 | *EST | 96-43-5 |
| $C_4H_3F_9N^+$ | | | | | | | |
| $(CF_3)_3CNH_3$ | | (−329) | (−1375) | | | | |
| | From proton affinity of $(CF_3)_3CNH_2$ (RN 2809-92-9). PA = (191.5) kcal/mol, (801.) kJ/mol. | | | | | | |
| $C_4H_3IS^+$ | | | | | | | |
|  | ≤8.46 | (≤242) | (≤1010) | 46 | 194 | *EST | 3437-95-4 |
|  | (≤8.46) | (≤241) | (≤1010) | 46 | 194 | *EST | 10486-61-0 |
| $C_4H_3N^+$ | | | | | | | |
| $CH_2=C=CHCN$ | (10.1) | (259) | (1084) | 26 | 110 | *EST | 1001-56-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3C\equiv CCN$ | 10.78±0.02 | (329) | (1378) | 81±0.7 | 338±3 | *EST | 13752-78-8 |
| $C_4H_3NO_3^+$ | | | | | | | |
|  | (≤9.75±0.05) | (≤218) | (≤910) | −7 | −31 | *EST | 609-39-2 |

**Table 1. Positive Ion Table - Continued**

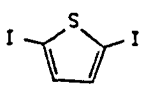
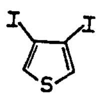
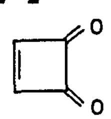
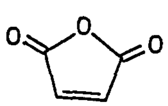
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_2F_9N^+$ | | | | | | | |
| $(CF_3)_3CNH_2$ | (10.4) | (−263) | (−1100) | −503 | −2104 | *EST | 2809-92-9 |
| | IP from 79AUE/BOW. | | | | | | |
| $C_4H_2F_9O^+$ | | | | | | | |
| $(CF_3)_3COH_2$ | | −346 | −1449 | | | | |
| | From proton affinity of $(CF_3)_3COH$ (RN 2378-02-1). PA = 163.1 kcal/mol, 682. kJ/mol. | | | | | | |
| $C_4H_2I_2S^+$ | | | | | | | |
|  | ≤8.28 | (≤256) | (≤1072) | 65 | 273 | *EST | 625-88-7 |
|  | (≤8.45) | (≤263) | (≤1099) | 68 | 284 | *EST | 19259-08-6 |
| $C_4H_2N_2^+$ | | | | | | | |
| (Z)-CH(CN)CH(CN) | (11.15) | (338) | (1416) | 81.3±0.5 | 340.2±1.9 | 77PED/RYL | 928-53-0 |
| (E)-CH(CN)CH(CN) | 11.16±0.03 | 338 | 1417 | 81 | 340 | 82CHU/NGU | 764-42-1 |
| $C_4H_2O_2^+$ | | | | | | | |
|  | (≤9.79) | (≤239) | (≤1002) | 14 | 57 | *EST | 32936-74-6 |
| $C_4H_2O_3^+$ | | | | | | | |
|  | (10.8) | (154) | (644) | −95±1 | −398±5 | 77PED/RYL | 108-31-6 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_4H_3^+$ | | | | | | | |
| $HCCCCH_2$ | | (291) | (1217) | | | | |
| | From proton affinity of HC≡CC≡CH (RN 460-12-8) (87DEA/MAU). PA = 180 kcal/mol, 753 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

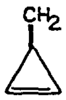
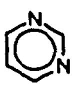
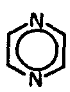
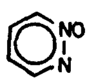
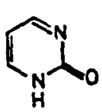
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_4^+$ | | | | | | | |
| $CH_2=C=C=CH_2$ | (9.15) | (294) | (1232) | 83 | 349 | 82ROS/DAN | 2873-50-9 |
| | See also: 85DEW/TIE. | | | | | | |
| $CH_2=CHC\equiv CH$ | 9.58±0.02 | (294) | (1229) | 73 | 305 | 69STU/WES | 689-97-4 |
|  | 8.15 | (289) | (1209) | 101 | 423 | 87STA/NOR | 4095-06-1 |
| | Heat of formation of ion from appearance potential measurements (82ROS/DAN); $\Delta_fH$(Neutral) is $\Delta_fH$(Ion) - IP (87STA/NOR). | | | | | | |
| $C_4H_4N_2^+$ | | | | | | | |
| $NCCH_2CH_2CN$ | 12.1±0.25 | 329 | 1377 | 50.1±0.1 | 209.7±0.6 | 77PED/RYL | 110-61-2 |
| | IP from 82CHE/LAP. | | | | | | |
|  | (8.64) | (266) | (1112) | 66.5±0.2 | 278.3±1 | 77PED/RYL | 289-80-5 |
|  | 9.23 | 260 | 1087 | 47.0±0.2 | 196.6±0.9 | 77PED/RYL | 289-95-2 |
| | See also: 83PIA/KEL. | | | | | | |
|  | 9.29±0.01 | 261 | 1092 | 46.8±0.3 | 196.0±1.3 | 77PED/RYL | 290-37-9 |
| | See also: 83PIA/KEL. | | | | | | |
| $C_4H_4N_2O^+$ | | | | | | | |
|  | (8.89±0.02) | (252) | (1056) | 47 | 198 | *EST | 1457-42-7 |
|  | (8.80±0.02) | (231) | (966) | 28 | 117 | *EST | 17043-94-6 |
|  | (10.06±0.05) | (221) | (924) | −11 | −47 | *EST | 557-01-7 |

Table 1. Positive Ion Table - Continued

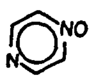
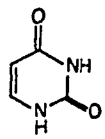
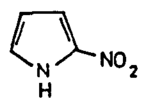
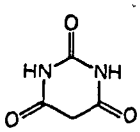
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_4N_2O^+$ | | | | | | | |
|  | (9.0) | (235) | (984) | 28 | 116 | *EST | 2423-65-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_4N_2O_2^+$ | | | | | | | |
|  | (9.2) | (140) | (585) | −72±0.5 | −303±2 | 77NAB/SAB | 66-22-8 |
| | IP is onset of photoelectron band. See also: 81YU/ODO. | | | | | | |
|  | (9.30±0.05) | (237) | (990) | 23 | 93 | *EST | 5919-26-6 |
| $C_4H_4N_2O_3^+$ | | | | | | | |
|  | (10.20) | (103) | (430) | −132 | −554 | 72DOM | 67-52-7 |
| $C_4H_4O^+$ | | | | | | | |
| $CH_3CH=C=C=O$ | 8.68±0.05 | (215) | (900) | 15 | 63 | *EST | 78957-08-1 |
| | IP from 83TER/HOL. See also: 79HOL/TER, 81MOH/HIR. | | | | | | |
| $(CH_2)_2C=C=O$ | | 198 | 828 | | | | |
| | From appearance potential determination (82BUR/HOL). | | | | | | |
| $CH_2=CHCH=C=O$ | 8.29±0.05 | (195) | (817) | 4 | 17 | *EST | 50888-73-8 |
| | IP from 79TER/BUR. See also: 82BUR/HOL, 81MOH/HIR, 79HOL/TER, 85MCN/SUF, 81BOC/HIR. | | | | | | |
| $CH_2=C=CHCHO$ | (9.5) | (236) | (987) | 18 | 75 | *EST | 53268-92-1 |
| | $\Delta_f H$(Ion) from 82BUR/HOL. IP from 79HOL/TER. | | | | | | |
| $HC\equiv CCH_2CHO$ | (9.85) | (247) | (1034) | 20 | 84 | *EST | 52844-23-2 |
| | IP estimated in 82BUR/HOL. | | | | | | |
| $CH_3C\equiv CCHO$ | 10.20±0.02 | (253) | (1057) | 17 | 73 | *EST | 1119-19-3 |
| | IP from 79CAR/MOU. See also: 79TER/BUR, 82BUR/HOL, 79HOL/TER. | | | | | | |
| $CH_3COC\equiv CH$ | 10.17±0.02 | (250.18) | (1046.75) | 15.6±.2 | 65.5±1 | 85FUC | 1423-60-5 |
| | IP from 79CAR/MOU. See also: 79TER/BUR, 82BUR/HOL, 79HOL/TER. | | | | | | |
| $CH_2=C=C=CHOH$ | | 222 | 931 | | | | |
| | From appearance potential determination(82BUR/HOL). | | | | | | |

**Table 1. Positive Ion Table - Continued**

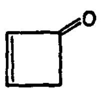
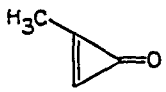
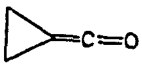
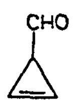
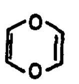
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_4O^+$ | | | | | | | |
| HC≡CCH=CHOH | | 220 | 922 | | | | 59095-55-5 |
| | From appearance potential determination(82BUR/HOL). | | | | | | |
| $CH_2$=C(OH)C≡CH | (8.92) | (226) | (944) | 20±2 | 83±7 | 86TUR/HAV2 | |
| | $\Delta_f H$(Ion) from appearance potential determination (86TUR/HAV2). See also: 82BUR/HOL, 79HOL/TER. | | | | | | |
| HC≡COCH=$CH_2$ | 9.40 | (273) | (1142) | 56 | 235 | *EST | |
| | IP from 82BUR/HOL. See also: 79HOL/TER. | | | | | | |
|  | 8.883±0.003 | 196.5 | 822.3 | -8.3±0.1 | -34.8±0.4 | 77PED/RYL | 110-00-9 |
| | See also: 82BUR/HOL, 82KOB/KUB, 79HOL/TER, 81GAL/KLA, 81KIM/KAT, 82BIE/ASB, 80TED/VID, 83BOC/ROT, 83ZYK/ERC, 82KLA/SAB. | | | | | | |
|  | (9.3) | (223) | (933) | 8 | 33 | *EST | 32264-87-2 |
| | From appearance potential determination; kinetic energy release = 0.19 eV (82BUR/HOL). IP from 79HOL/TER. | | | | | | |
|  | 9.15±0.05 | (240) | (1004) | 29 | 121 | *EST | 4883-96-9 |
| | See also: 79TER/BUR, 82BUR/HOL, 79HOL/TER. | | | | | | |
|  | (8.78) | (222) | (931) | 20 | 84 | *EST | |
| | IP from 81BOC/HIR. | | | | | | |
|  | (9.6) | (235) | (983) | 14 | 58 | *EST | 36998-21-7 |
| | IP from 79HOL/TER. | | | | | | |
| $C_4H_4O_2^+$ | | | | | | | |
| HC≡CCOOC$H_3$ | (10.3) | (214) | (894) | -24 | -100 | *EST | 922-67-8 |
| | IP is onset of photoelectron band (82BIE/ASB). | | | | | | |
|  | (7.75±0.02) | (152) | (633) | -27±1 | -115±5 | *EST | 290-67-5 |

Table 1. Positive Ion Table - Continued

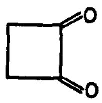
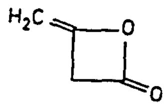
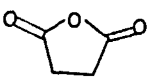
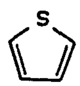
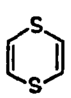
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_4O_2^+$ | | | | | | | |
|  | (9.4) | (178) | (745) | −39 | −163 | *EST | 33689-28-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.6±0.02) | (176) | (736) | −45.5±0.1 | −190.3±0.4 | 77PED/RYL | 674-82-8 |
| | IP from 84OLI/FLE. | | | | | | |
| $C_4H_4O_3^+$ | | | | | | | |
|  | (10.6) | (119) | (498) | −125 | −525 | 77PED/RYL | 108-30-5 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_4H_4O_4^+$ | | | | | | | |
| (E)-$HO_2CCH=CHCO_2H$ | (10.7) | (85) | (352) | −162±0.6 | −680±3 | 77PED/RYL | 110-17-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_4S^+$ | | | | | | | |
|  | 8.87±0.04 | 232 | 971 | 27.5±0.1 | 115.0±0.4 | 81KUD/KUD3 | 110-02-1 |
| | See also: 80TED/VID, 83BOC/ROT, 81GAL/KLA, 82KLA/SAB. | | | | | | |
| $C_4H_4S_2^+$ | | | | | | | |
|  | (7.7) | (233) | (976) | 56±3 | 233±13 | *EST | 290-79-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_5^+$ | | | | | | | |
| $CH_2=CCH=CH_2$ | | (246) | (1029) | | | | 62698-26-4 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
| $CH\equiv CCHCH_3$ | 7.97 | 257 | 1074 | 73 | 305 | 82MCM/GOL | 3315-42-2 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
| $CH_3C\equiv CCH_2$ | 7.95 | 252 | 1056 | 69 | 289 | 82MCM/GOL | 82252-88-8 ~~64235-83-2~~ |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |

**Table 1. Positive Ion Table - Continued**

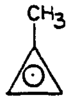
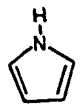
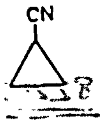
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_5^+$ | | | | | | | |
|  | | (237) | (992) | | | | 60824-24-0 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
| $C_4H_5ClO^+$ | | | | | | | |
| (E)-$CH_3CH=CHCOCl$ | (9.4) | (216) | (906) | -0.2 | -1 | *EST | 625-35-4 |
| | IP is onset of photoelectron band (81MOH/HIR). | | | | | | |
| $C_4H_5F_3O_2^+$ | | | | | | | |
| $CF_3COOC_2H_5$ | (11.0) | (5) | (19) | -249 | -1042 | *EST | 383-63-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_5F_4O_2^+$ | | | | | | | |
| $CF_3C(OH)OCH_2CH_2F$ | | -105 | -441 | | | | |
| | From proton affinity of $CF_3COOCH_2CH_2F$ (RN 1683-88-1). PA = 178.6 kcal/mol, 747. kJ/mol. | | | | | | |
| $C_4H_5F_6O^+$ | | | | | | | |
| $(CF_3)_2C(CH_3)OH_2$ | | -192 | -805 | | | | |
| | From proton affinity of $(CF_3)_2C(CH_3)OH$ (RN 1515-14-6). PA = 167.0 kcal/mol, 699. kJ/mol. | | | | | | |
| $C_4H_5N^+$ | | | | | | | |
| $CH_2=CHCH_2CN$ | 10.20±0.05 | 273 | 1140 | 37±0.5 | 156±2 | 77PED/RYL | 109-75-1 |
| | See also: 84OHN/MAT. | | | | | | |
| $CH_2C(CH_3)CN$ | 10.34 | 269 | 1128 | 31 | 130 | 80WIL/BAE | 126-98-7 |
| (E)-$CH_3CH=CHCN$ | (≤10.23±0.05) | (≤272) | (≤1137) | 36 | 150 | 82CHU/NGU | 627-26-9 |
|  | 8.208±0.005 | 215.2 | 900.2 | 25.9±0.1 | 108.3±0.4 | 80WIL/BAE | 109-97-7 |
| | See also: 81GAL/KLA, 82BIE/ASB, 80TED/VID, 82KLA/SAB. | | | | | | |
|  | 10.25 | 280 | 1172 | 44±0.2 | 183±1 | 82FUC/HAL | 5500-21-0 |

Table 1. Positive Ion Table - Continued

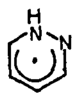
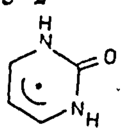
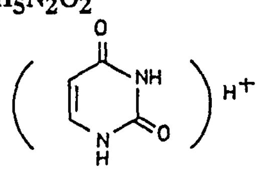
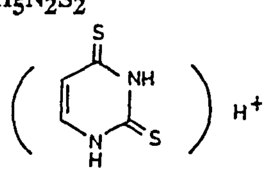
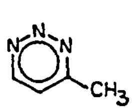
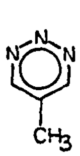
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_5N_2^+$ | | | | | | | |
|  | | 216 | 906 | | | | |
| | From proton affinity of pyridazine (RN 289-80-5). PA = 215.7 kcal/mol, 902 kJ/mol. | | | | | | |
|  | | 202 | 846 | | | | |
| | From proton affinity of pyrimidine (RN 289-95-2). PA = 210.8 kcal/mol, 882. kJ/mol. | | | | | | |
|  | | 203 | 852 | | | | |
| | From proton affinity of pyrazine (RN 290-37-9). PA = 209.0 kcal/mol, 874. kJ/mol. | | | | | | |
| $C_4H_5N_2O^+$ | | | | | | | |
|  | | 146 | 613 | | | | |
| | From proton affinity of 2(1H)-pyrimidinone (RN 557-01-7). PA = ~208 kcal/mol, ~870 kJ/mol. | | | | | | |
| $C_4H_5N_2O_2^+$ | | | | | | | |
|  | | (85) | (357) | | | | |
| | From proton affinity of uracil (RN 66-22-8). PA = ~208 kcal/mol, ~870 kJ/mol. | | | | | | |
| $C_4H_5N_2S_2^+$ | | | | | | | |
|  | | (200) | (836) | | | | |
| | From proton affinity of dithiouracil (RN 2001-93-6). PA = ~217 kcal/mol, ~907 kJ/mol. | | | | | | |
| $C_4H_5N_3^+$ | | | | | | | |
|  | (≤9.7) | (≤313) | (≤1311) | 90 | 375 | *EST | 77202-08-5 |
| | IP from 83GLE/SPA. | | | | | | |
|  | (9.1) | (301) | (1258) | 91 | 380 | *EST | 86402-30-4 |
| | IP is onset of photoelectron band (83GLE/SPA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

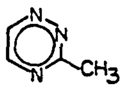
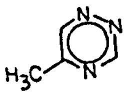
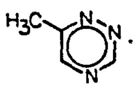
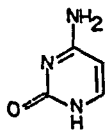
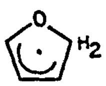
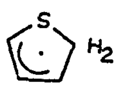
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_5N_3{}^+$ | | | | | | | |
|  | (8.6) | (268) | (1123) | 70 | 293 | *EST | 24108-33-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.31) | (≤285) | (≤1191) | 70 | 293 | *EST | 21134-95-2 |
|  | (≤9.35) | (≤286) | (≤1195) | 70 | 293 | *EST | 21134-96-3 |
| $C_4H_5N_3O^+$ | | | | | | | |
|  | (8.45) | (181) | (756) | −14±2 | −59±10 | 80SAB2 | 71-30-7 |
| $C_4H_5O^+$ | | | | | | | |
|  | | 165 | 691 | | | | |
| | From proton affinity of furan (RN 110-00-9). PA = 192.2 kcal/mol, 804. kJ/mol. | | | | | | |
| $C_4H_5O_2{}^+$ | | | | | | | |
| $CH_3C(OH)=CHCO$ | | 110 | 461 | | | | 43115-54-4 |
| | From appearance potential of 10.24 eV in $CH_3COCH_2COCH_3$. | | | | | | |
| $C_4H_5S^+$ | | | | | | | |
|  | | 197 | 826 | | | | |
| | From proton affinity of thiophene (RN 110-02-1) (86MAU, 84LIA/LIE). PA = 195.8 kcal/mol, 819. kJ/mol. | | | | | | |
| $C_4H_6{}^+$ | | | | | | | |
| $CH_2=C=CHCH_3$ | (9.03) | (247) | (1033) | 38.8±0.1 | 162.3±0.5 | 77PED/RYL | 590-19-2 |

**Table 1. Positive Ion Table - Continued**

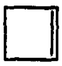
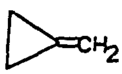
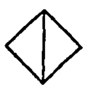
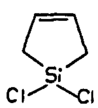
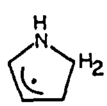
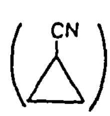
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6^+$ | | | | | | | |
| $CH_3C{\equiv}CCH_3$ | 9.562±0.005 | 255.2 | 1068 | 34.7±0.2 | 145.4±0.8 | 77PED/RYL | 503-17-3 |
|  | 9.43 | 255 | 1067 | 37.5±0.4 | 156.7±1.5 | 77PED/RYL | 822-35-5 |
|  | (9.57)<br>See also: 81KIM/KAT. | (269) | (1124) | 48±0.5 | 201±2 | 77PED/RYL | 6142-73-0 |
|  | 8.700±0.005<br>IP from 83BOM/DAN3. | 253 | 1057 | 51.9±0.2 | 217.2±0.8 | 77PED/RYL | 157-33-5 |
| $C_4H_6Cl_2Si^+$ | | | | | | | |
| $CH_2{=}CHSiCl_2CH{=}CH_2$ | (≤10.8)<br>IP from 81KHV/ZYK. | (≤192) | (≤802) | −57 | −240 | *EST | 1745-72-8 |
|  | ≤9.65<br>See also: 81KHV/ZYK. | (≤143) | (≤598) | −80 | −333 | *EST | 872-46-8 |
| $C_4H_6F_3O_2^+$ | | | | | | | |
| $CF_3C(OH)OC_2H_5$ | From proton affinity of $CF_3COOC_2H_5$ (RN 383-63-1). PA = 184.6 kcal/mol, 772. kJ/mol. | −68 | −284 | | | | |
| $C_4H_6N^+$ | | | | | | | |
| $(CH_3)_2CCN$ | (8.2)<br>IP is onset of photoelectron band. | (229) | (960) | 40.3±2.2 | 168.6±9.2 | 82MCM/GOL | 3225-31-8 |
|  | From proton affinity of pyrrole (RN 109-97-7). PA = 207.6 kcal/mol, 868 kJ/mol. | 184 | 769 | | | | |
|  $H^+$ | From proton affinity of cyclopropylcarbonitrile (RN 5500-21-0). PA = 195.4 kcal/mol, 817.5 kJ/mol. | 214 | 895 | | | | |

**Table 1. Positive Ion Table - Continued**

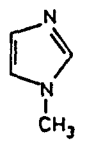
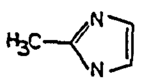
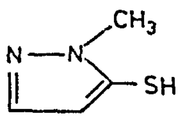
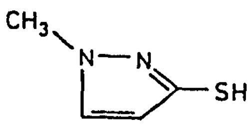
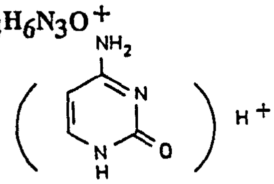
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6NO_2^+$ | | | | | | | |
| $(NCCOOC_2H_5)H$ | | 134 | 562 | | | | |
| | From proton affinity of $NCCOOC_2H_5$ (RN 623-49-4). PA = 179.5 kcal/mol, 751. kJ/mol. | | | | | | |
| $C_4H_6N_2^+$ | | | | | | | |
|  | (≤8.66) | ≤236 | ≤986 | 36 | 150 | *EST | 616-47-7 |
|  | (≤8.50) | ≤225 | ≤942 | 29 | 122 | *EST | 693-98-1 |
| $C_4H_6N_2S^+$ | | | | | | | |
|  | ≤9.1 | (≤265) | (≤1107) | 55 | 229 | *EST | |
| | IP from 83GUI/PFI. | | | | | | |
|  | (≤8.6) | (≤251) | (≤1049) | 52 | 219 | *EST | 79208-64-3 |
| | IP from 83GUI/PFI. | | | | | | |
| $C_4H_6N_3O^+$ | | | | | | | |
|  | | 128 | 535 | | | | |
| | From proton affinity of cytosine (RN 71-30-7). PA = 223.8 kcal/mol, 936. kJ/mol. | | | | | | |
| $C_4H_6O^+$ | | | | | | | |
| $C_2H_5CH=C=O$ | 8.80 | (171) | (714) | −32 | −135 | *EST | 20334-52-5 |
| | IP from 81BOC/HIR. | | | | | | |
| $(CH_3)_2C=C=O$ | (8.45) | (163) | (681) | −32±1 | −134±4 | 80DEM/WUL | 598-26-5 |
| | IP from 81BOC/HIR. | | | | | | |
| (E)-$CH_3CH=CHCHO$ | 9.73±0.01 | 200 | 835 | −24.8±0.4 | −103.6±1.5 | 79VAJ/HAR | 4170-30-3 |
| | See also: 78VAN/OSK. | | | | | | |
| $CH_2=C(CH_3)CHO$ | (9.86) | (199) | (834) | −28 | −117 | 79VAJ/HAR | 78-85-3 |
| | IP from 86HOL/LOS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

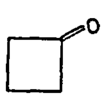
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6O^+$ | | | | | | | |
| $CH_2=CHCOCH_3$ | 9.64 | (189) | (792) | −33 | −138 | 79VAJ/HAR | 78-94-4 |
| | See also: 80TER/HEE, 82MOR/MER. | | | | | | |
| $CH_3C\equiv COCH_3$ | (8.79) | (206) | (860) | 2.9 | 12.1 | *EST | 13169-01-2 |
| | IP from 86HOL/LOS. | | | | | | |
| $CH_2=CHCH=CHOH$(E) | (8.51±0.03) | (175) | (733) | −21±1 | −88±5 | 86TUR/HAV | 70411-98-2 |
| | IP from 86TUR/HAV, 86TUR/HAV3. See also: 80TER/HEE. | | | | | | |
| $CH_2=CHCH=CHOH$(Z) | (8.47±0.03) | (174) | (728) | −21±2 | −89±9 | 86TUR/HEE | 70415-58-6 |
| | IP from 86TUR/HAV, 86TUR/HAV3. See also: 80TER/HEE. | | | | | | |
| $CH_2=C=CHCH_2OH$ | (8.74) | (206) | (861) | 4.3 | 18.0 | *EST | 18913-31-0 |
| | IP from 80TER/HEE. | | | | | | |
| $HC\equiv CCH_2CH_2OH$ | (9.66) | (226) | (945) | 3.2 | 13.4 | *EST | 927-74-2 |
| | IP from 86HOL/LOS. | | | | | | |
| $CH_3C\equiv CCH_2OH$ | (9.78) | (227) | (948) | 1.1 | 4.6 | *EST | 764-01-2 |
| | IP from 86HOL/LOS. | | | | | | |
| $HC\equiv CCH(CH_3)OH$ | (10.15) | (236) | (987) | 2 | 8 | *EST | 2028-63-9 |
| $CH_2=CHC(OH)=CH_2$ | 8.68±0.03 | 182 | 761 | −18 | −76 | 84TUR | 59120-04-6 |
| | $\Delta_f H$(Ion) from appearance potential determination(80TER/HEE). IP from 84TUR. | | | | | | |
| $CH_2=C=CHOCH_3$ | (8.64) | (207) | (866) | 7.7 | 32.2 | *EST | 13169-00-1 |
| | IP from 86HOL/LOS, onset of photoelectron band (86KAM/BOS). | | | | | | |
| $HC\equiv CCH_2OCH_3$ | (9.78) | (240) | (1005) | 14.7 | 61.5 | *EST | 627-41-8 |
| | IP from 86HOL/LOS. | | | | | | |
| $CH_2=CHOCH=CH_2$ | (8.7) | (197) | (824) | −3 | −13 | *EST | 109-93-3 |
| | $\Delta_f H$(Ion) from appearance potential determination (81HOL/BUR). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
|  | 9.14±0.02 | 195 | 816 | −16±1 | −66±3 | 81ALL/GLA | 1708-29-8 |
|  | 9.354 | (194) | (814) | −21 | −89 | *EST | 1191-95-3 |

Table 1. Positive Ion Table - Continued

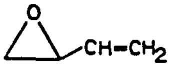
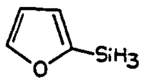
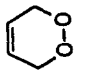
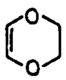
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6O^+$ | | | | | | | |
|  | 9.52 | (222) | (928) | 2 | 10 | *EST | 930-22-3 |
| | IP from 86HOL/LOS. | | | | | | |
| $C_4H_6OSi^+$ | | | | | | | |
|  | (<8.0) | (<183) | (<765) | −2 | −7 | *EST | 73726-79-1 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
| $C_4H_6O_2^+$ | | | | | | | |
| (Z)-$CH_3CH=CHCOOH$ | (10.08) | (150) | (626) | −83 | −346 | *EST | 503-64-0 |
| (E)-$CH_3CH=CHCOOH$ | (9.9) | (145) | (605) | −84 | −350 | *EST | 107-93-7 |
| | IP is onset of photoelectron band (78VAN/OSK, 81MOH/HIR). | | | | | | |
| $CH_2=CHCH_2COOH$ | (9.75) | (141) | (589) | −84 | −352 | *EST | 625-38-7 |
| | IP is onset of photoelectron band (81MOH/HIR). | | | | | | |
| $CH_2=C(CH_3)COOH$ | (10.15) | (146) | (610) | −88 | −369 | 84BOU/HOP | ~~3724-65-0~~ 79-41-4 |
| $CH_3CO_2CH=CH_2$ | 9.19 | 137 | 572 | −75.3±0.1 | −314.9±0.5 | 77PED/RYL | 108-05-4 |
| | "Doubtful" IP value reported in K. Watanabe, T. Nakayama, and J. R. Mottl, J. Quant. Spectrosc. Radiat. Transfer 2, 369 (1962) is in good agreement with onset of photoelectron band (78VAN/OSK). See also: 82LEV/LIA. | | | | | | |
| $CH_2=CHCOOCH_3$ | (9.9) | (154) | (643) | −75 | −312 | 80VIL/PER | 96-33-3 |
| | IP is onset of photoelectron band (78VAN/OSK). See also: 82LEV/LIA. | | | | | | |
| $(CH_3CO)_2$ | 9.24±0.04 | 135 | 564 | −78.2±0.3 | −327.1±1.1 | 77PED/RYL | 431-03-8 |
| | See also: 80VON/BIE, 81KIM/KAT. | | | | | | |
|  | (9.5) | (224) | (938) | 5 | 21 | *EST | 18715-02-1 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
|  | (8.07±0.02) | (131) | (549) | −55 | −230 | *EST | 543-75-9 |

Table 1. Positive Ion Table - Continued

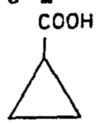
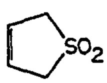
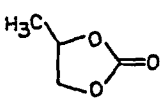
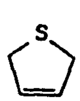
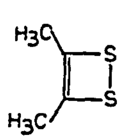
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6O_2^+$ | | | | | | | |
|  | 10.64 | (167) | (699) | −78 | −328 | *EST | 1759-53-1 |
| $C_4H_6O_2S^+$ | | | | | | | |
| $(CH_2=CH)_2SO_2$ | 10.59±0.03 | 208 | 871 | −36±0.9 | −151±4 | 77PED/RYL | 77-77-0 |
|  | (10.0) | (169) | (709) | −61±0.7 | −256±3 | 77PED/RYL | 77-79-2 |
| | IP is onset of photoelectron band (82LEV/LIA, 84AIT/GOS). | | | | | | |
| $C_4H_6O_3^+$ | | | | | | | |
| $(CH_3CO)_2O$ | (10.0) | (95) | (398) | −135.6±0.3 | −567.3±1.3 | 77PED/RYL | 108-24-7 |
| | IP is onset of photoelectron band (81BOC/HIR). | | | | | | |
|  | (10.52) | (103) | (432) | −139±0.5 | −583±2 | 77PED/RYL | 108-32-7 |
| $C_4H_6O_4^+$ | | | | | | | |
| $CH_3OCOCOOCH_3$ | (10.0) | (69) | (289) | −162 | −676 | 76ANT/CAR | 553-90-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_6S^+$ | | | | | | | |
| $(CH_2=CH)_2S$ | (8.25±0.01) | (232) | (970) | 42±2 | 174±9 | *EST | 627-51-0 |
|  | (8.4) | (215) | (897) | 20.8±0.3 | 87.0±1.1 | 81KUD/KUD3 | 1708-32-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_6S_2^+$ | | | | | | | |
| $CH_3SC{\equiv}CSCH_3$ | (7.8) | (238) | (995) | 58 | 242 | *EST | 59507-56-1 |
| | IP is onset of photoelectron band (81BOC/RIE). | | | | | | |
|  | (8.0) | (231) | (966) | 46 | 194 | *EST | 74378-81-7 |
| | IP is onset of photoelectron band (83SCH/SCH). | | | | | | |

**Table 1. Positive Ion Table - Continued**

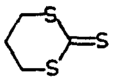
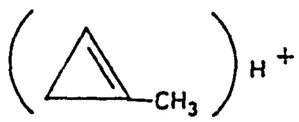
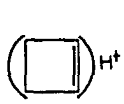
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_6S_3^+$ | | | | | | | |
|  | (8.2) | (208) | (869) | 19±0.7 | 78±3 | 77PED/RYL | 1748-15-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_7^+$ | | | | | | | |
| $CH_3CHCH=CH_2$ | (7.49±0.02) | 202 | 845 | 31.7 | 132.6 | 87LIA/AUS | 65338-31-0 |
| | | *206* | *863* | *35.7* | *149.4* | | |
| | IP from 84SCH/HOU2. Value of $\Delta_fH$(Ion) from proton affinity of 1,3-butadiene (RN 106-99-0). PA = 190 kcal/mol, 795 kJ/mol (87LIA/AUS). See also: 86TRA. | | | | | | |
| $CH_2C(CH_3)=CH_2$ | 7.90±0.02 | (211) | (883) | 29 | 121 | 87LIA/AUS | 15157-95-6 |
| | IP from 84SCH/HOU2. | | | | | | |
|  | | (218) | (912) | | | | 65338-31-0 |
| | From proton affinity of 1-methylcyclopropene (RN 3100-04-7). PA = (206) kcal/mol, (862) kJ/mol. | | | | | | |
| $CH_3CCHCH_3$ | | (213) | (893) | | | | |
| | | *(217)* | *(908)* | | | | |
| | From proton affinity of 2-butyne. (RN 503-17-3). PA = 188 kcal/mol, 787 kJ/mol (87LIA/AUS). | | | | | | |
| $CH_2=CHCH_2CH_2$ | 8.04 | (231) | (968) | 46 | 191 | 84SCH/HOU2 | 2154-62-3 |
| | IP from 84SCH/HOU2. | | | | | | |
|  | 7.54±0.02 | (225) | (941) | 51.2 | 214.2 | 82MCM/GOL | 4548-06-5 |
| | IP from 84SCH/HOU2. Value of $\Delta_fH$(Ion) formed by protonation of cyclobutene (RN 822-35-5) = 212 kcal/mol, 888 kJ/mol. | | | | | | |
| $C_4H_7F_3O^+$ | | | | | | | |
| $CF_3CH_2OC_2H_5$ | 10.27 | (21) | (86) | −216 | −905 | *EST | 461-24-5 |
| | IP from 83MOL/PIK. | | | | | | |
| $C_4H_7IO_2^+$ | | | | | | | |
| $CH_3CHICOOCH_3$ | (9.1) | (122) | (510) | −88 | −368 | *EST | 56905-18-1 |
| | IP from 83BUR/HOL3. | | | | | | |
| $C_4H_7N^+$ | | | | | | | |
| n-$C_3H_7CN$ | (11.2) | (266) | (1112) | 7 | 31 | 82CHU/NGU | 109-74-0 |
| | IP is onset of photoelectron band (84OHN/MAT, 81KIM/KAT). See also: 82CHE/LAP. | | | | | | |
| n-$C_3H_7NC$ | (11.8) | (302) | (1262) | 29.5 | 123.4 | *EST | 627-36-1 |
| | IP from 82CHE/LAP. | | | | | | |

**Table 1. Positive Ion Table - Continued**

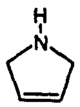
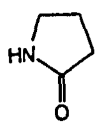
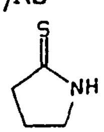
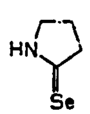
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_7N^+$ | | | | | | | |
| iso-$C_3H_7CN$ | (11.3) | (266) | (1115) | 5.8±0.2 | 24.5±0.7 | 77PED/RYL | 78-82-0 |
| | IP is onset of photoelectron band (84OHN/MAT, 81KIM/KAT). | | | | | | |
|  | (8.0) | (210) | (882) | 26±0.7 | 110±3 | *EST | 109-96-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.2) | (251) | (1048) | 61 | 257 | *EST | |
| | IP from 81MUL/PRE. | | | | | | |
| $C_4H_7NO^+$ | | | | | | | |
|  | (9.2) | (161) | (675) | −51 | −213 | 77PED/RYL | 616-45-5 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_4H_7NO_2^+$ | | | | | | | |
| $CH_2=CHCH_2CH_2ONO$ | (9.7) | (224) | (939) | 0.7 | 3 | *EST | 67428-02-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_7NO_3^+$ | | | | | | | |
| $CH_3CONHCH_2COOH$ | (9.4) | (72) | (303) | −144 | −604 | *EST | 543-24-8 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $C_4H_7NS^+$ | | | | | | | |
|  | (8.14) | (192) | (801) | 4 | 16 | *EST | 2295-35-4 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_4H_7NSe^+$ | | | | | | | |
|  | 7.6 | (196) | (819) | 21 | 86 | *EST | 23164-74-1 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |

**Table 1. Positive Ion Table - Continued**

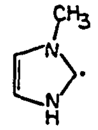
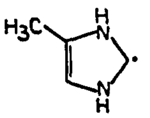
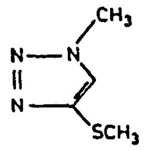
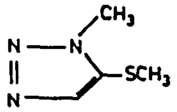
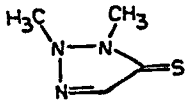
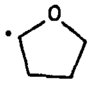
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_7N_2^+$ | | | | | | | |
|  | | (173) | (723) | | | | |
| | From proton affinity of 1-methylimidazole (RN 616-47-7). PA = 228.9 kcal/mol, 958. kJ/mol. | | | | | | |
|  | | (170) | (713) | | | | |
| | From proton affinity of 4-methylimidazole (RN 822-36-6). PA = 224.4 kcal/mol, 939. kJ/mol. | | | | | | |
| $C_4H_7N_3S^+$ | | | | | | | |
|  | ≤8.33 | (≤250) | (≤1047) | 58 | 243 | *EST | 36811-14-0 |
| | IP from 83GUI/PFI. | | | | | | |
|  | ≤8.65 | (≤258) | (≤1077) | 58 | 243 | *EST | 35262-23-8 |
| | IP from 83GUI/PFI. | | | | | | |
|  | (7.4) | (259) | (1084) | 88 | 370 | *EST | 64808-28-2 |
| | IP from 83GUI/PFI. | | | | | | |
| $C_4H_7O^+$ | | | | | | | |
| (E)-$CH_3CHCHCHOH$ | | 141 | 591 | | | | |
| | From proton affinity of (E)-$CH_3CH=CHCHO$ (RN 4170-30-3). PA = 199.7 kcal/mol, 835.5 kJ/mol. | | | | | | |
| $CH_2C(CH_3)CHOH$ | | 142 | 596 | | | | |
| | From proton affinity of $CH_2=C(CH_3)CHO$ (RN 78-85-3). PA = 195.2 kcal/mol, 817. kJ/mol. | | | | | | |
| $CH_2CHC(OH)CH_3$ | | 133 | 554 | | | | |
| | From proton affinity of $CH_2=CHCOCH_3$ (RN 78-94-4). PA = 200.2 kcal/mol, 838. kJ/mol. | | | | | | |
|  | | 141 | 589 | | | | |
| | From proton affinity of 2,3-dihydrofuran (RN 1191-99-7) (86BOU/DJA). PA = 206.8 kcal/mol, 865 kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

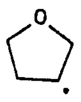
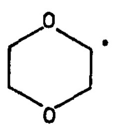
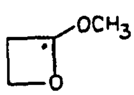
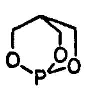
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_7O^+$ | | | | | | | |
|  | | 152 | 634 | | | | |
| | From proton affinity of 2,5-dihydrofuran (RN 1708-29-8) (86BOU/DJA). PA = 198.4 kcal/mol, 830. kJ/mol. | | | | | | |
| $C_4H_7O_2^+$ | | | | | | | |
| (Z)-$CH_3CH=CHC(OH)_2$ | | 78 | 327 | | | | |
| | From proton affinity of (Z)-$CH_3CH=CHCOOH$ (RN 503-64-0)(84BOU/HOP). PA = 199.7 kcal/mol, 836. kJ/mol. | | | | | | |
| $CH_3C(CH_2)C(OH)_2$ | | 81 | 338 | | | | |
| | From proton affinity of $CH_3C(=CH_2)COOH$ (RN 3724-65-0)(84BOU/HOP). PA = 196.8 kcal/mol, 823. kJ/mol. | | | | | | |
| $CH_2=CHC(OH)OCH_3$ | | 92 | 386 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83BUR/HOL3). | | | | | | |
| $CH_3CO_2CHCH_3$ | | 94 | 392 | | | | |
| | From proton affinity of $CH_3CO_2CH=CH_2$ (RN 108-05-4) (86MAU). PA = 196.7 kcal/mol, 823. kJ/mol. | | | | | | |
| $CH_3CHCOOCH_3$ | | 115 | 480 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83BUR/HOL3). | | | | | | |
| $CH_3COC(OH)CH_3$ | | 93 | 388 | | | | |
| | From proton affinity of $(CH_3CO)_2$ (RN 431-03-8). PA = 194.8 kcal/mol, 815. kJ/mol. | | | | | | |
|  | | 126 | 529 | | | | |
| | From proton affinity of dihydro-1,4-dioxin (RN 543-75-9) (86BOU/HAN). PA = 198.4 kcal/mol, 830. kJ/mol. | | | | | | |
|  | | 108 | 450 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (83BUR/HOL3). | | | | | | |
| $C_4H_7O_3P^+$ | | | | | | | |
|  | (9.42±0.1) | (89) | (371) | −129 | −538 | *EST | 280-45-5 |

Table 1. Positive Ion Table - Continued

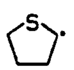
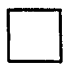
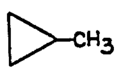
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_7S^+$ | | | | | | | |
|  | | 237 | 992 | | | | 39925-70-7 |
| | | *214* | *895* | | | | |
| | $\Delta_f H$(Ion) from appearance potential in tetrahydrothiophene (83BUT/BAE2). | | | | | | |
| $C_4H_8^+$ | | | | | | | |
| $1\text{-}C_4H_8$ | 9.58±0.02 | 221 | 924 | −0.1±0.1 | −0.4±0.5 | 77PED/RYL | 106-98-9 |
| | See also: 83HOL/LOS, 86TRA. | | | | | | |
| $(Z)\text{-}2\text{-}C_4H_8$ | 9.108±0.008 | 208 | 871 | −1.9±0.1 | −7.8±0.5 | 77PED/RYL | 590-18-1 |
| | IP from 78LIA/AUS. See also: 81KIM/KAT, 86TRA. | | | | | | |
| $(E)\text{-}2\text{-}C_4H_8$ | 9.100±0.008 | 207 | 866 | −2.9±0.2 | −12.2±0.5 | 77PED/RYL | 624-64-6 |
| | IP from 78LIA/AUS. See also: 81KIM/KAT, 86TRA. | | | | | | |
| $iso\text{-}C_4H_8$ | 9.239±0.003 | 209 | 874 | −4.0±0.1 | −16.9±0.6 | 77PED/RYL | 115-11-7 |
| | See also: 83HOL/LOS, 81KIM/KAT, 86TRA. | | | | | | |
|  | (9.92±0.05) | (235) | (985) | 6.8±0.2 | 28.4±0.5 | 77PED/RYL | 287-23-0 |
|  | (9.46) | (224) | (938) | 5.5 | 23 | 77PED/RYL | 594-11-6 |
| $C_4H_8Br_2^+$ | | | | | | | |
| $CH_3CHBrCHBrCH_3$-(R,R(±)) | (≤10.12) | (≤206) | (≤860) | −28 | −116 | *EST | 598-71-0 |
| $CH_3CHBrCHBrCH_3$-(R,S) | (≤10.16) | (≤207) | (≤864) | −28 | −116 | *EST | 5780-13-2 |
| $BrCH_2CH_2CH_2CH_2Br$ | (10.15) | (210) | (880) | −24 | −99 | 77PED/RYL | 110-52-1 |
| | IP from 77STA/WIE. | | | | | | |
| $C_4H_8F_3N^+$ | | | | | | | |
| $CF_3CH_2CH_2CH_2NH_2$ | (9.1) | (29) | (123) | −180 | −755 | *EST | 819-46-5 |
| | IP from 79AUE/BOW. | | | | | | |
| $(CH_3)_2NCH_2CF_3$ | (8.42) | (27) | (112) | −167 | −700 | 81LOG/TAK | 819-06-7 |
| | IP from 81LOG/TAK. See also: 79AUE/BOW. | | | | | | |

Table 1. Positive Ion Table - Continued

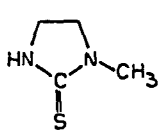
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8F_3O^+$ | | | | | | | |
| $C_2H_5OHCH_2CF_3$ | | -37 | -154 | | | | |
| | From proton affinity of $C_2H_5OCH_2CF_3$ (RN 461-24-5). PA = 186.4 kcal/mol, 780. kJ/mol. | | | | | | |
| $C_4H_8N^+$ | | | | | | | |
| n-$C_3H_7CNH$ | | 179 | 751 | | | | |
| | From proton affinity of n-$C_3H_7CN$ (RN 109-74-0). PA = 193.7 kcal/mol, 810. kJ/mol. | | | | | | |
| i-$C_3H_7CNH$ | | 177 | 740 | | | | |
| | From proton affinity of i-$C_3H_7CN$ (RN 78-82-0). PA = 194.3 kcal/mol, 813. kJ/mol. | | | | | | |
| i-$C_3H_7NCH$ | | 186 | 778 | | | | |
| | From proton affinity of i-$C_3H_7NC$ (RN 598-45-8) (86MAU/KAR). PA = 206. kcal/mol, 862. kJ/mol. | | | | | | |
| $C_4H_8NO_4^+$ | | | | | | | |
| $HOOCCH_2CH(NH_3)COOH$ | | -44 | -184 | | | | |
| | From proton affinity of L-aspartic acid (RN 617-45-8). PA = 216.7 kcal/mol, 907. kJ/mol. | | | | | | |
| $C_4H_8N_2^+$ | | | | | | | |
| $(CH_3)_2NCH_2CN$ | (8.72±0.05) | (228) | (953) | 27 | 112 | *EST | 926-64-7 |
| | See also: 83MOL/PIK2. | | | | | | |
| $C_4H_8N_2OS^+$ | | | | | | | |
| $(CH_3)_2NCSOCNH_2$ | (≤8.21) | (≤171) | (≤714) | -19 | -78 | *EST | 41168-96-1 |
| | IP from 81HEN/ISA. | | | | | | |
| $(CH_3)_2NCOCSNH_2$ | ≤8.37 | (≤168) | (≤704) | -25 | -104 | *EST | 18138-14-2 |
| | IP from 81HEN/ISA. | | | | | | |
| $C_4H_8N_2O_2^+$ | | | | | | | |
| $CH_3NHCOCONHCH_3$ | (9.33) | (121) | (504) | -95 | -396 | *EST | 615-35-0 |
| $C_4H_8N_2S^+$ | | | | | | | |
|  | (7.7) | (201) | (842) | 24 | 99 | *EST | 13431-10-2 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| $C_4H_8N_2S_2^+$ | | | | | | | |
| $CH_3NHCSCSNHCH_3$ | ≤8.23 | (≤163) | (≤684) | -26 | -110 | *EST | 120-79-6 |
| | IP from 81HEN/ISA. | | | | | | |
| $C_4H_8N_4^+$ | | | | | | | |
| $NCN=C(NHCH_3)_2$ | (8.5) | (234) | (977) | 38 | 157 | *EST | 31857-31-5 |
| | IP is onset of photoelectron band (80KLA/BUT). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8O^+$ | | | | | | | |
| n-$C_3H_7CHO$ | 9.84±0.02 | 177 | 742 | −49.6±0.4 | −207.5±1.5 | 77PED/RYL | 123-72-8 |
| | See also: 81ELS/ALL, 83MCA/HUD, 81KIM/KAT, 86TRA/MCA. | | | | | | |
| iso-$C_3H_7CHO$ | 9.705±0.005 | 172 | 721 | −51.5±0.1 | −215.6±0.6 | 77PED/RYL | 78-84-2 |
| | See also: 83MCA/HUD, 86TRA/MCA. | | | | | | |
| $C_2H_5COCH_3$ | 9.51±0.04 | 162 | 677 | −57.5±0.1 | −240.8±0.6 | 77PED/RYL | 78-93-3 |
| | See also: 72POT/SOR, 85TRA, 81KIM/KAT. | | | | | | |
| $CH_3CH_2CH=CHOH$ | (8.34±0.05) | (150) | (628) | −42 | −177 | *EST | 56640-69-8 |
| | $\Delta_f H$(Ion) from appearance potential determinations. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral) (83HOL/LOS). See also: 83MCA/HUD. | | | | | | |
| (E)-$CH_3CH=CHCH_2OH$ | (9.13±0.02) | (173) | (726) | −37 | −155 | *EST | |
| | IP from 86TRA/MCA. See also: 83MCA/HUD. | | | | | | |
| $CH_2=CHCH_2CH_2OH$ | (9.56±0.05) | (184) | (770) | −36 | −152 | *EST | 627-27-0 |
| | IP from 83HOL/LOS. | | | | | | |
| $CH_3CHCH_2CHOH$ | | (165) | (690) | | | | |
| | Based on appearance energy measurements of metastable processes (83MCA/HUD). | | | | | | |
| $CH_2=C(CH_3)CH_2OH$ | (9.26±0.02) | (176) | (734) | −38 | −159 | *EST | 513-42-8 |
| | IP is average of values from 83HOL/LOS and 86TRA/MCA. | | | | | | |
| $(CH_3)_2C=CHOH$ | (8.27±0.05) | (145) | (607) | −46 | −192 | *EST | 56640-70-1 |
| | $\Delta_f H$(Ion) from appearance potential determinations. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral)(83HOL/LOS). | | | | | | |
| $CH_2CH(CH_3)CHOH$ | | (154) | (644) | | | | |
| | Based on appearance energy measurements of metastable processes (83MCA/HUD). | | | | | | |
| $CH_3CH_2C(OH)=CH_2$ | (8.36±0.05) | (150) | (628) | −43 | −179 | *EST | 61923-55-5 |
| | $\Delta_f H$(Ion) from appearance potential determinations. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral)(83HOL/LOS). See also:83MCA/HUD. | | | | | | |
| $CH_3C(OH)=CHCH_3$ | | 139 | 581 | | | | 21411-38-1 |
| | $\Delta_f H$(Ion) from appearance potential determinations. See also: 83MCA/HUD. | | | | | | |
| $CH_2=CHCH(OH)CH_3$ | 9.50±0.05 | (180) | (756) | −38 | −161 | *EST | 598-32-3 |
| | IP from 83MCA/HUD, 83HOL/LOS, 86TRA/MCA. | | | | | | |
| $CH_3C(OH)CH_2CH_2$ | | (147) | (613) | | | | |
| | Based on appearance energy measurements of metastable processes (83MCA/HUD). | | | | | | |
| $CH_2=CHCH_2OCH_3$ | (9.56) | (195) | (817) | −25 | −105 | *EST | 627-40-7 |
| | IP from 86HOL/LOS. | | | | | | |

Table 1. Positive Ion Table - Continued

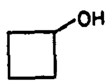
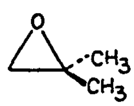
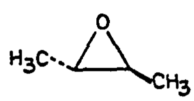
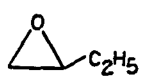
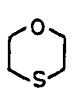
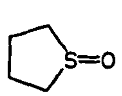
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8O^+$ | | | | | | | |
| $CH_2=CHOC_2H_5$ | (8.8) | (169) | (708) | −34 | −141 | 77PED/RYL | 109-92-2 |
| | IP from 86HOL/LOS. See also: 82MOR/MER. | | | | | | |
| $CH_2=C(CH_3)OCH_3$ | (8.64) | (164) | (688) | −35 | −146 | *EST | 116-11-0 |
| | IP from 82HOL/LOS2. | | | | | | |
|  | 9.41±0.02 | 173 | 724 | −44.0±0.2 | −184.2±0.7 | 77PED/RYL | 109-99-9 |
| | See also: 81KIM/KAT. | | | | | | |
|  | 9.25 | (181) | (756) | −32 | −136 | *EST | 2919-23-5 |
| | IP from 83MCA/HUD, 86TRA/MCA. | | | | | | |
|  | (10.00) | (198) | (830) | −32 | −135 | *EST | 558-30-5 |
|  | (9.98) | (199) | (832) | −31 | −131 | *EST | 21490-63-1 |
|  | (10.15) | (206) | (864) | −28 | −115 | *EST | 106-88-7 |
| $C_4H_8OS^+$ | | | | | | | |
| $CH_3COSC_2H_5$ | (9.2) | (158) | (660) | −54±0.2 | −228±1 | 66WAD | 625-60-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.67) | (164) | (688) | −36 | −149 | *EST | 15980-15-1 |
|  | 8.5 | (161) | (674) | −35 | −146 | *EST | 1600-44-8 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

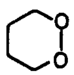
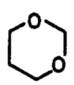
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8O_2{}^+$ | | | | | | | |
| n-$C_3H_7COOH$ | 10.17±0.05 | 121 | 507 | −113±1 | −473±4 | 82BUT/FRA | 107-92-6 |
| | | *127* | *533* | *−107* | *−447* | | |
| | See also: 82BUT/FRA, 81HOL/FIN. | | | | | | |
| iso-$C_3H_7COOH$ | 10.33±0.03 | (123) | (517) | −115 | −480 | *EST | 79-31-2 |
| $HCOOCH_2CH_2CH_3$ | 10.52±0.02 | 132 | 553 | −110 | −462 | 77PED/RYL | 110-74-7 |
| $HCOOCH(CH_3)_2$ | 10.44±0.05 | (144) | (602) | −97 | −405 | *EST | 625-55-8 |
| $CH_3COOC_2H_5$ | 10.01±0.05 | 125 | 523 | −106.1±0.1 | −443.9±0.4 | 77PED/RYL | 141-78-6 |
| | | *131* | *548* | *−99.9±0.1* | *−418.0±0.4* | | |
| | IP from 82FRA/FRA2. | | | | | | |
| $C_2H_5COOCH_3$ | 10.15±0.03 | (131) | (547) | −103 | −432 | *EST | 554-12-1 |
| $CH_3CH_2CH=C(OH)_2$ | | 97 | 405 | | | | 12542-32-4 |
| | From appearance potential of 10.14 eV in $(C_2H_5)_2CHCOOH$ (RN 88-09-5). | | | | | | |
| $(CH_3)_2C=C(OH)_2$ | | 92 | 387 | | | | |
| | From appearance potentials of 10.02 eV in $C_2H_5C(CH_3)_2COOH$ (RN 595-37-9) and 9.96 eV in n-$C_3H_7C(CH_3)_2COOH$ (RN 1185-39-3). | | | | | | |
| $CH_2=C(OH)OC_2H_5$ | | 104 | 433 | | | | |
| | From appearance potential of 10.06 eV in n-$C_3H_7COOC_2H_5$ (RN 105-54-4) and 9.96 eV in n-$C_5H_{11}COOC_2H_5$ (RN 123-66-0). | | | | | | |
| $CH_3CH=C(OH)OCH_3$ | | 99 | 413 | | | | |
| | From appearance potential of 9.81 eV in sec-$C_4H_9COOCH_3$ (RN 868-57-5). | | | | | | |
| $CH_3COCH_2OCH_3$ | ≤9.66 | (≤143) | (≤598) | −80 | −334 | *EST | 5878-19-3 |
| | IP from 84OLI/GUE. | | | | | | |
|  | (≤10.0) | (≤195) | (≤816) | −36 | −149 | *EST | 5703-46-8 |
|  | 9.8 | 145 | 608 | −81±0.2 | −338±1 | 82BYS/MAN | 505-22-6 |
| | See also: 84ASF/ZYK. | | | | | | |

**Table 1. Positive Ion Table - Continued**

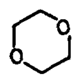
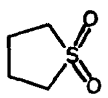
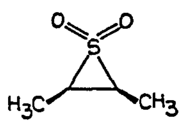
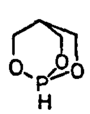
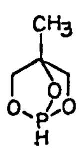
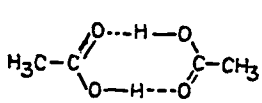
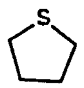
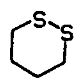
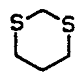
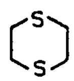
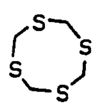
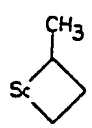
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8O_2^+$ | | | | | | | |
|  | 9.19±0.01 | 136 | 571 | −75.5±0.2 | −316.0±0.7 | 82BYS/MAN | 123-91-1 |
| | | *144* | *602* | *−68.2±0.2* | *−285.3±0.8* | | |
| | IP from 82FRA/FRA. See also: 81KIM/KAT, 73GOL/KOR, 82BIE/ASB. | | | | | | |
| $C_4H_8O_2S^+$ | | | | | | | |
|  | (9.8) | (138) | (577) | −88 | −369 | *EST | 126-33-0 |
| | IP is onset of photoelectron band. See also: 84AIT/GOS. | | | | | | |
|  | (9.5) | (142) | (593) | −77 | −324 | *EST | 54697-52-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_8O_3^+$ | | | | | | | |
| $(CH_3)_2COHCOOH$ | ≤10.9 | (≤96) | (≤404) | −155 | −648 | *EST | 594-61-6 |
| | IP from 73GOL/KOR. | | | | | | |
| $C_4H_8O_3P^+$ | | | | | | | |
|  | | 30 | 126 | | | | |
| | From proton affinity of 2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane (RN 280-45-5). PA = 207.1 kcal/mol, 866.5 kJ/mol. | | | | | | |
|  | | 13 | 55 | | | | |
| | From proton affinity of 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.1]heptane (RN 61580-09-4). PA = 198.1 kcal/mol, 829. kJ/mol. | | | | | | |
| $C_4H_8O_4^+$ | | | | | | | |
|  | (≤10.6) | (≤22) | (≤94) | −222 | −929 | *EST | 6993-75-5 |
| $C_4H_8S^+$ | | | | | | | |
| $CH_3SCH_2CH=CH_2$ | 8.6 | (210) | (880) | 12±2 | 50±9 | *EST | 10152-76-8 |
| $CH_2=CHSC_2H_5$ | (8.21±0.01) | (201) | (840) | 11±1 | 48±6 | *EST | 627-50-9 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_8S^+$ | | | | | | | |
|  | 8.47 | 187.1 | 782.8 | −8.2±0.2 | −34.1±0.9 | 81KUD/KUD3 | 110-01-0 |
| | | *193.8* | *810.8* | *−1.5* | *−6.2* | | |
| | Results from 83BUT/BAE2. | | | | | | |
| $C_4H_8S_2^+$ | | | | | | | |
| (Z)-$CH_3SCH=CHSCH_3$ | (≤7.80) | (≤203) | (≤849) | 23 | 96 | *EST | 764-44-3 |
| (E)-$CH_3SCH=CHSCH_3$ | (≤7.85) | (≤204) | (≤853) | 23 | 96 | *EST | 764-45-4 |
| $CH_2=C(SCH_3)_2$ | (≤8.2) | (≤212) | (≤887) | 23 | 96 | *EST | 51102-74-0 |
|  | 8.1 | (178) | (746) | −9 | −36 | *EST | 505-20-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.2 | (188) | (786) | −1 | −5 | *EST | 505-23-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.4) | (193) | (805) | −1 | −5 | *EST | 505-29-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_8S_4^+$ | | | | | | | |
|  | (7.8) | (197) | (825) | 17 | 72 | *EST | 2373-00-4 |
| | IP is onset of photoelectron band (81BOC/SCH). | | | | | | |
| $C_4H_8Sc^+$ | | | | | | | |
| ((E)-$CH_3CH=CHCH_3$)Sc | | (191) | (799) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
|  | | (179) | (749) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |

✓

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_4H_9^+$ | | | | | | | |
| n-$C_4H_9$ | 8.02 | (203) | (849) | 18 | 74 | *EST | 2492-36-6 |
| | IP from 84SCH/HOU. Error limits +0.04-0.1. $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | | | | | | |
| sec-$C_4H_9$ | 7.25±0.02 | 183 | 766 | 17.0±0.4 | 71.0±1.6 | 85TSA | 2348-55-2 ~~4630-45-9~~ |
| | IP from 84SCH/HOU. Heat of formation of ion at 298 K from appearance potential measurements (81TRA). $\Delta_f H$(Neutral) based on D[C-H] = 99 kcal/mol. $\Delta_f H$(Ion) - IP leads to $\Delta_f H$(Neutral) = 16 kcal/mol, 66 kJ/mol. | | | | | | |
| iso-$C_4H_9$ | 7.93 | (199) | (832) | 16 | 70 | 81TSA | 1630-45-9 ~~65114-21-8~~ |
| | IP from 84SCH/HOU. Error limits +0.03-0.1. $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | | | | | | |
| tert-$C_4H_9$ | 6.70±0.03 | 165.8 | 693.7 | 11.0±0.6 | 46.2±2.5 | 85TSA | 1605-73-8 |
| | Same value is obtained for heat of formation of ion from appearance potential measurements (81TRA/MCL). Neutral $\Delta_f H$ based on D[C-H] = 95.5 kcal/mol. $\Delta_f H$(Ion) - IP leads to $\Delta_f H$(Neutral) = 11.3 kcal/mol, 47.2 kJ/mol. | | | | | | |
| $C_4H_9Br^+$ | | | | | | | |
| n-$C_4H_9Br$ | 10.13 | 208 | 870 | −25.6±0.3 | −107.1±1.3 | 77PED/RYL | 109-65-9 |
| | See: 81KIM/KAT. | | | | | | |
| sec-$C_4H_9Br$ | 9.98±0.01 | 201 | 842 | −28.9±0.1 | −120.9±0.4 | 77PED/RYL | 78-76-2 |
| | See also: 81TRA, 81KIM/KAT. | | | | | | |
| iso-$C_4H_9Br$ | 10.09±0.02 | (205) | (858) | −27 | −115 | *EST | 78-77-3 |
| | See: 81KIM/KAT. | | | | | | |
| tert-$C_4H_9Br$ | 9.92±0.03 | 197 | 824 | −32 | −133 | 79WIB/SQU | 507-19-7 |
| | See: 81KIM/KAT. | | | | | | |
| $C_4H_9Cl^+$ | | | | | | | |
| n-$C_4H_9Cl$ | 10.67±0.03 | 209 | 874 | −36.9±0.2 | −154.5±1 | 78SEL/STR | 109-69-3 |
| | See also: 81KIM/KAT. | | | | | | |
| sec-$C_4H_9Cl$ | 10.53 | 204 | 855 | −38±2 | −161±8 | 77PED/RYL | 78-86-4 |
| | See also: 81KIM/KAT. | | | | | | |
| iso-$C_4H_9Cl$ | 10.66±0.03 | 208 | 869 | −38±2 | −159±8 | 77PED/RYL | 513-36-0 |
| | See also: 81KIM/KAT. | | | | | | |
| tert-$C_4H_9Cl$ | 10.61±0.03 | 201 | 842 | −43.5±0.3 | −182.1±1.2 | 77PED/RYL | 507-20-0 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_4H_9ClHg^+$ | | | | | | | |
| n-$C_4H_9HgCl$ | ≤10.08 | (≤206) | (≤864) | −26 | −109 | *EST | 543-63-5 |
| | IP from 81BAI/CHI2. | | | | | | |
| sec-$C_4H_9HgCl$ | 9.5 | (194) | (814) | −25 | −103 | *EST | 38455-12-8 |
| | IP is onset of photoelectron band (81BAI/CHI2). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_9ClHg^+$ | | | | | | | |
| iso-$C_4H_9HgCl$ | ≤10.04 | (≤204) | (≤852) | −28 | −117 | *EST | 27151-74-2 |
| | IP from 81BAI/CHI2. | | | | | | |
| tert-$C_4H_9HgCl$ | ≤9.52 | (≤198) | (≤830) | −21 | −89 | *EST | 38442-51-2 |
| | IP from 81BAI/CHI2. | | | | | | |
| $C_4H_9ClO^+$ | | | | | | | |
| tert-$C_4H_9OCl$ | ≤9.91 | ≤188 | ≤788 | −40 | −168 | 68WAL/PAP | 507-40-4 |
| | IP from 81COL/FRO. | | | | | | |
| $C_4H_9Cl_2P^+$ | | | | | | | |
| tert-$C_4H_9PCl_2$ | (9.0) | (136) | (570) | −71 | −298 | *EST | 25979-07-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_9F_2P^+$ | | | | | | | |
| tert-$C_4H_9PF_2$ | (9.2) | (34) | (143) | −178 | −745 | *EST | 29149-32-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_9F_3N^+$ | | | | | | | |
| $CF_3CH_2NH(CH_3)_2$ | | −17 | −69 | | | | |
| | From proton affinity of $CF_3CH_2N(CH_3)_2$ (RN 819-06-7). PA = 215.0 kcal/mol, 900. kJ/mol. | | | | | | |
| $CF_3CH_2CH_2CH_2NH_3$ | | −29 | −122 | | | | |
| | From proton affinity of $CF_3CH_2CH_2CH_2NH_2$ (RN 819-46-5). PA = 214.3 kcal/mol, 897 kJ/mol. | | | | | | |
| $C_4H_9I^+$ | | | | | | | |
| n-$C_4H_9I$ | 9.229 | (200) | (838) | −12 | −52 | *EST | 542-69-8 |
| | See: 81KIM/KAT. | | | | | | |
| sec-$C_4H_9I$ | 9.09±0.02 | (195) | (815) | −15 | −62 | *EST | 513-48-4 |
| | See also: 81TRA, 81KIM/KAT. | | | | | | |
| iso-$C_4H_9I$ | 9.202 | (197) | (826) | −15 | −62 | *EST | 513-38-2 |
| | See also: 81KIM/KAT. | | | | | | |
| tert-$C_4H_9I$ | 9.02±0.03 | 191 | 798 | −17.2±0.5 | −72.0±2.2 | 77PED/RYL | 558-17-8 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_4H_9N^+$ | | | | | | | |
| $CH_2=C(CH_3)CH_2NH_2$ | (8.8) | (207) | (866) | 5 | 21 | *EST | 2878-14-0 |
| | IP from 79AUE/BOW. | | | | | | |
| (E)-$CH_3CH=NC_2H_5$ | (9.29) | (218) | (914) | 4±0.2 | 18±1 | *EST | 1190-79-0 |
| | See also: 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

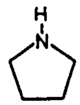
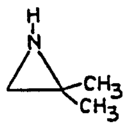
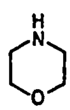
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_4H_9N^+$** | | | | | | | |
|  | (8.0) | (184) | (771) | −0.8±0.1 | −3.4±0.6 | 77PED/RYL | 123-75-1 |
| | IP from 79AUE/BOW. Predicted $\Delta_f H$(Ion) based on hydrogen affinities of homologous series is 186 kcal/mol, 778 kJ/mol corresponding to IP of 8.1 eV. | | | | | | |
|  | (8.94) | (222) | (929) | 16±0.5 | 66±2 | *EST | 2658-24-4 |
| **$C_4H_9NO^+$** | | | | | | | |
| tert-$C_4H_9NO$ | (7.5) | (163) | (681) | −10±1 | −43±6 | 74CHO/MEN | 917-95-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $CH_3CON(CH_3)_2$ | 8.81 | 147 | 617 | −56 | −233 | 78BEA/LEE | 127-19-5 |
| (E)-$CH_3(CH_2)_2CH=NOH$ | (9.5) | (203) | (849) | −16 | −68 | *EST | 110-69-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.2) | (201) | (842) | 12 | 51 | *EST | 110-91-8 |
| **$C_4H_9NOS^+$** | | | | | | | |
| $(CH_3)_3CNSO$ | (10.0) | (166) | (695) | −65 | −270 | *EST | 38662-39-4 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_4H_9NO_2^+$** | | | | | | | |
| $H_2NCH_2CH_2CH_2COOH$ | (8.7) | (95) | (398) | −105±0.5 | −441±2 | 83SKO/SAB | 56-12-2 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $C_2H_5CH(NH_2)COOH$ | (8.70) | (97) | (402) | −104±2 | −437±10 | *EST | 80-60-4 |
| $H_2NCH_2COOC_2H_5$ | (8.8) | (107) | (447) | −96 | −402 | *EST | 459-73-4 |
| n-$C_4H_9NO_2$ | (10.71±0.01) | (213) | (889) | −34.4±0.3 | −143.9±1.4 | 77PED/RYL | 627-05-4 |
| sec-$C_4H_9NO_2$ | (10.71±0.01) | (208) | (870) | −39.1±0.4 | −163.6±1.6 | 77PED/RYL | 600-24-8 |
| **$C_4H_9NO_2S^+$** | | | | | | | |
| L-$CH_3SCH_2CH(NH_2)COOH$ | (8.4) | (99) | (412) | −95 | −398 | *EST | 1187-84-9 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_9NO_3{}^+$ | | | | | | | |
| L-$CH_3CH(OH)CH(NH_2)COOH$ | (≤10.2) | (≤94) | (≤392) | −141 | −592 | *EST | 72-19-5 |
| | IP from 83CAN/HAM. | | | | | | |
| $C_4H_9N_2{}^+$ | | | | | | | |
| $NCCH_2\dot{N}H(CH_3)_2$ | | (188) | (788) | | | | |
| | From proton affinity of $NCCH_2N(CH_3)_2$ (RN 926-64-7). PA = 211.1 kcal/mol, 883. kJ/mol. | | | | | | |
| $C_4H_9N_2O_3{}^+$ | | | | | | | |
| L-$H_2NCOCH_2CH(NH_3)COOH$ | | 5 | 19 | | | | |
| | From proton affinity of L-asparagine (RN 3130-87-8). PA = 219.8 kcal/mol, 920. kJ/mol. | | | | | | |
| $C_4H_9O^+$ | | | | | | | |
| n-$C_4H_9O$ | (9.22) | (196) | (820) | −17 | −69 | 82MCM/GOL | 21576-64-7 |
| n-$C_3H_7CHOH$ | | 124 | 521 | | | | |
| | From proton affinity of n-$C_3H_7CHO$ (RN 123-72-8). PA = 191.5 kcal/mol, 801. kJ/mol. | | | | | | |
| i-$C_3H_7CHOH$ | | 121 | 508 | | | | |
| | From proton affinity of i-$C_3H_7CHO$ (RN 78-84-2). PA = 192.6 kcal/mol, 806. kJ/mol. | | | | | | |
| $(CH_3)(C_2H_5)COH$ | | 109 | 455 | | | | |
| | From proton affinity of $CH_3COC_2H_5$ (RN 78-93-3). PA = 199.8 kcal/mol, 836. kJ/mol. See 82MAC for appearance potential determination. | | | | | | |
| $C_2H_5OCHCH_3$ | | 125 | 521 | | | | |
| | From proton affinity of $C_2H_5OCH=CH_2$ (RN 109-92-2). PA = 207.4 kcal/mol, 868. kJ/mol (86BOU/DJA). See also: 82MAC. | | | | | | |
| $(CH_3)_2COCH_3$ | | (114) | (477) | | | | |
| | From appearance potential determination (82MAC). | | | | | | |
|  $H^+$ | | 123 | 514 | | | | |
| | From proton affinity of tetrahydrofuran (RN 109-99-9). PA = 198.8 kcal/mol, 831. kJ/mol. | | | | | | |
| $C_4H_9O_2{}^+$ | | | | | | | |
| $1HOH(O$-n-$C_3H_7)$ | | 61 | 256 | | | | |
| | From proton affinity of $HCOO(n$-$C_3H_7)$ (RN 110-74-7). PA = 194.2 kcal/mol, 812.5 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

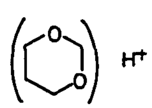
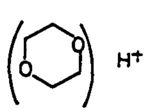
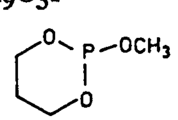
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_9O_2^+$ | | | | | | | |
| $HCOH(O\text{-}i\text{-}C_3H_7)$ | | 73 | 305 | | | | |
| | From proton affinity of $HCOOCH(CH_3)_2$ (RN 625-55-8). PA = 196.0 kcal/mol, 820. kJ/mol. | | | | | | |
| $CH_3COH(O\text{-}C_2H_5)$ | | 59 | 247 | | | | |
| | From proton affinity of $CH_3COOC_2H_5$ (RN 141-78-6). PA = 200.7 kcal/mol, 840. kJ/mol. | | | | | | |
| $C_2H_5COH(O\text{-}CH_3)$ | | 62 | 260 | | | | |
| | From proton affinity of $C_2H_5COOCH_3$ (RN 554-12-1). PA = 200.2 kcal/mol, 838. kJ/mol. | | | | | | |
|  | | 86 | 360 | | | | |
| | From proton affinity of 1,3-dioxane (RN 505-22-6). PA = 198.8 kcal/mol, 832. kJ/mol. | | | | | | |
|  | | 96 | 403 | | | | |
| | From proton affinity of 1,4-dioxane (RN 123-91-1). PA = 193.8 kcal/mol, 811. kJ/mol. | | | | | | |
| $C_4H_9O_2S^+$ | | | | | | | |
| $C_2H_5S(OCH_3)COH$ | | 64 | 269 | | | | |
| | From proton affinity of $C_2H_5S(OCH_3)CO$ (RN 38103-96-7). PA = 201.0 kcal/mol, 841. kJ/mol. | | | | | | |
| $C_4H_9O_3^+$ | | | | | | | |
| $C(OCH_3)_3$ | | 53 | 223 | | | | |
| | From appearance potential of 10.22 eV in $CH(OCH_3)_3$, and appearance potential of 9.86 eV in $CH_3C(OCH_3)_3$ (82HOL/LOS2). | | | | | | |
| $C_2H_5OC(OH)OCH_3$ | | 22 | 90 | | | | |
| | From proton affinity of $C_2H_5OCOOCH_3$ (RN 623-53-0). PA = 202.7 kcal/mol, 848 kJ/mol. | | | | | | |
| $C_4H_9O_3P^+$ | | | | | | | |
|  | (8.74±0.1) | (26) | (110) | −175 | −733 | *EST | 31121-06-9 |

**Table 1. Positive Ion Table - Continued**

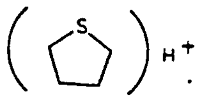
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_9S^+$ | | | | | | | |
|  | | 153 | 640 | | | | |
| | From proton affinity of tetrahydrothiophene (RN 110-01-0) (83CAS/KIM). PA = 204.6 kcal/mol, 856. kJ/mol. | | | | | | |
| $C_4H_{10}^+$ | | | | | | | |
| n-$C_4H_{10}$ | 10.53±0.10 | 213 | 889 | −30.2±0.1 | −126.5±0.4 | 77PED/RYL | 106-97-8 |
| | IP based on charge transfer equilibrium constant in cyclopentane: n-butane system. IP (c-$C_5H_{10}$) = 10.51 eV (81MAU/SIE). Threshold value = 10.55 eV. See also: 81KIM/KAT. | | | | | | |
| iso-$C_4H_{10}$ | 10.57 | (212) | (885) | −32.1±0.1 | −134.5±0.5 | 77PED/RYL | 75-28-5 |
| | See also: 81KIM/KAT. | | | | | | |
| $C_4H_{10}Cd^+$ | | | | | | | |
| $(C_2H_5)_2Cd$ | (8.0) | (210) | (877) | 25±0.7 | 105±3 | 77PED/RYL | 592-02-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_{10}Cl^+$ | | | | | | | |
| $(CH_3)_2CHClCH_3$ | | (150) | (628) | | | | |
| | From equilibrium constant determination (85SHA/HOJ). | | | | | | |
| $C_4H_{10}Cl_2Si^+$ | | | | | | | |
| $(CH_3)_3SiCHCl_2$ | (9.7) | (163) | (683) | −60 | −253 | *EST | 5926-38-5 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| $(CH_3)_2Si(CH_2Cl)_2$ | (9.7) | (165) | (689) | −59 | −247 | *EST | 2917-46-6 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| $C_4H_{10}Hg^+$ | | | | | | | |
| $(C_2H_5)_2Hg$ | ≤8.45 | ≤212 | ≤887 | 17.3±0.2 | 72.3±0.8 | 77PED/RYL | 627-44-1 |
| $C_4H_{10}N^+$ | | | | | | | |
| $CH_2C(CH_3)CH_2NH_3$ | | (152) | (638) | | | | |
| | From proton affinity of $CH_2=C(CH_3)CH_2NH_2$ (RN 2878-14-0). PA = (218.2) kcal/mol, (913.) kJ/mol. | | | | | | |
| $CH_3CHN(CH_3)_2$ | | 153 | 639 | | | | |
| | From proton affinity of $(CH_3)_2NCH=CH_2$ (RN 5763-87-1). PA = 227.8 kcal/mol, 953. kJ/mol. | | | | | | |
| $CH_3CHNHC_2H_5$ | | 147 | 616 | | | | |
| | From proton affinity of $CH_3CH=NC_2H_5$ (RN 1190-79-0). PA = 222.7 kcal/mol, 932. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

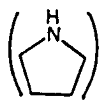
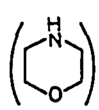
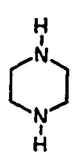
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{10}N^+$ | | | | | | | |
|  H+ | | 140 | 585 | | | | |
| | From proton affinity of pyrrolidine (RN 123-75-1). PA = 225.2 kcal/mol, 942. kJ/mol. | | | | | | |
| $C_4H_{10}NO^+$ | | | | | | | |
| $CH_3C(OH)N(CH_3)_2$ | | 94 | 392 | | | | |
| | From proton affinity of $CH_3CON(CH_3)_2$ (RN 127-19-5) (86TAF/GAL). PA = 216.2 kcal/mol, 905. kJ/mol. | | | | | | |
| n-$C_3H_7$NHCHOH | | 95 | 395 | | | | |
| | From proton affinity of n-$C_3H_7$NHCHO (RN 6281-94-3). PA = (210.0) kcal/mol, (879.) kJ/mol. | | | | | | |
|  H+ | | 158 | 663 | | | | |
| | From proton affinity of morpholine (RN 110-91-8). PA = 219.4 kcal/mol, 918. kJ/mol. | | | | | | |
| $C_4H_{10}NO_2^+$ | | | | | | | |
| t-$C_4H_9$ONHO | | 119 | 497 | | | | |
| | From proton affinity of t-$C_4H_9$ONO (RN 540-80-7). PA = 205.7 kcal/mol, 861. kJ/mol. | | | | | | |
| $C_4H_{10}NO_3^+$ | | | | | | | |
| $CH_3CH(OH)CH(NH_3)COOH$ | | (6) | (23) | | | | |
| | From proton affinity of L-threonine (RN 72-19-5). PA = 218.6 kcal/mol, 915. kJ/mol. | | | | | | |
| $C_4H_{10}N_2^+$ | | | | | | | |
| $(CH_3)_2NN=CHCH_3$ | (7.54) | (176) | (736) | 2 | 9 | 80LEB/MAS | 7422-90-4 |
|  | (≤8.72) | (≤207) | (≤866) | 6±0.2 | 25±1 | *EST | 110-85-0 |
| $C_4H_{10}N_2O^+$ | | | | | | | |
| $(CH_3)_2NCONHCH_3$ | (≤8.80) | (≤146) | (≤609) | −57 | −240 | *EST | 632-14-4 |
| $C_4H_{10}O^+$ | | | | | | | |
| n-$C_4H_9$OH | 10.06±0.03 | 166 | 696 | −65.7±0.1 | −275.0±0.4 | 77PED/RYL | 71-36-3 |
| | See also: 81KIM/KAT, 80BAC/MOU, 84BOW/MAC. | | | | | | |
| sec-$C_4H_9$OH | 9.88 | 158 | 660 | −70.5±0.1 | −295.0±0.4 | 77PED/RYL | 78-92-2 |
| | IP from 81HOL/FIN, 84BOW/MAC. See also: 80BAC/MOU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

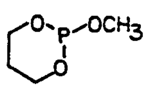
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{10}O^+$ | | | | | | | |
| iso-$C_4H_9OH$ | 10.12±0.04 | 166 | 692 | −67.8±0.1 | −283.6±0.4 | 77PED/RYL | 78-83-1 |
| | IP from 81HOL/FIN, 84BOW/MAC, 77ROS/DRA. | | | | | | |
| tert-$C_4H_9OH$ | 9.97±0.02 | 155 | 650 | −74.7±0.7 | −312.5±2.9 | 77PED/RYL | 75-65-0 |
| | See also: 84BOW/MAC. | | | | | | |
| $(C_2H_5)_2O$ | 9.51±0.03 | 159 | 666 | −60.1±0.1 | −251.7±0.3 | 77PED/RYL | 60-29-7 |
| | See also: 81KIM/KAT, 80BAC/MOU, 84BOW/MAC. | | | | | | |
| n-$C_3H_7OCH_3$ | (9.42) | (160) | (671) | −56.8±0.1 | −237.9±0.5 | 77PED/RYL | 557-17-5 |
| | IP from 84BOW/MAC. See also: 80BAC/MOU. | | | | | | |
| i-$C_3H_7OCH_3$ | 9.42 | 157 | 657 | −60.2±0.2 | −252.0±0.9 | 77PED/RYL | 598-53-8 |
| | IP from 81HOL/FIN, 84BOW/MAC. | | | | | | |
| $C_4H_{10}OS^+$ | | | | | | | |
| $(CH_3CH_2)_2SO$ | ≤8.76 | ≤153 | ≤640 | −49.1±0.4 | −205.6±1.5 | 77PED/RYL | 70-29-1 |
| $C_4H_{10}O_2^+$ | | | | | | | |
| n-$C_4H_9OOH$ | (9.36±0.03) | (166) | (696) | −49 | −207 | *EST | 4813-50-7 |
| | IP from 77ASH/BUR. | | | | | | |
| tert-$C_4H_9OOH$ | (≤10.24) | (≤178) | (≤744) | −58±1 | −244±6 | 77PED/RYL | 75-91-2 |
| $HOCH_2CH_2CH_2OCH_3$ | (9.3) | (122) | (509) | −93 | −388 | *EST | 1320-67-8 |
| | IP is onset of photoelectron band (83BIE/MOR). | | | | | | |
| $HOCH_2CH_2OC_2H_5$ | (9.6) | (126) | (528) | −95 | −398 | *EST | 110-80-5 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $CH_3OCH_2CH_2OCH_3$ | (9.3) | (133) | (557) | −81 | −340 | 67LOU/LAI | 110-71-4 |
| | IP is onset of photoelectron band (83BAK/ARM, 81KIM/KAT). | | | | | | |
| $CH_3CH(OCH_3)_2$ | (9.65±0.03) | (129) | (541) | −93.1±0.2 | −389.7±0.8 | 77PED/RYL | 534-15-6 |
| $C_4H_{10}O_2S^+$ | | | | | | | |
| $(C_2H_5)_2SO_2$ | (9.96±0.03) | (127) | (532) | −103±0.7 | −429±3 | 77PED/RYL | 597-35-3 |
| $C_4H_{10}O_3^+$ | | | | | | | |
| $CH(OCH_3)_3$ | (9.5) | (89) | (372) | −130±0.2 | −545±1 | 77PED/RYL | 149-73-5 |
| | IP from 82HOL/LOS2. | | | | | | |
| $C_4H_{10}O_3P^+$ | | | | | | | |
|  | | (−29) | (−121) | | | | |
| | From proton affinity of 2-methoxy-1,3,2-dioxaphosphorinane (RN 31121-06-9). PA = 219.4 kcal/mol, 918. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

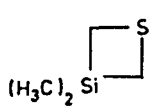
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{10}O_3S^+$ | | | | | | | |
| $(C_2H_5O)_2SO$ | (9.68) | (91) | (382) | −132±0.5 | −552±2 | 77PED/RYL | 623-81-4 |
| $C_4H_{10}S^+$ | | | | | | | |
| n-$C_4H_9SH$ | 9.14±0.02 | 190 | 794 | −21.1±0.3 | −88.1±1.2 | 77PED/RYL | 109-79-5 |
| sec-$C_4H_9SH$ | (9.10) | (187) | (781) | −23.2±0.2 | −96.9±0.8 | 77PED/RYL | 513-53-1 |
| iso-$C_4H_9SH$ | (9.12) | (187) | (783) | −23.3±0.2 | −97.3±0.8 | 77PED/RYL | 513-44-0 |
| tert-$C_4H_9SH$ | (9.03) | (182) | (762) | −26.2±0.2 | −109.6±0.8 | 77PED/RYL | 75-66-1 |
| n-$C_3H_7SCH_3$ | (8.8±0.2) | (183) | (767) | −19.6±0.2 | −82.2±0.9 | 77PED/RYL | 3877-15-4 |
| iso-$C_3H_7SCH_3$ | (8.7±0.2) | (179) | (748) | −21.6±0.2 | −90.5±0.7 | 77PED/RYL | |
| $(C_2H_5)_2S$ | 8.43±0.01 | 174 | 729 | −20±0.2 | −84±1 | 77PED/RYL | 352-93-2 |
| | | *181* | *757* | *−13* | *−56* | | |
| $C_4H_{10}SSi^+$ | | | | | | | |
| $(C_2H_5)_2Si=S$ | | (188) | (787) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (81GUS/VOL). | | | | | | |
|  | (8.25±0.03) | (193) | (806) | (2) | (10) | 81GUS/VOL | 77205-52-8 |
| | IP from 81GUS/VOL | | | | | | |
| $C_4H_{10}S_2^+$ | | | | | | | |
| $(C_2H_5S)_2$ | ≤8.27±0.03 | ≤173 | ≤723 | −17.8±0.3 | −74.7±1.1 | 77PED/RYL | 110-81-6 |
| | Dialkyl disulfides undergo a change in the dihedral CSSC angle from 90° to 180°. upon ionization; adiabatic ionization potentials are probably well below the the experimentally observed ionization onset. | | | | | | |
| $CH_3SCH_2CH_2SCH_3$ | (≤8.64) | (≤190) | (≤797) | −9 | −37 | *EST | 6628-18-8 |
| $C_4H_{10}Sc^+$ | | | | | | | |
| $HScCH(CH_3)C_2H_5$ | | (195) | (816) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $CH_3ScC_3H_7$ | | (174) | (728) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $C_2H_4Sc(CH_3)_2$ | | (175) | (732) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $(CH_3CH=CH_2)ScH(CH_3)$ | | (184) | (770) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

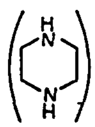
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_4H_{10}Sc^+$ | | | | | | | |
| $(CH_3CH=CHCH_3)ScH_2$ | | (195) | (816) | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). | | | | | | |
| $C_4H_{10}Se^+$ | | | | | | | |
| $(C_2H_5)_2Se$ | (8.3±0.3) | (178) | (743) | −14±1 | −58±5 | 77PED/RYL | 627-53-2 |
| $C_4H_{10}Zn^+$ | | | | | | | |
| $(C_2H_5)_2Zn$ | (≤8.6) | (≤212) | (≤888) | 14±0.7 | 58±3 | 77PED/RYL | 557-20-0 |
| $C_4H_{11}^+$ | | | | | | | |
| $((CH_3)_3CH)H$ | | 170 | 712 | | | | |
| | From proton affinity of iso-$C_4H_{10}$. (RN 75-28-5). PA = 163.3 kcal/mol, 683. kJ/mol. | | | | | | |
| $C_4H_{11}ClO_3Si^+$ | | | | | | | |
| $(CH_3O)_3SiCH_2Cl$ | (10.0) | (4) | (17) | −226 | −948 | *EST | 5926-26-1 |
| | IP is onset of photoelectron band (81ZYK/KHV). | | | | | | |
| $C_4H_{11}ClSi^+$ | | | | | | | |
| $(CH_3)_3SiCH_2Cl$ | (9.4) | (159) | (667) | −57 | −240 | *EST | 2344-80-1 |
| | IP is onset of photoelectron band (81ZYK/KHV, 82LEV/LIA). | | | | | | |
| $C_4H_{11}N^+$ | | | | | | | |
| n-$C_4H_9NH_2$ | 8.71±0.03 | 179 | 748 | −22±0.2 | −92±1 | 77PED/RYL | 109-73-9 |
| | See also: 81KIM/KAT, 79AUE/BOW. | | | | | | |
| sec-$C_4H_9NH_2$ | (8.70) | (176) | (734) | −25.0±0.2 | −104.8±0.9 | 77PED/RYL | 13952-84-6 |
| iso-$C_4H_9NH_2$ | (8.70) | (177) | (741) | −23.6±0.1 | −98.8±0.4 | 77PED/RYL | 78-81-9 |
| tert-$C_4H_9NH_2$ | (8.64) | (170) | (713) | −28.9±0.1 | −120.9±0.4 | 77PED/RYL | 75-64-9 |
| $(C_2H_5)_2NH$ | 8.01±0.01 | 167 | 700 | −17.4±0.5 | −72.6±2 | 77PED/RYL | 109-89-7 |
| $C_2H_5N(CH_3)_2$ | (7.74±0.05) | (167) | (701) | −11 | −48 | *EST | 598-56-1 |
| | IP is onset of photoelectron band. See also: 81LOG/TAK, 79AUE/BOW. | | | | | | |
| $C_4H_{11}NO^+$ | | | | | | | |
| $(CH_3)_2NCH_2CH_2OH$ | (8.2) | (140) | (587) | −49 | −204 | 81LOS/LAM | 108-01-0 |
| | IP is onset of photoelectron band (82LEV/LIA, 86VOR/BRO). | | | | | | |
| $C_4H_{11}N_2^+$ | | | | | | | |
|  $H^+$ | | 147 | 617 | | | | |
| | From proton affinity of piperazine (RN 110-85-0). PA = 224.2 kcal/mol, 938. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

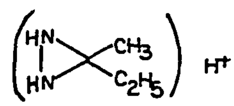
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_4H_{11}N_2^+$** | | | | | | | |
|  | | (182) | (764) | | | | |
| | From proton affinity of 3-ethyl-3-methyldiaziridine (RN 4901-75-1). PA = (214.9) kcal/mol, (899) kJ/mol. | | | | | | |
| **$C_4H_{11}O^+$** | | | | | | | |
| n-$C_4H_9OH_2$ | | 109 | 456 | | | | |
| | From proton affinity of n-$C_4H_9OH$ (RN 71-36-3). PA = 191.1 kcal/mol, 799.5 kJ/mol. | | | | | | |
| sec-$C_4H_9OH_2$ | | (101) | (421) | | | | |
| | From proton affinity of sec-$C_4H_9OH$ (RN 78-92-2) (78PAU/KIM). PA = (195) kcal/mol, (816) kJ/mol. | | | | | | |
| iso-$C_4H_9OH_2$ | | 105 | 441 | | | | |
| | From proton affinity of iso-$C_4H_9OH$ (RN 78-83-1) (78TAF/TAA). PA = 192.4 kcal/mol, 805. kJ/mol. | | | | | | |
| tert-$C_4H_9OH_2$ | | 97 | 408 | | | | |
| | From proton affinity of tert-$C_4H_9OH$ (RN 75-65-0). PA = 193.7 kcal/mol, 810. kJ/mol. | | | | | | |
| $(C_2H_5)_2OH$ | | 105 | 440 | | | | |
| | From proton affinity of $(C_2H_5)_2O$ (RN 60-29-7) (86KNI/FRE, 86MAU/LIE). PA = 200.2 kcal/mol, 838 kJ/mol. | | | | | | |
| **$C_4H_{11}O_2^+$** | | | | | | | |
| $HO(CH_2)_4OH_2$ | | 52 | 216 | | | | |
| | From proton affinity of $HO(CH_2)_4OH$ (RN 110-63-4). PA = (212) kcal/mol, (887) kJ/mol. | | | | | | |
| $CH_3OCH_2CH_2OHCH_3$ | | 80 | 333 | | | | |
| | From proton affinity of $CH_3OCH_2CH_2OCH_3$ (RN 110-71-4). PA = 204.9 kcal/mol, 857. kJ/mol. | | | | | | |
| **$C_4H_{11}O_3P^+$** | | | | | | | |
| $OPH(OC_2H_5)_2$ | (10.31) | (19) | (79) | −219 | −916 | *EST | 762-04-9 |
| | See also: 80ZVE/VIL. | | | | | | |
| **$C_4H_{11}P^+$** | | | | | | | |
| tert-$C_4H_9PH_2$ | (8.9) | (181) | (757) | −24 | −102 | *EST | 2501-94-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $(C_2H_5)_2PH$ | (8.69) | (176) | (736) | −24 | −102 | *EST | 627-49-6 |
| **$C_4H_{11}S^+$** | | | | | | | |
| $(C_2H_5)_2SH$ | | 141 | 588 | | | | |
| | From proton affinity of $(C_2H_5)_2S$ (RN 352-93-2). PA = 205.0 kcal/mol, 858. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

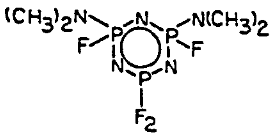
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{11}S^+$ | | | | | | | |
| tert-$C_4H_9SH_2$ | | 143 | 596 | | | | |
| | From proton affinity of t-$C_4H_9SH$ (RN 75-66-1). PA = 196.9 kcal/mol, 824. kJ/mol. | | | | | | |
| sec-$C_4H_9SH_2$ | | (148) | (621) | | | | |
| | From proton affinity of sec-$C_4H_9SH$ (RN 513-53-1) (78PAU/KIM). PA = (194.0) kcal/mol, (812.) kJ/mol. | | | | | | |
| $C_4H_{11}SSi^+$ | | | | | | | |
| $(C_2H_5)_2SiSH$ | | (157) | (657) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (81GUS/VOL). | | | | | | |
| $C_4H_{12}BClN_2^+$ | | | | | | | |
| $B(N(CH_3)_2)_2Cl$ | 8.08 | 106 | 445 | −80±1 | −335±5 | 77PED/RYL | 6562-41-0 |
| $C_4H_{12}ClN_2OP^+$ | | | | | | | |
| $((CH_3)_2N)_2POCl$ | (8.61) | (75) | (316) | −123 | −515 | *EST | 1605-65-8 |
| $C_4H_{12}ClN_2P^+$ | | | | | | | |
| $((CH_3)_2N)_2PCl$ | (7.6) | (127) | (531) | −48 | −202 | *EST | 3348-44-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_{12}F_4N_5P_3^+$ | | | | | | | |
|  | (8.96) | (−169) | (−706) | −375.5 | −1571 | *EST | 30004-14-9 |
| | IP from 81CLA/SOW. | | | | | | |
| $C_4H_{12}Ge^+$ | | | | | | | |
| $(CH_3)_4Ge$ | 9.33±0.05 | 198 | 828 | −17±2 | −72±9 | 77PED/RYL | 865-52-1 |
| $C_4H_{12}N^+$ | | | | | | | |
| n-$C_4H_9NH_3$ | | 122 | 524 | | | | |
| | From proton affinity of n-$C_4H_9NH_2$ (RN 109-73-9). PA = 218.4 kcal/mol, 914. kJ/mol. | | | | | | |
| sec-$C_4H_9NH_3$ | | 120 | 502 | | | | |
| | From proton affinity of sec-$C_4H_9NH_2$ (RN 13952-84-6). PA = 220.5 kcal/mol, 922. kJ/mol. | | | | | | |
| iso-$C_4H_9NH_3$ | | 123 | 515 | | | | |
| | From proton affinity of iso-$C_4H_9NH_2$ (RN 78-81-9). PA = 218.8 kcal/mol, 915. kJ/mol. | | | | | | |
| tert-$C_4H_9NH_3$ | | 116 | 485 | | | | |
| | From proton affinity of tert-$C_4H_9NH_2$ (RN 75-64-9). PA = 220.8 kcal/mol, 924. kJ/mol. | | | | | | |
| $(C_2H_5)_2NH_2$ | | 125 | 512 | | | | |
| | From proton affinity of $(C_2H_5)_2NH$ (RN 109-89-7). PA = 225.9 kcal/mol, 945. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{12}N^+$ | | | | | | | |
| $(CH_3)_2(C_2H_5)NH$ | | 127 | 531 | | | | |
| | From proton affinity of $(CH_3)_2(C_2H_5)N$ (RN 598-56-1). PA = 227.5 kcal/mol, 952. kJ/mol. | | | | | | |
| $C_4H_{12}NO^+$ | | | | | | | |
| $NH_3(CH_2)_4OH$ | | 75 | 312 | | | | |
| | From proton affinity of $NH_2(CH_2)_4OH$ (RN 13325-10-5). PA = 233.8 kcal/mol, 978. kJ/mol. | | | | | | |
| $C_4H_{12}NO_2P^+$ | | | | | | | |
| $(CH_3O)_2PN(CH_3)_2$ | (8.1) | (71) | (296) | -116 | -486 | *EST | 597-07-9 |
| | IP is onset of photoelectron band (82WOR/HAR). | | | | | | |
| $C_4H_{12}N_2{}^+$ | | | | | | | |
| $(CH_3)_2NN(CH_3)_2$ | (6.87) | (175) | (732) | 16 | 69 | 61GOW/JON | 6415-12-9 |
| | IP from charge transfer equilibrium constant determination (86RUM). Reference standard: IP($C_6H_5N(CH_3)_2$) = 7.12 eV. See also: 84MAU/NEL. | | | | | | |
| $C_4H_{12}N_2S_2{}^+$ | | | | | | | |
| $(CH_3)_2NSSN(CH_3)_2$ | (7.2) | (163) | (683) | -3 | -12 | *EST | 928-05-2 |
| | IP is onset of photoelectron band (81BOC/SCH). | | | | | | |
| $C_4H_{12}N_4{}^+$ | | | | | | | |
| (E)-$(CH_3)NN=NN(CH_3)_2$ | (7.0) | (227) | (948) | 65±0.7 | 273±3 | 77PED/RYL | 6130-87-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_{12}OSi^+$ | | | | | | | |
| $(CH_3)_3SiOCH_3$ | 9.61 | (110) | (459) | -112±2 | -468±8 | *EST | 1825-61-2 |
| | IP from 83MOL/PIK. | | | | | | |
| $C_4H_{12}Pb^+$ | | | | | | | |
| $(CH_3)_4Pb$ | (8.50) | (229) | (956) | 33±1 | 136±4 | 82PIL/SKI | 75-74-1 |
| $C_4H_{12}Si^+$ | | | | | | | |
| $(CH_3)_4Si$ | 9.80±0.04 | 170 | 711 | -55.7±0.7 | -233.0±2.9 | 83STE2 | 75-76-3 |
| | | *178* | *743* | *-48* | *-202* | | |
| $(C_2H_5)_2SiH_2$ | (9.8) | (182) | (763) | -44±1 | -183±6 | 77PED/RYL | 542-91-6 |
| $C_4H_{12}SiS^+$ | | | | | | | |
| $(CH_3)_3SiSCH_3$ | (8.4) | (128) | (534) | -66 | -276 | *EST | 3908-55-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_4H_{12}Sn^+$ | | | | | | | |
| $(CH_3)_4Sn$ | 8.89±0.05 | 200 | 838 | -5±0.5 | -20±2 | 77PED/RYL | 594-27-4 |

**Table 1. Positive Ion Table - Continued**

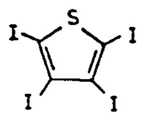
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_4H_{13}N_2^+$ | | | | | | | |
| $NH_2(CH_2)_4NH_3$ | | 115 | 483 | | | | |
| | From proton affinity of $NH_2(CH_2)_4NH_2$ (RN 110-60-1). PA = 237.6 kcal/mol, 994 kJ/mol. | | | | | | |
| $(CH_3)_2NNH(CH_3)_2$ | | 157 | 658 | | | | |
| | From proton affinity of $(CH_3)_2NN(CH_3)_2$ (RN 6415-12-9) (84MAU/NEL). PA = 224.8 kcal/mol, 941. kJ/mol. | | | | | | |
| $C_4H_{13}OSi^+$ | | | | | | | |
| $(CH_3)_3Si(OH)CH_3$ | | (51) | (213) | | | | |
| | From proton affinity of $(CH_3)_3SiOCH_3$ (RN 1825-61-2). PA = ~203 kcal/mol, ~849 kJ/mol. | | | | | | |
| $C_4H_{14}N_3OP^+$ | | | | | | | |
| $((CH_3)_2N)_2(NH_2)PO$ | (8.60±0.05) | (83) | (348) | −115 | −482 | *EST | 3732-86-3 |
| $C_4H_{15}N_3OP^+$ | | | | | | | |
| $((CH_3)_2N)_2(NH_2)POH$ | | 26 | 109 | | | | |
| | From proton affinity of $((CH_3)_2N)_2(NH_2)PO$ (RN 3732-86-3) (85BOL/HOU). PA = 224.4 kcal/mol, 939. kJ/mol. | | | | | | |
| $C_4H_{15}OSi_2^+$ | | | | | | | |
| $((CH_3)_2SiH)_2OH$ | | (6) | (26) | | | | |
| | From proton affinity of $((CH_3)_2SiH)_2O$ (RN 3277-26-7). PA = ~203 kcal/mol, ~849 kJ/mol. | | | | | | |
| $C_4I_4S^+$ | | | | | | | |
|  | (≤8.27) | (≤302) | (≤1262) | 111 | 464 | *EST | 19259-11-1 |
| $C_4La^+$ | | | | | | | |
| $LaC_4$ | (4.7±0.5) | (288) | (1207) | 180±2 | 754±8 | 81GIN/PEL | 12603-31-5 |
| $C_4N_2^+$ | | | | | | | |
| NCC≡CCN | 11.81±0.01 | 400 | 1673 | 128 | 534 | 82CHU/NGU | 1071-98-3 |
| | See also: 82MAI/MIS. | | | | | | |
| $C_4N_2O^+$ | | | | | | | |
| $(NC)_2C=C=O$ | (10.56) | (300) | (1255) | 56.5 | 236 | *EST | 4361-47-1 |
| | IP is onset of photoelectron band (80HOT/NEI). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_4N_2S^+$ | | | | | | | |
| $(NC)_2C=C=S$ | (9.94) | (339) | (1419) | 110 | 460 | 80SCH/SCH2 | 54856-36-9 |
| | IP is onset of photoelectron band (80SCH/SCH2). | | | | | | |
| $C_4NiO_4^+$ | | | | | | | |
| $Ni(CO)_4$ | 8.27±0.04 | 48 | 200 | −143±1 | −598±4 | 77PED/RYL | 13463-39-3 |
| | See also: 86REU/WAN. | | | | | | |
| $C_4Sc^+$ | | | | | | | |
| $ScC_4$ | (6.7±1.0) | (339) | (1418) | 184±4 | 772±18 | 81HAQ/GIN | 12547-95-4 |
| | IP from 81HAQ/GIN. | | | | | | |
| $C_5BrMnO_5^+$ | | | | | | | |
| $Mn(CO)_5Br$ | 8.4 | (−16) | (−65) | −209±1 | −876±5 | 82CON/ZAF | 14516-54-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5BrO_5Re^+$ | | | | | | | |
| $Re(CO)_5Br$ | 8.5 | (−9) | (−38) | −205±1 | −858±5 | 83ALT/CON | 14220-21-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5ClMnO_5^+$ | | | | | | | |
| $Mn(CO)_5Cl$ | 8.6 | (−21) | (−88) | −219±2 | −918±10 | 82CON/ZAF | 14100-30-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5ClO_5Re^+$ | | | | | | | |
| $Re(CO)_5Cl$ | 8.55 | (−12) | (−52) | −210±4 | −877±18 | 83ALT/CON | 14099-01-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5FeO_4S^+$ | | | | | | | |
| $Fe(CO)_4CS$ | (7.8) | (65) | (273) | −115 | −480 | *EST | 66517-47-3 |
| | IP is onset of photoelectron band (82BOH/GLE). | | | | | | |
| $C_5FeO_5^+$ | | | | | | | |
| $Fe(CO)_5$ | 7.96±0.01 | 10 | 43 | −173±2 | −725±7 | 82PIL/SKI | 13463-40-6 |
| | See also: 83HAR/OHN. | | | | | | |
| $C_5HFeO_5^+$ | | | | | | | |
| $HFe(CO)_5$ | | (−10) | (−40) | | | | |
| | From proton affinity of $Fe(CO)_5$ (RN 13463-40-6). PA = ~202 kcal/mol, ~845 kJ/mol. | | | | | | |
| $C_5HMnO_5^+$ | | | | | | | |
| $Mn(CO)_5H$ | 8.5±0.1 | 19 | 80 | −177±2 | −740±10 | 82CON/ZAF | 16972-33-1 |
| $C_5HN_3^+$ | | | | | | | |
| $C(CN)_2=CHCN$ | (~11.55) | (390) | (1632) | 124 | 518 | 82CHU/NGU | 997-76-2 |
| $C_5H_2MnO_5^+$ | | | | | | | |
| $H_2Mn(CO)_5$ | | (−12) | (−51) | | | | |
| | From proton affinity of $HMn(CO)_5$ (RN 16972-33-1). PA = (201) kcal/mol, (841) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

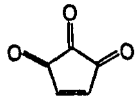
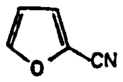
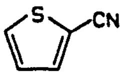
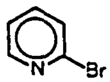
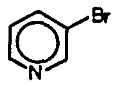
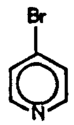
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_2O_3{}^+$ | | | | | | | |
|  | (9.3) | (144) | (603) | −70 | −294 | *EST | 15548-56-8 |
| | IP is onset of photoelectron band (82GLE/DOB). | | | | | | |
| $C_5H_3Cl^+$ | | | | | | | |
| $CH_3C{\equiv}CC{\equiv}CCl$ | 9.19±0.01 | (321) | (1342) | 110±0.2 | 459±1 | *EST | |
| | IP from 84KLA/KUH. | | | | | | |
| $C_5H_3NO^+$ | | | | | | | |
|  | (≤9.47±0.05) | (≤243) | (≤1018) | 25 | 104 | *EST | 617-90-3 |
| $C_5H_3NS^+$ | | | | | | | |
|  | (9.83±0.05) | (293) | (1226) | 66 | 278 | *EST | 1003-31-2 |
| $C_5H_4{}^+$ | | | | | | | |
| $CH_2{=}C{=}C{=}C{=}CH_2$ | (8.67) | (315) | (1318) | 115 | 481 | *EST | 21986-03-8 |
| $CH{\equiv}CCH_2C{\equiv}CH$ | 10.1 | (338) | (1413) | 105 | 439 | *EST | 24442-69-1 |
| | IP from 83HOL. | | | | | | |
| $CH_3C{\equiv}CC{\equiv}CH$ | 9.4 | (318) | (1332) | 101 | 425 | *EST | 4911-55-1 |
| | IP from 81FOR/MAI. See also: 81MAI. | | | | | | |
| $C_5H_4BrN^+$ | | | | | | | |
|  | 9.65±0.05 | (261) | (1092) | 38 | 161 | *EST | 109-04-6 |
|  | (9.75±0.1) | (263) | (1102) | 38 | 161 | *EST | 626-55-1 |
|  | 9.94±0.05 | (268) | (1120) | 38 | 161 | *EST | 1120-87-2 |

Table 1. Positive Ion Table - Continued

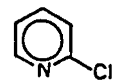
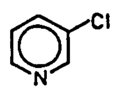
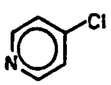
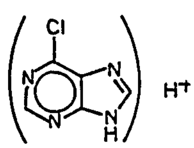
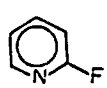
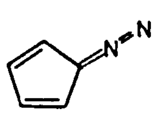
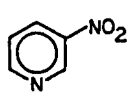
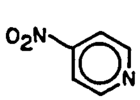
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_4ClN^+$ | | | | | | | |
|  | 9.0 | (232) | (971) | 25 | 103 | *EST | 109-09-1 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | 9.1 | (236) | (986) | 26 | 108 | *EST | 626-60-8 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | 9.5 | (245) | (1025) | 26 | 108 | *EST | 626-61-9 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
| $C_5H_4ClN_4^+$ | | | | | | | |
|  | | (200) | (839) | | | | |
| | From proton affinity of 6-chloropurine (RN 87-42-3). PA = ~208 kcal/mol, ~870 kJ/mol. | | | | | | |
| $C_5H_4FN^+$ | | | | | | | |
|  | (9.4) | (201) | (839) | −16 | −68 | *EST | 372-48-5 |
| | IP is onset of photoelectron band (83PIA/KEL). | | | | | | |
| $C_5H_4N_2^+$ | | | | | | | |
|  | (8.09±0.01) | (277) | (1161) | 91±4 | 380±16 | *EST | 1192-27-4 |
| $C_5H_4N_2O_2^+$ | | | | | | | |
|  | (10.3±0.1) | (270) | (1130) | 33 | 136 | *EST | 2530-26-9 |
|  | (10.4) | (273) | (1140) | 33 | 137 | *EST | 1122-61-8 |

**Table 1. Positive Ion Table - Continued**

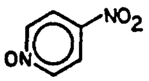
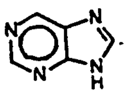
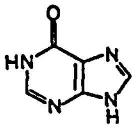
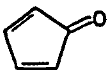
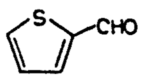
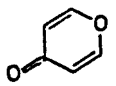
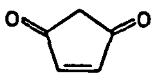
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_4N_2O_3{}^+$ | | | | | | | |
|  | (9.03±0.02) | (222) | (930) | 14 | 59 | *EST | 1124-82-9 |
| $C_5H_4N_4{}^+$ | | | | | | | |
|  | (≤9.52±0.03) | (≤275) | (≤1149) | 55 | 230 | *EST | 120-73-0 |
| $C_5H_4N_4O^+$ | | | | | | | |
|  | (≤8.55±0.03) | (≤209) | (≤875) | 12 | 50 | 77PED/RYL | 68-94-0 |
| $C_5H_4O^+$ | | | | | | | |
|  | (9.49) | (211) | (881) | −8±8 | −35±35 | *EST | 13177-38-3 |
| $C_5H_4OS^+$ | | | | | | | |
|  | (≤9.37±0.05) | (≤222) | (≤928) | 6 | 24 | *EST | 98-03-3 |
| $C_5H_4O_2{}^+$ | | | | | | | |
|  | 9.35±0.05 | (176) | (733) | −40 | −169 | *EST | 108-97-4 |
|  | (9.6)<br>IP is onset of photoelectron band (82GLE/DOB). | (168) | (704) | −53 | −222 | *EST | 930-60-9 |

Table 1. Positive Ion Table - Continued

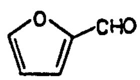
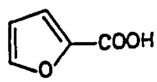
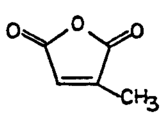
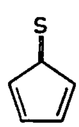
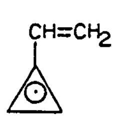
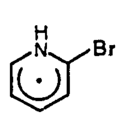
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_5H_4O_2^+$ | | | | | | | |
|  | 9.21±0.01 | 176 | 738 | −36±1 | −151±5 | 77PED/RYL | 98-01-1 |
| $C_5H_4O_3^+$ | | | | | | | |
|  | (≤9.16±0.05) | (≤118) | (≤493) | −93±0.7 | −391±3 | 77PED/RYL | 488-93-7 |
|  | (10.7) | (140) | (585) | −106.9±0.6 | −447.2±2.5 | 77PED/RYL | 616-02-4 |
| | IP is onset of photoelectron band (81KIM/KAT). | | | | | | |
| $C_5H_4S^+$ | | | | | | | |
|  | (8.4) | (239) | (1000) | 45 | 190 | *EST | 77825-99-1 |
| | IP is onset of photoelectron band (81SCH/SCH). | | | | | | |
| $C_5H_5^+$ | | | | | | | |
| $HC{\equiv}CCHCH=CH_2$ | 7.88 | 271 | 1132 | 89 | 372 | 82MCM/GOL | 50706-18-8 |
| | IP from 84LOS/HOL. | | | | | | |
|  | 8.41 | (252) | (1052) | 58±1 | 241±6 | 82MCM/GOL | 62744-94-9 |
|  | | (242) | (1012) | | | | |
| | From appearance energy from $C_6H_5CH_2^+$ precursor, 3.55 eV (78MCC/FRE). | | | | | | |
| $C_5H_5BrN^+$ | | | | | | | |
|  | | 189 | 793 | | | | |
| | From proton affinity of 2-bromopyridine (RN 109-04-6). | | | | | | |

Table 1. Positive Ion Table - Continued

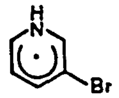
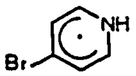
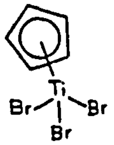
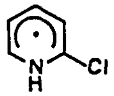
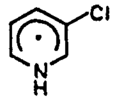
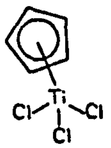
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_5BrN^+$ | | | | | | | |
|  | | 189 | 791 | | | | |
| | From proton affinity of 3-bromopyridine (RN 626-55-1). | | | | | | |
|  | | 186 | 779 | | | | |
| | From proton affinity of 4-bromopyridine (RN 1120-87-2). | | | | | | |
| $C_5H_5Br_3Ti^+$ | | | | | | | |
|  | (9.1) | (102) | (428) | −108 | −450 | •EST | 12240-42-5 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |
| $C_5H_5ClN^+$ | | | | | | | |
|  | | 176 | 736 | | | | |
| | From proton affinity of 2-chloropyridine (RN 109-09-1). PA = 214.4 kcal/mol, 897. kJ/mol. | | | | | | |
|  | | 177 | 739 | | | | |
| | From proton affinity of 3-chloropyridine (RN 626-60-8). PA = 214.8 kcal/mol, 899. kJ/mol. | | | | | | |
|  | | 174 | 727 | | | | |
| | From proton affinity of 4-chloropyridine (RN 626-61-9). PA = 217.8 kcal/mol, 911 kJ/mol. | | | | | | |
| $C_5H_5Cl_3Ti^+$ | | | | | | | |
|  | (9.1) | (76) | (319) | −133±3 | −559±12 | 77PED/RYL | 1270-98-0 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |

**Table 1. Positive Ion Table - Continued**

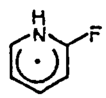
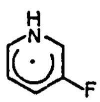
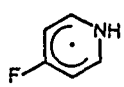
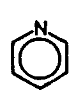
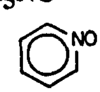
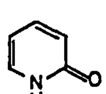
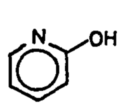
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_5FN^+$** | | | | | | | |
|  | | 139 | 581 | | | | |
| | From proton affinity of 2-fluoropyridine (RN 372-48-5). PA = 210.6 kcal/mol, 881 kJ/mol. | | | | | | |
|  | | 138 | 577 | | | | |
| | From proton affinity of 3-fluoropyridine (RN 372-47-4). PA = 214.3 kcal/mol, 897. kJ/mol. | | | | | | |
|  | | 135 | 567 | | | | |
| | From proton affinity of 4-fluoropyridine (RN 694-52-0). PA = 216.6 kcal/mol, 906. kJ/mol. | | | | | | |
| **$C_5H_5F_3O_2^+$** | | | | | | | |
| $CF_3COH=CHCOCH_3$ | (9.5) | (−20.7) | (−86.7) | −239.8 | −1003.3 | 84ERA/KOL | 367-57-7 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_5H_5N^+$** | | | | | | | |
|  | 9.25 | 247 | 1032 | 33±0.2 | 140±1 | 79KUD/KUD3 | 110-86-1 |
| | See also: 83PIA/KEL, 82LIF, 81KIM/KAT. | | | | | | |
| **$C_5H_5NO^+$** | | | | | | | |
|  | 8.38±0.02 | (207) | (869) | 14 | 61 | *EST | 694-59-7 |
|  | (8.4) | (176) | (733) | −18±0.5 | −77±2 | 82SUR/ELS | 142-08-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.6 | (179) | (750) | −19±0.5 | −80±2 | 82SUR/ELS | 109-10-4 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

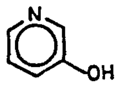
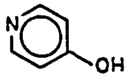
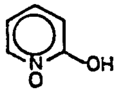
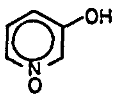
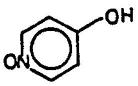
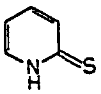
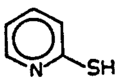
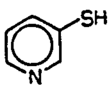
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_5NO^+$ | | | | | | | |
|  | (≤9.15±0.03) | (≤200) | (≤839) | −11±0.5 | −44±2 | 82SUR/ELS | 109-00-2 |
|  | 9.75±0.11 | (215) | (900) | −10±0.5 | −41±2 | 82SUR/ELS | 626-64-2 |
| $C_5H_5NO_2^+$ | | | | | | | |
|  | (8.90±0.05) | (167) | (699) | −38 | −160 | *EST | |
|  | (8.60±0.05) | (168) | (706) | −30 | −124 | *EST | 6602-28-4 |
|  | (8.18±0.05) | (160) | (668) | −29 | −121 | *EST | 6890-62-6 |
| $C_5H_5NS^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band. | (220) | (921) | 43 | 178 | *EST | 2637-34-5 |
|  | ≤8.7<br>IP from 81DRE/BEC, 82LEV/LIA. | (≤230) | (≤963) | 30 | 124 | *EST | 73018-10-7 |
|  | (≤8.89±0.03) | (≤239) | (≤999) | 34 | 141 | *EST | 16133-26-9 |

**Table 1. Positive Ion Table - Continued**

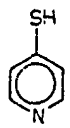
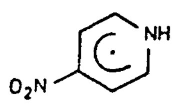
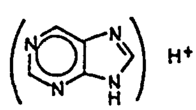
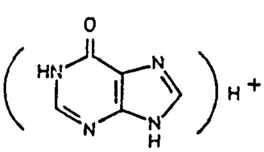
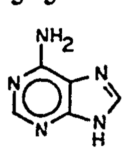
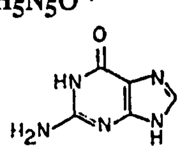
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_5NS^+$ | | | | | | | |
|  | ≤9.25±0.03 | (≤247) | (≤1033) | 34 | 141 | *EST | 4556-23-4 |
| $C_5H_5N_2O_2^+$ | | | | | | | |
|  | | 190 | 795 | | | | |
| | From proton affinity of 4-nitropyridine (RN 1122-61-8). PA = 208.5 kcal/mol, 872. kJ/mol. | | | | | | |
| $C_5H_5N_4^+$ | | | | | | | |
|  | | 201 | 843 | | | | |
| | From proton affinity of 9H-purine (RN 120-73-0). PA = 219.3 kcal/mol, 917.5 kJ/mol. | | | | | | |
| $C_5H_5N_4O^+$ | | | | | | | |
|  | | (161) | (673) | | | | |
| | From proton affinity of hypoxanthine (RN 68-94-0). PA = ~217 kcal/mol, ~907 kJ/mol. | | | | | | |
| $C_5H_5N_5^+$ | | | | | | | |
|  | (7.8) | (229) | (960) | 49±2 | 207±8 | 83KIR/DOM | 73-24-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5H_5N_5O^+$ | | | | | | | |
|  | (7.85) | (181) | (759) | 0.5 | 2 | 77PED/RYL | 73-40-5 |
| $C_5H_6^+$ | | | | | | | |
| $CH_2=C=CHCH=CH_2$ | (8.88) | (265) | (1108) | 60 | 251 | *EST | 10563-01-6 |
| (Z)-$CH_3CH=CHC\equiv CH$ | 9.14±0.04 | 272 | 1138 | 61±1 | 256±6 | 78SHA | 1574-40-9 |
| (E)-$CH_3CH=CHC\equiv CH$ | (9.05) | (270) | (1130) | 61±0.7 | 257±3 | 78SHA | 2004-69-5 |
| $CH_2=CHC\equiv CCH_3$ | 9.00±0.01 | (267) | (1118) | (60) | (250) | *EST | 646-05-9 |

**Table 1. Positive Ion Table - Continued**

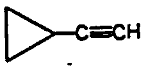
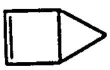
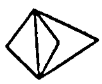
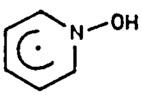
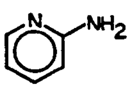
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_6^+$ | | | | | | | |
| $CH_2=C(CH_3)C\equiv CH$ | 9.23±0.01 | 275 | 1148 | 62 | 258 | 77LEB/RYA | 78-80-8 |
|  | 8.56±0.01 | 229 | 957 | 31±1 | 131±4 | 77PED/RYL | 542-92-7 |
|  | (8.7) | (275) | (1152) | 75 | 313 | *EST | 6746-94-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.0) | (264) | (1103) | 79 | 331 | *EST | 5164-35-2 |
|  | 9.74 | 308 | 1291 | 84±1 | 351±4 | 85WIB/DAI | 35634-10-7 |
| | IP from 85HON/HUB. | | | | | | |
| $C_5H_6N^+$ | | | | | | | |
|  | | 178 | 746 | | | | |
| | From proton affinity of pyridine (RN 110-86-1). PA = 220.8 kcal/mol, 924 kJ/mol. | | | | | | |
| $C_5H_6NO^+$ | | | | | | | |
|  | | 160 | 669 | | | | |
| | From proton affinity of pyridine-N-oxide (RN 694-59-7). PA = 220.3 kcal/mol, 922. kJ/mol. | | | | | | |
| $C_5H_6N_2^+$ | | | | | | | |
|  | (8.0) | (213) | (890) | 28±0.2 | 118±1 | 84BIC/PIL | 504-29-0 |
| | IP is onset of photoelectron band (82LEV/LIA, 82GUI/KHA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

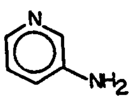
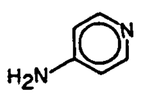
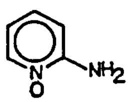
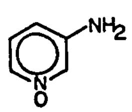
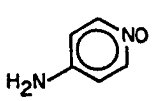
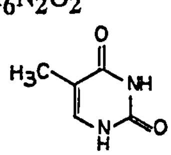
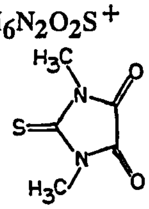
| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_5H_6N_2^+$ | | | | | | | |
|  | (8.1) | (221) | (926) | 34±0.5 | 144±2 | 84BIC/PIL | 462-08-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.4) | (225) | (940) | 31±0.2 | 130±1 | 84BIC/PIL | 504-24-5 |
| | IP is onset of photoelectron band. Value of $\Delta_fH$(Ion) predicted from hydrogen affinity considerations: 214 kcal/mol, 895 kJ/mol, corresponding to IP of 7.9 eV. | | | | | | |
| $C_5H_6N_2O^+$ | | | | | | | |
|  | (8.04±0.05) | (197) | (825) | 12 | 49 | *EST | 14150-95-9 |
|  | (8.21±0.05) | (204) | (853) | 15 | 61 | *EST | 1657-32-5 |
|  | (7.67±0.05) | (191) | (797) | 14 | 57 | *EST | 3535-75-9 |
| $C_5H_6N_2O_2^+$ | | | | | | | |
|  | (8.8) | (124) | (520) | −79±1 | −329±4 | 77NAB/SAB | 65-71-4 |
| | IP from onset of photoelectron band. | | | | | | |
| $C_5H_6N_2O_2S^+$ | | | | | | | |
|  | 8.6 | (152) | (635) | −47 | −195 | *EST | 21035-65-4 |

**Table 1. Positive Ion Table - Continued**

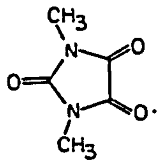
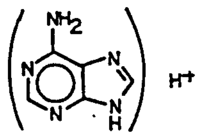
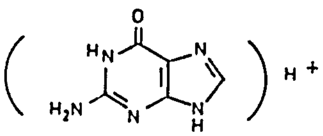
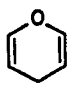
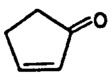
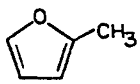
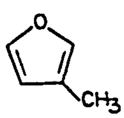
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_5H_6N_2O_3^+$ | | | | | | | |
|  | 10.19 | (≤124) | (≤519) | −111 | −464 | *EST | 5176-82-9 |
| | IP from 85ROT/BOC. | | | | | | |
| $C_5H_6N_5^+$ | | | | | | | |
|  | | 191 | 802 | | | | |
| | From proton affinity of adenine (RN 73-24-5). PA = 223.5 kcal/mol, 935. kJ/mol. | | | | | | |
| $C_5H_6N_5O^+$ | | | | | | | |
|  | | (143) | (599) | | | | |
| | From proton affinity of guanine (RN 73-40-5). PA = ~223 kcal/mol, ~933 kJ/mol. | | | | | | |
| $C_5H_6O^+$ | | | | | | | |
|  | 8.4 | (192) | (803) | −2±1 | −7±5 | *EST | 289-65-6 |
| | IP from 86SPI/GRU. | | | | | | |
|  | ≤9.34±0.02 | (≤196) | (≤823) | −19 | −78 | *EST | 930-30-3 |
|  | 8.39±0.01 | (174) | (730) | −19 | −80 | *EST | 534-22-5 |
| | IP from 78LIA/AUS, 77ROS/DRA. See also: 83ZYK/ERC, 86SPI/GRU. | | | | | | |
|  | (8.64) | (182) | (763) | −17 | −71 | *EST | 930-27-8 |
| | IP from 86SPI/GRU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

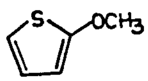
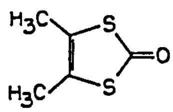
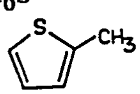
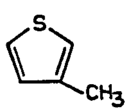
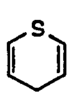
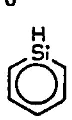
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_6OS^+$ | | | | | | | |
|  | (7.8) | (131) | (547) | −49 | −206 | *EST | 16839-97-7 |
| | IP is onset of photoelectron band (85BAJ/HUM). | | | | | | |
| $C_5H_6OS_2^+$ | | | | | | | |
|  | (≤8.5) | (≤177) | (≤740) | −19 | −80 | *EST | 49675-88-9 |
| | IP from 83SCH/SCH. | | | | | | |
| $C_5H_6O_3^+$ | | | | | | | |
| $CH_3(CO)_3CH_3$ | (≤9.52) | (≤115) | (≤482) | −104 | −437 | *EST | 921-11-9 |
| $C_5H_6S^+$ | | | | | | | |
|  | 8.61±0.02 | 218 | 914 | 20.0±0.2 | 83.5±0.8 | 77PED/RYL | 554-14-3 |
|  | (8.40) | (213) | (893) | 19.7±0.2 | 82.6±0.8 | 77PED/RYL | 616-44-4 |
|  | (7.9) | (224) | (940) | 42±2 | 178±8 | *EST | 289-70-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5H_6Si^+$ | | | | | | | |
|  | (7.8) | (197) | (824) | 17 | 71 | 83GOR/BOU | 289-77-0 |
| | IP is onset of photoelectron band (84BOC/ROS). | | | | | | |
| $C_5H_7^+$ | Fw says KN goes with | | | $CH_2=CH_2CHCH=CH\bullet$ | | | |
| $CH_2=CHCHCH=CH_2$ | (7.25) | (220) | (922) | 53 | 222 | 69GOL/BEN | 14362-08-4 |
| | See also: 80WOL/HOL. | | | | | | |
| $HC\equiv CC(CH_3)_2$ | (7.44) | (234) | (981) | 63 | 263 | 76LOS/TRA | 56897-57-5 |
| | See also: 80WOL/HOL. | | | | | | |

Table 1. Positive Ion Table - Continued

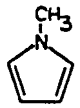
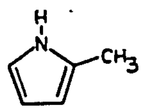
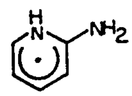
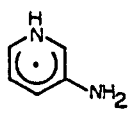
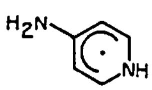
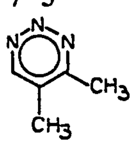
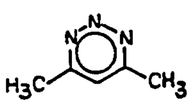
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_7^+$ | | | | | | | |
|  | 7.00 | 199 | 833 | 38 | 159 | 70FUR/GOL | 54846-63-8 |
| | Proton affinity of cyclopentadiene (RN 542-92-7) (PA = 199.6 kcal/mol, 835. kJ/mol) leads to $\Delta_f H$(Ion) = 197 kcal/mol, 826 kJ/mol. IP from 80WOL/HOL. | | | | | | |
| $C_5H_7N^+$ | | | | | | | |
|  | 7.94±0.02 | 207.6 | 869.2 | 24.6±0.1 | 103.1±0.5 | 77PED/RYL | 96-54-8 |
|  | (7.78±0.01) | (197) | (825) | 18±0.2 | 74±1 | *EST | 636-41-9 |
| $C_5H_7N_2^+$ | | | | | | | |
|  | | 170 | 711 | | | | |
| | From proton affinity of 2-pyridinamine (RN 504-29-0). PA = 223.8 kcal/mol, 936. kJ/mol. | | | | | | |
|  | | 179 | 747 | | | | |
| | From proton affinity of 3-pyridinamine (RN 462-08-8). PA = 221.0 kcal/mol, 925. kJ/mol. | | | | | | |
|  | | (169) | (706) | | | | |
| | From proton affinity of 4-pyridinamine (RN 504-24-5). PA = (230) kcal/mol, (962) kJ/mol. | | | | | | |
| $C_5H_7N_3^+$ | | | | | | | |
|  | (≤9.5) | (≤302) | (≤1263) | 83 | 346 | *EST | 86402-31-5 |
| | IP from 83GLE/SPA. | | | | | | |
|  | (≤9.5) | (≤300) | (≤1257) | 81 | 340 | *EST | 77202-09-6 |
| | IP from 83GLE/SPA. | | | | | | |

**Table 1. Positive Ion Table - Continued**

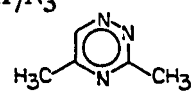
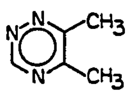
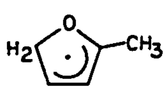
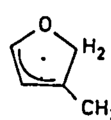
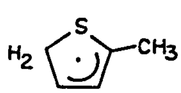
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_7N_3$ +** | | | | | | | |
|  | (≤9.02) | (≤268) | (≤1123) | 60 | 253 | *EST | 24108-34-7 |
|  | (≤9.15) | (≤274) | (≤1145) | 63 | 262 | *EST | 21134-90-7 |
| **$C_5H_7O$ +** | | | | | | | |
| $(CH_3)_2C=CHCO$ | | (138) | (577) | | | | 44391-34-6 |
| | $\Delta_f H$(Ion) from appearance potential determination (85ALA/ATT). | | | | | | |
|  | | 140 | 587 | | | | |
| | From proton affinity of 2-methylfuran (RN 534-22-5) (85HOU/ROL, 86MAU/LIE, 86SAN/BAL). PA = 206.2 kcal/mol, 863. kJ/mol. | | | | | | |
|  | | 145 | 606 | | | | |
| | From proton affinity of 3-methylfuran (RN 930-27-8) (85HOU/ROL). PA = 204.0 kcal/mol, 853. kJ/mol. | | | | | | |
| **$C_5H_7S$ +** | | | | | | | |
|  | | 180 | 754 | | | | |
| | From proton affinity of 2-methylthiophene (RN 554-14-3) (86MAU). PA = 205.4 kcal/mol, 859. kJ/mol. | | | | | | |
| **$C_5H_8$ +** | | | | | | | |
| $CH_2=C=CHCH_2CH_3$ | 9.22 | 246 | 1030 | 33.6±0.2 | 140.7±0.6 | 77PED/RYL | 591-95-7 |
| (Z)-$CH_2=CHCH=CHCH_3$ | 8.63±0.03 | 218 | 914 | 19.4±0.2 | 81.1±1.0 | 77PED/RYL | 1574-41-0 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_2=CHCH=CHCH_3$ | 8.59±0.02 | 216 | 905 | 18.2±0.1 | 76.3±0.6 | 77PED/RYL | 2004-70-8 |
| | IP from 81MAS/MOU. | | | | | | |
| $CH_2=CHCH_2CH=CH_2$ | (9.62±0.02) | (247) | (1034) | 25.3±0.2 | 105.7±0.6 | 77PED/RYL | 591-93-5 |
| $CH_3CH=C=CHCH_3$ | (8.7) | (232) | (972) | 31.8±0.2 | 133.1±0.7 | 77PED/RYL | 591-96-8 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

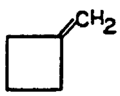
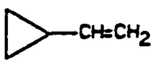
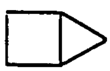
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_5H_8^+$ | | | | | | | |
| $CH_2=C(CH_3)CH=CH_2$ | 8.84±0.01 | 221.8 | 927.9 | 17.9±.2 | 75±1 | 77PED/RYL | 78-79-5 |
| | See also: 81MAS/MOU. | | | | | | |
| $C_3H_7C\equiv CH$ | 10.05 | 266 | 1114 | 34.4±1 | 144±4 | 79ROG/DAG | 627-19-0 |
| | IP from 81HOL/FIN. | | | | | | |
| $C_2H_5C\equiv CCH_3$ | 9.44±0.01 | 248 | 1039 | 30.6±1 | 128±4 | 79ROG/DAG | 627-21-4 |
| $(CH_3)_2CHC\equiv CH$ | 9.97 | 262 | 1098 | 32.5 | 136 | 69BEN/CRU | 598-23-2 |
| | IP from 81HOL/FIN. | | | | | | |
|  | 9.01±0.02 | 216 | 905 | 8.6 | 36 | 82ALL/DOD | 142-29-0 |
| | See also: 81KIM/KAT. | | | | | | |
|   | 9.16±0.02 | 241 | 1008 | 29.6±.2 | 124±1 | 78LEB/TSV | 1120-56-5 |
|   | (8.7) | (236) | (988) | 35.6±.2 | 149±1 | 77PED/RYL | 693-86-7 |
|  | (8.7±0.1) | (238) | (997) | 37.8 | 158 | 82WIB/WEN | 185-94-4 |
|  | (9.65) | (272) | (1139) | 49.7 | 208 | 82WIB/WEN | 311-75-1 |
|  | 9.26 | 258 | 1078 | 44.2±0.2 | 185.1±0.7 | 77PED/RYL | 157-40-4 |
| | See also: 86GLE/KRE. | | | | | | |

Table 1. Positive Ion Table - Continued

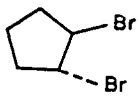
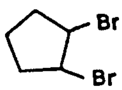
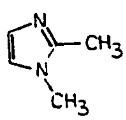
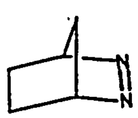
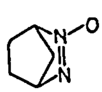
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_8Br_2{}^+$ | | | | | | | |
|  | 10.06 | (218) | (913) | −14 | −58 | *EST | 10230-26-9 |
|  | (10.02±0.02) | (217) | (909) | −14 | −58 | *EST | 33547-17-0 |
| $C_5H_8F_3O_2{}^+$ | | | | | | | |
| $CF_3C(OH)O(n\text{-}C_3H_7)$ | | −74 | −311 | | | | |
| | From proton affinity of $CF_3COO(n\text{-}C_3H_7)$ (RN 383-66-4). | | | | | | |
| $C_5H_8N_2{}^+$ | | | | | | | |
|  | (≤8.38) | (≤224) | (≤936) | 30 | 127 | *EST | 1739-84-0 |
|  | 8.45±0.04 | 244 | 1022 | 49±0.7 | 207±3 | 80ENG | 2721-32-6 |
| $C_5H_8N_2O^+$ | | | | | | | |
|  | (9.2) | (243) | (1015) | 30.55±0.3 | 127.8±1.4 | 83BYS | 22509-00-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_5H_8O^+$ | | | | | | | |
| (E)-$CH_3CH_2CH=CHCHO$ | (9.70) | (194) | (810) | −30 | −126 | 83HOL | 764-39-6 |
| $CH_3CH=C(CH_3)CHO$ | (9.60) | (188) | (787) | −33 | −139 | 83HOL | 497-03-0 |
| $C_2H_5COCH=CH_2$ | (9.50) | (186) | (781) | −33 | −136 | 83HOL | 1629-58-9 |
| (E)-$CH_3CH=CHC(=O)CH_3$ | (9.39) | (175) | (732) | −42 | −174 | 84BOU/HOP | 625-33-2 |
| $CH_2=C(CH_3)C(=O)CH_3$ | (9.50) | (177) | (741) | −42 | −176 | 84BOU/HOP | 814-78-8 |

Table 1. Positive Ion Table - Continued

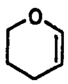
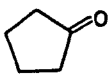
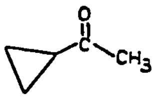
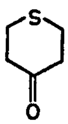
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_8O^+$** | | | | | | | |
| (E)-$CH_3OCH=CHCH=CH_2$ | (8.03) | (222) | (931) | 37 | 156 | *EST | 10034-09-0 |
|  | 8.34±0.01 | 162 | 679 | −29.9±0.4 | −125.2±1.5 | 77PED/RYL | 110-87-2 |
|  | 9.25±0.01 | 167 | 698 | −46±0.5 | −194±2 | 77PED/RYL | 120-92-3 |
| | See also: 82BIE/ASB. | | | | | | |
|  | 9.46 | 190 | 794 | −28±0.2 | −119±1 | 83FUC/SMI | 765-43-5 |
| **$C_5H_8OS^+$** | | | | | | | |
| (Z)-$CH_3C(=S)CH=C(OH)CH_3$ | (8.4) | (160) | (670) | −33 | −140 | *EST | 73059-87-7 |
| | IP is onset of photoelectron band (81JOR/CAR). | | | | | | |
| (Z)-$CH_3C=(SH)CHC(=O)CH_3$ | (≤8.73) | (≤168) | (≤702) | −33 | −140 | *EST | 65581-04-6 |
| | IP from 81JOR/CAR. | | | | | | |
|  | (8.90±0.05) | (168) | (704) | −37±0.7 | −155±3 | 77PED/RYL | 1072-72-6 |
| **$C_5H_8O_2^+$** | | | | | | | |
| $C_2H_5CH=CHCOOH$ | (10.14) | (144) | (601) | −90±2 | −377±8 | *EST | 626-98-2 |
| $(CH_3)_2C=CHCOOH$ | (9.63) | (124) | (519) | −98 | −410 | *EST | 541-47-9 |
| $CH_3CH=C(CH_3)COOH$ | (9.50) | (121) | (507) | −98 | −410 | *EST | 13201-46-2 |
| $CH_2=C(C_2H_5)COOH$ | (10.06) | (139) | (582) | −93 | −389 | *EST | 3586-58-1 |
| $CH_2=C(CH_3)CH_2COOH$ | (9.52) | (128) | (536) | −92 | −383 | *EST | 53774-20-2 |

**Table 1. Positive Ion Table - Continued**

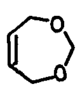
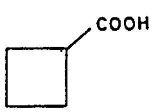
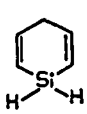
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_8O_2{}^+$ | | | | | | | |
| $CH_3CH=CHCH_2COOH$ | (9.41) | (126) | (527) | −91 | −381 | *EST | 1617-32-9 |
| $CH_2=CHCOOC_2H_5$ | (>10.3) | (>147) | (>617) | −90 | −377 | *EST | 140-88-5 |
| | IP from 82MOR/MER. | | | | | | |
| $CH_2=C(CH_3)COOCH_3$ | (9.7) | (141) | (588) | −83 | −348 | 80VIL/PER | 80-62-6 |
| | IP is onset of photoelectron band(78VAN/OSK). | | | | | | |
| $CH_3COCH_2COCH_3$ | 8.85±0.02 | 112 | 470 | −92±0.2 | −384±1 | 79HAC/PIL | 123-54-6 |
| | Enol form, $CH_3COCH=C(OH)CH_3$, is preferred. | | | | | | |
| $CH_2=C(CH_3)OC(=O)CH_3$ | 9.1 | 126 | 529 | −83 | −349 | 77PED/RYL | 108-22-5 ~~591-87-7~~ |
| | IP is onset of photoelectron band (78VAN/OSK). See also: 82LEV/LIA. | | | | | | |
|  | ≤9.54 | (≤163) | (≤682) | −57 | −238 | *EST | 5417-32-3 |
| | IP from 82ZVE/VIL. | | | | | | |
|  | (10.35) | (154) | (645) | −85 | −354 | *EST | 3721-95-7 |
| $C_5H_8Si^+$ | | | | | | | |
|  | (9.1) | (238) | (997) | 28 | 119 | *EST | 81200-77-3 |
| | IP is onset of photoelectron band (84BOC/ROS). | | | | | | |
| $C_5H_9{}^+$ | | | | | | | |
| $CH_2=CHCHCH_2CH_3$ | (7.30) | (193) | (810) | 25 | 106 | 76LOS/TRA | 17829-37-7 |
| $CH_3CHCH=CHCH_3$ | (7.07) | (182) | (763) | (22) | (92) | 76LOS/TRA | 51685-67-7 |
| | Heat of formation of ion from proton affinity of (E)-1,3-pentadiene (RN 2004-70-8). PA = (201.8) kcal/mol, (844.) kJ/mol. | | | | | | |
| $CH_3CH=CC_2H_5$ | | 200 | 838 | | | | |
| | From proton affinity of 2-pentyne (RN 627-21-4). PA = (196) kcal/mol, (820) kJ/mol. | | | | | | |
| $(CH_3)_2CCH=CH_2$ | (7.13) | (183) | (767) | 19 | 81 | 76LOS/TRA | 29791-12-6 |
| | Heat of formation of ion from proton affinity of 2-methyl-1,3-butadiene (RN 78-79-5). PA = (200.4) kcal/mol, (838.) kJ/mol. See also: 85LAD/HAR. | | | | | | |

Table 1. Positive Ion Table - Continued

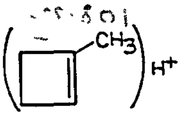
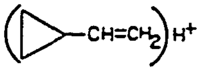
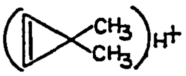
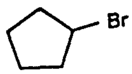
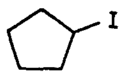
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_9^+$** | | | | | | | |
| $(CH_3)_2CHC=CH_2$ | | (200) | (838) | | | | |
| | From proton affinity of 3-methyl-1-butyne (RN 598-23-2). PA = (198) kcal/mol, (828) kJ/mol. | | | | | | |
| $CH_3CH=C(CH_3)CH_2$ | | 190 | 797 | | | | 60288-51-9 |
| | Heat of formation of ion from appearance potential measurements (84LOS/HOL). | | | | | | |
|  | 7.21 | 191.4 | 800.8 | 24±1 | 102±4 | 82MCM/GOL | 3889-74-5 |
| | Value of $\Delta_f H$(Ion) from hydride and chloride transfer equilibrium constant determinations (76SOL/FIE, 85SHA/SHA), and from proton affinity of cyclopentene (84LIA/LIE). PA = 183.4 kcal/mol, 767.5 kJ/mol. IP from 79HOU. $\Delta_f H$(Ion)-IP leads to $\Delta_f H$(Neutral) = 25 kcal/mol, 105 kJ/mol. | | | | | | |
|  | | (193) | (807) | | | | 53249-17-5 |
| | From proton affinity of 1-methylcyclobutene (RN 1489-60-7). PA = 201 kcal/mol, 841 kJ/mol. | | | | | | |
|  | | 204 | 852 | | | | |
| | From proton affinity of vinylcyclopropane (RN 693-86-7). PA = 197.6 kcal/mol, 827. kJ/mol. | | | | | | |
|  | | (213) | (890) | | | | 63974-90-3 |
| | From proton affinity of 3,3-dimethylcyclopropene (RN 3907-06-0). PA = 203 kcal/mol, 849 kJ/mol. | | | | | | |
| **$C_5H_9Br^+$** | | | | | | | |
|  | (9.94±0.02) | (213) | (891) | −16 | −68 | *EST | 137-43-9 |
| **$C_5H_9BrO^+$** | | | | | | | |
| $(CH_3)_2CBrCOCH_3$ | (9.35) | (154) | (646) | −61 | −256 | *EST | 26497-[illegible]1-7 |
| | IP from 84BOU/DAG. | | | | | | |
| **$C_5H_9I^+$** | | | | | | | |
|  | 9.07 | (206) | (861) | −3 | −14 | *EST | 1556-18-9 |

Table 1. Positive Ion Table - Continued

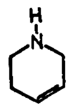
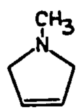
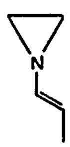
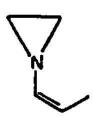
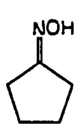
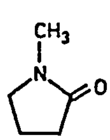
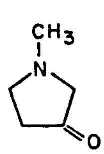
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_9N^+$ | | | | | | | |
| n-$C_4H_9NC$ | (11.1) | (280) | (1173) | 24±0.5 | 102±2 | *EST | 2769-64-4 |
| $(CH_3)_2NCH_2C{\equiv}CH$ | (8.17) | (242) | (1013) | 54±1 | 225±5 | *EST | 7223-38-3 |
| | See also: 81LOG/TAK. | | | | | | |
|  | (8.0) | (201) | (845) | 17 | 73 | 74PIH/TAS | 694-05-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.21±0.05) | (≤216) | (≤907) | 27±0.5 | 115±2 | *EST | 554-15-4 |
|  | (7.9) | (224) | (939) | 42 | 177 | *EST | |
| | IP is onset of photoelectron band (81MUL/PRE). | | | | | | |
|  | (8.0) | (227) | (949) | 42 | 177 | *EST | |
| | IP from 81MUL/PRE. | | | | | | |
| $C_5H_9NO^+$ | | | | | | | |
| n-$C_4H_9NCO$ | (10.14±0.05) | (186) | (776) | −48 | −202 | *EST | 111-36-4 |
| tert-$C_4H_9CNO$ | ≤9.55±0.005 | (≤223) | (≤931) | 2 | 10 | *EST | 27143-81-3 |
|  | (8.92±0.03) | (193) | (809) | −12 | −52 | *EST | 1192-28-5 |
| | IP from 79GOL/KUL. | | | | | | |
|  | ≤9.17 | ≤161 | ≤674 | −50 | −211 | 77PED/RYL | 872-50-4 |
| | IP from 85TRE/RAD. | | | | | | |
|  | (8.3) | (165) | (691) | −26 | −110 | *EST | 68165-06-0 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

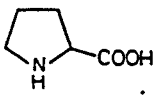
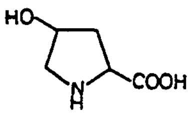
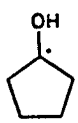
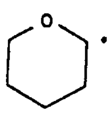
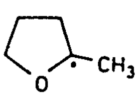
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_9NO_2^+$ | | | | | | | |
|  | (8.3) | (104) | (435) | -87±1 | -366±4 | 78SAB/LAF | 609-36-9 |
| | IP is onset of photoelectron band(83CAN/HAM). | | | | | | |
| $C_5H_9NO_3^+$ | | | | | | | |
| $CH_3CONHCH(CH_3)COOH$ | (9.2) | (62) | (260) | -150 | -628 | *EST | 97-69-8 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
|  | (≤9.1) | (≤87) | (≤362) | -123 | -516 | 77PED/RYL | 51-35-4 |
| | IP from 83CAN/HAM. | | | | | | |
| $C_5H_9O^+$ | | | | | | | |
| $CH_3C(OH)C(CH_2)CH_3$ | | 121 | 507 | | | | |
| | From proton affinity of $CH_3C(=O)C(=CH_2)CH_3$ (RN 814-78-8) (84BOU/HOP). PA = 202.4 kcal/mol, 847. kJ/mol. | | | | | | |
| (E)-$CH_3CHCHC(OH)CH_3$ | | 117 | 491 | | | | |
| | From proton affinity of (E)-$CH_3CH=CHC(=O)CH_3$ (RN 625-33-2) (84BOU/HOP). PA = 206.7 kcal/mol, 865. kJ/mol. | | | | | | |
|  | | 121 | 506 | | | | |
| | From proton affinity of cyclopentanone (RN 120-92-3). PA = 198.8 kcal/mol, 832. kJ/mol. | | | | | | |
|  | | 129 | 539 | | | | |
| | From proton affinity of 3,4-dihydro-4H-pyran (RN 110-87-2) (86BOU/HAN). PA = 206.9 kcal/mol, 866. kJ/mol. | | | | | | |
|  | | 121 | 507 | | | | |
| | From proton affinity of 2-methyl-4,5-dihydrofuran (RN 1487-15-6) (86BOU/DJA). PA = 215.6 kcal/mol, 902. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

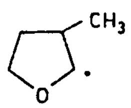
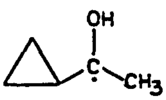
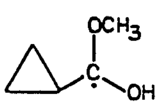
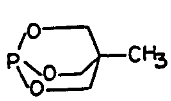
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_9O^+$** | | | | | | | |
|  | | 132 | 552 | | | | |
| | From proton affinity of 3-methyl-4,5-dihydrofuran (RN 557-31-3) (86BOU/DJA). PA = 207.0 kcal/mol, 866. kJ/mol. | | | | | | |
|  | | 133 | 555 | | | | |
| | From proton affinity of 1-cyclopropylethanone (RN 765-43-5). PA = 205.1 kcal/mol, 858. kJ/mol. | | | | | | |
| **$C_5H_9O_2^+$** | | | | | | | |
| $CH_3C(OH)CHC(OH)CH_3$ | | 66 | 277 | | | | |
| | From proton affinity of $CH_3COCH=C(OH)CH_3$ (RN 123-54-6). PA = 207.8 kcal/mol, 869. kJ/mol. | | | | | | |
|  | | 89 | 373 | | | | |
| | From proton affinity of methylcyclopropane carboxylate (RN 2868-37-3). PA = 202.9 kcal/mol, 849. kJ/mol. | | | | | | |
| **$C_5H_9O_3P^+$** | | | | | | | |
|  | (9.2) | (76) | (317) | −136 | −571 | *EST | 1449-91-8 |
| | IP is onset of photoelectron band. (77COW/GOO). | | | | | | |
| **$C_5H_{10}^+$** | | | | | | | |
| $1\text{-}C_5H_{10}$ | 9.52±0.02 | 214 | 897 | −5.1±0.1 | −21.4±0.4 | 84WIB/WAS | 109-67-1 |
| | | *221.5* | *926.9* | *2.0* | *8.4* | | |
| | See also: 83HOL/LOS, 86TRA, 84BRA/BAE. | | | | | | |
| $2\text{-}(Z)\text{-}C_5H_{10}$ | 9.036±0.005 | 202.0 | 845.3 | −6.3±0.1 | −26.5±0.4 | 84WIB/WAS | 627-20-3 |
| | See also: 86TRA. | | | | | | |
| $2\text{-}(E)\text{-}C_5H_{10}$ | 9.036±0.005 | 200.8 | 840.3 | −7.5±0.1 | −31.5±0.4 | 84WIB/WAS | 646-04-8 |
| | | *208.0* | *870.1* | *−0.4* | *−1.7* | | |
| | See also: 84BRA/BAE. | | | | | | |
| $(CH_3)_2CHCH=CH_2$ | 9.52±0.02 | 213 | 891 | −6.5±0.2 | −27.4±0.6 | 77PED/RYL | 563-45-1 |
| | | *220.3* | *921.6* | *0.7* | *3.1* | | |
| | See also: 84BRA/BAE. | | | | | | |
| $C_2H_5C(CH_3)=CH_2$ | 9.13±0.03 | 202 | 845 | −8.5±0.2 | −35.6±0.7 | 77PED/RYL | 563-46-2 |
| | | *209.3* | *875.8* | *−1.2* | *−5.1* | | |
| | See also: 86TRA, 84BRA/BAE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

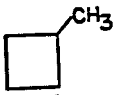
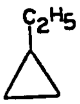
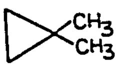
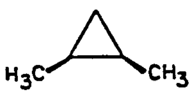
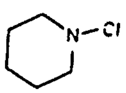
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_5H_{10}^+$ | | | | | | | |
| $(CH_3)_2C=CHCH_3$ | 8.68±0.01 | 190 | 795 | −10.1±0.1 | −42.1±0.6 | 77PED/RYL | 513-35-9 |
| | | *197.4* | *825.8* | *−2.8* | *−11.6* | | |
| | See also: 86TRA, 84BRA/BAE. | | | | | | |
|  | 10.51±0.05 | 224 | 936 | −18.7±0.2 | −78.4±0.8 | 77PED/RYL | 287-92-3 |
| | | *231.8* | *969.8* | *−10.6* | *−44.2* | | |
| | See also: 81MAU/SIE, 81KIM/KAT, 86TRA, 84BRA/BAE. | | | | | | |
|  | (9.60) | (221) | (923) | −0.7 | −3 | *EST | 598-61-8 |
|  | (9.50) | (218) | (912) | −1 | −5 | 77PED/RYL | 1191-96-4 |
|  | (9.08) | (207) | (868) | −2 | −8 | 77PED/RYL | 1630-94-0 |
| | See also: 81PLE/VIL. | | | | | | |
|  | (9.76±0.02) | (225) | (942) | 0 | 0 | 77PED/RYL | 930-18-7 |
|  | (9.73±0.02) | (223) | (934) | −1 | −5 | 77PED/RYL | 2402-06-4 |
| $C_5H_{10}Br_2^+$ | | | | | | | |
| $Br(CH_2)_5Br$ | (≤10.23) | (≤207) | (≤868) | −28 | −119 | *EST | 111-24-0 |
| $C_5H_{10}ClN^+$ | | | | | | | |
|  | (8.5) | (208) | (871) | 12 | 51 | *EST | 2156-71-0 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

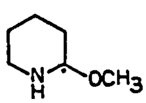
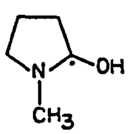
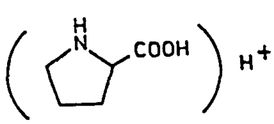
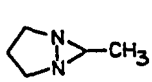
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{10}N^+$** | | | | | | | |
| n-$C_4H_9$CNH | | 174 | 728 | | | | |
| | From proton affinity of n-$C_4H_9$CN (RN 110-59-8). PA = 194.0 kcal/mol, 812. kJ/mol. | | | | | | |
| t-$C_4H_9$CNH | | 169 | 709 | | | | |
| | From proton affinity of t-$C_4H_9$CN (86MAR/TOP, 86MAU/KAR). PA = 195.7 kcal/mol, 819. kJ/mol. | | | | | | |
| t-$C_4H_9$NCH | | 178 | 744 | | | | |
| | From proton affinity of t-$C_4H_9$NC (RN 7188-38-7) (86MAU/KAR). PA = 207.5 kcal/mol, 868 kJ/mol. | | | | | | |
| **$C_5H_{10}NO^+$** | | | | | | | |
|  | | 103 | 433 | | | | |
| | From proton affinity of 2-methoxy-1-pyrroline (RN 5264-35-7). PA = 225.9 kcal/mol, 945. kJ/mol. | | | | | | |
|  | | 98 | 412 | | | | |
| | From proton affinity of 1-methyl-2-pyrrolidinone (RN 872-50-4). PA = 216.8 kcal/mol, 907. kJ/mol. | | | | | | |
| **$C_5H_{10}NO_2^+$** | | | | | | | |
|  | | 58 | 243 | | | | |
| | From proton affinity of L-proline (RN 609-36-9). PA = 220.2 kcal/mol, 921. kJ/mol. | | | | | | |
| **$C_5H_{10}NO_3^+$** | | | | | | | |
| $CH_3C(OH)NHCH_2COOCH_3$ | | 8 | 34 | | | | |
| | From proton affinity of $CH_3CONHCH_2COOCH_3$. PA = 217.7 kcal/mol, 911. kJ/mol. | | | | | | |
| **$C_5H_{10}NO_4^+$** | | | | | | | |
| L-$HOOC(CH_2)_2CH(NH_3)COOH$ | | 29 | 121 | | | | |
| | From proton affinity of L-$HOOC(CH_2)_2CH(NH_2)COOH$ (RN 617-65-2). PA = 216.5 kcal/mol, 906. kJ/mol. | | | | | | |
| **$C_5H_{10}N_2^+$** | | | | | | | |
|  | (≤8.78) | (≤264) | (≤1108) | 62 | 261 | *EST | 6794-96-3 |

**Table 1. Positive Ion Table - Continued**

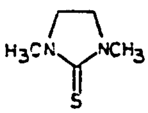
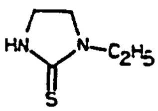
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{10}N_2S^+$** | | | | | | | |
|  | ≤7.95 | (≤208) | (≤869) | 24 | 102 | *EST | 13461-16-0 |
| | See also: 80AND/DEV. | | | | | | |
|  | (7.7) | (194) | (813) | 17 | 70 | *EST | 29704-02-7 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |
| **$C_5H_{10}N_4^+$** | | | | | | | |
| $NCN=C(N(CH_3)_2)(NHCH_3)$ | (8.2) | (227) | (950) | 38 | 159 | *EST | 17686-53-2 |
| | IP is onset of photoelectron band (80KLA/BUT). | | | | | | |
| **$C_5H_{10}O^+$** | | | | | | | |
| n-$C_4H_9CHO$ | 9.74±0.04 | 169 | 709 | −55.1±0.5 | −230.5±2 | 77PED/RYL | 110-62-3 |
| | See also: 81HOL/FIN. | | | | | | |
| sec-$C_4H_9CHO$ | (9.59±0.01) | (165) | (689) | −56 | −236 | *EST | 96-17-3 |
| iso-$C_4H_9CHO$ | 9.70±0.02 | (167) | (699) | −57 | −237 | *EST | 590-86-3 |
| | See also: 81HOL/FIN. | | | | | | |
| tert-$C_4H_9CHO$ | 9.50 | (161) | (673) | −58 | −244 | *EST | 630-19-3 |
| n-$C_3H_7COCH_3$ | 9.38±0.01 | 154.4 | 645.9 | −61.9±0.2 | −259.1±0.8 | 77PED/RYL | 107-87-9 |
| | See also: 84OLI/GUE. | | | | | | |
| $(C_2H_5)_2CO$ | 9.31±0.01 | 153.0 | 639.9 | −61.7±0.2 | −258.4±0.7 | 77PED/RYL | 96-22-0 |
| | See also: 81HOL/FIN. | | | | | | |
| iso-$C_3H_7COCH_3$ | 9.30±0.01 | 151.8 | 634.9 | −62.7±0.2 | −262.4±0.8 | 77PED/RYL | 563-80-4 |
| $CH_2=CHCH_2CH_2CH_2OH$ | (9.42±0.05) | (176) | (737) | −41 | −172 | *EST | 821-09-0 |
| | IP from 83HOL/LOS. | | | | | | |
| $CH_2=CHC(CH_3)_2OH$ | (≤9.90) | (≤198) | (≤830) | −30 | −125 | 84GUB/GER | 115-18-4 |
| $CH_2=CHCH_2CH(OH)CH_3$ | (9.38±0.05) | (171) | (717) | −45 | −188 | *EST | 625-31-0 |
| | IP from 83HOL/LOS. | | | | | | |
| $CH_2=CHCH(OH)CH_2CH_3$ | 9.40±0.05 | (173) | (725) | −43 | −182 | *EST | 616-25-1 |
| | IP from 83HOL/LOS. See also: 84ZWI/HAR. | | | | | | |

Table 1. Positive Ion Table – Continued

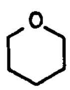
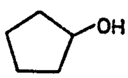
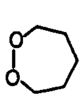
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_{10}O^+$ | | | | | | | |
| $CH_2{=}CHOCH(CH_3)_2$ | | | | | | | |
| | (≤8.90) | (≤164) | (≤685) | −42±1 | −174±5 | 81TRO/NED | 926-65-8 |
|  | 9.25±0.01<br>See also: 81KIM/KAT. | 160 | 669 | −53.3±0.2 | −223.0±0.7 | 77PED/RYL | 142-68-7 |
|  | 9.72<br>IP from 85TRA. | 166 | 695 | −58.0±0.3 | −242.6±1.2 | 77PED/RYL | 96-41-3 |
| $C_5H_{10}OS^+$ | | | | | | | |
| $CH_3COCH_2SCH_2CH_3$ | | | | | | | |
| | (≤8.72)<br>IP from 84OLI/GUE. | (≤153) | (≤638) | −49 | −203 | *EST | 20996-62-7 |
| $C_5H_{10}O_2^+$ | | | | | | | |
| n-$C_4H_9COOH$ | (≤10.53) | (≤126) | (≤526) | −117±0.5 | −490±2 | 77PED/RYL | 109-52-4 |
| iso-$C_4H_9COOH$ | (≤10.51) | (≤119) | (≤499) | −123±1 | −515±6 | 77PED/RYL | 503-74-2 |
| tert-$C_4H_9COOH$ | (10.08)<br>IP from 81HOL/FIN. | (110) | (460) | −122 | −512 | *EST | 75-98-9 |
| $HCOO(CH_2)_3CH_3$ | 10.50±0.02 | (139) | (583) | −103 | −430 | *EST | 592-84-7 |
| $CH_3COOCH_2CH_2CH_3$ | | | | | | | |
| | 10.04±0.03 | (123) | (515) | −109 | −454 | *EST | 109-60-4 |
| $CH_3COOCH(CH_3)_2$ | 9.99±0.03 | 115 | 482 | −115.1±0.1 | −481.5±0.6 | 77PED/RYL | 108-21-4 |
| $C_2H_5COOC_2H_5$ | (10.00±0.02) | (120) | (501) | −111±0.5 | −464±2 | 77PED/RYL | 105-37-3 |
| n-$C_3H_7COOCH_3$ | 10.07±0.03 | (124) | (520) | −108 | −452 | *EST | 623-42-7 |
| iso-$C_3H_7COOCH_3$ | 9.86<br>IP from 83BUR/HOL3. | 118 | 495 | −109±0.2 | −456±1 | 83FUC/SMI | 547-63-1 |
|  | (≤9.75) | (≤190) | (≤797) | −34 | −144 | *EST | 505-63-5 |

**Table 1. Positive Ion Table - Continued**

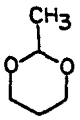
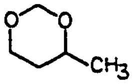
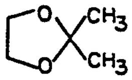
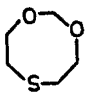
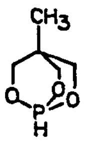
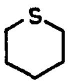
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_{10}O_2{}^+$ | | | | | | | |
|  | (9.45) | (135) | (565) | −83±0.5 | −347±2 | 77PED/RYL | 505-65-7 |
|  | (≤10.03)<br>IP from 84ASF/ZYK | (≤136) | (≤570) | −95.1±0.07 | −397.8±2.9 | 77PED/RYL | 626-68-6 |
|  | (≤10.04)<br>IP from 84ASF/ZYK. | (≤141) | (≤592) | −90.1±0.7 | −376.9±3.1 | 77PED/RYL | 1120-97-4 |
|  | (9.2)<br>IP is onset of photoelectron band. | (120) | (502) | −92±0.2 | −386±1 | *EST | 2916-31-6 |
| $C_5H_{10}O_2S^+$ | | | | | | | |
|  | 8.67±0.05<br>IP from 72CON/COL. | 128 | 537 | −72 | −300 | 72CON/COL | 2094-92-0 |
| $C_5H_{10}O_3P^+$ | | | | | | | |
|  | From proton affinity of 4-methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane (RN 1449-91-8). PA = 210.0 kcal/mol, 879. kJ/mol. | 19 | 80 | | | | |
| $C_5H_{10}S^+$ | | | | | | | |
| $CH_2{=}CHCH_2SC_2H_5$ | (8.51±0.01) | (200) | (839) | 4±0.7 | 18±3 | 77PED/RYL | 5296-62-8 |
|  | (8.2)<br>IP is onset of photoelectron band (80SAR/WOR, 82LEV/LIA). | (174) | (730) | −15.2±0.2 | −63.5±0.7 | 77PED/RYL | 1613-51-0 |

Table 1. Positive Ion Table - Continued

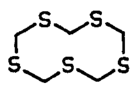
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_{10}S_5^+$ | | | | | | | |
|  | (7.6) | (197) | (823) | 22 | 90 | *EST | 2372-99-8 |
| | IP is onset of photoelectron band (81BOC/SCH). | | | | | | |
| $C_5H_{11}^+$ | | | | | | | |
| 1-$C_5H_{11}$ | (7.85) | (194) | (812) | 13 | 56 | *EST | 2672-01-7 |
| | $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. IP estimated by J.L. Holmes, personal communication. | | | | | | |
| $CH_3CH_2CH_2CHCH_3$ | (7.1) | (175) | (732) | 12 | 50 | *EST | 2492-34-4 |
| | Cited ionization potential is difference between heats of formation of ion and neutral. $\Delta_f H$(Neutral) based on D[C-H] = 99 kcal/mol. Experimental value = 7.41 eV. | | | | | | |
| $(CH_3)_2CCH_2CH_3$ | 6.6 | 158±1 | 661±4 | 6.5 | 27 | *EST | 4348-35-0 |
| | $\Delta_f H$(Ion) from hydride transfer equilibrium constant determinations (75SOL/FIE, 76GOR/MUN). $\Delta_f H$(Neutral) based on D[C-H] = 95.5 kcal/mol. IP given is $\Delta_f H$(Ion) -$\Delta_f H$(Neutral). Experimental IP of radical = 6.65 eV (86KRU/BEA). | | | | | | |
| $(CH_3)_3CCH_2$ | 7.88±0.05 | (190) | (795) | 8 | 33 | *EST | 3744-21-6 |
| | IP from 84SCH/HOU. $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | | | | | | |
| $C_5H_{11}Br^+$ | | | | | | | |
| n-$C_5H_{11}Br$ | 10.09±0.02 | 202 | 844 | −30.8±0.3 | −129.1±1.4 | 77PED/RYL | 110-53-2 |
| $(CH_3)_3CCH_2Br$ | 10.04 | 196 | 822 | −35 | −147 | 81HOL/FIN | 630-17-1 |
| $C_5H_{11}ClHg^+$ | | | | | | | |
| n-$C_5H_{11}HgCl$ | ≤9.99 | (≤200) | (≤835) | −31 | −129 | *EST | 544-15-0 |
| | IP from 81BAI/CHI2. | | | | | | |
| iso-$C_5H_{11}HgCl$ | ≤9.95 | (≤197) | (≤823) | −33 | −137 | *EST | 17774-08-2 |
| | IP from 81BAI/CHI2. | | | | | | |
| $C_5H_{11}I^+$ | | | | | | | |
| n-$C_5H_{11}I$ | 9.201 | (195) | (816) | −17 | −72 | *EST | 628-17-1 |
| $(CH_3)_2C(C_2H_5)I$ | (8.93) | (184) | (769) | −22 | −93 | *EST | 594-38-7 |
| $CH_2ICH_2CH(CH_3)_2$ | 9.192 | (193) | (807) | −19 | −80 | *EST | 541-28-6 |
| $C_5H_{11}N^+$ | | | | | | | |
| $C_2H_5CH=NC_2H_5$ | (8.7) | (201) | (839) | 0 | 0 | 69BEN/CRU | 18328-91-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $(CH_3)_2C=NC_2H_5$ | (8.83) | (195) | (816) | −9±2 | −36±9 | *EST | 15673-04-8 |
| | See also: 79AUE/BOW. | | | | | | |

Table 1. Positive Ion Table - Continued

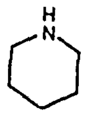
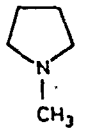
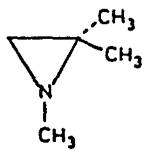
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{11}N^+$** | | | | | | | |
| $(CH_3)_2NCH_2CH=CH_2$ | | | | | | | |
| | 7.84 | 195 | 813 | 14 | 57 | 70BEN/O'N | 2155-94-4 |
| | See also: 81LOG/TAK. | | | | | | |
|  | 8.05±0.05 | 174 | 728 | −11.7±0.4 | −48.9±1.5 | 77PED/RYL | 110-89-4 |
| | See also: 82ROZ/HOU. | | | | | | |
|  | (≤8.41±0.02) | (≤193) | (≤809) | −0.5±0.5 | −2±2 | *EST | 120-94-5 |
| | $\Delta_f H$(Ion) from hydrogen affinities of homologues, 178kcal/mol; 746 kJ/mol; corresponding IP, 7.8 eV. | | | | | | |
|  | (≤8.68±0.02) | (≤201) | (≤842) | 1 | 5 | *EST | 23132-47-0 |
| **$C_5H_{11}NO^+$** | | | | | | | |
| $(CH_3)_2NCH_2COCH_3$ | | | | | | | |
| | (7.71) | (135) | (567) | −42 | −177 | 81LOG/TAK | 15364-56-4 |
| | IP from 81LOG/TAK. See also: 84OLI/GUE. | | | | | | |
| **$C_5H_{11}NO_2^+$** | | | | | | | |
| $H_2N(CH_2)_4COOH$ | (≤9.4) | (≤107) | (≤447) | −110±.7 | −460±3 | 83SKO/SAB | 660-88-8 |
| n-$C_3H_7CH(NH_2)COOH$ | | | | | | | |
| | (8.53) | (87) | (364) | −110±2 | −459±10 | *EST | 6600-40-4 |
| L-iso-$C_3H_7CH(NH_2)COOH$ | | | | | | | |
| | (8.71) | (92) | (385) | −108.8±0.2 | −455.1±1.0 | 77PED/RYL | 72-18-4 |
| $(CH_3)_2NCH_2COOCH_3$ | | | | | | | |
| | (7.96) | (98) | (411) | −85 | −357 | 81LOG/TAK | 7148-06-3 |
| | IP from 81LOG/TAK. | | | | | | |
| **$C_5H_{11}NO_2S^+$** | | | | | | | |
| L-$CH_3SCH_2CH_2CH(NH_2)COOH$ | | | | | | | |
| | (8.3) | (92) | (387) | −99±1 | −414±4 | 81SAB/MIN | 59-51-8 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| **$C_5H_{11}N_2O_3^+$** | | | | | | | |
| L-$H_2NCO(CH_2)_2CH(NH_3)COOH$ | | | | | | | |
| | | 73 | 304 | | | | |
| | From proton affinity of L-$H_2NCO(CH_2)_2CH(NH_2)COOH$ (RN 585-21-7). PA = 218.4 kcal/mol, 914. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

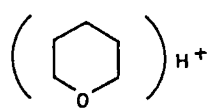
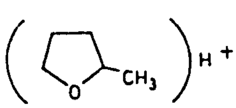
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{11}O^+$** | | | | | | | |
| i-$C_3H_7C(OH)CH_3$ | | 102 | 427 | | | | |
| | From proton affinity of i-$C_3H_7COCH_3$ (RN 563-80-4). PA = 201.1 kcal/mol, 841. kJ/mol. | | | | | | |
| n-$C_4H_9CHOH$ | | 118 | 493 | | | | |
| | From proton affinity of n-$C_4H_9CHO$ (RN 110-62-3). PA = 192.6 kcal/mol, 806. kJ/mol. | | | | | | |
| $(CH_3)_2COC_2H_5$ | | (104) | (435) | | | | |
| | From appearance potential determination (82MAC). | | | | | | |
| $(C_2H_5)_2COH$ | | 102 | 429 | | | | |
| | From proton affinity of $(C_2H_5)_2CO$ (RN 96-22-0). PA = 201.4 kcal/mol, 843. kJ/mol. | | | | | | |
| $C_2H_5OCHCH_2CH_3$ | | (114) | (476) | | | | |
| | From proton affinity of $C_2H_5OCH{=}CHCH_3$ (86BOU/DJA). PA = (210.) kcal/mol, (880.) kJ/mol. ← needs RN check with Rhoda | | | | | | |
| $C_2H_5O(H)CH_2CHCH_2$ | | (132) | (552) | | | | |
| | From proton affinity of $C_2H_5OCH_2CH{=}CH_2$. (PA = ?)/(RN = ?) ← RHODA | | | | | | |
|  | | 113 | 472 | | | | |
| | From proton affinity of tetrahydropyran (RN 142-68-7). PA = 199.7 kcal/mol, 835.5 kJ/mol. | | | | | | |
|  | | 110 | 461 | | | | |
| | From proton affinity of 2-methyltetrahydrofuran (RN 96-47-9). PA = 203.6 kcal/mol, 852. kJ/mol. | | | | | | |
| **$C_5H_{11}O_2^+$** | | | | | | | |
| $HC(OH)(O\text{-}n\text{-}C_4H_9)$ | | 68 | 285 | | | | |
| | From proton affinity of $HCOO(n\text{-}C_4H_9)$ (RN 592-84-7). PA = 194.8 kcal/mol, 815. kJ/mol. | | | | | | |
| n-$C_3H_7C(OH)(OCH_3)$ | | 57 | 241 | | | | |
| | From proton affinity of $C_3H_7COOCH_3$ (RN 623-42-7). PA = 200.1 kcal/mol, 837. kJ/mol. | | | | | | |
| $CH_3C(OH)(O\text{-}C_3H_7)$ | | 57 | 237 | | | | |
| | From proton affinity of $CH_3COOC_3H_7$ (RN 109-60-4). PA = 200.6 kcal/mol, 839. kJ/mol. | | | | | | |
| i-$C_3H_7C(OH)OCH_3$ | | 55 | 231 | | | | |
| | From proton affinity of i-$C_3H_7COOCH_3$ (RN 547-63-7). PA = 201.6 kcal/mol, 843. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

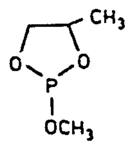
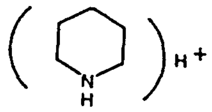
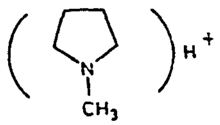
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_{11}O_3P^+$ | | | | | | | |
|  | (8.7) | (22) | (93) | −178 | −746 | *EST | 33892-95-4 |
| | IP is onset of photoelectron band (81ARS/ZVE). | | | | | | |
| $C_5H_{12}^+$ | | | | | | | |
| n-$C_5H_{12}$ | 10.35±0.01 | 204 | 852 | −35.0±0.1 | −146.5±0.4 | 77PED/RYL | 109-66-0 |
| | | *211* | *884* | *−27.3±0.1* | *−114.2±0.4* | | |
| | See also: 81MAU/SIE, 82LIA, 81KIM/KAT. | | | | | | |
| iso-$C_5H_{12}$ | ≤10.22 | ≤199 | ≤832 | −36.7±0.1 | −153.8±0.5 | 77PED/RYL | 78-78-4 |
| | | *≤207* | *≤867* | *−28.4* | *−118.8* | | |
| | IP from 81TRA. See also: 81KIM/KAT. | | | | | | |
| neo-$C_5H_{12}$ | ≤10.21±0.04 | ≤195 | ≤818 | −40.0±0.1 | −167.4±0.7 | 77PED/RYL | 463-82-1 |
| | | *≤203* | *≤850* | *−32.4* | *−135.6* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $C_5H_{12}Cl^+$ | | | | | | | |
| $(CH_3)_3CClCH_3$ | | (137) | (572) | | | | |
| | From equilibrium constant determination (85SHA/HOJ). | | | | | | |
| $C_5H_{12}N^+$ | | | | | | | |
| $(CH_3)_2CNHC_2H_5$ | | (128) | (534) | | | | |
| | From proton affinity of $(CH_3)_2C=NC_2H_5$ (RN 15673-04-8). PA = (229.5) kcal/mol, (960.) kJ/mol. | | | | | | |
| $CH_3CH_2CHN(CH_3)_2$ | | 142 | 596 | | | | |
| | From proton affinity of $CH_3CH=CHN(CH_3)_2$ (RN 6163-56-0). PA = 229.4 kcal/mol, 960. kJ/mol. | | | | | | |
|  | | 128 | 535 | | | | |
| | From proton affinity of piperidine (RN 110-89-4). PA = 226.4 kcal/mol, 947. kJ/mol. | | | | | | |
|  | | 136 | 571 | | | | |
| | From proton affinity of N-methylpyrrolidine (RN 120-94-5). PA = 228.7 kcal/mol, 957. kJ/mol. | | | | | | |
| $C_5H_{12}NO_2^+$ | | | | | | | |
| $(CH_3)_2NC(OH)OC_2H_5$ | | 43 | 180 | | | | |
| | From proton affinity of $(CH_3)_2NCOOC_2H_5$ (RN 687-48-9). PA = 213.7 kcal/mol, 894. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

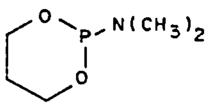
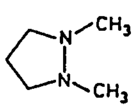
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{12}NO_2{}^+$** | | | | | | | |
| L-i-$C_3H_7CH(NH_3)COOH$ | | 40 | 167 | | | | |
| | From proton affinity of L-i-$C_3H_7CH(NH_2)COOH$ (RN 72-18-4). PA = 217.0 kcal/mol, 908. kJ/mol. | | | | | | |
| **$C_5H_{12}NO_2P^+$** | | | | | | | |
|  | 7.8 | (50) | (208) | −130 | −545 | *EST | 17454-25-0 |
| | IP from 81ARS/ZVE. | | | | | | |
| **$C_5H_{12}NO_2S^+$** | | | | | | | |
| L-$CH_3SCH_2CH_2CH(NH_3)COOH$ | | 45 | 190 | | | | |
| | From proton affinity of L-$CH_3SCH_2CH_2CH(NH_2)COOH$ (RN 59-51-8). PA = 221.4 kcal/mol, 926. kJ/mol. | | | | | | |
| **$C_5H_{12}N_2{}^+$** | | | | | | | |
|  | 6.66 | (180) | (754) | 27 | 111 | *EST | 38704-89-1 |
| | IP from charge transfer equilibrium constant determination (86RUM). Reference standard: IP ($C_6H_5N(CH_3)_2$) = 7.12 eV. See also: 84NEL. | | | | | | |
| **$C_5H_{12}N_2O^+$** | | | | | | | |
| $((CH_3)_2N)_2CO$ | ≤8.64 | (≤142) | (≤595) | −57 | −238 | *EST | 632-22-4 |
| **$C_5H_{12}N_2S^+$** | | | | | | | |
| $((CH_3)_2N)_2CS$ | (7.5) | (184) | (769) | 11±0.5 | 45±2 | 82INA/MUR2 | 2782-91-4 |
| | IP is onset of photoelectron band. See also: 85ROT/BOC. | | | | | | |
| **$C_5H_{12}O^+$** | | | | | | | |
| n-$C_5H_{11}OH$ | 10.00±0.03 | 160 | 668 | −70.9±0.4 | −296.7±1.6 | 77PED/RYL | 71-41-0 |
| | IP from 77ASH/BUR. See also: 80BAC/MOU. | | | | | | |
| $CH_3CH_2CH(CH_3)CH_2OH$ | (9.86) | (155) | (649) | −72.2±0.3 | −302.0±1.4 | 77PED/RYL | 137-32-6 |
| | IP from 81HOL/FIN. | | | | | | |
| n-$C_3H_7CH(OH)CH_3$ | (9.78±0.03) | (151) | (630) | −75.0±0.2 | −313.8±0.8 | 77PED/RYL | 6032-29-7 |
| | IP from 77ASH/BUR, 84BOW/MAC. | | | | | | |
| $(C_2H_5)_2CHOH$ | 9.78 | 150 | 628 | −75.4±0.2 | −315.5±0.9 | 77PED/RYL | 584-02-1 |
| | IP from 81HOL/FIN, 84BOW/MAC. See also: 77ASH/BUR. | | | | | | |
| $(CH_3)_2CHCH(OH)CH_3$ | (10.01) | (155) | (650) | −75.4±0.3 | −315.7±1.1 | 77PED/RYL | 598-75-4 |
| | IP from 84BOW/MAC. | | | | | | |

Table 1. Positive Ion Table - Continued

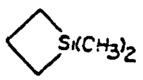
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_5H_{12}O^+$ | | | | | | | |
| $C_2H_5C(CH_3)_2OH$ | 9.80 | 147 | 615 | −79.1±0.3 | −330.8±1.3 | 77PED/RYL | 75-85-4 |
| | IP from 84BOW/MAC, 82LEV/LIA. | | | | | | |
| n-$C_4H_9OCH_3$ | (9.54) | (158) | (662) | −61.7±0.3 | −258.1±1.1 | 77PED/RYL | 628-28-4 |
| | IP from 81HOL/FIN. | | | | | | |
| n-$C_3H_7OC_2H_5$ | (9.45±0.1) | (153) | (640) | −65.0±0.2 | −272.2±1 | 77PED/RYL | 628-32-0 |
| | IP cited in 81HOL/FIN. | | | | | | |
| tert-$C_4H_9OCH_3$ | (9.24) | (145) | (608) | −67.8±0.2 | −283.6±1 | 77PED/RYL | 1634-04-4 |
| | IP from 84BOW/MAC. See also: 80BAC/MOU. | | | | | | |
| $C_5H_{12}O_2^+$ | | | | | | | |
| n-$C_3H_7CH(CH_3)OOH$ | (9.35±0.03) | (159) | (666) | −56 | −236 | *EST | 14018-58-7 |
| | IP from 77ASH/BUR. | | | | | | |
| $CH_3O(CH_2)_3OCH_3$ | (9.3) | (126) | (526) | −89 | −371 | *EST | 17081-21-9 |
| | IP is onset of photoelectron band (83BIE/MOR). | | | | | | |
| n-$C_5H_{11}OOH$ | (9.50±0.03) | (167) | (698) | −52 | −219 | *EST | 74-80-6 |
| | IP from 77ASH/BUR. | | | | | | |
| $C_5H_{12}O_3^+$ | | | | | | | |
| $CH_3C(OCH_3)_3$ | (9.65) | (82) | (343) | −140±0.5 | −588±2 | 77PED/RYL | 1445-45-0 |
| | IP from 82HOL/LOS2. | | | | | | |
| $C_5H_{12}S^+$ | | | | | | | |
| n-$C_3H_7SC_2H_5$ | (8.50±0.05) | (171) | (715) | −25.0±0.2 | −104.7±0.7 | 77PED/RYL | 4110-50-3 |
| $(CH_3)_3CSCH_3$ | (8.38±0.05) | (164) | (687) | −29.0±0.2 | −121.3±0.7 | 77PED/RYL | 6163-64-0 |
| $C_2H_5S$(iso-$C_3H_7$) | (8.35±0.01) | (165) | (689) | −28±0.6 | −117±2 | 77PED/RYL | 5145-99-3 |
| $C_5H_{12}S_2^+$ | | | | | | | |
| $C_2H_5SCH_2SC_2H_5$ | (8.22±0.02) | (179) | (750) | −10 | −43 | *EST | 4396-19-4 |
| $C_5H_{12}Si^+$ | | | | | | | |
| $CH_2=CHSi(CH_3)_3$ | (9.5) | (190) | (794) | −29 | −123 | *EST | 754-05-2 |
| | IP is onset of photoelectron band (81KHV/ZYK, 82LEV/LIA). | | | | | | |
|  | 8.83±0.07 | 184 | 769 | −19.8 | −82.8 | 81GUS/VOL2 | 2295-12-7 |
| | See also: 82DYK/JOS, 81KOE/MCK, 81GUS/VOL2. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{12}Sn^+$** | | | | | | | |
| $CH_2=CHSn(CH_3)_3$ | (≤9.7) | (≤246) | (≤1028) | 22±3 | 92±13 | 77PED/RYL | 754-06-3 |
| **$C_5H_{13}N^+$** | | | | | | | |
| n-$C_5H_{11}NH_2$ | (8.67) IP from 79AUE/BOW. | (174) | (726) | −26 | −110 | *EST | 110-58-7 |
| tert-$C_5H_{11}NH_2$ | (8.46±0.1) | (165) | (689) | −30 | −127 | *EST | 594-39-8 |
| neo-$C_5H_{11}NH_2$ | (8.54±0.1) | (166) | (692) | −31 | −132 | *EST | 5813-64-9 |
| $(C_2H_5)_2(CH_3)N$ | (7.50±0.1) IP from 79AUE/BOW. | (156) | (654) | −17 | −70 | *EST | 616-39-7 |
| $(CH_3)_2(i-C_3H_7)N$ | (7.3) $\Delta_f H$(Ion) from hydrogen affinities of homologous series. IP cited is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). See also: 84NEL. | (150) | (628) | −18 | −76 | *EST | 996-35-0 |
| **$C_5H_{13}N_2O^+$** | | | | | | | |
| $[(CH_3)_2N]_2COH$ | From proton affinity of $[(CH_3)_2N]_2C=O$ (RN 632-22-4) (86TAF/GAL). PA = 221.1 kcal/mol, 925. kJ/mol. | 88 | 367 | | | | |
| **$C_5H_{13}O^+$** | | | | | | | |
| neo-$C_5H_{11}OH_2$ | From proton affinity of neo-$C_5H_{11}OH$ (RN 75-84-3) (78TAF/TAA). PA = 193.6 kcal/mol, 810. kJ/mol. | 97 | 406 | | | | |
| $C_2H_5OH(i-C_3H_7)$ | From proton affinity of $C_2H_5O(i-C_3H_7)$ (RN 625-54-7). PA = 203.5 kcal/mol, 851. kJ/mol. | 94 | 393 | | | | |
| t-$C_4H_9OHCH_3$ | From proton affinity of t-$C_4H_9OCH_3$ (RN 1634-04-4). PA = 202.2 kcal/mol, 846. kJ/mol. | 96 | 400 | | | | |
| **$C_5H_{14}N^+$** | | | | | | | |
| n-$C_5H_{11}NH_3$ | From proton affinity of n-$C_5H_{11}NH_2$ (RN 110-58-7). PA = 218.9 kcal/mol, 916. kJ/mol. | 121 | 504 | | | | |
| tert-$C_5H_{11}NH_3$ | From proton affinity of tert-$C_5H_{11}NH_2$ (RN 594-39-8). PA = 222.3 kcal/mol, 930. kJ/mol. | 112 | 468 | | | | |
| neo-$C_5H_{11}NH_3$ | From proton affinity of neo-$C_5H_{11}NH_2$ (RN 5813-64-9). PA = 219.3 kcal/mol, 917.5 kJ/mol. | 115 | 481 | | | | |

**Table 1. Positive Ion Table - Continued**

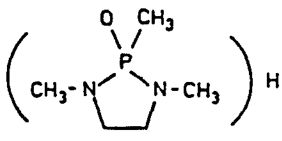
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{14}N^+$** | | | | | | | |
| $(C_2H_5)(i\text{-}C_3H_7)NH_2$ | | 113 | 474 | | | | |
| | From proton affinity of $(C_2H_5)(i\text{-}C_3H_7)NH$ (RN 19961-27-4). PA = 227.4 kcal/mol, 951. kJ/mol. | | | | | | |
| $(CH_3)(C_2H_5)_2NH$ | | 119 | 498 | | | | |
| | From proton affinity of $(CH_3)(C_2H_5)_2N$ (RN 616-39-7). PA = 230.0 kcal/mol, 962. kJ/mol. | | | | | | |
| $(CH_3)_2(i\text{-}C_3H_7)NH$ | | 118 | 493 | | | | |
| | From proton affinity of $(CH_3)_2(i\text{-}C_3H_7)N$ (RN 996-35-0). PA = 229.8 kcal/mol, 961. kJ/mol. | | | | | | |
| **$C_5H_{14}N_2^+$** | | | | | | | |
| $(C_2H_5)(CH_3)NN(CH_3)_2$ | (8.18) | (201) | (839) | 12 | 50 | *EST | 50599-41-2 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |
| $((CH_3)_2N)_2CH_2$ | (7.74±0.05) | (174) | (729) | −4.2±0.3 | −17.6±1.4 | 77PED/RYL | 51-80-9 |
| | See also: 81LOG/TAK. | | | | | | |
| **$C_5H_{14}N_2OP^+$** | | | | | | | |
|  | | 42 | 176 | | | | |
| | From proton affinity of 2,5-dimethyl-1,3,2-diazaphospholidine-2-oxide (RN 16606-18-1) (84MAU/NEL). PA = 224.8 kcal/mol, 941. kJ/mol. | | | | | | |
| **$C_5H_{14}N_3^+$** | | | | | | | |
| $[(CH_3)_2N]_2CNH_2$ | | 192 | 803 | | | | |
| | From proton affinity of $[(CH_3)_2N]_2C{=}NH$ (RN 31081-16-0) (86TAF/GAL). PA = 241.0 kcal/mol, 1008. kJ/mol. | | | | | | |
| **$C_5H_{14}Si^+$** | | | | | | | |
| $(CH_3)_3SiC_2H_5$ | (9.6) | (164) | (685) | −58 | −241 | *EST | 3439-38-1 |
| **$C_5H_{14}Sn^+$** | | | | | | | |
| $(CH_3)_3SnC_2H_5$ | (8.6) | (191) | (800) | −7±0.7 | −30±3 | 77PED/RYL | 3531-44-0 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_5H_{15}N_2^+$** | | | | | | | |
| $NH_2(CH_2)_5NH_3$ | | 110 | 461 | | | | |
| | From proton affinity of $NH_2(CH_2)_5NH_2$ (RN 462-94-2). PA = 238.1 kcal/mol, 996. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

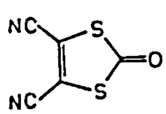
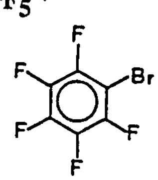
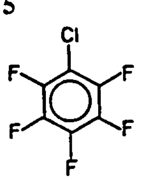
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_5H_{15}N_2^+$** | | | | | | | |
| $(CH_3)_2NH(CH_2)_3NH_2$ | | | | | | | |
| | | 118 | 494 | | | | |
| | From proton affinity of $(CH_3)_2N(CH_2)_3NH_2$ (RN 109-55-7). Data re-evaluated. PA = 241. kcal/mol, 1006. kJ/mol. | | | | | | |
| **$C_5H_{15}Si_2^+$** | | | | | | | |
| $(CH_3)_3SiSi(CH_3)_2$ | | | | | | | |
| | | *117* | *489* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (84SZE/BAE, 84SZE/BAE2). 0 K values. | | | | | | |
| **$C_5H_{15}Ta^+$** | | | | | | | |
| $Ta(CH_3)_5$ | 8.25 | 241 | 1007 | 51±6 | 212±26 | 82PIL/SKI | 53378-72-6 |
| | IP is onset of photoelectron band (75GAL/WIL, 82LEV/LIA). | | | | | | |
| **$C_5H_{16}NSi^+$** | | | | | | | |
| $(CH_3)_3SiNH(CH_3)_2$ | | | | | | | |
| | | (81) | (336) | | | | |
| | From proton affinity of $(CH_3)_3SiN(CH_3)_2$ (RN 18135-05-2). PA = (226) kcal/mol, (946) kJ/mol. | | | | | | |
| **$C_5IMnO_5^+$** | | | | | | | |
| $Mn(CO)_5I$ | (8.1) | (−13) | (−52) | −199±1 | −834±5 | 82CON/ZAF | 14879-42-6 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_5N_2OS_2^+$** | | | | | | | |
|  | ≤9.94 | (≤294) | (≤1229) | 65 | 270 | *EST | 934-31-6 |
| | IP from 83SCH/SCH. | | | | | | |
| **$C_5N_4^+$** | | | | | | | |
| $C(CN)_4$ | (13.94) | (482) | (2018) | 161±2 | 673±9 | 82CHU/NGU | 24331-09-7 |
| **$C_6BrF_5^+$** | | | | | | | |
|  | 9.57±0.02 | 51 | 211 | −170±4 | −712±17 | 77KRE/PRI | 344-04-7 |
| **$C_6ClF_5^+$** | | | | | | | |
|  | (9.72±0.02) | (30) | (128) | −194±3 | −810±11 | 77PED/RYL | 344-07-0 |

**Table 1. Positive Ion Table - Continued**

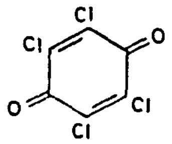
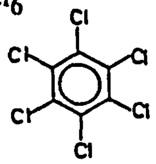
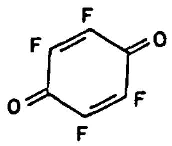
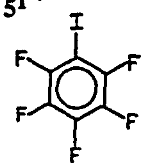
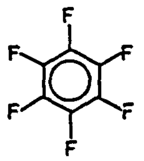
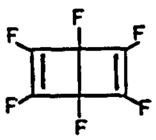
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6Cl_4O_2^+$ | | | | | | | |
|  | 9.74 | 180 | 754 | −44.4±2.8 | −185.7±11 | 77PED/RYL | 118-75-2 |
| | IP from 81SAT/SEK. | | | | | | |
| $C_6Cl_6^+$ | | | | | | | |
|  | 8.98 | 196.4 | 821.7 | −10.7 | −44.7 | 83PLA/SIM | 118-74-1 |
| | IP from 81SAT/SEK. See also: 81RUS/KLA, 81KIM/KAT. | | | | | | |
| $C_6CrO_6^+$ | | | | | | | |
| $Cr(CO)_6$ | 8.142±0.017 | −29 | −122 | −217.0±0.3 | −908±1.2 | 77PED/RYL | 13007-92-6 |
| | See also: 82HUB/LIC, 85DAS/NIS. | | | | | | |
| $C_6F_3MnO_5^+$ | | | | | | | |
| $CF_3Mn(CO)_5$ | 8.8 | −128 | −537 | −331±1 | −1386±4 | 82CON/ZAF | 13601-14-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6F_4O_2^+$ | | | | | | | |
|  | (10.7) | (52) | (216) | −195.0±9.9 | −816±41 | *EST | 527-21-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6F_5I^+$ | | | | | | | |
|  | 9.54 | 87 | 362 | −133±3 | −558±13 | 77PED/RYL | 827-15-6 |
| | See also: 81BIE/ASB. | | | | | | |
| $C_6F_6^+$ | | | | | | | |
| $CF_3C{\equiv}CC{\equiv}CCF_3$ | (10.99±0.01) | (78) | (326) | −175 | −734 | 77PRA/HUB | 10524-09-1 |
|  | 9.906 | 2 | 10 | −226±2 | −946±8 | 79PRI/SAP | 392-56-3 |
| | IP from 81BIE/ASB. A value of 9.91 eV is assigned to the ionization potential at 300 K based on determinations of charge transfer equilibrium constants (reference standard, ionization potential of $C_6H_5CF_3$ = 9.685 eV). See also: 81MAI/THO. | | | | | | |
|  | 10.08±0.05 | 62 | 260 | −170 | −713 | 77PRA/HUB | 6733-01-3 |

Table 1. Positive Ion Table - Continued

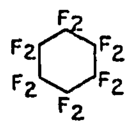
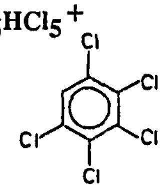
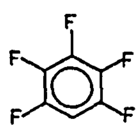
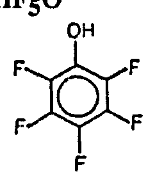
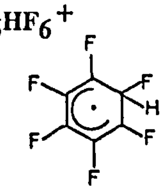
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6F_{12}^+$  | (13.2) | (-262) | (-1095) | -566±2 | -2369±8 | 79PRI/SAP | 355-68-0 |
| $C_6HCl_5^+$  | (8.9) | (195.7) | (818.7) | -9.6±2.1 | -40.0±8.7 | 85PLA/SIM2 | 608-93-5 |
| | IP is onset of photoelectron band (81RUS/KLA3). | | | | | | |
| $C_6HCrO_6^+$ HCr(CO)$_6$ | | (-31) | (-131) | | | | |
| | From proton affinity of Cr(CO)$_6$ (RN 13007-92-6). PA = (180) kcal/mol, (753) kJ/mol. | | | | | | |
| $C_6HF_5^+$  | 9.63 | 29 | 123 | -193±2 | -806±7 | 77PED/RYL | 363-72-4 |
| | Ionization potential from charge transfer equilibrium constant determinations (standard: $C_6H_5CF_3$, 9.685 eV)(78LIA/AUS). Value of 9.64 eV reported from photoelectron spectroscopy measurement. See also: 81BIE/ASB. | | | | | | |
| $C_6HF_5O^+$  | 9.20±0.02 | -17 | -69 | -229±0.5 | -957±2 | 77PED/RYL | 771-61-9 |
| $C_6HF_6^+$  | | -38 | -159 | | | | |
| | From proton affinity of $C_6F_6$ (RN 392-56-3). PA = 177.7 kcal/mol, 743. kJ/mol. | | | | | | |
| $C_6HMoO_6^+$ HMo(CO)$_6$ | | -38 | -160 | | | | |
| | From proton affinity of Mo(CO)$_6$ (RN 13939-06-5). PA = (185) kcal/mol, (774) kJ/mol. | | | | | | |
| $C_6HO_6V^+$ HV(CO)$_6$ | | (-33) | (-138) | | | | |
| | From proton affinity of V(CO)$_6$ (RN 20644-87-5). PA = (194.5) kcal/mol, (814) kJ/mol. | | | | | | |
| $C_6HO_6W^+$ HW(CO)$_6$ | | -30 | -127 | | | | |
| | From proton affinity of W(CO)$_6$ (RN 14040-11-0). PA = (184) kcal/mol, (770) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

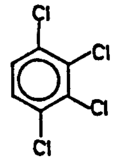
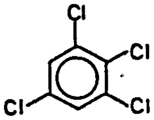
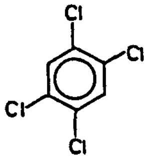
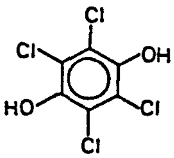
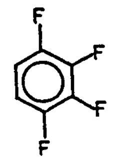
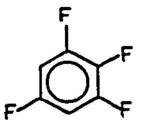
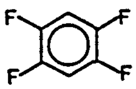
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_2^+$ | | | | | | | |
| HC≡CC≡CC≡CH | (9.50) | (375) | (1569) | 155 | 652 | *EST | 3161-99-7 |
| $C_6H_2Cl_4^+$ | | | | | | | |
|  | (8.9)<br>IP is onset of photoelectron band (81RUS/KLA3). | (199.1) | (833.3) | −6.1 | −25.4 | 85PLA/SIM | 634-66-2 |
|  | (9.0)<br>IP is onset of photoelectron band (81RUS/KLA3). | (199) | (833) | −8.3 | −34.9 | 85PLA/SIM | 634-90-2 |
|  | 8.9<br>IP is onset of photoelectron band (81RUS/KLA3, 81KIM/KAT). | 197.4 | 826.1 | −7.8 | −32.6 | 83PLA/SIM | 95-94-3 |
| $C_6H_2Cl_4O_2^+$ | | | | | | | |
|  | (8.30±0.05) | (104) | (437) | −87 | −364 | 77PED/RYL | 87-87-6 |
| $C_6H_2F_4^+$ | | | | | | | |
|  | 9.53±0.01<br>Ionization potential from charge transfer equilibrium constant determinations (standard: IP of $C_6H_5CF_3$, 9.685 eV)(78LIA/AUS). Value of ionization potential from photoelectron spectroscopy, 9.56 eV. See also: 81BIE/ASB. | (68) | (281) | −152±0.2 | −638±1 | *EST | 551-62-2 |
|  | 9.53±0.01<br>Ionization potential from charge transfer equilibrium constant determinations (standard: ionization potential of $C_6H_5CF_3$, 9.685 eV)(78LIA/AUS). Value of ionization potential from photoionization, 9.55 eV; from photoelectron spectroscopy, 9.56 eV. See also: 81BIE/ASB. | (63) | (262) | −157±0.2 | −657±1 | *EST | 2367-82-0 |
|  | 9.35±0.01<br>Ionization potential from charge transfer equilibrium constant determinations (standard: ionization potential of $C_6H_5CF_3$, 9.685 eV)(78LIA/AUS). Value of IP from photoelectron spectroscopy, 9.36 eV (82LEV/LIA, 81BIE/ASB). | 61 | 255 | −155±1 | −647±3 | 78HAR/HEA | 327-54-8 |

Table 1. Positive Ion Table - Continued

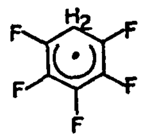
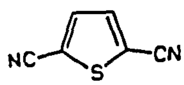
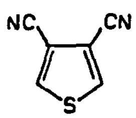
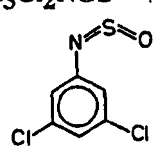
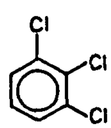
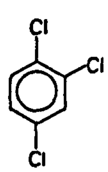
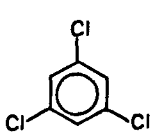
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_2F_5^+$ | | | | | | | |
|  | | -7 | -29 | | | | |
| | From proton affinity of $C_6HF_5$ (RN 363-72-4). PA = 179.9 kcal/mol, 753. kJ/mol. | | | | | | |
| $C_6H_2N_2S^+$ | | | | | | | |
|  | ≤9.76 | (≤319) | (≤1337) | 94 | 395 | *EST | 18853-40-2 |
| | IP from 83BOC/ROT. | | | | | | |
|  | (≤10.20) | (≤331) | (≤1384) | 96 | 400 | *EST | 18853-32-2 |
| | IP from 83BOC/ROT. | | | | | | |
| $C_6H_3Cl_2NOS^+$ | | | | | | | |
|  | (≤9.46) | (≤197) | (≤826) | -21 | -87 | *EST | |
| | IP from 82LOU/VAN. | | | | | | |
| $C_6H_3Cl_3^+$ | | | | | | | |
|  | 9.18 | 209.8 | 877.6 | -1.9 | -8.1 | 85PLA/SIM | 87-61-6 |
| | IP from 81RUS/KLA3. | | | | | | |
|  | 9.04 | 210 | 880 | 1.9 | 8.1 | 85PLA/SIM | 120-82-1 |
| | IP from 81RUS/KLA3 | | | | | | |
|  | 9.32±0.02 | 215 | 899 | 0 | 0 | 82SHA | 108-70-3 |
| | IP from 81RUS/KLA(3), onset of photoelectron band (81KIM/KAT). See also: 82MAI/THO2. | | | | | | |

**Table 1. Positive Ion Table - Continued**

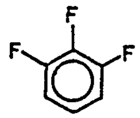
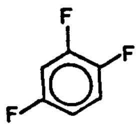
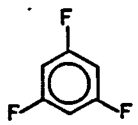
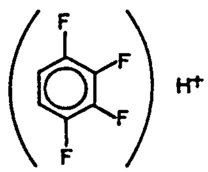
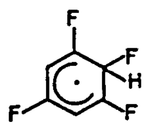
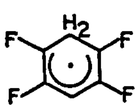
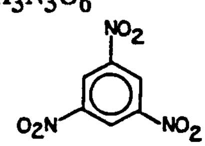
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_3F_3^+$ | | | | | | | |
|  | (9.7) | (107) | (448) | −117 | −488 | *EST | 1489-53-8 |
| | IP from 81BIE/ASB. | | | | | | |
|  | 9.30±0.05 | (96) | (401) | −119 | −496 | *EST | 367-23-7 |
| | IP from charge transfer equilibrium constant determinations (standard: IP of $C_6H_5CF_3$, 9.685 eV)(78LIA/AUS) and from photoelectron spectroscopy (81BIE/ASB, 77ROS/DRA). | | | | | | |
|  | 9.64 | (100) | (418) | −122±0.7 | −512±3 | *EST | 372-38-3 |
| | See also: 81BIE/ASB. | | | | | | |
| $C_6H_3F_4^+$ | | | | | | | |
|  | | 32 | 134 | | | | |
| | From proton affinity of 1,2,3,4-$C_6F_4H_2$ (RN 551-62-2). PA = 181.1 kcal/mol, 758. kJ/mol. | | | | | | |
|  | | 28 | 117 | | | | |
| | From proton affinity of 1,2,3,5-$C_6F_4H_2$ (RN 2367-82-0). PA = 180.6 kcal/mol, 756. kJ/mol. | | | | | | |
|  | | 31 | 131 | | | | |
| | From proton affinity of 1,2,4,5-$C_6F_4H_2$ (RN 327-54-8). PA = 179.7 kcal/mol, 752. kJ/mol. | | | | | | |
| $C_6H_3MnO_5^+$ | | | | | | | |
| $CH_3(CO)_5Mn$ | (8.4) | (14) | (57) | −180±1 | −753±4 | 82CON/ZAF | 13601-24-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_3N_3O_6^+$ | | | | | | | |
|  | (10.96±0.02) | (268) | (1119) | 15±0.5 | 62±2 | 77PED/RYL | 99-35-4 |

**Table 1. Positive Ion Table - Continued**

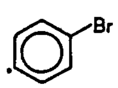
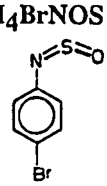
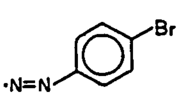
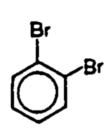
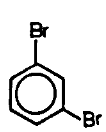
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_3O_5Re^+$ | | | | | | | |
| $(CO)_5CH_3Re$ | 8.5 | 14 | 60 | −182±1 | −760±6 | 82PIL/SKI | 14524-92-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_4^+$ | | | | | | | |
| (Z)-HC≡CCH=CHC≡CH | (9.10±0.02) | (333) | (1394) | 123 | 516 | *EST | 16668-67-0 |
| (E)-HC≡CCH=CHC≡CH | (9.07±0.02) | (334) | (1400) | 125 | 525 | *EST | 16668-68-1 |
|  | 8.6 | 313 | 1311 | 115 | 481 | 80POL/HEH | 462-80-6 |
| | | *316* | *1321* | *118* | *492* | | |
| | $\Delta_f H$(Ion) from 80ROS/STO2. Cited IP = $\Delta_f H$(Ion) - $\Delta_f H$(Neutral); a value of 8.95 eV has been estimated (80ROS/STO2). See also: 82ROS/DAN, 85DEW/TIE. | | | | | | |
| $C_6H_4Br^+$ | | | | | | | |
|  | 9.04 | 298 | 1247 | 89.6 | 374.9 | 77NUY/MES | 2973-43-5 |
| | $\Delta_f H$(Ion) from 77NUY/MES. IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). | | | | | | |
| $C_6H_4BrNOS^+$ | | | | | | | |
|  | (≤8.91) | (≤203) | (≤851) | −2 | −9 | *EST | 26516-62-1 |
| | IP from 82LOU/VAN. | | | | | | |
| $C_6H_4BrN_2^+$ | | | | | | | |
|  | (8.18) | (276) | (1155) | 87 | 366 | *EST | |
| | $\Delta_f H$(Ion) from 77NUY/MES. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $C_6H_4Br_2^+$ | | | | | | | |
|  | 8.8 | (234) | (981) | 31.5 | 132 | *EST | 583-53-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.85 | 235 | 985 | 31 | 131 | 83DEW/HEA | 108-36-1 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

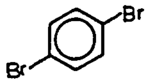
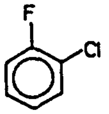
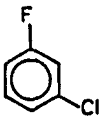
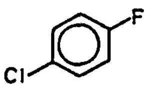
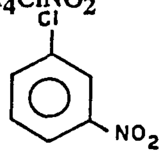
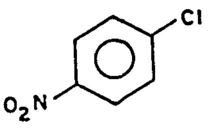
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4Br_2^+$ | | | | | | | |
|  | 8.7<br>IP is onset of photoelectron band. | (232) | (970) | 31 | 131 | *EST | 106-37-6 |
| $C_6H_4ClF^+$ | | | | | | | |
|  | 9.18±0.01<br>See also: 78LIA/AUS. | (181) | (756) | −31 | −130 | *EST | 348-51-6 |
|  | 9.21±0.01 | (179) | (749) | −33 | −140 | *EST | 625-98-9 |
|  | 9.01±0.01<br>IP from 78LIA/AUS. | (174) | (728) | −34 | −141 | *EST | 352-33-0 |
| $C_6H_4ClNOS^+$ | | | | | | | |
|  | (8.8)<br>IP is onset of photoelectron band (82LOU/VAN). | (188) | (787) | (−15) | (−62) | ? | |
| $C_6H_4ClNO_2^+$ | | | | | | | |
|  | (9.92±0.1) | (238) | (995) | 9.1±2.0 | 38.1±8.4 | *EST | 121-73-3 |
|  | 9.96±0.1 | (239) | (999) | 9.1±2.0 | 38.1±8.4 | *EST | 100-00-5 |

**Table 1. Positive Ion Table - Continued**

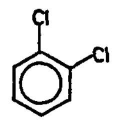
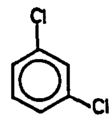
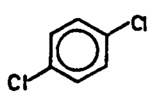
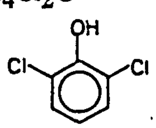
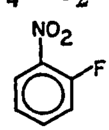
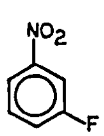
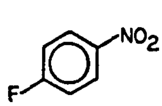
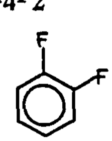
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4Cl_2{}^+$ | | | | | | | |
|  | 9.08±0.01 | 217.3 | 909.1 | 7.9 | 33.0 | 84PLA/SIM | 95-50-1 |
| | IP from charge transfer equilibrium constant determination (78LIA/AUS). See also: 81RUS/KLA2, 81KIM/KAT. | | | | | | |
|  | 9.11±0.01 | 216.8 | 907.1 | 6.7 | 28.1 | 84PLA/SIM | 541-73-1 |
| | IP from charge transfer equilibrium constant determination(78LIA/AUS). See also: 82LEV/LIA, 81RUS/KLA2, 81KIM/KAT. | | | | | | |
|  | 8.89±0.01 | 210.9 | 882.3 | 5.9 | 24.6 | 84PLA/SIM | 106-46-7 |
| | IP from 81RUS/KLA2 (onset of photoelectron band), and 78LIA/AUS (charge transfer equilibrium constant determination). See also: 81KIM/KAT. | | | | | | |
| $C_6H_4Cl_2O^+$ | | | | | | | |
|  | (8.65±0.02) | (174) | (729) | −25 | −106 | 82SHA | 87-65-0 |
| $C_6H_4FNO_2{}^+$ | | | | | | | |
|  | (≤9.86) | (≤199) | (≤833) | −28 | −118 | *EST | 1493-27-2 |
|  | 9.88 | (198) | (827) | −30 | −126 | *EST | 402-67-5 |
|  | 9.90 | (197) | (824) | −31 | −131 | *EST | 350-46-9 |
| $C_6H_4F_2{}^+$ | | | | | | | |
|  | (9.28±0.01) | (144) | (602) | −70.2±0.2 | −293.8±1.0 | 77PED/RYL | 367-11-3 |
| | Ionization potential from charge transfer equilibrium constant determinations (standard: ionization potential of $C_6H_5CF_3$, 9.685 eV). Value of ionization potential from Rydberg series and from photoelectron spectroscopy (81BIE/ASB) = 9.30 eV. | | | | | | |

**Table 1. Positive Ion Table - Continued**

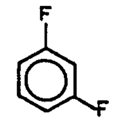
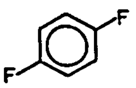
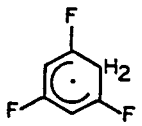
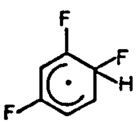
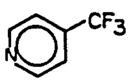
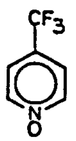
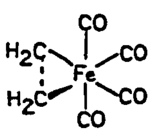
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4F_2^+$ | | | | | | | |
|  | 9.33±0.01 | 141 | 591 | −73.9±0.3 | −309.2±1.1 | 77PED/RYL | 372-18-9 |
| | Ionization potential from charge transfer equilibrium constant determinations (standard: ionization potential of $C_6H_5CF_3$, 9.685 eV). Value of ionization potential from Rydberg series, 9.35 eV, from photoelectron spectroscopy, 9.32 eV. See also: 81BIE/ASB. | | | | | | |
|  | 9.14±0.01 | 137 | 575 | −73.3±0.3 | −306.6±1.1 | 77PED/RYL | 540-36-3 |
| | Ionization potential from charge transfer equilibrium constant determinations (standard: ionization potential of $C_6H_5CF_3$, 9.685 eV). Value of ionization potential from Rydberg series, 9.18 eV, from photoionization and photoelectron spectroscopy, 9.14 eV(81BIE/ASB). | | | | | | |
| $C_6H_4F_3^+$ | | | | | | | |
|  | | 62 | 261 | | | | |
| | From proton affinity of 1,3,5-$C_6F_3H_3$ (RN 372-38-3). PA = 181. kcal/mol, 757. kJ/mol. | | | | | | |
|  | | 69 | 289 | | | | |
| | From proton affinity of 1,2,4-$C_6F_3H_3$ (RN 367-23-7). PA = 181.4 kcal/mol, 759. kJ/mol. | | | | | | |
| $C_6H_4F_3N^+$ | | | | | | | |
|  | (≤10.1) | (≤105) | (≤438) | −128 | −536 | *EST | 3796-24-5 |
| $C_6H_4F_3NO^+$ | | | | | | | |
|  | (≤8.90) | (≤58) | (≤243) | −147 | −616 | *EST | |
| $C_6H_4FeO_4^+$ | | | | | | | |
|  | (7.6) | (46) | (192) | −129±2 | −541±10 | 82PIL/SKI | 32799-25-0 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

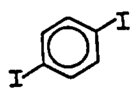
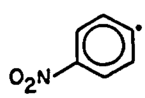
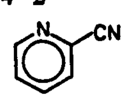
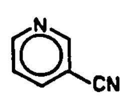
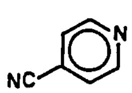
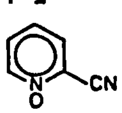
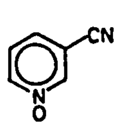
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4I_2^+$ | | | | | | | |
|  | 8.45 | (252) | (1056) | 58 | 241 | *EST | 624-38-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_4MnO_5^+$ | | | | | | | |
| $CH_3MnH(CO)_5$ | | 3 | 11 | | | | |
| | From proton affinity of $CH_3Mn(CO)_5$ (RN 13601-24-6). PA = 183 kcal/mol, 766 kJ/mol. | | | | | | |
| $C_6H_4NO_2^+$ | | | | | | | |
|  | (9.06) | (283) | (1183) | 74 | 309 | *EST | 2395-99-5 |
| | IP from 77NUY/MES. | | | | | | |
| $C_6H_4N_2^+$ | | | | | | | |
|  | 10.12 | 301 | 1260 | 67±0.5 | 281±2 | 84BIC/PIL | 100-70-9 |
|  | (10.0) | (297) | (1243) | 66±0.5 | 278±2 | 84BIC/PIL | 100-54-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.9) | (296) | (1239) | 68±0.2 | 284±1 | 84BIC/PIL | 100-48-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_4N_2O^+$ | | | | | | | |
|  | (8.96±0.02) | (256) | (1069) | 49 | 204 | *EST | 2402-98-4 |
|  | (≤8.93±0.02) | (≤254) | (≤1064) | 48 | 202 | *EST | 14906-64-0 |

**Table 1. Positive Ion Table - Continued**

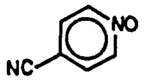
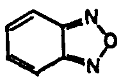
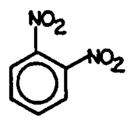
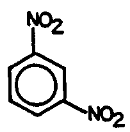
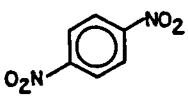
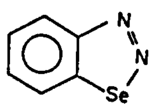
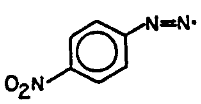
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4N_2O^+$ | | | | | | | |
|  | 8.95±0.02 | (255) | (1068) | 49 | 204 | *EST | 14906-59-3 |
|  | (9.37) | (288) | (1205) | 72±0.5 | 301±2 | 80ARS | 273-09-6 |
| $C_6H_4N_2O_4^+$ | | | | | | | |
|  | (≤10.71) | (≤267) | (≤1119) | 21±0.5 | 86±2 | 76FER/PIA | 528-29-0 |
|  | 10.43±0.02 | 255 | 1065 | 14±0.2 | 59±1 | 76FER/PIA | 99-65-0 |
|  | 10.3±0.1 | 251 | 1051 | 14±0.7 | 57±3 | 76FER/PIA | 100-25-4 |
| $C_6H_4N_2Se^+$ | | | | | | | |
|  | (8.5)<br>IP is onset of photoelectron band. | (292) | (1223) | 96 | 403 | *EST | 273-92-7 |
| $C_6H_4N_3O_2^+$ | | | | | | | |
|  | (7.89)<br>IP from 77NUY/MES. | (258) | (1079) | 76 | 318 | *EST | |

**Table 1. Positive Ion Table - Continued**

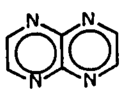
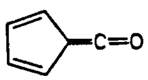
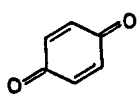
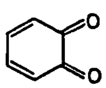
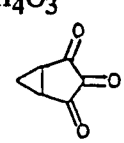
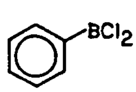
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_4N_4^+$ | | | | | | | |
|  | (8.9) | (295) | (1233) | 89 | 374 | *EST | 255-53-8 |
| | IP is onset of photoelectron band (84GLE/SPA2). | | | | | | |
| $C_6H_4O^+$ | | | | | | | |
|  | 8.2 | (214) | (895) | 25±1 | 104±6 | *EST | 4727-22-4 |
| | IP is onset of photoelectron band (79SCH/SCH, 81BOC/HIR). | | | | | | |
| $C_6H_4O_2^+$ | | | | | | | |
|  | 10.04±0.18 | 202 | 846 | −29±1 | −123±4 | 77PED/RYL | 106-51-4 |
| | See also: 83BOC/MOH. | | | | | | |
|  | (9.3) | (189) | (791) | −25±1 | −106±4 | *EST | 583-63-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_4O_3^+$ | | | | | | | |
|  | (9.0) | (119) | (498) | −88 | −370 | *EST | 81640-31-5 |
| | IP is onset of photoelectron band (81BEC/HOF). | | | | | | |
| $C_6H_5^+$ | | | | | | | |
|  | 8.25 | 269.3 | 1126.9 | 79±1 | 329±4 | 82MCM/GOL | 2396-01-2 |
| | | *272.8* | *1141.3* | | | | |
| | $\Delta_f H$(Ion) from appearance potential measurements(86MAL/LIF). See also: 83DAN/ROS, 85MAL/ARA, 76BAE/TSA, 84LIF/MAL, 80ROS/STO, 81PRA/CHU, 84GEF/LIF, 85DUN, 74BEA, 84PAN/BAE, 85PAN/BAE, 85PAN/BAE2, 86NIS/DAS and 84BUR/HOL. IP given is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). Experimental IP of radical = 8.1-8.2 eV. | | | | | | |
| $C_6H_5BCl_2^+$ | | | | | | | |
|  | (9.3) | (151) | (631) | −64±0.5 | −266±2 | 77PED/RYL | 873-51-8 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

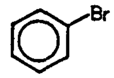
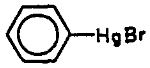
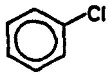
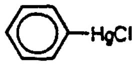
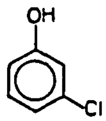
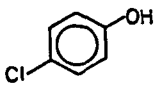
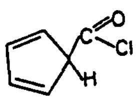
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_5Br^+$ | | | | | | | |
|  | 8.98±0.02 | 232 | 971 | 24.9±0.7 | 104.3±3.1 | 77PED/RYL | 108-86-1 |
| | | *237* | *993* | *30.1±0.7* | *126.1±3.1* | | |
| | IP from 78LIA/AUS, 82LEV/LIA, onset of photoelectron band in 81KIM/KAT. See also: 82VON/ASB, 83KLA/KOV, 86FUJ/OHN. | | | | | | |
| $C_6H_5BrHg^+$ | | | | | | | |
|  | (9.1) | (248) | (1037) | 38 | 159 | *EST | 1192-89-8 |
| | IP is onset of photoelectron band (81BAI/CHI). | | | | | | |
| $C_6H_5Cl^+$ | | | | | | | |
|  | 9.06±0.02 | 222 | 929 | 13.0±0.2 | 54.4±0.9 | 85PLA/SIM | 108-90-7 |
| | See also: 78LIA/AUS, 81RUS/KLA2, 82VON/ASB, 83KLA/KOV, 81KIM/KAT, 86FUJ/OHN. | | | | | | |
| $C_6H_5ClHg^+$ | | | | | | | |
|  | 9.14±0.04 | 240.5 | 1006.2 | 29.7 | 124.3 | 85DEW/GRA | 100-56-1 |
| | See also: 81BAI/CHI. | | | | | | |
| $C_6H_5ClO^+$ | | | | | | | |
|  | (8.65) | (163) | (682) | −37±2 | −153±9 | 77PED/RYL | 108-43-0 |
| | IP from 85OIK/ABE. | | | | | | |
|  | (≤8.69) | (≤165) | (692) | −35±2 | −146±9 | 77PED/RYL | 106-48-9 |
|  | (8.9) | (194) | (813) | −11 | −46 | *EST | 78957-21-8 |
| | IP is onset of photoelectron band (81BOC/HIR). | | | | | | |

**Table 1. Positive Ion Table - Continued**

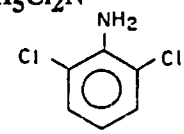
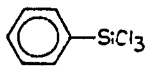
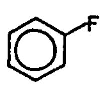
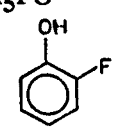
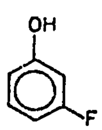
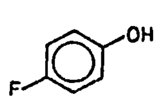
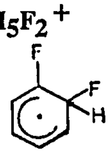
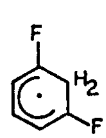
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_5Cl_2N^+$ | | | | | | | |
|  | (7.60±0.02) | (182) | (763) | 7 | 30 | *EST | 608-31-1 |
| $C_6H_5Cl_3Si^+$ | | | | | | | |
|  | (9.10)<br>IP from 84VES/HAR. | (115) | (481) | −95 | −397 | *EST | 98-13-5 |
| $C_6H_5F^+$ | | | | | | | |
|  | 9.200±0.005<br>See also: 81BIE/ASB, 81KIM/KAT, 86FUJ/OHN. | 184.4 | 771.6 | −27.7±0.3 | −116.0±1.4 | 77PED/RYL | 462-06-6 |
| $C_6H_5FO^+$ | | | | | | | |
|  | 8.68±0.02<br>IP from 85OIK/ABE. | (131) | (548) | −69 | −289 | *EST | 367-12-4 |
|  | 8.73±0.02<br>IP from 85OIK/ABE. | (131) | (547) | −71 | −295 | *EST | 372-20-3 |
|  | (8.5)<br>IP is onset of photoelectron band. | (126) | (529) | −70 | −291 | *EST | 371-41-5 |
| $C_6H_5F_2^+$ | | | | | | | |
|  | From proton affinity of 1,2-difluorobenzene (RN 367-11-3). PA = 181.8 kcal/mol, 761. kJ/mol. | 114 | 475 | | | | |
|  | From proton affinity of 1,3-difluorobenzene (RN 372-18-9) (82MAS/BOH). PA = 181.9 kcal/mol, 761. kJ/mol. | 110 | 460 | | | | |

**Table 1. Positive Ion Table - Continued**

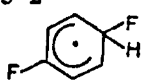
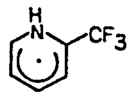
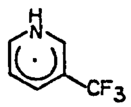
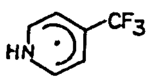
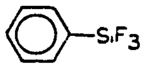
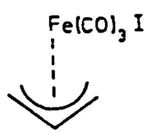
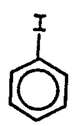
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_5F_2{}^+$ | | | | | | | |
|  | | 111 | 465 | | | | |
| | From proton affinity of 1,4-difluorobenzene (RN 540-36-3). PA = 181.2 kcal/mol, 758. kJ/mol. | | | | | | |
| $C_6H_5F_3N^+$ | | | | | | | |
|  | | 27 | 113 | | | | |
| | From proton affinity of 2-trifluoromethylpyridine (RN 368-48-9). PA = 211.5 kcal/mol, 885. kJ/mol. | | | | | | |
|  | | 25 | 104 | | | | |
| | From proton affinity of 3-trifluoromethylpyridine (RN 3796-23-4). PA = 212.6 kcal/mol, 889. kJ/mol. | | | | | | |
|  | | 25 | 104 | | | | |
| | From proton affinity of 4-trifluoromethylpyridine (RN 3796-24-5). PA = 212.8 kcal/mol, 890. kJ/mol. | | | | | | |
| $C_6H_5F_3Si^+$ | | | | | | | |
|  | (9.18) | (-50) | (-207) | -261 | -1093 | *EST | 368-47-8 |
| | IP from 84VES/HAR. | | | | | | |
| $C_6H_5FeIO_3{}^+$ | | | | | | | |
|  | 8.17 | 106 | 444 | -82±3 | -344±11 | 82PIL/SKI | 12189-10-5 |
| | IP is onset of photoelectron band (82LOU/HAR). | | | | | | |
| $C_6H_5I^+$ | | | | | | | |
|  | 8.685 | 240 | 1003 | 39.4±1.4 | 164.9±5.9 | 77PED/RYL | 591-50-4 |
| | | *243* | *1019* | *43.2±1.4* | *180.9±5.9* | | |
| | See also: 83KLA/KOV, 83DAN/ROS, 81KIM/KAT, 86FUJ/OHN. | | | | | | |

Table 1. Positive Ion Table – Continued

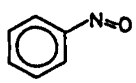
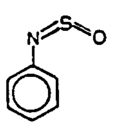
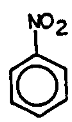
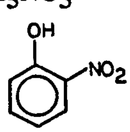
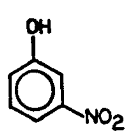
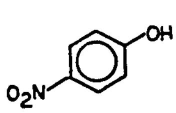
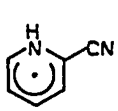
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_5NO^+$ | | | | | | | |
|  | (8.09) | (235) | (982) | 48±1 | 201±4 | 75CHO/GOL | 586-96-9 |
| $C_6H_5NOS^+$ | | | | | | | |
|  | (8.8) | (196) | (819) | −7 | −30 | *EST | 1122-83-4 |
| | IP is onset of photoelectron band (82LOU/VAN). | | | | | | |
| $C_6H_5NO_2^+$ | | | | | | | |
|  | 9.86±0.02 | 243 | 1019 | 16.1±0.2 | 67.6±1 | 77PED/RYL | 98-95-3 |
| | | *250* | *1045* | *22* | *92* | | |
| | See also: 83KLA/KOV, 81KIM/KAT, 81ALL/MIG, 82ALL/MIG, 73GOL/KOR.<br>0 K values from 84PAN/BAE, 85PAN/BAE2. | | | | | | |
| $C_6H_5NO_3^+$ | | | | | | | |
|  | (9.1) | (187) | (780) | −23 | −98 | *EST | 88-75-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.0) | (181) | (757) | −27 | −111 | *EST | 554-84-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.1) | (182) | (762) | −28 | −116 | *EST | 100-02-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_5N_2^+$ | | | | | | | |
|  | | 225 | 943 | | | | |
| | From proton affinity of 2-pyridinecarbonitrile. (RN 100-70-9).<br>208.1 kcal/mol, 871. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

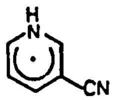
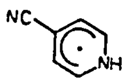
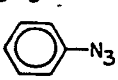
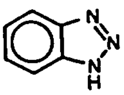
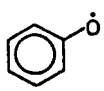
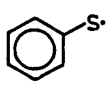
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_5N_2^+$ | | | | | | | |
|  | | 222 | 932 | | | | |
| | From proton affinity of 3-pyridinecarbonitrile (RN 100-54-9). PA = 209.3 kcal/mol, 876. kJ/mol. | | | | | | |
|  | | 223 | 934 | | | | |
| | From proton affinity of 4-pyridinecarbonitrile (RN 100-48-1). PA = 210.3 kcal/mol, 880 kJ/mol. | | | | | | |
| $C_6H_5N_3^+$ | | | | | | | |
|  | (8.4) | (286) | (1195) | 92 | 385 | 29ROT/MUE | 622-37-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.20±0.05) | (295) | (1236) | 83 | 348 | 61ZIM/GEI | 95-14-7 |
| $C_6H_5O^+$ | | | | | | | |
|  | (8.56) | (208) | (870) | 11.4 | 48 | 82MCM/GOL | 2122-46-5 |
| | | *(212)* | *(888)* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (84LOS/HOL). IP from 80DEW/DAV. See also: 84PAN/BAE, 85PAN/BAE, 85PAN/BAE2, 86DAS/GIL. | | | | | | |
| $C_6H_5S^+$ | | | | | | | |
|  | (8.63±0.10) | (254) | (1063) | 55±2 | 230±8 | 82MCM/GOL | 4985-62-0 |
| $C_6H_6^+$ | | | | | | | |
| $CH_2{=}C{=}CHCH{=}C{=}CH_2$ | (8.53) | (295) | (1234) | 98 | 411 | 82ROS/DAN | 29776-96-3 |
| | | *(299)* | *(1251)* | *102* | *428* | | |
| $HC{\equiv}CCH_2CH{=}C{=}CH_2$ | (9.40) | (316) | (1321) | 99 | 414 | 82ROS/DAN | 33142-15-3 |
| | | *(320)* | *(1339)* | *103* | *432* | | |
| | IP from 82ROS/DAN (onset of photoelectron band). | | | | | | |

Table 1. Positive Ion Table - Continued

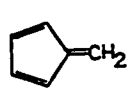
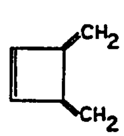
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6H_6^+$ | | | | | | | |
| $HC{\equiv}CCH=CHCH=CH_2$ | | | | | | | |
| | (9.20) | (299) | (1253) | 87 | 365 | 82ROS/DAN | 10420-90-3 |
| | | *(303)* | *(1270)* | *91* | *382* | | |
| | IP from 82ROS/DAN. | | | | | | |
| $CH_2=CHC{\equiv}CCH=CH_2$ | | | | | | | |
| | (8.50±0.02) | (280) | (1172) | 84 | 352 | 82ROS/DAN | 821-08-9 |
| | | *(284)* | *(1189)* | *88* | *369* | | |
| | See also: 85DEW/TIE. | | | | | | |
| $HC{\equiv}CC{\equiv}CC_2H_5$ | (9.41) | (312) | (1306) | 95 | 398 | 82ROS/DAN | 4447-21-6 |
| | | *(316)* | *(1323)* | *99* | *415* | | |
| | IP from 82ROS/DAN. | | | | | | |
| $HC{\equiv}CCH_2C{\equiv}CCH_3$ | (9.50) | (317) | (1328) | 98 | 411 | 82ROS/DAN | 10420-91-4 |
| | | *(321)* | *(1345)* | *102* | *428* | | |
| | IP from 82ROS/DAN (onset of photoelectron band). | | | | | | |
| $HC{\equiv}CCH_2CH_2C{\equiv}CH$ | 9.90 | 327 | 1369 | 99 | 414 | 82ROS/DAN | 628-16-0 |
| | | *331* | *1387* | *103* | *432* | | |
| | See also: 82ROS/DAN. | | | | | | |
| $CH_3C{\equiv}CC{\equiv}CCH_3$ | 8.92±0.05 | 296 | 1238 | 90 | 377 | 82ROS/DAN | 2809-69-0 |
| | | *299* | *1255* | *94* | *394* | | |
| | See also: 82ROS/DAN. | | | | | | |
|  | 9.2459±0.0002 | 233.2 | 975.8 | 19.8±0.1 | 82.9±0.3 | 77PED/RYL | 71-43-2 |
| | | *237.2* | *992.6* | *24.0±0.2* | *100.4±1* | | |
| | IP from 84GRU/WHE. IP at 298 K = 9.225±0.005 (78LIA/AUS). See also: 81KIM/KAT, duplicate 81KIM/KAT, 84HOW/GON. | | | | | | |
|  | (8.36) | (246) | (1030) | 53.5 | 223.8 | 84ROT | 497-20-1 |
| | | *(251)* | *(1048)* | *57.8* | *241.9* | | |
|  | (8.80) | (283) | (1184) | 80.4 | 335.5 | 86ROT/LEN | 5291-90-7 |
| | | *(286)* | *(1198)* | *83* | *349* | | |

**Table 1. Positive Ion Table - Continued**

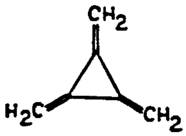
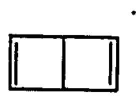
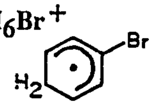
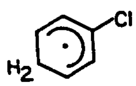
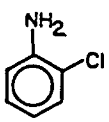
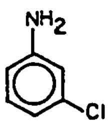
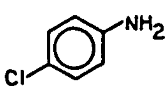
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_6^+$ | | | | | | | |
|  | (8.80) | (298) | (1245) | 95 | 396 | 82ROS/DAN | 3227-90-5 |
| | | *(302)* | *(1263)* | *99* | *414* | | |
| | IP from 82ROS/DAN (onset of photoelectron band). | | | | | | |
|  | (9.0) | (294) | (1232) | 87 | 364 | 82ROS/DAN | 5649-95-6 |
| | | *(298)* | *(1250)* | *91* | *382* | | |
| | IP from 82ROS/DAN (onset of photoelectron band). | | | | | | |
|  | 8.1 | (274) | (1144) | 87 | 363 | 82ROS/DAN | 659-85-8 |
| | | *(278)* | *(1163)* | *91* | *381* | | |
| | IP from 82ROS/DAN (onset of photoelectron band). | | | | | | |
| $C_6H_6Br^+$ | | | | | | | |
|  | | 208 | 871 | | | | |
| | From proton affinity of $C_6H_5Br$ (RN 108-86-1). PA = 182.4 kcal/mol, 763. kJ/mol. | | | | | | |
| $C_6H_6Cl^+$ | | | | | | | |
|  | | 196 | 821 | | | | |
| | From proton affinity of $C_6H_5Cl$ (RN 108-90-7). PA = 181.7 kcal/mol, 760. kJ/mol. | | | | | | |
| $C_6H_6ClN^+$ | | | | | | | |
|  | (8.50) | (211) | (881) | 15 | 61 | *EST | 95-51-2 |
|  | (8.09±0.1) | (200) | (836) | 13 | 55 | *EST | 108-42-9 |
|  | (≤8.18) | (≤202) | (≤844) | 13 | 55 | *EST | 106-47-8 |

Table 1. Positive Ion Table - Continued

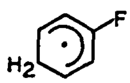
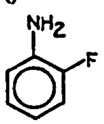
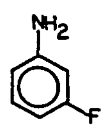
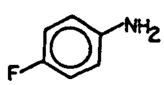
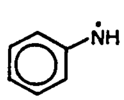
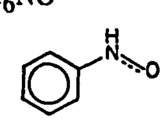
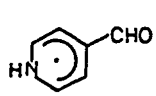
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_6F^+$ | | | | | | | |
|  | | 155 | 650 | | | | |
| | From proton affinity of $C_6H_5F$ (RN 462-06-6). PA = 182.6 kcal/mol, 764. kJ/mol. | | | | | | |
| $C_6H_6FN^+$ | | | | | | | |
|  | (≤8.18) | (≤164) | (≤683) | −25 | −106 | *EST | 348-54-9 |
|  | (≤8.32) | (≤165) | (≤691) | −27 | −112 | *EST | 372-19-0 |
|  | (≤8.18) | (≤163) | (≤680) | −26 | −109 | *EST | 371-40-4 |
| $C_6H_6Hg^+$ | | | | | | | |
| $(CH_3C{\equiv}C)_2Hg$ | 8.98±0.07 | (323) | (1351) | 116 | 485 | *EST | 64705-15-3 |
| | IP is onset of photoelectron band (81FUR/PIA). | | | | | | |
| $C_6H_6N^+$ | | | | | | | |
|  | (8.26±0.1) | (247) | (1034) | 57±2 | 237±8 | 82MCM/GOL | 2835-77-0 |
| $C_6H_6NO^+$ | | | | | | | |
|  | | 209 | 874 | | | | |
| | From proton affinity of nitrosobenzene (RN 586-96-9). PA = 204.8 kcal/mol, 857. kJ/mol. | | | | | | |
|  | | (156) | (654) | | | | |
| | From proton affinity of 4-pyridinecarboxaldehyde (RN 872-85-5). PA = (215.2) kcal/mol, (900.) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

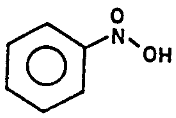
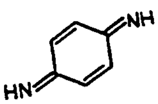
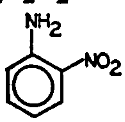
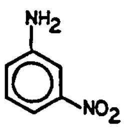
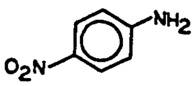
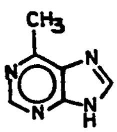
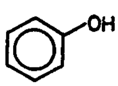
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_6NO_2^+$ | | | | | | | |
|  | | 189 | 789 | | | | |
| | From proton affinity of nitrobenzene (RN 98-95-3). PA = 193.4 kcal/mol, 809. kJ/mol. | | | | | | |
| $C_6H_6N_2^+$ | | | | | | | |
|  | (9.36±0.03) | (294) | (1229) | 78±1 | 326±5 | *EST | 4377-73-5 |
| $C_6H_6N_2O_2^+$ | | | | | | | |
|  | 8.27±0.01 | 206 | 862 | 15±1 | 64±4 | 77PED/RYL | 88-74-4 |
|  | 8.31±0.02 | 207 | 864 | 15±0.5 | 62±2 | 83NIS/SAK | 99-09-2 |
|  | 8.34±0.01 | 205 | 860 | 13±0.5 | 55±2 | 83NIS/SAK | 100-01-6 |
| $C_6H_6N_4^+$ | | | | | | | |
|  | (8.9) | (248) | (1037) | 43 | 178 | *EST | 2004-03-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_6O^+$ | | | | | | | |
|  | 8.47 | 173 | 722 | −23.0±0.2 | −96.3±0.8 | 78KUD/KUD | 108-95-2 |
| | | *175* | *732* | *−20.4* | *−85.2* | | |
| | IP from 84FRA/FRA. See also: 84FUK/YOS, 83KLA/KOV, 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

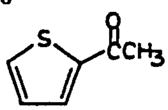
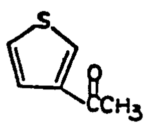
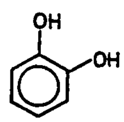
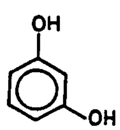
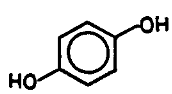
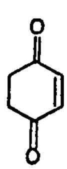
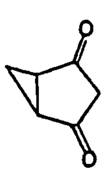
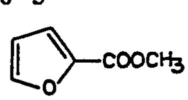
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_6OS^+$ | | | | | | | |
|  | (9.20±0.05) | (206) | (862) | −6 | −26 | *EST | 88-15-3 |
|  | (9.32±0.05) | (209) | (875) | −6 | −24 | *EST | 1468-83-3 |
| $C_6H_6O_2^+$ | | | | | | | |
|  | (8.15)<br>IP is onset of photoelectron band. | (123) | (514) | −65±1 | −272±5 | 79KUD/KUD | 120-80-9 |
|  | (8.2)<br>IP is onset of photoelectron band. | (123) | (514) | −65.6±0.5 | −274.7±2.1 | 79KUD/KUD | 108-46-3 |
|  | 7.95±0.03<br>IP from 85OIK/ABE. | 121 | 505 | −63±0.5 | −262±2 | 79KUD/KUD | 123-31-9 |
|  | (9.77)<br>IP is onset of photoelectron band (85GLE/JAH). | (205) | (859) | −20 | −84 | *EST | 4505-38-8 |
|  | (9.4)<br>IP is onset of photoelectron band (81BEC/HOF). | (170) | (713) | −46 | −194 | *EST | 29798-87-6 |
| $C_6H_6O_3^+$ | | | | | | | |
|  | (≤9.00±0.05) | (≤110) | (≤463) | −97 | −405 | 80BAL/LEB | 611-13-2 |

**Table 1. Positive Ion Table - Continued**

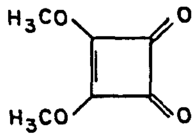
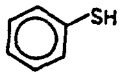
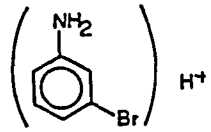
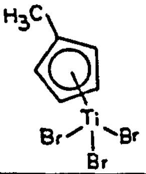
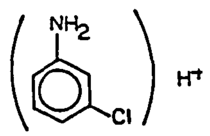
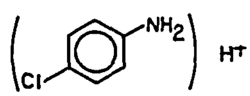
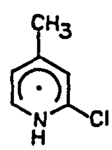
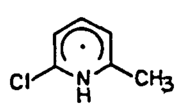
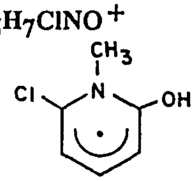
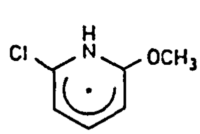
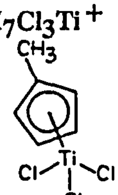
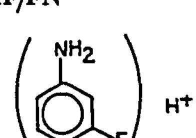
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_6O_4{}^+$ | | | | | | | |
|  | ≤9.20 | (≤107) | (≤447) | −105 | −441 | *EST | 5222-73-1 |
| $C_6H_6S^+$ | | | | | | | |
|  | 8.30±0.02 | 218 | 913 | 26.9±0.2 | 112.4±0.8 | 77PED/RYL | 108-98-5 |
| | See also: 82CAR/KIB, 81KIM/KAT. | | | | | | |
| $C_6H_6Se^+$ | | | | | | | |
|  | (≤7.7) | (≤217) | (≤906) | 39 | 163 | *EST | 645-96-5 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
| $C_6H_7{}^+$ | | | | | | | |
|  | | 204 | 854 | | | | |
| | From proton affinity of benzene. (RN 71-43-2). PA = 181.3 kcal/mol, 759. kJ/mol. | | | | | | |
| $(HC\equiv CCH_2CH_2C\equiv CH)H$ | | | | | | | |
| | | 269 | 1124 | | | | |
| | From proton affinity of $HC\equiv C(CH_2)_2C\equiv CH$ (RN 628-16-0) (85LIA/AUS). PA = 196 kcal/mol, 819 kJ/mol. | | | | | | |
| $(CH_3C\equiv CC\equiv CCH_3)H$ | | | | | | | |
| | | 260 | 1087 | | | | |
| | From proton affinity of $CH_3C\equiv CC\equiv CCH_3$ (RN 2809-69-0) (85LIA/AUS). PA = 196 kcal/mol, 819 kJ/mol. | | | | | | |
| $C_6H_7BrN^+$ | | | | | | | |
|  | | 183 | 767 | | | | |
| | From proton affinity of $3\text{-}BrC_6H_4NH_2$ (RN 591-19-5). | | | | | | |
| $C_6H_7Br_3Ti^+$ | | | | | | | |
|  | (8.6) | (80) | (337) | −118 | −493 | *EST | 1277-45-8 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_7ClN^+$ | | | | | | | |
|  | | 172 | 718 | | | | |
| | From proton affinity of 3-$ClC_6H_4NH_2$ (RN 108-42-9). PA = 207.2 kcal/mol, 867. kJ/mol. | | | | | | |
|  | | 170 | 712 | | | | |
| | From proton affinity of 4-$ClC_6H_4NH_2$ (RN 106-47-8). PA = 208.6 kcal/mol, 873. kJ/mol. | | | | | | |
|  | | (163) | (681) | | | | |
| | From proton affinity of 2-chloro-4-methylpyridine (RN 3678-62-4). (218.6) kcal/mol, (915.) kJ/mol. | | | | | | |
|  | | (161) | (675) | | | | |
| | From proton affinity of 2-chloro-6-methylpyridine (RN 18368-63-3). PA = (219) kcal/mol, (916) kJ/mol. | | | | | | |
| $C_6H_7ClNO^+$ | | | | | | | |
|  | | 127 | 531 | | | | |
| | From proton affinity of 6-chloro-1-methyl-2(1H)pyridinone (RN 17228-63-6). PA = 217.8 kcal/mol, 911. kJ/mol. | | | | | | |
|  | | 129 | 538 | | | | |
| | From proton affinity of 2-chloro-6-methoxypyridine (RN 17228-64-7). PA = 215.9 kcal/mol, 903. kJ/mol. | | | | | | |
| $C_6H_7Cl_3Ti^+$ | | | | | | | |
|  | (9.1) | (66) | (276) | -144 | -602 | *EST | 1282-31-1 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |
| $C_6H_7FN^+$ | | | | | | | |
|  | | 132 | 552 | | | | |
| | From proton affinity of 3-fluorobenzeneamine (RN 372-19-0). PA = 207.0 kcal/mol, 866. kJ/mol. | | | | | | |

### Table 1. Positive Ion Table - Continued

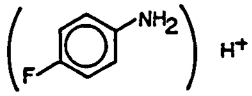
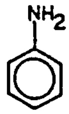
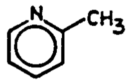
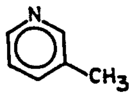
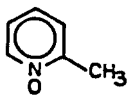
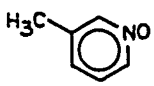
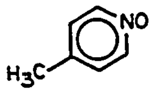
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_7FN^+$ | | | | | | | |
|  | | 132 | 550 | | | | |
| | From proton affinity of 4-fluorobenzeneamine (RN 371-40-4). PA = 208.1 kcal/mol, 871. kJ/mol. | | | | | | |
| $C_6H_7N^+$ | | | | | | | |
|  | 7.720±0.002 | 198 | 829 | 20.8±0.2 | 87.1±0.8 | 77PED/RYL | 62-53-3 |
| | IP from 84SMI/HAG. See also: 83KLA/KOV, 81KIM/KAT, 85MEE/SEK, 85HAG/SMI. | | | | | | |
|  | 9.02±0.03 | 232 | 969 | 23.7±0.2 | 99.2±0.7 | 77PED/RYL | 109-06-8 |
| | See also: 81KIM/KAT. | | | | | | |
|  | 9.04±0.03 | 234 | 979 | 25.4±0.1 | 106.4±0.5 | 77PED/RYL | 108-99-6 |
| | See also: 81MOD/DIS2, 81KIM/KAT. | | | | | | |
|  | 9.04±0.03 | 233 | 976 | 24.8±0.3 | 103.8±1.2 | 77PED/RYL | 108-89-4 |
| $C_6H_7NO^+$ | | | | | | | |
|  | ≤8.21±0.02 | (≤194) | (≤811) | 5 | 19 | *EST | 931-19-1 |
|  | (≤8.20±0.02) | (≤195) | (≤817) | 6 | 26 | *EST | 1003-73-2 |
|  | 8.12±0.02 | (193) | (807) | 6 | 24 | *EST | 1003-67-4 |

Table 1. Positive Ion Table - Continued

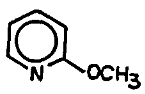
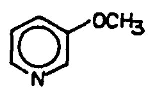
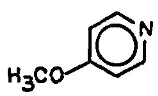
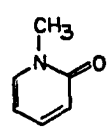
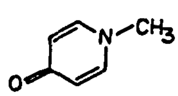
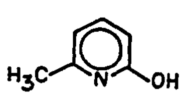
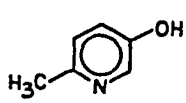
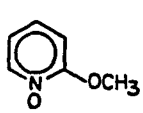
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_7NO^+$ | | | | | | | |
|  | (8.7) | (189) | (787) | −12 | −52 | *EST | 1628-89-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.34±0.02) | (211) | (885) | −4 | −16 | *EST | 7295-76-3 |
|  | (9.58±0.02) | (218) | (911) | −3 | −13 | *EST | 620-08-6 |
|  | (8.2) | (169) | (706) | −20±2 | −85±10 | *EST | 694-85-9 |
| | IP is onset of photoelectron band. See also: 81DRE/BEC. | | | | | | |
|  | (≤8.20±0.03) | (≤186) | (≤778) | −3±2 | −13±8 | *EST | 695-19-2 |
|  | (8.33) | (163) | (684) | −29±0.7 | −120±3 | 82SUR/ELS | 73229-70-6 |
|  | (9.15±0.05) | (194) | (813) | −17±0.7 | −70±3 | 82SUR/ELS | 1121-78-4 |
| $C_6H_7NO_2^+$ | | | | | | | |
|  | (7.5) | (151) | (631) | −22 | −93 | *EST | 1122-96-9 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

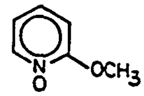
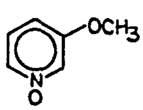
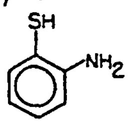
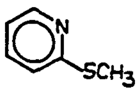
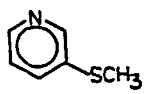
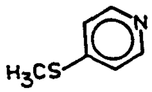
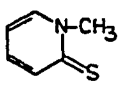
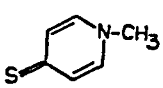
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_7NO_2^+$ | | | | | | | |
|  | (8.21±0.05) | (158) | (660) | −32 | −132 | *EST | 20773-98-2 |
|  | (8.40±0.05) | (171) | (714) | −23 | −96 | *EST | 14906-61-7 |
| $C_6H_7NS^+$ | | | | | | | |
|  | (7.6) | (203) | (849) | 28 | 116 | *EST | 137-07-5 |
| | IP is onset of photoelectron band (82ZVE/ASH). | | | | | | |
|  | (8.24±0.03) | (223) | (933) | 33 | 138 | *EST | 18438-38-5 |
| | See also: 81DRE/BEC. | | | | | | |
|  | (≤8.41±0.03) | (≤231) | (≤966) | 37 | 155 | *EST | 18794-33-7 |
|  | (≤8.73±0.03) | (≤238) | (≤997) | 37 | 155 | *EST | 22581-72-2 |
|  | (7.69±0.03) | (218) | (912) | 41 | 170 | *EST | 2044-27-1 |
| | See also: 81DRE/BEC. | | | | | | |
|  | 7.54±0.02 | (239) | (999) | 65 | 272 | *EST | 6887-59-8 |

Table 1. Positive Ion Table - Continued

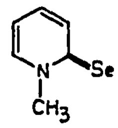
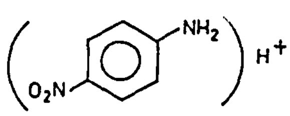
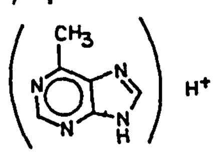
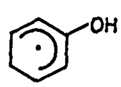
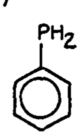
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_7NSe^+$ | | | | | | | |
|  | ≤7.22 | (≤224) | (≤937) | 57 | 240 | *EST | 2240-85-9 |
| | IP from 81DRE/BEC. | | | | | | |
| $C_6H_7N_2O_2^+$ | | | | | | | |
|  | | 172 | 719 | | | | |
| | From proton affinity of 4-$NO_2C_6H_4NH_2$ (RN 100-01-6) (84ROL/HOU). PA = 207.0 kcal/mol, 866. kJ/mol. | | | | | | |
| $C_6H_7N_4^+$ | | | | | | | |
|  | | 185 | 775 | | | | |
| | From proton affinity of 6-methylpurine (RN 2004-03-7). PA = (223) kcal/mol, (933) kJ/mol. | | | | | | |
| $C_6H_7O^+$ | | | | | | | |
|  | | 146 | 613 | | | | |
| | From proton affinity of $C_6H_5OH$ (RN 108-95-2). PA = 196.3 kcal/mol, 821. kJ/mol. | | | | | | |
| $(HC{\equiv}CCH_2)_2OH$ | | (246) | (1031) | | | | |
| | From proton affinity of $(HC{\equiv}CCH_2)_2O$ (RN 6921-27-3). PA = 190.8 kcal/mol, 798. kJ/mol. | | | | | | |
| $C_6H_7P^+$ | | | | | | | |
|  | (8.47±0.01) | (226) | (945) | 31 | 128 | *EST | 638-21-1 |
| | See also: 81CAB/COW2. | | | | | | |
| $C_6H_8^+$ | | | | | | | |
| (E)-$CH_2{=}C{=}CHCH{=}CHCH_3$ | (8.32) | (244) | (1020) | 52 | 217 | *EST | 20130-95-4 |
| (Z)-$CH_2{=}CHCH{=}CHCH{=}CH_2$ | 8.31±0.01 | 233 | 973 | 41 | 171 | 70BEN/O'N | 2612-46-6 |
| (E)-$CH_2{=}CHCH{=}CHCH{=}CH_2$ | 8.28±0.02 | (231) | (965) | 40 | 166 | *EST | 821-07-8 |
| | | *(237)* | *(991)* | *46* | *192* | | |
| $CH_3CH{=}C{=}CHCH{=}CH_2$ | (8.56) | (250) | (1048) | 53 | 222 | *EST | 33755-64-5 |

**Table 1. Positive Ion Table - Continued**

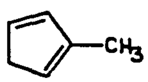
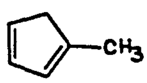
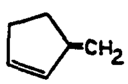
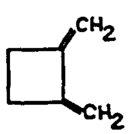
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8^+$ | | | | | | | |
| $CH_2=C=C(CH_3)CH=CH_2$ | (8.54) | (249) | (1040) | 52 | 216 | *EST | 25054-29-9 |
| $CH_2=C=CHC(CH_3)=CH_2$ | (8.54) | (249) | (1040) | 52 | 216 | *EST | 14763-81-6 |
| $C_2H_5C\equiv CCH=CH_2$ | (8.91±0.01) | (260) | (1090) | 55 | 230 | *EST | 13721-54-5 |
| $CH_3C\equiv CC(CH_3)=CH_2$ | (8.72±0.01) | (253) | (1058) | 52 | 217 | *EST | 926-55-6 |
|  | 8.25±0.02 | 215.6<br>*221.3* | 902.3<br>*926.1* | 25.4±0.1<br>*31.1±0.1* | 106.3±0.5<br>*130.1±0.5* | 77PED/RYL | 592-57-4 |
| | See also: 81KIM/KAT. | | | | | | |
|  | 8.82±0.02 | 229<br>*235* | 959<br>*985* | 25.8±0.5<br>*32.0±0.5* | 107.9±2<br>*133.9±2* | 77SHA/GOL | 628-41-1 |
| | See also: 81KIM/KAT. | | | | | | |
|  | 8.40±0.05 | (217) | (907) | 23 | 97 | *EST | 96-39-9 |
|  | 8.45±0.05 | (218) | (911) | 23 | 96 | *EST | 3727-31-9 |
|  | (8.40) | (223) | (931) | 29 | 121 | *EST | 930-26-7 |
|  | (8.4) | (242) | (1011) | 48 | 201 | 80GAJ | 14296-80-1 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

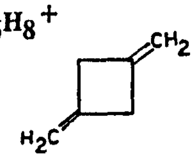
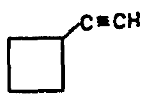
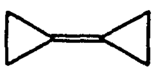
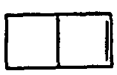
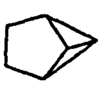
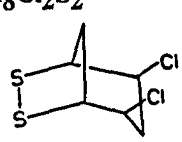
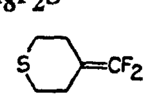
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8^+$ | | | | | | | |
|  | (8.7) | (254) | (1063) | 54 | 224 | 80GAJ | 2045-78-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.6) | (284) | (1188) | 63 | 262 | *EST | 50786-62-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.5) | (280) | (1170) | 84 | 350 | *EST | 27567-82-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.1) | (271) | (1135) | 61 | 257 | 80ROT/KLA | 3097-63-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.43) | (≤272) | (≤1138) | 54.5 | 228.0 | 85SVY/IOF | 287-12-7 |
| $C_6H_8Cl_2S_2^+$ | | | | | | | |
|  | (7.8) | (158) | (660) | -22 | -93 | *EST | 74796-12-6 |
| | IP is onset of photoelectron band (83JOR/MCC). | | | | | | |
| $C_6H_8F_2S^+$ | | | | | | | |
|  | (9.34) | (129) | (538) | -87 | -363 | *EST | 77471-71-7 |
| | IP from 80SAR/WOR. | | | | | | |
| $C_6H_8N^+$ | | | | | | | |
| $(HC{\equiv}CCH_2)_2NH_2$ | | 262 | 1098 | | | | |
| | From proton affinity of $(HC{\equiv}CCH_2)_2NH$ (RN 6921-28-4). PA = 216.1 kcal/mol, 904. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

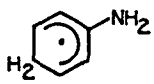
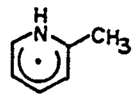
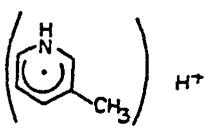
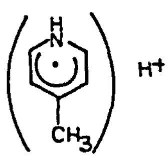
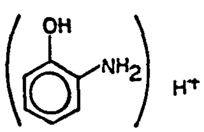
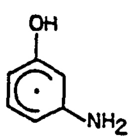
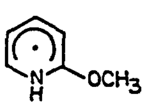
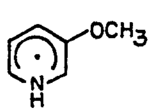
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8N^+$ | | | | | | | |
|  | | 177 | 740 | | | | |
| | From proton affinity of $C_6H_5NH_2$ (RN 62-53-3). PA = 209.5 kcal/mol, 876. kJ/mol. | | | | | | |
|  | | 164 | 688 | | | | |
| | From proton affinity of 2-methylpyridine (RN 109-06-8). PA = 225.0 kcal/mol, 942. kJ/mol. | | | | | | |
|  | | 167 | 698 | | | | |
| | From proton affinity of 3-methylpyridine (RN 108-99-6). PA = 224.1 kcal/mol, 938. kJ/mol. | | | | | | |
|  | | 165 | 692 | | | | |
| | From proton affinity of 4-methylpyridine (RN 108-89-4). PA = 225.2 kcal/mol, 942. kJ/mol. | | | | | | |
| $C_6H_8NO^+$ | | | | | | | |
|  | | 131 | 547 | | | | |
| | From proton affinity of 2-$HOC_6H_4NH_2$. PA = 214.2 kcal/mol, 896. kJ/mol. | | | | | | |
|  | | 130 | 545 | | | | |
| | From proton affinity of 3-$(OH)C_6H_4NH_2$ (RN 591-27-5). PA = 214.2 kcal/mol, 896. kJ/mol. | | | | | | |
|  | | 131 | 550 | | | | |
| | From proton affinity of 2-methoxypyridine (RN 1628-89-3). PA = 221.9 kcal/mol, 928. kJ/mol. | | | | | | |
|  | | 138 | 579 | | | | |
| | From proton affinity of 3-methoxypyridine (RN 7295-76-3). PA = 223.6 kcal/mol, 935. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

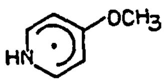
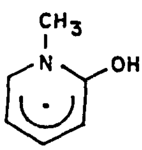
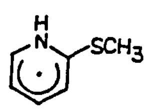
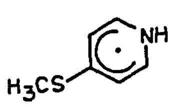
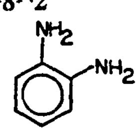
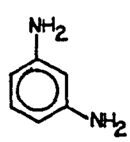
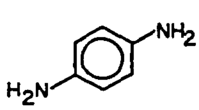
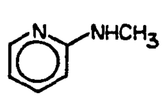
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8NO^+$ | | | | | | | |
|  | | 135 | 565 | | | | |
| | From proton affinity of 4-methoxypyridine (RN 620-08-6). PA = 227.6 kcal/mol, 952. kJ/mol. | | | | | | |
|  | | 125 | 524 | | | | |
| | From proton affinity of 1-methyl-2-pyridinone (RN 694-85-9). PA = 220.2 kcal/mol, 921. kJ/mol. | | | | | | |
| $C_6H_8NS^+$ | | | | | | | |
|  | | 177 | 739 | | | | |
| | From proton affinity of 2-(methylthio)pyridine (RN 18438-38-5). PA = 222.0 kcal/mol, 929. kJ/mol. | | | | | | |
|  | | (177) | (742) | | | | |
| | From proton affinity of 4-(methylthio)pyridine (RN 22581-72-2). PA = (225.5) kcal/mol, (943.) kJ/mol. | | | | | | |
| $C_6H_8N_2^+$ | | | | | | | |
|  | 7.2 | (188) | (787) | 22±1 | 92±5 | *EST | 95-54-5 |
| | See also: 81NEL/GRE. | | | | | | |
|  | 7.14 | (186) | (777) | 21 | 88 | *EST | 108-45-2 |
|  | 6.87±0.05 | (181) | (760) | 23 | 97 | *EST | 106-50-3 |
| | See also: 81CAB/COW2. | | | | | | |
|  | (8.26±0.05) | (220) | (924) | 30 | 127 | *EST | 4597-87-9 |

**Table 1. Positive Ion Table - Continued**

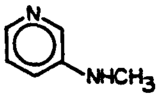
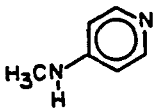
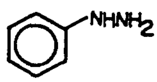
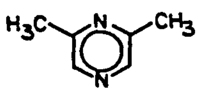
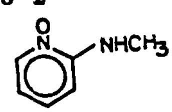
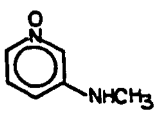
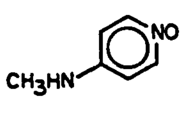
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8N_2^+$ | | | | | | | |
|  | (8.53±0.05) | (231) | (965) | 34 | 142 | *EST | 18364-47-1 |
|  | (8.75±0.05) | (233) | (972) | 31 | 128 | *EST | 1121-58-0 |
|  | | | | 48.6±0.2 | 203.5±0.8 | 77PED/RYL | 100-63-0 |
| | Values of 7.64 and 7.74 have been reported for the adiabatic IP of this compound. Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. | | | | | | |
|  | (8.80) | (270) | (1128) | 67±0.7 | 279±3 | *EST | 108-50-9 |
| $C_6H_8N_2O^+$ | | | | | | | |
|  | (7.67±0.05) | (188) | (787) | 11 | 47 | *EST | 54818-70-1 |
|  | (7.97±0.05) | (198) | (829) | 14 | 60 | *EST | 54818-71-2 |
|  | (7.45±0.05) | (185) | (775) | 13 | 56 | *EST | 1122-92-5 |
| $C_6H_8O^+$ | | | | | | | |
| $HC{\equiv}CCOCH_2CH_2CH_3$ | (10.00±0.04) | (233) | (975) | 2.5 | 10.5 | *EST | |
| | IP from 86TUR/HAV2. | | | | | | |

Table 1. Positive Ion Table - Continued

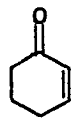
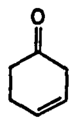
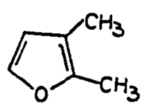
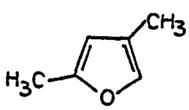
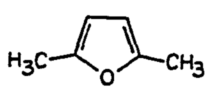
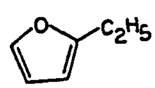
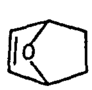
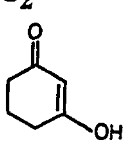
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8O^+$ | | | | | | | |
|  | 9.23±0.05 | (185) | (775) | −28±0.7 | −116±3 | *EST | 930-68-7 |
|  | (≤9.42) | (≤185) | (≤773) | −33±0.7 | −136±3 | *EST | 4096-34-8 |
|  | (8.25±0.10)<br>IP from 85GRU/SPI. | (166) | (694) | −24 | −102 | *EST | |
|  | (8.39±0.10)<br>IP from 85GRU/SPI. | (166) | (694) | −28 | −116 | *EST | 3710-43-8 |
|  | (8.25±0.10)<br>IP from 85GRU/SPI. | (165) | (690) | −25 | −106 | *EST | 625-86-5 |
|  | (8.45±0.05) | (171) | (715) | −24 | −100 | *EST | 3208-16-0 |
|  | (≤9.44±0.02) | (≤207) | (≤867) | −11 | −44 | *EST | 6705-50-6 |
| $C_6H_8O_2^+$ | | | | | | | |
|  | 9.52±0.05 | (141) | (589) | −79 | −330 | *EST | 504-02-9 |

**Table 1. Positive Ion Table - Continued**

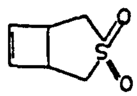
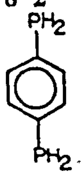
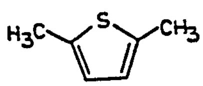
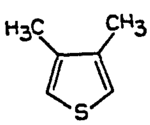
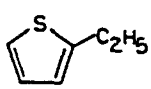
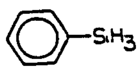
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_8O_2S^+$ | | | | | | | |
|  | <9.6 | (<187) | (<784) | −34 | −142 | *EST | 84451-42-3 |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
| $C_6H_8P_2^+$ | | | | | | | |
|  | ≤8.78 | (≤237) | (≤990) | 34 | 143 | *EST | 78550-67-1 |
| | IP from 81CAB/COW2. | | | | | | |
| $C_6H_8S^+$ | | | | | | | |
|  | (8.10) | (199) | (832) | 12 | 50 | *EST | 638-02-8 |
| | See also: 83BOC/ROT. | | | | | | |
|  | (≤8.55) | (≤209) | (≤875) | 12 | 50 | *EST | 632-15-5 |
| | IP from 83BOC/ROT. | | | | | | |
|  | (8.67±0.05) | (215) | (898) | 15 | 61 | *EST | 872-55-9 |
| $C_6H_8Si^+$ | | | | | | | |
|  | (9.09) | (236) | (988) | 27 | 111 | *EST | 694-53-1 |
| $C_6H_9^+$ | | | | | | | |
| $CH_3C{\equiv}CC(CH_3)_2$ | | 216 | 904 | | | | 77920-98-0 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
|  | | 191 | 800 | | | | |
| | From proton affinities of 1,3-c-$C_6H_8$ (RN 592-57-4) PA = (200) kcal/mol, (837) kJ/mol and 1,4-c-$C_6H_8$ (RN 628-41-1) (83GAU/HOU) PA = (200) kcal/mol, (837) kJ/mol. Value derived from appearance potential measurements (84LOS/HOL) is the same. | | | | | | |

Table 1. Positive Ion Table - Continued

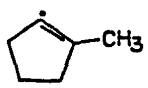
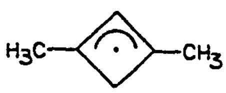
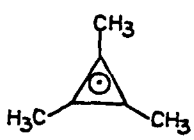
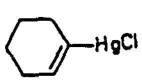
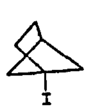
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_9^+$ | | | | | | | |
|  | | 190 | 795 | | | | 72026-92-7 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
|  | | (202) | (845) | | | | |
| | From proton affinity of 1-methyl-3-methylenecyclobutene. (RN 15082-13-0). PA = (212) kcal/mol, (887) kJ/mol. | | | | | | |
|  | | 199 | 833 | | | | 26827-04-3 |
| | From appearance potential measurements (84LOS/HOL). | | | | | | |
| $C_6H_9Br^+$ | | | | | | | |
|  | (9.5) | (235) | (983) | 16 | 66 | *EST | 77379-00-1 |
| | IP is onset of photoelectron band (84DEL/ABE). | | | | | | |
| $C_6H_9ClHg^+$ | | | | | | | |
|  | (8.8) | (212) | (887) | 9 | 38 | *EST | 10080-39-4 |
| | IP is onset of photoelectron band (81BAI/CHI). | | | | | | |
| $C_6H_9Cl_2P^+$ | | | | | | | |
| $(CH_3)_3CC{\equiv}CPCl_2$ | (≤9.58) | (≤211) | (≤883) | −10 | −41 | *EST | 77376-08-0 |
| | IP from 81CAB/COW. | | | | | | |
| $C_6H_9I^+$ | | | | | | | |
|  | (8.8) | (233) | (976) | 30 | 127 | *EST | 74725-75-0 |
| | IP is onset of photoelectron band (84DEL/ABE). | | | | | | |
| $C_6H_9N^+$ | | | | | | | |
| (E)-$(CH_3)_2NCH{=}CHC{\equiv}CH$ | (7.7) | (260) | (1087) | 82±1 | 344±6 | *EST | 2206-24-8 |

**Table 1. Positive Ion Table - Continued**

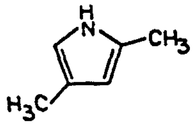
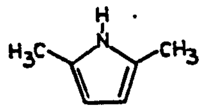
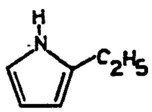
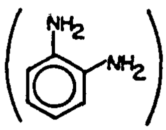
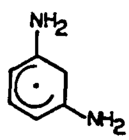
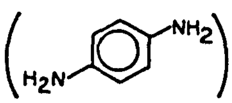
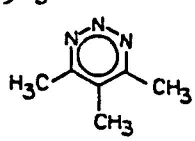
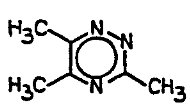
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_9N^+$ | | | | | | | |
|  | (7.54±0.02) | (184) | (767) | 10 | 40 | *EST | 625-82-1 |
|  | (≤7.69) | (≤187) | (≤782) | 9.5±0.2 | 39.8±0.8 | 77PED/RYL | 625-84-3 |
|  | (7.97±0.05) | (197) | (823) | 13 | 54 | *EST | 1551-06-0 |
| $C_6H_9N_2^+$ | | | | | | | |
|  H+ | From proton affinity of 1,2-$C_6H_4(NH_2)_2$ (RN 95-54-5). PA = 212.8 kcal/mol, 890. kJ/mol. | 175 | 732 | | | | |
|  | From proton affinity of 1,3-$C_6H_4(NH_2)_2$ (RN 108-45-2). PA = 222.4 kcal/mol, 930.5 kJ/mol. | 164 | 688 | | | | |
|  H+ | From proton affinity of 1,4-$C_6H_4(NH_2)_2$ (RN 106-50-3). PA = 215.9 kcal/mol, 903. kJ/mol. | 173 | 723 | | | | |
| $C_6H_9N_3^+$ | | | | | | | |
|  | ≤9.4<br>IP from 83GLE/SPA. | (≤267) | (≤1118) | 50 | 211 | *EST | 33209-85-7 |
|  | (≤8.84) | (≤274) | (≤1146) | 70 | 293 | *EST | 24108-36-9 |

Table 1. Positive Ion Table - Continued

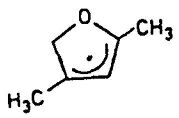
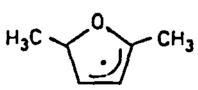
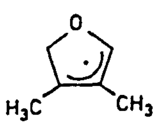
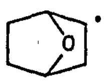
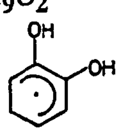
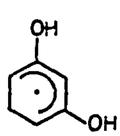
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_9O^+$ | | | | | | | |
|  | | 125 | 523 | | | | |
| | From proton affinity of 2,4-dimethylfuran (RN 3710-43-8) (85HOU/ROL). PA = 213.0 kcal/mol, 819. kJ/mol. | | | | | | |
|  | | 131 | 550 | | | | |
| | From proton affinity of 2,5-dimethylfuran (RN 625-86-5) (85HOU/ROL, 86MAU). PA = 209.0 kcal/mol, 874. kJ/mol. | | | | | | |
|  | | 133 | 556 | | | | |
| | From proton affinity of 3,4-dimethylfuran (RN 20843-07-6) (85HOU/ROL). PA = 207.1 kcal/mol, 867. kJ/mol. | | | | | | |
|  | | 155 | 649 | | | | |
| | From proton affinity of bicyclo[2.2.1]hept-2-ene, 7-oxa- (RN 6705-50-6) (86HOU/SCH). PA = 200.0 kcal/mol, 837. kJ/mol. | | | | | | |
| $C_6H_9O_2^+$ | | | | | | | |
|  | | 92 | 384 | | | | |
| | From proton affinity of 1,2-cyclohexanedione (RN 765-87-7) (83MAU). PA = 203.9 kcal/mol, 853. kJ/mol. | | | | | | |
|  | | 76 | 318 | | | | |
| | From proton affinity of 1,3-cyclohexanedione (RN 504-02-9). PA = 210.8 kcal/mol, 882. kJ/mol. | | | | | | |
| $C_6H_{10}^+$ | | | | | | | |
| $CH_2=C=CHCH_2C_2H_5$ | (9.00±0.05) | (237) | (990) | 29 | 122 | *EST | 592-44-9 |
| (E)-$CH_2=CHCH=CHC_2H_5$ | 8.51 | (210) | (878) | 14 | 57 | *EST | 20237-34-7 |
| | IP from 81MAS/MOU. | | | | | | |
| (Z)-$CH_2=CHCH_2CH=CHCH_3$ | (9.04±0.05) | (227) | (950) | 19 | 80 | *EST | 7318-67-4 |
| (E)-$CH_2=CHCH_2CH=CHCH_3$ | (8.98±0.05) | (225) | (940) | 18 | 74 | *EST | 7319-00-8 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}^+$ | | | | | | | |
| $CH_2=CHCH_2CH_2CH=CH_2$ | 9.29±0.05 | 234 | 980 | 20.1±0.1 | 84.1±0.6 | 77PED/RYL | 592-42-7 |
| $CH_3CH=C=CHC_2H_5$ | (8.76±0.05) | (228) | (955) | 26 | 110 | *EST | 592-49-4 |
| (Z),(Z)-$CH_3CH=CHCH=CHCH_3$ | (8.27) | (203) | (850) | 12 | 52 | *EST | 6108-61-8 |
| | See also: 81MAS/MOU. | | | | | | |
| (E),(Z)-$CH_3CH=CHCH=CHCH_3$ | 8.24±0.02 | (202) | (844) | 12 | 49 | *EST | 5194-50-3 |
| | See also: 81MAS/MOU. | | | | | | |
| (E),(E)-$CH_3CH=CHCH=CHCH_3$ | 8.18±0.06 | (199) | (832) | 11 | 43 | *EST | 5194-51-4 |
| | See also: 81MAS/MOU. | | | | | | |
| $CH_2=C=CHCH(CH_3)_2$ | (9.06±0.05) | (236) | (987) | 27 | 113 | *EST | 13643-05-5 |
| $CH_2=C=C(CH_3)C_2H_5$ | (8.74±0.05) | (227) | (951) | 26 | 108 | *EST | 7417-48-3 |
| $(CH_3)_2C=CHCH=CH_2$ | 8.25 | (201) | (839) | 10 | 43 | 70BEN/O'N | 926-56-7 |
| | IP from 81MAS/MOU, 82LEV/LIA. | | | | | | |
| (Z)-$CH_2=CHC(CH_3)=CHCH_3$ | 8.42 | (205) | (859) | 11 | 47 | *EST | 2787-43-1 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_2=CHC(CH_3)=CHCH_3$ | (8.38) | (204) | (852) | 10 | 43 | *EST | 2787-45-3 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_2=C(CH_3)CH=CHCH_3$ | 8.43 | (205) | (856) | 10 | 43 | *EST | 926-54-5 |
| | IP from 81MAS/MOU. | | | | | | |
| $CH_2=C(CH_3)CH_2CH=CH_2$ | (9.16±0.05) | (228) | (956) | 17 | 72 | *EST | 763-30-4 |
| $CH_2=CHCH(CH_3)CH=CH_2$ | (9.40±0.05) | (235) | (985) | 19 | 78 | *EST | 1115-08-8 |
| $(CH_3)_2C=C=CHCH_3$ | 8.64±0.05 | (222) | (930) | 23 | 96 | *EST | 3043-33-2 |
| $CH_2=C(CH_3)C(CH_3)=CH_2$ | 8.71 | 211 | 884 | 10±0.2 | 44±1 | 77PED/RYL | 513-81-5 |
| | See also: 81MAS/MOU. | | | | | | |

Table 1. Positive Ion Table - Continued

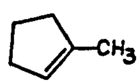
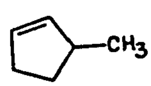
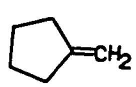
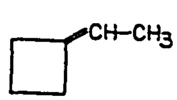
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}^+$ | | | | | | | |
| $C_2H_5C(=CH_2)CH=CH_2$ | (8.79±0.02)<br>See also: 81MAS/MOU. | (216) | (904) | 13 | 56 | *EST | 3404-63-5 |
| $C_4H_9C \equiv CH$ | (9.95±0.05)<br>See 81HOL/FIN. | (258) | (1082) | 29±0.2 | 122±1 | 79ROG/DAG | 693-02-7 |
| $C_3H_7C \equiv CCH_3$ | 9.366±0.005 | 242 | 1012 | 26±0.5 | 108±2 | 79ROG/DAG | 764-35-2 |
| $C_2H_5C \equiv CC_2H_5$ | 9.323±0.005 | 240 | 1005 | 25±0.5 | 106±2 | 79ROG/DAG | 928-49-4 |
| $(CH_3)_2CHCH_2C \equiv CH$ | (9.83±0.05) | (254) | (1064) | 28 | 116 | *EST | 7154-75-8 |
| $CH_3CH_2CH(CH_3)C \equiv CH$ | 9.79±0.05 | 253 | 1058 | 27±0.2 | 113±1 | 79ROG/DAG | 922-59-8 |
| $(CH_3)_3CC \equiv CH$ | (9.80±0.05)<br>See also: 81CAB/COW, 85ORL/BOG. | (251) | (1051) | 25±0.7 | 106±3 | 77KUP/SHI | 917-92-0 |
| $(CH_3)_2CHC \equiv CCH_3$ | 9.31±0.05 | (238) | (995) | 23 | 97 | *EST | 21020-27-9 |
|  | 8.945±0.01<br>See also: 81KIM/KAT. | 205.2 | 858.4 | −1.1±0.1 | −4.6±0.5 | 77PED/RYL | 110-83-8 |
|  | 8.55±0.05 | 196 | 821 | −1±0.2 | −4±1 | 82ALL/DOD | 693-89-0 |
|  | 8.95±0.01 | 208 | 871 | 2±0.5 | 7±2 | 79FUC/PEA | 1120-62-3 |
|  | 8.55±0.01 | 200 | 837 | 3±0.5 | 12±2 | 82ALL/DOD | 1528-30-9 |
|  | (8.70±0.05) | (221) | (925) | 21 | 86 | *EST | 1528-21-8 |

**Table 1. Positive Ion Table - Continued**

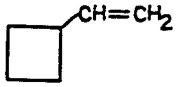
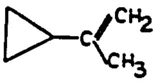
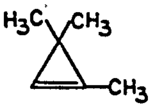
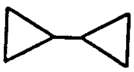
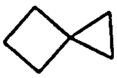
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}^+$ | | | | | | | |
|  | (≤9.44) | (≤242) | (≤1010) | 24 | 99 | *EST | 2597-49-1 |
|  | (8.66±0.05) | (222) | (930) | 22 | 94 | 82KOZ/MAS | 4663-22-3 |
|  | (8.58±0.05)<br>See also: 81PLE/VIL. | (239) | (1001) | 41 | 173 | *EST | 3664-56-0 |
|  | (9.16±0.02) | (220.4) | (922.1) | 9.2±0.1 | 38.3±0.4 | 77PED/RYL | 285-58-5 |
|  | (9.0)<br>IP is onset of photoelectron band. | (237) | (993) | 30 | 125 | 82WIB/WEN | 186-04-9 |
|  | (9.7)<br>IP is onset of photoelectron band (84DEL/PIG). | (239) | (1000) | 15.3 | 64.0 | 82WIB/WEN | 285-86-9 |
|  | (8.9)<br>IP is onset of photoelectron band (82SPA/GLE). | (236) | (988) | 31±1 | 129±4 | 77PED/RYL | 5685-46-1 |
|  | (9.1)<br>IP is onset of photoelectron band. | (250) | (1045) | 40 | 167 | *EST | 157-45-9 |

**Table 1. Positive Ion Table - Continued**

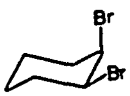
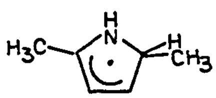
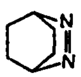
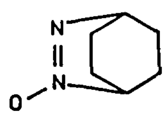
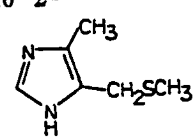
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}Br_2^+$ | | | | | | | |
|  | 10.02±0.02 | (206) | (863) | −25 | −104 | *EST | 7429-37-0 |
|  | (9.94±0.02) | (204) | (855) | −25 | −104 | *EST | 19246-38-9 |
| $C_6H_{10}F_3O_2^+$ | | | | | | | |
| $CF_3C(OH)O(n\text{-}C_4H_9)$ | | −79 | −332 | | | | |
| | From proton affinity of $CF_3COO(n\text{-}C_4H_9)$ (RN 367-64-6). PA = 185.8 kcal/mol, 777. kJ/mol. | | | | | | |
| $C_6H_{10}N^+$ | | | | | | | |
|  | | 157 | 656 | | | | |
| | From proton affinity of 2,5-dimethylpyrrole (RN 625-84-3) (86MAU/LIE). PA = 218.2 kcal/mol, 913. kJ/mol. | | | | | | |
| $C_6H_{10}N_2^+$ | | | | | | | |
|  | (7.79±0.04) | (218) | (913) | 38 | 161 | 77OTH/OLS | 3310-62-1 |
| $C_6H_{10}N_2O^+$ | | | | | | | |
|  | (≤9.30±0.03) | (≤237) | (≤990) | 22.08±.44 | 92.38±1.84 | 83BYS | 25926-96-9 |
| $C_6H_{10}N_2S^+$ | | | | | | | |
|  | (7.9) | (208) | (869) | 26 | 107 | *EST | 75899-43-3 |
| | IP is onset of photoelectron band (80KLA/BUT). | | | | | | |

Table 1. Positive Ion Table - Continued

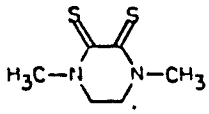
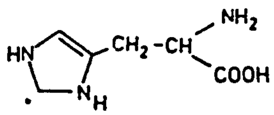
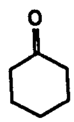
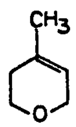
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}N_2S_2^+$ | | | | | | | |
|  | ≤7.82 | (≤236) | (≤986) | 55 | 232 | *EST | 78134-03-9 |
| | IP from 81HEN/ISA. | | | | | | |
| $C_6H_{10}N_3O_2^+$ | | | | | | | |
|  | | 103 | 431 | | | | |
| | From proton affinity of L-histidine. PA = 231.9 kcal/mol, 970. kJ/mol. | | | | | | |
| $C_6H_{10}O^+$ | | | | | | | |
| (E)-n-$C_3H_7CH=CHCHO$ | (9.65) | (187) | (782) | -36 | -149 | *EST | 505-57-7 |
| $CH_3CH_2CH=C(CH_3)CHO$ | (9.54) | (181) | (758) | -39 | -162 | *EST | 623-36-9 |
| $CH_3CH=C(C_2H_5)CHO$ | (9.53) | (181) | (757) | -39 | -162 | *EST | 19780-25-7 |
| iso-$C_3H_7COCH=CH_2$ | (9.39) | (177) | (741) | -39 | -165 | *EST | 1606-47-9 |
| (E)-$CH_3CH=CHC(=O)C_2H_5$ | (9.32) | (175) | (730) | -40 | -169 | *EST | 2497-21-4 |
| $CH_3CH=C(CH_3)C(=O)CH_3$ | (9.35) | (172) | (719) | -44 | -183 | *EST | 565-62-8 |
| $(CH_3)_2C=CHC(=O)CH_3$ | 9.08±0.03 | (165) | (693) | -44 | -183 | *EST | 141-79-7 |
|  | 9.14±0.01 | 157 | 656 | -54±0.5 | -226±2 | 77PED/RYL | 108-94-1 |
| | See also: 86SPA/RAD. | | | | | | |
|  | (8.88) | (173) | (724) | -32 | -133 | *EST | 2270-61-3 |
| | IP from 84ALA/RYE. | | | | | | |

Table 1. Positive Ion Table - Continued

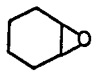
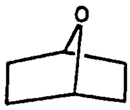
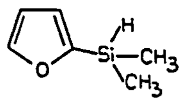
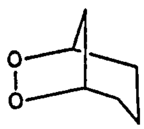
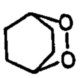
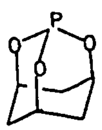
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}O^+$ | | | | | | | |
|  | (9.82)<br>IP from 84ALA/RYE. | (197) | (822) | −30 | −125 | *EST | 286-20-4 |
|  | (≤9.57±0.02) | (≤177) | (≤740) | −44 | −183 | 74PIH/TAS | 279-49-2 |
| $C_6H_{10}OS^+$ | | | | | | | |
| $CH_3SC(CH_3)=CHC(=O)CH_3$ | (8.15)<br>IP is onset of photoelectron band (81JOR/CAR). | (152) | (636) | −36 | −150 | *EST | 60887-86-7 |
| $C_6H_{10}OSi^+$ | | | | | | | |
|  | ≤8.62<br>IP from 83ZYK/ERC. | (≤165) | (≤689) | −34 | −143 | *EST | 13271-68-6 |
| $C_6H_{10}O_2^+$ | | | | | | | |
| (E)-$CH_3CH=CHCOOC_2H_5$ | (≤10.11) | (≤143) | (≤599) | −90±0.5 | −376±2 | 77PED/RYL | 623-70-1 |
|  | (8.6)<br>IP is onset of photoelectron band (84GLE/DOB). | (163) | (683) | −35 | −147 | *EST | 51272-66-3 |
|  | 8.4<br>IP is onset of photoelectron band. | (159) | (663) | −35 | −147 | *EST | 280-53-5 |
| $C_6H_{10}O_3P^+$ | | | | | | | |
|  | From proton affinity of 2,8,9-trioxa-1-phosphaadamantane (RN 281-33-4).<br>PA = 213.8 kcal/mol, 894. kJ/mol. | −14 | −58 | | | | |

**Table 1. Positive Ion Table - Continued**

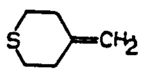
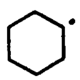
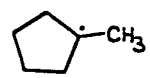
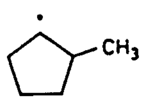
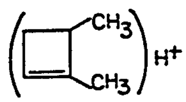
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6H_{10}O_4{}^+$ | | | | | | | |
| $C_2H_5OCOCOOC_2H_5$ | (9.8) | (49) | (206) | −177±2 | −740±9 | 77PED/RYL | 95-92-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_{10}S^+$ | | | | | | | |
|  | 9.22 | (221) | (923) | 8 | 34 | *EST | 50550-56-6 |
| | IP from 80SAR/WOR. | | | | | | |
| $C_6H_{11}{}^+$ | | | | | | | |
| $CH_3CH=CHC(CH_3)_2$ | | (169) | (706) | | | | |
| | From proton affinity of $CH_3CH=CHC(CH_3)=CH_2$. (RN 1118-58-7). PA = (207.9) kcal/mol, (870.) kJ/mol. | | | | | | |
| $C_2H_5C(CH_3)CH=CH_2$ | | (170) | (712) | | | | |
| | From proton affinity of $CH_3CH=C(CH_3)CH=CH_2$. (RN 4549-74-0). PA = (205.7) kcal/mol, (860.6) kJ/mol. | | | | | | |
| $(CH_3)_2CC(CH_3)=CH_2$ | | (174) | (728) | | | | |
| | From proton affinity of $CH_2=C(CH_3)C(CH_3)=CH_2$. (RN 513-81-5). PA = (202.1) kcal/mol, (846.) kJ/mol. | | | | | | |
|  | | (175) | (733) | 18 | 77 | 81TSA | 3170-58-9 |
| | From proton affinity of cyclohexene (RN 110-83-8). PA = (189) kcal/mol, (792) kJ/mol. | | | | | | |
|  | | 167 | 698 | | | | |
| | From proton affinities of methylenecyclopentane (RN 1528-30-9) PA = 200.8 kcal/mol, 840. kJ/mol and 1-methylcyclopentene (RN 693-89-0), PA = 196.9 kcal/mol, 824. kJ/mol, and from hydride and chloride transfer equilibrium constant determinations (76SOL/FIE, 76GOR/MUN, 85SHA/SHA). | | | | | | |
|  | | (179) | (747) | | | | |
| | From appearance potential measurements (81HER/SIC). | | | | | | |
|  | | (182) | (762) | | | | |
| | From proton affinity of 1,2-dimethylcyclobutene. (RN 1501-58-2). PA = (201) kcal/mol, (841) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

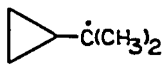
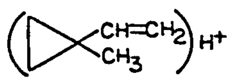
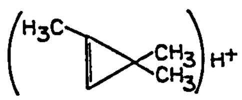
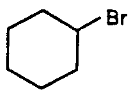
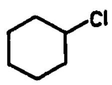
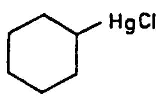
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_6H_{11}^+$** | | | | | | | |
|  | | 179 | 750 | | | | |
| | From proton affinity of 2-cyclopropylpropene (RN 4663-22-3). PA = 209.0 kcal/mol, 874. kJ/mol. | | | | | | |
|  | | (181) | (756) | | | | |
| | From proton affinity of 1-methyl-1-vinylcyclopropane (RN 16906-27-7). PA = (206) kcal/mol, (862) kJ/mol. | | | | | | |
|  | | (193) | (808) | | | | |
| | From proton affinity of 1,3,3-trimethylcyclopropene. (RN 3664-56-0). PA = (214) kcal/mol, (895) kJ/mol. | | | | | | |
| **$C_6H_{11}Br^+$** | | | | | | | |
|  | (9.85±0.01) | (200) | (835) | −27 | −115 | *EST | 108-85-0 |
| **$C_6H_{11}Cl^+$** | | | | | | | |
|  | (10.10±0.01) | (194) | (810) | −39±1 | −164±4 | 77PED/RYL | 542-18-7 |
| **$C_6H_{11}ClHg^+$** | | | | | | | |
|  | 9.2 | (188) | (787) | −24 | −101 | *EST | 24371-94-6 |
| | IP is onset of photoelectron band (81BAI/CHI2). | | | | | | |
| **$C_6H_{11}F_3NO^+$** | | | | | | | |
| $CF_3C(OH)NH(n\text{-}C_4H_9)$ | | −54 | −226 | | | | |
| | From proton affinity of $CF_3CONH(n\text{-}C_4H_9)$ (RN 400-59-9). PA = 203.6 kcal/mol, 852. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

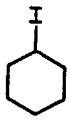
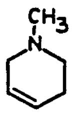
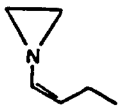
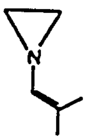
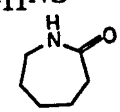
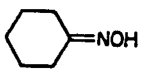
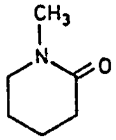
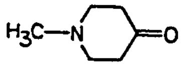
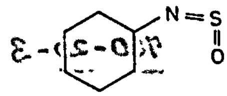
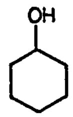
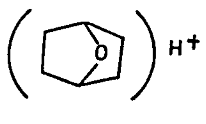
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{11}I^+$ | | | | | | | |
|  | 9.003 | 195 | 818 | −12±1 | −51±4 | 77PED/RYL | 626-62-0 |
| $C_6H_{11}N^+$ | | | | | | | |
| (E)-$CH_3CH=CHCH=NC_2H_5$ | (8.9) | (225) | (941) | 20±1 | 82±6 | *EST | 3653-19-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $(CH_2=CHCH_2)_2NH$ | (8.2) | (224) | (937) | 35±1 | 146±6 | *EST | 124-02-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.67±0.05) | (≤219) | (≤914) | 19±2 | 78±10 | *EST | 694-55-3 |
|  | (7.9) | (220) | (919) | 38 | 157 | *EST | |
| | IP from onset of photoelectron band (81MUL/PRE). | | | | | | |
|  | (7.7) | (215) | (900) | 38 | 157 | *EST | |
| | IP is onset of photoelectron band (81MUL/PRE, 81MUL/PRE2). | | | | | | |
|  | (7.6) | (220) | (919) | 44 | 186 | *EST | |
| | IP is onset of photoelectron band (81MUL/PRE, 81MUL/PRE2). | | | | | | |
| $C_6H_{11}NO^+$ | | | | | | | |
|  | (9.07±0.02) | (150) | (629) | −58.8±0.3 | −246.2±1.2 | 77PED/RYL | 105-60-2 |
|  | (8.97±0.03) | (186) | (779) | −21 | −86 | *EST | 100-64-1 |
| | IP from 79GOL/KUL. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_6H_{11}NO^+$** | | | | | | | |
|  | ≤8.92 | ≤149 | ≤624 | −57±0.7 | −237±3 | 77PED/RYL | 931-20-4 |
| | IP from 85TRE/RAD. | | | | | | |
|  | (8.3) | (155) | (648) | −37 | −153 | *EST | 1445-73-4 |
| | IP from 80SAR/WOR. See also: 86SPA/RAD. | | | | | | |
| **$C_6H_{11}NOS^+$** | | | | | | | |
|  | (≤10.0) | (≤169) | (≤707) | −62 | −258 | *EST | 30980-11-1 |
| **$C_6H_{11}O^+$** | | | | | | | |
| $(CH_3)_2CCHC(OH)CH_3$ | | (112) | (470) | | | | |
| | From proton affinity of $(CH_3)_2C=CHC(=O)CH_3$ (RN 141-79-7). PA = (210) kcal/mol, (877) kJ/mol. | | | | | | |
| $(CH_2CHCH_2)_2OH$ | | 158 | 661 | | | | |
| | From proton affinity of $(CH_2=CHCH_2)_2O$ (RN 557-40-4). PA = 200.4 kcal/mol, 838. kJ/mol. | | | | | | |
|  | | 111 | 466 | | | | |
| | From proton affinity of cyclohexanone (RN 108-94-1) (86SAN/BAL). PA = 201.4 kcal/mol, 843. kJ/mol. | | | | | | |
|  | | 119 | 498 | | | | |
| | From proton affinity of bicyclo[2.2.1]heptane, 7-oxa- (RN 279-49-2). PA = 203 kcal/mol, 849 kJ/mol. | | | | | | |
| **$C_6H_{11}O_2^+$** | | | | | | | |
| $CH_3C(OH)CH_2CH_2COCH_3$ | | 64 | 269 | | | 83MAU | |
| | From proton affinity of $CH_3COCH_2CH_2COCH_3$ (RN 110-13-4). PA = 213.2 kcal/mol, 892. kJ/mol. | | | | | | |
| **$C_6H_{11}P^+$** | | | | | | | |
| $(CH_3)_3CC{\equiv}CPH_2$ | ≤9.05 | (≤246) | (≤1028) | 37 | 155 | *EST | 77376-07-9 |
| | IP from 81CAB/COW. | | | | | | |

## Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{12}^+$ | | | | | | | |
| 1-$C_6H_{12}$ | 9.44±0.04 | 207.7 | 869.0 | −10.0±0.2 | −41.8±1 | 81WIB/WAS | 592-41-6 |
| (Z)-2-$C_6H_{12}$ | (8.97±0.01) | (195.5) | (817.8) | −11.4±0.2 | −47.7±1 | 81WIB/WAS | 7688-21-3 |
| (E)-2-$C_6H_{12}$ | (8.97±0.01) | (194.5) | (814.0) | −12.3±0.2 | −51.5±1 | 81WIB/WAS | 4050-45-7 |
| (Z)-3-$C_6H_{12}$ | (8.95±0.01) | (195.2) | (816.7) | −11.2±0.2 | −46.8±0.8 | 81WIB/WAS | 7642-09-3 |
| (E)-3-$C_6H_{12}$ | 8.96±0.02 | 194.5 | 813.9 | −12.1±0.2 | −50.6±1 | 81WIB/WAS | 13269-52-8 |
| $C_2H_5CH_2C(CH_3)=CH_2$ | (9.08±0.01) | (195) | (817) | −14.2±0.3 | −59.4±1 | 77PED/RYL | 763-29-1 |
| $C_2H_5CH(CH_3)CH=CH_2$ | (9.44) | (206) | (861) | −11.8±0.4 | −49.5±1.5 | 77PED/RYL | 760-20-3 ~~29564-68-9~~ |
| | IP from 81HOL/FIN. | | | | | | |
| $(CH_3)_2CHCH_2CH=CH_2$ | (9.45±0.01) | (206) | (861) | −12±0.5 | −51±2 | 77PED/RYL | 691-37-2 |
| $(C_2H_5)_2C=CH_2$ | (9.06±0.02) | (196) | (818) | −13.4±0.3 | −56.0±1 | 77PED/RYL | 760-21-4 |
| $(CH_3)_2CHC(CH_3)=CH_2$ | (9.07±0.01) | (194) | (812) | −15.1±0.2 | −63.3±0.8 | 77PED/RYL | 563-78-0 |
| $(CH_3)_3CCH=CH_2$ | 9.45±0.01 | 203 | 851 | −14.5±0.2 | −60.7±0.9 | 77PED/RYL | 558-37-2 |
| (Z)-$CH_3CH=C(CH_3)C_2H_5$ | (8.58) | (183) | (766) | −14.9±0.4 | −62.3±1 | 77PED/RYL | 922-61-2 |
| | IP from 81HOL/FIN. | | | | | | |
| (Z)-$(CH_3)_2CHCH=CHCH_3$ | (8.98±0.01) | (193) | (809) | −13.7±0.2 | −57.5±1 | 77PED/RYL | 691-38-3 |
| (E)-$(CH_3)_2CHCH=CHCH_3$ | (8.97±0.01) | (192) | (804) | −14.7±0.3 | −61.5±1 | 77PED/RYL | 674-76-0 |
| $(CH_3)_2C=CHC_2H_5$ | (8.58) | (182) | (761) | −16.0±0.3 | −66.8±1 | 77PED/RYL | 625-27-4 |
| | IP from 81HOL/FIN. | | | | | | |
| $(CH_3)_2C=C(CH_3)_2$ | 8.27±0.01 | 174 | 729 | −16.6±0.2 | −69.3±0.8 | 77PED/RYL | 563-79-1 |
|  | 9.86±0.03 | 198 | 828 | −29.5±0.1 | −123.3±0.3 | 77PED/RYL | 110-82-7 |
| | From charge transfer equilibria relative to fluorobenzenes; data re-interpreted. (82SIE/MAU; 82LIA). Threshold measurement leads to IP = 9.88 eV. See also: 81KIM/KAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

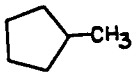
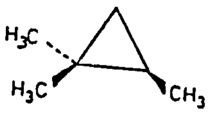
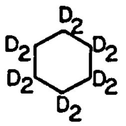
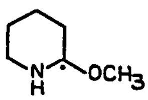
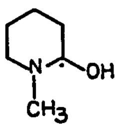
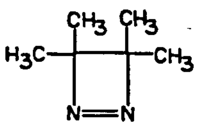
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_6H_{12}^+$** | | | | | | | |
|  | 9.85±0.03 | 202 | 844 | −25.3±0.1 | −105.9±0.4 | 77PED/RYL | 96-37-7 |
| | From charge transfer equilibrium constant relative to cyclohexane (76LIA/AUS). | | | | | | |
|  | (8.90) | (197) | (825) | −8.0 | −33.5 | *EST | |
| | IP from 85LAD/HAR. | | | | | | |
| **$C_6D_{12}^+$** | | | | | | | |
|  | 9.89 | | | | | | 1735-17-7 |
| | From charge transfer equilibria relative to fluorobenzenes; data re-interpreted. (82SIE/MAU; 82LIA). Threshold measurement leads to IP = 9.88 eV. | | | | | | |
| **$C_6H_{12}N^+$** | | | | | | | |
| $(CH_2CHCH_2)_2NH_2$ | | 175 | 735 | | | | |
| | From proton affinity of $(CH_2=CHCH_2)_2NH$ (RN 124-02-7). PA = 224.7 kcal/mol, 940. kJ/mol. | | | | | | |
| **$C_6H_{12}NO^+$** | | | | | | | |
|  | | 96 | 400 | | | | |
| | From proton affinity of 2,3,4,5-tetrahydro-6-methoxypyridine (RN 53687-79-9). PA = 228.1 kcal/mol, 954. kJ/mol. | | | | | | |
|  | | 90 | 376 | | | | |
| | From proton affinity of 1-methylpiperidine-2-one (RN 931-20-4). PA = 219.3 kcal/mol, 917.5 kJ/mol. | | | | | | |
| **$C_6H_{12}NO_3^+$** | | | | | | | |
| $CH_3C(OH)NHCH(CH_3)COOCH_3$ | | −4 | −18 | | | | |
| | From proton affinity of $CH_3CONHCH(CH_3)COOCH_3$. (RN 3619-02-1). PA = 224.5 kcal/mol, 939. kJ/mol. | | | | | | |
| **$C_6H_{12}N_2^+$** | | | | | | | |
|  | (8.2) | (225) | (941) | 36±0.7 | 150±3 | 80ENG | 54166-22-2 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

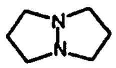
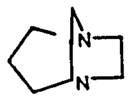
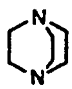
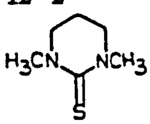
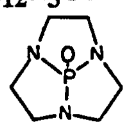
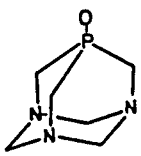
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{12}N_2{}^+$ | | | | | | | |
|  | (7.87) | (219) | (915) | 37 | 156 | *EST | 5397-67-1 |
| | IP from 82LEV/LIA. See also: 84NEL. | | | | | | |
|  | ≤8.24 | (≤210) | (≤878) | 20 | 83 | *EST | 280-28-4 |
|  | 7.197±0.001 | 187 | 784 | 21±2 | 89±7 | 71RAP/WES | 280-57-9 |
| | IP from 84SMI/HAG2. | | | | | | |
| $C_6H_{12}N_2O_2{}^+$ | | | | | | | |
| $(CH_3)_2NCOCON(CH_3)_2$ | 9.02 | (132) | (554) | −76 | −316 | *EST | 1608-14-6 |
| | IP from 82LEV/LIA, 85ROT/BOC. | | | | | | |
| $C_6H_{12}N_2S^+$ | | | | | | | |
|  | (7.3) | (192) | (802) | 23 | 98 | *EST | 16597-35-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_{12}N_2S_2{}^+$ | | | | | | | |
| $(CH_3)_2NC(=S)C(=S)N(CH_3)_2$ | ≤7.75 | (≤222) | (≤930) | 43 | 182 | *EST | 35840-78-9 |
| | IP from 81HEN/ISA. | | | | | | |
| $C_6H_{12}N_3OP^+$ | | | | | | | |
|  | ≤8.89 | (≤190) | (≤794) | −15 | −64 | *EST | 71771-37-4 |
| | IP from 82COW/LAT. | | | | | | |
|  | ≤8.19±0.10 | (≤151) | (≤631) | −38 | −159 | *EST | 53597-70-9 |
| | IP from 82COW/LAT. | | | | | | |

**Table 1. Positive Ion Table - Continued**

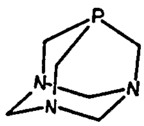
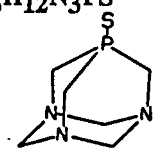
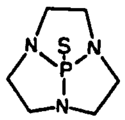
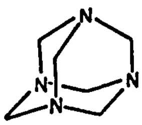
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{12}N_3P^+$ | | | | | | | |
|  | ≤8.05±0.10 | (≤227) | (≤952) | 42 | 175 | *EST | 53597-69-6 |
| | IP from 82COW/LAT. | | | | | | |
| $C_6H_{12}N_3PS^+$ | | | | | | | |
|  | ≤8.02±0.10 | (≤205) | (≤857) | 20 | 83 | *EST | 56796-56-6 |
| | IP from 82COW/LAT. | | | | | | |
|  | ≤8.43±0.10 | (≤237) | (≤991) | 43 | 178 | *EST | |
| | IP from 82COW/LAT. | | | | | | |
| $C_6H_{12}N_4^+$ | | | | | | | |
|  | (≤8.53) | (≤244) | (≤1022) | 47±0.7 | 199±3 | 77PED/RYL | 100-97-0 |
| | See also: 82COW/LAT. | | | | | | |
| $C_6H_{12}O^+$ | | | | | | | |
| n-$C_5H_{11}$CHO | 9.67±0.05 | 164 | 686 | −59 | −247 | 78TRC | 66-25-1 |
| n-$C_3H_7CH(CH_3)$CHO | (9.70) | (163) | (679) | −61 | −257 | *EST | 123-15-9 |
| $(C_2H_5)_2$CHCHO | (9.54) | (158) | (663) | −61 | −257 | *EST | 97-96-1 |
| | IP from 81HOL/FIN. | | | | | | |
| $C_2H_5CH(CH_3)CH_2$CHO | (9.68) | (161) | (676) | −62 | −258 | *EST | 15877-57-3 |
| | IP from 81HOL/FIN. | | | | | | |
| neo-$C_5H_{11}$CHO | 9.61±0.01 | (158) | (658) | −64 | −269 | *EST | 2987-16-8 |
| n-$C_4H_9COCH_3$ | 9.35±0.02 | 150 | 624 | −66±0.2 | −278±1 | 77PED/RYL | 591-78-6 |
| n-$C_3H_7COC_2H_5$ | 9.12±0.02 | 143 | 601 | −67±0.2 | −279±1 | 77PED/RYL | 589-38-8 |
| | See also: 81HOL/FIN. | | | | | | |
| sec-$C_4H_9COCH_3$ | 9.21±0.01 | (144) | (602) | −69 | −287 | *EST | 565-61-7 |
| | IP from 81HOL/FIN, 82LEV/LIA, 84BOU/FLA. | | | | | | |
| iso-$C_4H_9COCH_3$ | 9.30±0.01 | (145) | (610) | −69 | −287 | *EST | 108-10-1 |

Table 1. Positive Ion Table - Continued

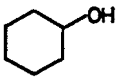
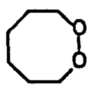
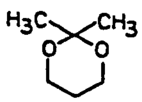
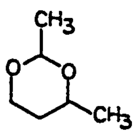
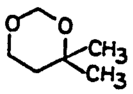
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{12}O^+$ | | | | | | | |
| tert-$C_4H_9COCH_3$ | 9.11±0.02 | 141 | 589 | −69.3±0.2 | −289.8±0.9 | 77PED/RYL | 75-97-8 |
| iso-$C_3H_7COC_2H_5$ | 9.10±0.01 | 141 | 592 | −68.3±0.2 | −286.1±0.9 | 77PED/RYL | 565-69-5 |
|  | (9.75) | (155.5) | (650.7) | −69.3±0.2 | −290.0±0.9 | 85WIB/WAS | 108-93-0 |
| | IP from 83RAB/SEL. | | | | | | |
| $C_6H_{12}O_2^+$ | | | | | | | |
| $CH_3(CH_2)_4COOH$ | ≤10.12 | ≤111 | ≤463 | −122.8±0.4 | −513.6±1.6 | 77PED/RYL | 142-62-1 |
| | IP from 81HOL/FIN. | | | | | | |
| $CH_3COO(CH_2)_3CH_3$ | 10.0 | 114 | 479 | −116.1±0.1 | −485.6±0.5 | 77PED/RYL | 123-86-4 |
| $CH_3COOCH(CH_3)C_2H_5$ | 9.90 | 109 | 454 | −120 | −501 | 82GRE/MCC | 105-46-4 |
| | IP from 82GRE/MCC. | | | | | | |
| $CH_3(CH_2)_3COOCH_3$ | (10.4±0.2) | (127) | (532) | −112.7±0.3 | −471.5±1.4 | 77PED/RYL | 624-24-8 |
| tert-$C_4H_9COOCH_3$ | (9.90±0.04) | (111) | (464) | −117±0.2 | −491±1 | 77PED/RYL | 598-98-1 |
|  | (≤9.29) | (≤178) | (≤746) | −36 | −150 | *EST | 6572-89-0 |
|  | ≤9.84 | (≤124) | (≤519) | −103 | −430 | 77PED/RYL | 695-30-7 |
| | IP from 84ASF/ZYK. | | | | | | |
|  | (≤9.90) | (≤127) | (≤530) | −102±1 | −425±4 | 77PED/RYL | 766-20-1 |
| | IP from 84ASF/ZYK. | | | | | | |
|  | ≤9.80 | (≤124) | (≤521) | −102 | −425 | *EST | 766-15-4 |
| | IP from 84ASF/ZYK. | | | | | | |

Table 1. Positive Ion Table - Continued

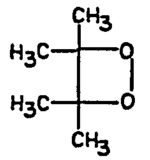
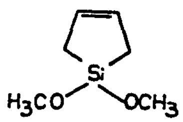
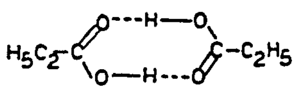
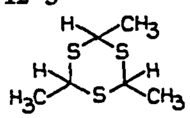
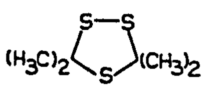
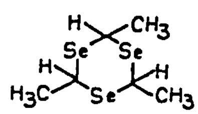
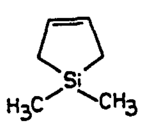
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{12}O_2^+$ | | | | | | | |
|  | (8.53) | (156) | (653) | −41 | −170 | 78GRE/LIE | 35856-82-7 |
| $C_6H_{12}O_2Si^+$ | | | | | | | |
|  | ≤9.59<br>IP from 81KHV/ZYK. | (≤39) | (≤163) | −182 | −762 | *EST | 61667-33-2 |
| $C_6H_{12}O_4^+$ | | | | | | | |
|  | (≤10.4) | (≤10) | (≤40) | −230 | −963 | *EST | |
| $C_6H_{12}S_3^+$ | | | | | | | |
|  | (8.0)<br>IP is onset of photoelectron band. | (178) | (746) | −6 | −26 | *EST | 2765-04-0 |
|  | 8.0<br>IP is onset of photoelectron band. | (151) | (633) | −33 | −139 | *EST | 38348-31-1 |
| $C_6H_{12}Se_3^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band (84BOC/AYG). | (211) | (882) | 33 | 139 | *EST | 15732-69-1 |
| $C_6H_{12}Si^+$ | | | | | | | |
|  | ≤9.0 | (≤182) | (≤760) | −26 | −108 | *EST | 16054-12-9 |
| $C_6H_{13}^+$ | | | | | | | |
| 1-$C_6H_{13}$ | 7.92±0.06<br>$\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | (191) | (800) | 8 | 33 | *EST | 2679-29-0 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{13}^+$ | | | | | | | |
| $2\text{-}C_6H_{13}$ | 7.0 | (168) | (704) | 7 | 29 | *EST | 2493-44-9 |
| | $\Delta_fH$(Neutral) based on D[C-H] = 99 kcal/mol. | | | | | | |
| $n\text{-}C_3H_7C(CH_3)_2$ | | 152 | 636 | | | | 21058-26-4 |
| | From hydride transfer equilibrium constant (75SOL/FIE and 76GOR/MUN); Heat of formation relative to $\Delta_fH$(tert-$C_4H_9^+$). | | | | | | |
| $(CH_3)_2CHC(CH_3)_2$ | | 150 | 628 | | | | 24436-98-4 |
| | From hydride transfer equilibrium constant (75SOL/FIE and 76GOR/MUN); Heat of formation relative to $\Delta_fH$(tert-$C_4H_9^+$). | | | | | | |
| $(C_2H_5)_2(CH_3)C$ | | 152 | 638 | | | | 23088-03-1 |
| | From proton affinity of $CH_3CH=C(CH_3)C_2H_5$. (RN 922-61-2). PA = 198.2 kcal/mol, 829. kJ/mol. | | | | | | |
|  $H^+$ | | (167) | (700) | | | | |
| | From proton affinity of cyclohexane. (RN 110-82-7). PA = (169) kcal/mol, (707) kJ/mol. | | | | | | |
| $C_6H_{13}ClHg^+$ | | | | | | | |
| $n\text{-}C_6H_{13}HgCl$ | ≤9.96 | (≤194) | (≤811) | −36 | −150 | *EST | 17774-09-3 |
| | IP from 81BAI/CHI2. | | | | | | |
| $C_6H_{13}I^+$ | | | | | | | |
| $n\text{-}C_6H_{13}I$ | 9.179 | 190 | 794 | −22 | −92 | 81HOL/FIN | 638-45-9 |
| $C_6H_{13}N^+$ | | | | | | | |
| $n\text{-}C_3H_7CH=NC_2H_5$ | (9.00) | (203) | (847) | −5 | −21 | *EST | 1611-12-7 |
| | See also: 79AUE/BOW. | | | | | | |
| $(iso\text{-}C_3H_7)CH=NC_2H_5$ | (8.7) | (192) | (805) | −8 | −34 | *EST | 1743-56-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $n\text{-}C_3H_7N=CHCH_2CH_3$ | (8.55±0.2) | (192) | (802) | −5 | −23 | *EST | 7707-70-2 |
| $n\text{-}C_3H_7N=C(CH_3)_2$ | (8.31±0.2) | (178) | (742) | −14±2 | −60±8 | *EST | 22023-64-9 |
| $iso\text{-}C_3H_7N=CHCH_2CH_3$ | (8.50±0.2) | (186) | (780) | −10 | −40 | 69BEN/CRU | 28916-23-6 |
| $(CH_3)_2NCH=CHC_2H_5$ | ≤7.57 | (≤174) | (≤730) | 0 | 0 | *EST | 14548-12-0 |
| | IP from 81MUL/PRE2. | | | | | | |

Table 1. Positive Ion Table - Continued

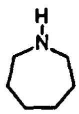
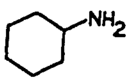
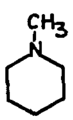
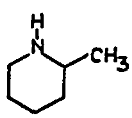
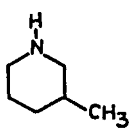
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{13}N^+$ | | | | | | | |
| $(CH_3)_2NCH=C(CH_3)_2$ | ≤8.15 | (≤189) | (≤791) | 1 | 5 | *EST | 6906-32-7 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | (≤8.41±0.02) | (≤183) | (≤767) | −10 | −44 | *EST | 111-49-9 |
|  | (8.62±0.24) | (174) | (727) | −25±0.2 | −105±1 | 79STE | 108-91-8 |
| | See also: 79AUE/BOW. | | | | | | |
|  | 7.74 | (166) | (697) | −12±1 | −50±4 | *EST | 626-67-5 |
| | See also: 82ROZ/HOU, 80SAR/WOR, 86SPA/RAD, 86CAU/DIV. | | | | | | |
|  | 7.76±0.05 | 159 | 664 | −20.2±0.2 | −84.4±1.0 | 77PED/RYL | 109-05-7 |
| | See also: 82ROZ/HOU. | | | | | | |
|  | 7.94±0.05 | (164) | (685) | −19±0.4 | −81±2 | *EST | 626-56-2 |
| | See also: 82ROZ/HOU. | | | | | | |
|  | 8.01±0.05 | (166) | (692) | −19±0.4 | −81±2 | *EST | 626-58-4 |
| | See also: 82ROZ/HOU. | | | | | | |
| $C_6H_{13}NO^+$ | | | | | | | |
|  | (≤9.49) | (≤186) | (≤777) | −33 | −139 | *EST | 6982-39-4 |
| $CH_3CON(C_2H_5)_2$ | (8.60±0.02) | (130) | (543) | −69 | −287 | *EST | 685-91-6 |

**Table 1. Positive Ion Table - Continued**

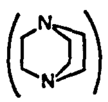
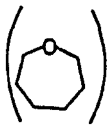
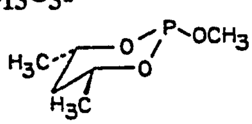
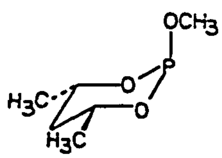
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{13}NO_2^+$ | | | | | | | |
| n-$C_4H_9CH(NH_2)COOH$ | (8.52) | (82) | (343) | −114±2 | −479±10 | *EST | 327-57-1 |
| sec-$C_4H_9CH(NH_2)COOH$ | (8.66) | (83) | (349) | −116±2 | −487±10 | *EST | 73-32-5 |
| iso-$C_4H_9CH(NH_2)COOH$ | (8.51) | (80) | (333) | −117±0.7 | −488±3 | 77PED/RYL | 61-90-5 |
| $C_6H_{13}N_2^+$ | | | | | | | |
|  $H^+$ | | 158 | 661 | | | | |
| | From proton affinity of 1,4-diazabicyclo[2.2.2]octane (RN 280-57-9). PA = 229.0 kcal/mol, 958. kJ/mol. | | | | | | |
| $C_6H_{13}O^+$ | | | | | | | |
| t-$C_4H_9C(OH)CH_3$ | | 94 | 394 | | | | |
| | From proton affinity of t-$C_4H_9COCH_3$ (RN 75-97-8). PA = 202.3 kcal/mol, 846. kJ/mol. | | | | | | |
|  $H^+$ | | (161) | (674) | | | | |
| | From proton affinity of oxepane (RN 592-90-5). PA = (202) kcal/mol, (845) kJ/mol. | | | | | | |
| $C_6H_{13}O_2^+$ | | | | | | | |
| t-$C_4H_9C(OH)OCH_3$ | | 46 | 191 | | | | |
| | From proton affinity of t-$C_4H_9COOCH_3$ (RN 598-98-1). PA = 202.8 kcal/mol, 848.5 kJ/mol. | | | | | | |
| $C_6H_{13}O_3P^+$ | | | | | | | |
|  | (8.34±0.1) | (11) | (45) | −182 | −760 | *EST | 7735-82-2 |
|  | (8.69±0.1) | (19) | (78) | −182 | −760 | *EST | 41821-91-4 |

**Table 1. Positive Ion Table - Continued**

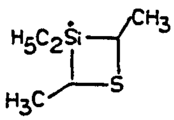
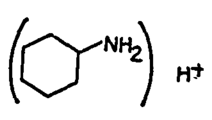
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{13}SSi^+$ | | | | | | | |
|  | | (162) | (679) | | | | 79126-87-7 |
| | $\Delta_f H$(Ion) from appearance potential determination (81GUS/VOL). | | | | | | |
| $C_6H_{14}^+$ | | | | | | | |
| n-$C_6H_{14}$ | 10.13 | 194 | 810 | −39.9±0.1 | −167.1±0.4 | 74SCO | 110-54-3 |
| | | *202* | *847* | *−31.1±0.1* | *−130.1±0.4* | | |
| | From charge transfer equilibrium constant determinations relative to fluorobenzenes; data re-interpreted (81MAU/SIE; 82LIA). Threshold measurement leads to IP = 10.2 eV. | | | | | | |
| $(CH_3)_2CH(CH_2)_2CH_3$ | (10.12) | (191) | (802) | −41.6±0.2 | −173.8±0.9 | 74SCO | 107-83-5 |
| | | *(201±0.2)* | *(842±0.9)* | *−32.2±0.2* | *−134.6±0.9* | | |
| $(C_2H_5)_2CHCH_3$ | (10.08) | (191) | (801) | −40.9±0.2 | −171.3±0.9 | 74SCO | 96-14-0 |
| | | *(201)* | *(841)* | *−31.5±0.2* | *−131.9±0.9* | | |
| $(CH_3)_2CHCH(CH_3)_2$ | (10.02) | (189) | (791) | −42.1±0.2 | −176.2±0.9 | 74SCO | 79-29-8 |
| | | *(199)* | *(832)* | *−32.3±0.2* | *−135.1±0.9* | | |
| $(CH_3)_3CCH_2CH_3$ | (10.06) | (188) | (787) | −43.9±0.2 | −183.9±0.9 | 74SCO | 75-83-2 |
| | | *(198)* | *(827)* | *−34.3±0.2* | *−143.5±0.9* | | |
| $C_6H_{14}Hg^+$ | | | | | | | |
| (n-$C_3H_7)_2Hg$ | (≤8.29) | (≤200) | (≤836) | 9±2 | 36±6 | 77PED/RYL | 628-85-3 |
| (iso-$C_3H_7)_2Hg$ | (≤8.03) | (≤195) | (≤815) | 10±1 | 40±6 | 77PED/RYL | 1071-39-2 |
| $C_6H_{14}N^+$ | | | | | | | |
| n-$C_3H_7CHNHC_2H_5$ | | (135) | (566) | | | | |
| | From proton affinity of n-$C_3H_7CH=NC_2H_5$ (RN 1611-12-7). PA = (225.3) kcal/mol, (943) kJ/mol. | | | | | | |
| $(CH_3)_2NC(CH_3)CH_2CH_3$ | | 129 | 539 | | | | |
| | From proton affinity of $(CH_3)_2NC(CH_3)=CHCH_3$ (RN 52113-79-8). PA = 237 kcal/mol, 992 kJ/mol. | | | | | | |
|  | | 120 | 500 | | | | |
| | From proton affinity of cyclohexanamine (RN 108-91-8). PA = 221.2 kcal/mol, 925.5 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

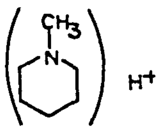
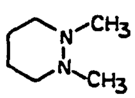
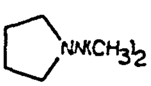
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{14}N^+$ | | | | | | | |
|  | | 124 | 519 | | | | |
| | From proton affinity of 1-methylpiperidine (RN 626-67-5). PA = 229.7 kcal/mol, 961 kJ/mol. | | | | | | |
| $C_6H_{14}NO_2^+$ | | | | | | | |
| L-$C_2H_5CH(CH_3)CH(NH_3)COOH$ | | 30 | 127 | | | | |
| | From proton affinity of L-$C_2H_5CH(CH_3)CH(NH_2)COOH$ (RN 73-32-5). PA = 218.9 kcal/mol, 916. kJ/mol. | | | | | | |
| L-$(CH_3)_2CHCH_2CH(NH_3)COOH$ | | 31 | 130 | | | | |
| | From proton affinity of L-$(CH_3)_2CHCH_2CH(NH_2)COOH$ (RN 61-90-5). PA = 218.1 kcal/mol, 912.5 kJ/mol. | | | | | | |
| $C_6H_{14}N_2^+$ | | | | | | | |
| (E)-$(C_3H_7)_2NN$ | (8.1) | (199) | (833) | 12±1 | 51±4 | 80ENG | 55204-42-7 |
| | IP is onset of photoelectron band. | | | | | | |
| (Z)-iso-$(C_3H_7)_2NN$ | (≤8.24) | (≤210) | (≤879) | 20 | 84 | *EST | 23201-84-5 |
| (E)-(iso-$C_3H_7)_2NN$ | (8.0) | (193) | (808) | 9±0.5 | 36±2 | 80ENG | 15464-00-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 6.54 | (167) | (699) | 16 | 68 | *EST | 26163-37-1 |
| | IP from charge transfer equilibrium constant determinations (84MAU/NEL). Reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV.) See also: 82LEV/LIA, 84NEL, 80SCH/THO. | | | | | | |
|  | (≤7.97) | (≤207) | (≤865) | 23 | 96 | *EST | 53779-90-1 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 82LEV/LIA, 84NEL. | | | | | | |
| $C_6H_{14}N_2O_2^+$ | | | | | | | |
| L-$H_2N(CH_2)_4CH(NH_2)COOH$ | (8.6) | (74) | (308) | -125 | -522 | *EST | 56-87-1 |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $C_6H_{14}O^+$ | | | | | | | |
| n-$C_6H_{13}OH$ | (9.89±0.03) | (153) | (639) | -75.3±0.3 | -315.1±1.4 | 77PED/RYL | 111-27-3 |
| | IP from 77ASH/BUR. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{14}O^+$ | | | | | | | |
| n-$C_4H_9CH(OH)CH_3$ | (9.80±0.03) | (146) | (612) | −80 | −334 | 84WIB/WAS | 626-93-7 |
| | IP from 77ASH/BUR. | | | | | | |
| $C_2H_5CH(OH)C_3H_7$ | (9.63±0.03) | (143) | (597) | −79 | −332 | *EST | 623-37-0 |
| | IP from 77ASH/BUR. | | | | | | |
| n-$C_5H_{11}OCH_3$ | (≤9.67) | (≤157) | (≤656) | −66 | −277 | *EST | 628-80-8 |
| | IP from 80BAC/MOU. | | | | | | |
| $(CH_3)_2CHCH_2CH_2OCH_3$ | (≤9.65) | (≤154) | (≤646) | −68 | −285 | *EST | 626-91-5 |
| | IP from 80BAC/MOU. | | | | | | |
| $(CH_3)_3CCH_2OCH_3$ | (≤9.41) | (≤146) | (≤611) | −71 | −297 | *EST | 1118-00-9 |
| | IP from 80BAC/MOU. | | | | | | |
| n-$C_4H_9OC_2H_5$ | 9.36 | 146 | 609 | −70 | −294 | 81HOL/FIN | 628-81-9 |
| | IP from 81HOL/FIN. See also: 82AUD/BOU, 80BAC/MOU. | | | | | | |
| sec-$C_4H_9OC_2H_5$ | (9.32) | (140) | (587) | −75 | −312 | 81HOL/FIN | 2679-87-0 |
| | IP from 81HOL/FIN. See also: 82AUD/BOU. | | | | | | |
| $(CH_3)_2CHCH_2OC_2H_5$ | (9.30) | (140) | (585) | −75 | −312 | *EST | 627-02-1 |
| | IP from 82AUD/BOU. | | | | | | |
| tert-$C_4H_9OC_2H_5$ | (≤9.39±0.015) | (≤139) | (≤582) | (−77) | (−324) | *EST | 637-92-3 |
| $(n\text{-}C_3H_7)_2O$ | 9.27±0.05 | 144 | 601 | −70±0.5 | −293±2 | 77PED/RYL | 111-43-3 |
| | See also: 80BAC/MOU. | | | | | | |
| $(iso\text{-}C_3H_7)_2O$ | 9.20±0.05 | 136 | 569 | −76.2±0.4 | −318.8±1.8 | 77PED/RYL | 108-20-3 |
| | See also: 80BAC/MOU. | | | | | | |
| $C_6H_{14}OS^+$ | | | | | | | |
| $(n\text{-}C_3H_7)_2SO$ | (≤8.60) | (≤137) | (≤575) | −60.9±0.4 | −254.9±1.5 | 77PED/RYL | 4253-91-2 |
| $[(CH_3)_2CH]_2SO$ | (≤8.46) | (≤134) | (≤562) | −61 | −254 | *EST | 2211-89-4 |
| $C_6H_{14}O_2^+$ | | | | | | | |
| n-$C_4H_9CH(CH_3)OOH$ | 9.25±0.03 | (152) | (636) | −61 | −256 | *EST | 24254-55-5 |
| | IP from 77ASH/BUR. | | | | | | |
| n-$C_6H_{13}OOH$ | (9.47±0.03) | (162) | (677) | −57 | −237 | *EST | 4312-76-9 |
| | IP from 77ASH/BUR. | | | | | | |
| $(iso\text{-}C_3H_7O)_2$ | (≤9.16) | (≤147) | (≤614) | −65 | −270 | 74BAT/CHR | 16642-57-2 |

**Table 1. Positive Ion Table - Continued**

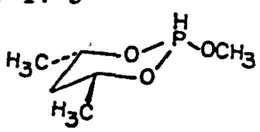
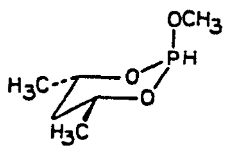
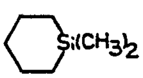
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{14}O_2^+$ | | | | | | | |
| $CH_3CH(OC_2H_5)_2$ | ≤9.78 | ≤117 | ≤490 | −108.4±0.6 | −453.5±2.4 | 77PED/RYL | 105-57-7 |
| | IP from 82ZVE/VIL. | | | | | | |
| $C_6H_{14}O_3^+$ | | | | | | | |
| $CH_3OCH_2CH_2OCH_2CH_2OCH_3$ | ≤9.8 | (≤107) | (≤448) | −119 | −498 | *EST | 111-96-6 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_6H_{14}O_3P^+$ | | | | | | | |
|  | | −42 | −176 | | | | |
| | From proton affinity of 2-eq-methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane (RN 7735-82-2). PA = 226.2 kcal/mol, 946 kJ/mol. | | | | | | |
|  | | −41 | −171 | | | | |
| | From proton affinity of 2-ax-methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane (RN 41821-91-4). PA = 225 kcal/mol, 941 kJ/mol. | | | | | | |
| $C_6H_{14}S^+$ | | | | | | | |
| $(n-C_3H_7)_2S$ | 8.30±0.02 | 161 | 676 | −29.9±0.2 | −125.3±0.8 | 77PED/RYL | 111-47-7 |
| $(i-C_3H_7)_2S$ | 8.0 | (150) | (630) | −33.9±0.2 | −141.9±0.9 | 77PED/RYL | 625-80-9 |
| | IP is onset of photoelectron spectrum. See also: 82HIR/MOH. | | | | | | |
| $C_6H_{14}S_2^+$ | | | | | | | |
| $(n-C_3H_7S)_2$ | (≤8.62) | (≤171) | (≤714) | −28.0±0.3 | −117.3±1.1 | 77PED/RYL | 629-19-6 |
| | Dialkyl disulfides undergo a change in the CSSC bond angle from 90° to 180° upon ionization; adiabatic ionization potentials are probably well below the experimentally observed ionization onset. | | | | | | |
| $(i-C_3H_7S)_2$ | ≤8.51 | (≤164) | (≤688) | −32 | −133 | *EST | 4253-89-8 |
| | Dialkyl disulfides undergo a change in the CSSC bond angle from 90° to 180° upon ionization; adiabatic ionization potentials are probably well below the experimentally observed ionization onset. | | | | | | |
| $C_6H_{14}Si^+$ | | | | | | | |
| $(C_2H_5)_2Si=CHCH_3$ | | (201) | (839) | | | | 2372-29-4 |
| | $\Delta_f H$(Ion) from appearance potential determination (81GUS/VOL). | | | | | | |
|  | (9.0) | (164) | (686) | −43±3 | −182±12 | 77PED/RYL | 1072-54-4 |
| | IP is onset of photoelectron band. See also: 81GUS/VOL2. | | | | | | |

Table 1. Positive Ion Table - Continued

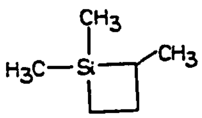
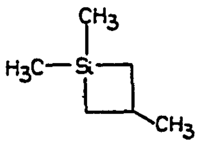
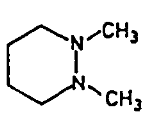
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{14}Si^+$ | | | | | | | |
|  | 8.59±0.03 | (167) | (699) | −31 | −130 | 81GUS/VOL2 | 30681-90-4 |
| | IP from 81GUS/VOL2. | | | | | | |
|  | (8.67±0.03) | (170) | (709) | −30 | −127 | 81GUS/VOL2 | 2295-13-8 |
| | IP from 81GUS/VOL2. | | | | | | |
| $C_6H_{15}B^+$ | | | | | | | |
| $(C_2H_5)_3B$ | 9.6 | (186) | (777) | −36±1 | −149±6 | 77PED/RYL | 97-94-9 |
| $C_6H_{15}BO_3^+$ | | | | | | | |
| $B(OC_2H_5)_3$ | (10.13) | (−6) | (−25) | −239±0.5 | −1002±2 | 77PED/RYL | 150-46-9 |
| $C_6H_{15}N^+$ | | | | | | | |
| n-$C_6H_{13}NH_2$ | (8.63±0.05) | (167) | (700) | −32±0.7 | −133±3 | *EST | 111-26-2 |
| | See also: 79AUE/BOW. | | | | | | |
| (n-$C_3H_7)_2NH$ | 7.84±0.02 | 153 | 640 | −27.7±0.1 | −116.0±1.4 | 77PED/RYL | 142-84-7 |
| (iso-$C_3H_7)_2NH$ | (7.73±0.03) | (144) | (602) | −34.4±0.1 | −144.0±0.4 | 77PED/RYL | 108-18-9 |
| n-$C_4H_9N(CH_3)_2$ | ≤8.35 | (≤172) | (≤722) | −20 | −84 | *EST | 927-62-8 |
| | IP from 84NEL. | | | | | | |
| i-$C_4H_9N(CH_3)_2$ | ≤8.31 | (≤170) | (≤711) | −22 | −91 | *EST | ? Same as above. |
| | IP from 84NEL. | | | | | | |
| t-$C_4H_9N(CH_3)_2$ | ≤8.08 | (≤166) | (≤694) | −21 | −86 | *EST | 918-02-5 |
| | IP from 84NEL. | | | | | | |
| $(C_2H_5)_3N$ | 7.50 | 151 | 631 | −22.1±0.1 | −92.8±0.6 | 77PED/RYL | 121-44-8 |
| | IP values of 7.11 and 7.20 eV have also been reported; selected value gives hydrogen affinity value consistent with other tertiary amine ions. | | | | | | |
| $C_6H_{15}NO_3^+$ | | | | | | | |
| $N(CH_2CH_2OH)_3$ | (7.9) | (49) | (205) | −133±0.7 | −558±3 | 82MIN/SAB | 102-71-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_6H_{15}N_2^+$ | | | | | | | |
|  | | 152 | 637 | | | | |
| | From proton affinity of hexahydro-1,2-dimethylpyridazine (RN 26163-37-1) (84MAU/NEL). PA = 229.8 kcal/mol, 961. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

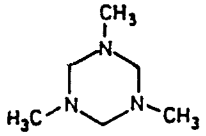
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{15}N_2O_2^+$ | | | | | | | |
| L-$H_3N(CH_2)_4CH(NH_2)COOH$ | | 11 | 45 | | | | |
| | From proton affinity of L-$H_2N(CH_2)_4CH(NH_2)COOH$ (RN 56-87-1). PA = 230.3 kcal/mol, 963.5 kJ/mol. | | | | | | |
| $C_6H_{15}N_3^+$ | | | | | | | |
|  | 7.6 | 185 | 772 | 9.4 | 39 | 69BEN/CRU | 108-74-7 |
| | IP is onset of photoelectron band (86BEC/HUN). | | | | | | |
| $C_6H_{15}O^+$ | | | | | | | |
| $(n\text{-}C_3H_7)_2OH$ | | 93 | 391 | | | | |
| | From proton affinity of $(n\text{-}C_3H_7)_2O$ (RN 111-43-3). PA = 202.3 kcal/mol, 846. kJ/mol. | | | | | | |
| $(i\text{-}C_3H_7)_2OH$ | | 84 | 350 | | | | |
| | From proton affinity of $(i\text{-}C_3H_7)_2O$ (RN 108-20-3). PA = 206.0 kcal/mol, 862. kJ/mol. | | | | | | |
| $C_2H_5OH(t\text{-}C_4H_9)$ | | 83 | 347 | | | | |
| | From proton affinity of $C_2H_5O(t\text{-}C_4H_9)$ (RN 637-92-3). PA = 205.3 kcal/mol, 859. kJ/mol. | | | | | | |
| $C_6H_{15}OSi^+$ | | | | | | | |
| $(CH_3)_2COSi(CH_3)_3$ | | 40 | 168 | | | | |
| | From proton affinity of $CH_2=C(CH_3)OSi(CH_3)_3$ (RN 1833-53-0). PA = 221. kcal/mol, 925. kJ/mol. | | | | | | |
| $C_6H_{15}O_2^+$ | | | | | | | |
| $CH_3OH(CH_2)_4OCH_3$ | | 46 | 194 | | | | |
| | From proton affinity of $CH_3O(CH_2)_4OCH_3$ (RN 13179-96-9). PA = 221.8 kcal/mol, 928. kJ/mol. | | | | | | |
| $C_6H_{15}O_3^+$ | | | | | | | |
| $(CH_3OCH_2CH_2)_2OH$ | | 27 | 114 | | | | |
| | From proton affinity of $CH_3(OCH_2CH_2)_2OCH_3$ (RN 111-96-6). PA = 219.4 kcal/mol, 918. kJ/mol. | | | | | | |
| $C_6H_{15}O_3P^+$ | | | | | | | |
| $(C_2H_5O)_3P$ | (8.4) | (0.6) | (2.5) | −193±1 | −808±5 | 80TEL/RAB | 122-52-1 |
| | IP is onset of photoelectron band (81ARS/ZVE, 81CHA/FIN, 82LEV/LIA). | | | | | | |
| $C_6H_{15}O_3PS^+$ | | | | | | | |
| $(C_2H_5O)_3PS$ | (8.49±0.02) | (−35) | (−148) | −231 | −967 | *EST | 126-68-1 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{15}O_3PSe^+$ | | | | | | | |
| $(C_2H_5O)_3PSe$ | (<7.9) | (<−27) | (<−113) | −209 | −875 | *EST | 2651-89-0 |
| | IP from 81ZVE/VIL. | | | | | | |
| $C_6H_{15}O_4P^+$ | | | | | | | |
| $(C_2H_5O)_3PO$ | (9.79) | (−58) | (−242) | −284±1 | −1187±6 | 77PED/RYL | 78-40-0 |
| | See also: 81CHA/FIN. | | | | | | |
| $C_6H_{15}P^+$ | | | | | | | |
| $(C_2H_5)_3P$ | 8.15±0.11 | (134) | (561) | −54 | −225 | *EST | 554-70-1 |
| | See also: 77COW/GOO, 69BOG/GRI, 79AUE/BOW. | | | | | | |
| $C_6H_{15}S^+$ | | | | | | | |
| $(n\text{-}C_3H_7)_2SH$ | | 129 | 541 | | | | |
| | From proton affinity of $(n\text{-}C_3H_7)_2S$ (RN 111-47-7). PA = 206.5 kcal/mol, 864. kJ/mol. | | | | | | |
| $(i\text{-}C_3H_7)_2SH$ | | 122 | 511 | | | | |
| | From proton affinity of $(i\text{-}C_3H_7)_2S$ (RN 625-80-9). PA = 209.6 kcal/mol, 877. kJ/mol. | | | | | | |
| $C_6H_{15}Sb^+$ | | | | | | | |
| $(C_2H_5)_3Sb$ | (9.2±0.3) | (224) | (937) | 12±3 | 49±11 | 82TN270 | 617-85-6 |
| $C_6H_{16}N^+$ | | | | | | | |
| $n\text{-}C_6H_{13}NH_3$ | | 116 | 484 | | | | |
| | From proton affinity of $n\text{-}C_6H_{13}NH_2$ (RN 111-26-2). PA = 218.9 kcal/mol, 916. kJ/mol. | | | | | | |
| $(n\text{-}C_3H_7)_2NH_2$ | | 110 | 462 | | | | |
| | From proton affinity of $(n\text{-}C_3H_7)_2NH$ (RN 142-84-7). PA = 227.5 kcal/mol, 952. kJ/mol. | | | | | | |
| $(i\text{-}C_3H_7)_2NH_2$ | | 101 | 423 | | | | |
| | From proton affinity of $(i\text{-}C_3H_7)_2NH$ (RN 108-18-9). PA = 230.2 kcal/mol, 963. kJ/mol. | | | | | | |
| $(CH_3)_2(tert\text{-}C_4H_9)NH$ | | 109 | 457 | | | | |
| | From proton affinity of $(CH_3)_2(tert\text{-}C_4H_9)N$ (RN 918-02-5). PA = 232.0 kcal/mol, 971. kJ/mol. | | | | | | |
| $(C_2H_5)_3NH$ | | 111 | 465 | | | | |
| | From proton affinity of $(C_2H_5)_3N$ (RN 121-44-8). PA = 232.3 kcal/mol, 972. kJ/mol. | | | | | | |
| $C_6H_{16}NO^+$ | | | | | | | |
| $NH_3(CH_2)_6OH$ | | (68) | (285) | | | | |
| | From proton affinity of $NH_2(CH_2)_6OH$ (RN 4048-33-3). PA = (231.0) kcal/mol, (966.5) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

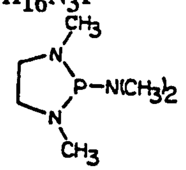
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{16}N_2^+$ | | | | | | | |
| $(CH_3)_2NCH_2CH_2N(CH_3)_2$ | 7.59±0.3 | 170 | 713 | −4.7 | −19.7 | 81LOG/TAK | 110-18-9 |
| | IP from 81LOG/TAK, 82LEV/LIA. | | | | | | |
| $(C_2H_5)_2NN(CH_3)_2$ | ≤8.10 | (≤196) | (≤819) | 9 | 37 | *EST | 21849-74-1 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 82LEV/LIA, 84NEL. | | | | | | |
| $(n\text{-}C_3H_7)(CH_3)NN(CH_3)_2$ | (6.63) | (160) | (671) | 7 | 31 | *EST | 60678-65-1 |
| | IP from charge transfer equilibrium determinations (84MAU/NEL). Reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV.) See also: 84NEL. | | | | | | |
| $(C_2H_5)(CH_3)NN(CH_3)(C_2H_5)$ | 6.75 | (164) | (686) | 8 | 35 | *EST | 23337-93-1 |
| | IP from charge transfer equilibrium constant determinations (86RUM). See also: 82LEV/LIA, 84NEL. | | | | | | |
| $C_6H_{16}N_3P^+$ | | | | | | | |
|  | (7.1) | (159) | (666) | −4 | −19 | *EST | 6069-38-1 |
| | IP is onset of photoelectron band (82WOR/HAR). | | | | | | |
| $C_6H_{16}OP^+$ | | | | | | | |
| $(C_2H_5)_3POH$ | | 70 | 292 | | | | |
| | From proton affinity of $(C_2H_5)_3PO$ (RN 597-50-2) (85BOL/HOU). PA = 222.6 kcal/mol, 931. kJ/mol. | | | | | | |
| $C_6H_{16}O_4P^+$ | | | | | | | |
| $HOP(OC_2H_5)_3$ | | −135 | −565 | | | | |
| | From proton affinity of $OP(OC_2H_5)_3$ (RN 78-40-0). PA = (217) kcal/mol, (910) kJ/mol. | | | | | | |
| $C_6H_{16}P^+$ | | | | | | | |
| $(C_2H_5)_3PH$ | | 80 | 336 | | | | |
| | From proton affinity of $(C_2H_5)_3P$ (RN 554-70-1). PA = (231.7) kcal/mol, (969.) kJ/mol. | | | | | | |
| $C_6H_{16}Si^+$ | | | | | | | |
| $(C_2H_5)_3SiH$ | 9.5 | 171 | 716 | −48±4 | −201±15 | 77PED/RYL | 617-86-7 |
| | See also: 81HOT. | | | | | | |

Table 1. Positive Ion Table - Continued

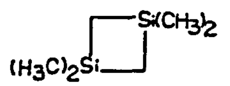
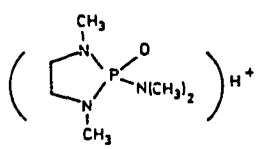
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_6H_{16}Si_2^+$** | | | | | | | |
|  | (8.56±0.07) | (125) | (525) | −72±3 | −301±14 | 77PED/RYL | 1627-98-1 |
| | See also: 81KHV/ZYK. | | | | | | |
| **$C_6H_{16}Sn^+$** | | | | | | | |
| $(C_2H_5)_3SnH$ | (≤9.1) | (≤210) | (≤878) | 0±2 | 0±8 | 80TEL/RAB | 997-50-2 |
| i-$C_3H_7Sn(CH_3)_3$ | 8.2 | (178) | (744) | −11±1 | −47±5 | 77PED/RYL | 3531-46-2 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_6H_{17}NSi^+$** | | | | | | | |
| $(CH_3)_2NCH_2Si(CH_3)_3$ | 7.61 | (126) | (527) | −49 | −207 | *EST | 18182-40-6 |
| | See also: 81LOG/TAK. | | | | | | |
| **$C_6H_{17}N_2^+$** | | | | | | | |
| $NH_3(CH_2)_6NH_2$ | | 106 | 442 | | | | |
| | From proton affinity of $NH_2(CH_2)_6NH_2$ (RN 124-09-4). PA = 237.7 kcal/mol, 994.4 kJ/mol. | | | | | | |
| $(n\text{-}C_3H_7)(CH_3)HNN(CH_3)_2$ | | 145 | 605 | | | | |
| | From proton affinity of $(n\text{-}C_3H_7)(CH_3)NN(CH_3)_2$ (RN 60678-65-1) (84MAU/NEL). PA = 229.1 kcal/mol, 959. kJ/mol. | | | | | | |
| $(CH_3)_2NH(CH_2)_2N(CH_3)_2$ | | 121 | 507 | | | | |
| | From proton affinity of $(CH_3)_2N(CH_2)_2N(CH_3)_2$ (RN 110-18-9) re-evaluated. PA = 240 kcal/mol, 1003 kJ/mol. | | | | | | |
| **$C_6H_{17}N_3OP^+$** | | | | | | | |
|  | | 37 | 154 | | | | |
| | From proton affinity of 1,3,2-Diazaphospholidine-2-amine,N,N',1,3-tetramethyl-2-oxide- (RN 7778-06-5) (85BOL/HOU). PA = 226.9 kcal/mol, 949. kJ/mol. | | | | | | |
| **$C_6H_{18}BN_3^+$** | | | | | | | |
| $B(N(CH_3)_2)_3$ | 7.60 | 116 | 487 | −59 | −246 | 82HOL/SMI | 4375-83-1 |
| **$C_6H_{18}NSi^+$** | | | | | | | |
| $(CH_3)_3SiCH_2NH(CH_3)_2$ | | 85 | 354 | | | | |
| | From proton affinity of $(CH_3)_3SiCH_2N(CH_3)_2$ (RN 18182-40-6). PA = 231.5 kcal/mol, 968. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

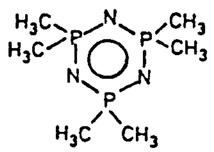
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_6H_{18}N_3OP^+$ | | | | | | | |
| $((CH_3)_2N)_3PO$ | 7.82 | 66 | 277 | −114 | −477 | 69BEN/CRU | 630-31-9 |
| | IP is onset of photoelectron band. (82LEV/LIA, 82WOR/HAR). See also: 82COW/LAT. | | | | | | |
| $C_6H_{18}N_3P^+$ | | | | | | | |
| $((CH_3)_2N)_3P$ | 6.75 | (124) | (517) | −32 | −134 | 69BEN/CRU | 1608-26-0 |
| | IP is onset of photoelectron band (82LEV/LIA, 82WOR/HAR, 77COW/GOO). See also: 82COW/LAT. | | | | | | |
| $C_6H_{18}N_3PS^+$ | | | | | | | |
| $SP[N(CH_3)_2]_3$ | ≤8.63±0.10 | (≤162) | (≤677) | −37 | −156 | •EST | 3732-82-9 |
| | IP from 82COW/LAT. | | | | | | |
| $C_6H_{18}N_3P_3^+$ | | | | | | | |
|  | (8.35±0.05) | (64) | (268) | −129±5 | −538±23 | 77PED/RYL | 6607-30-3 |
| $C_6H_{18}OSi_2^+$ | | | | | | | |
| $((CH_3)_3Si)_2O$ | 9.64±0.01 | 36 | 153 | −186±1 | −777±6 | 77PED/RYL | 107-46-0 |
| | | *(48)* | *(202)* | *−174* | *−728* | | |
| | IP from 83MOL/PIK, 85SEE/MOL. | | | | | | |
| $C_6H_{18}Si_2^+$ | | | | | | | |
| $(CH_3)_6Si_2$ | 8.27±0.05 | 110 | 459 | −81±2 | −339±8 | 81WAL | 1450-14-2 |
| | | *122* | *513* | *−68±2* | *−285±8* | | |
| | IP from 84SZE/BAE, 81SZE/KOR. See also: 81KHV/ZYK, 85MOC/WOR. | | | | | | |
| $C_6H_{18}Sn_2^+$ | | | | | | | |
| $((CH_3)_3Sn)_2$ | (7.8) | (173) | (726) | −6±2 | −27±8 | 77PED/RYL | 661-69-8 |
| | IP is onset of photoelectron band (85GRA/BER, 81SZE/KOR). See also: 85MOC/WOR. | | | | | | |
| $C_6H_{18}W^+$ | | | | | | | |
| $(CH_3)_6W$ | (8.3) | (376) | (1572) | 185±8 | 772±35 | 82PIL/SKI | 36133-73-0 |
| | IP is onset of photoelectron band (82LEV/LIA, 75GAL/WIL). | | | | | | |
| $C_6H_{19}NSi_2^+$ | | | | | | | |
| $((CH_3)_3Si)_2NH$ | ≤8.55 | ≤83 | ≤348 | −114±1 | −477±6 | 77PED/RYL | 999-97-3 |
| | IP from 83MOL/PIK3. | | | | | | |
| $C_6H_{19}N_3P^+$ | | | | | | | |
| $HP(N(CH_3)_2)_3$ | | 113 | 472 | | | | |
| | From proton affinity of $P(N(CH_3)_2)_3$ (RN 1608-26-0). PA = 220.9 kcal/mol, 924. kJ/mol. | | | | | | |
| $C_6H_{19}OSi_2^+$ | | | | | | | |
| $((CH_3)_3Si)_2OH$ | | (−23) | (−96) | | | | |
| | From proton affinity of $((CH_3)_3Si)_2O$ (RN 107-46-0). PA = (203) kcal/mol, (849) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

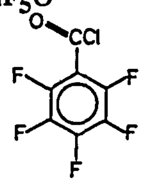
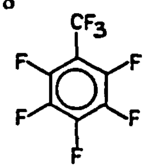
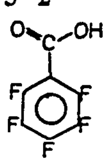
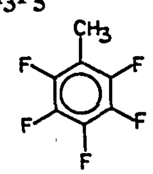
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_6MoO_6{}^+$ | | | | | | | |
| $Mo(CO)_6$ | 8.227±0.011 | −28 | −118 | −218 | −912 | 77ROS/DRA | 13939-06-5 |
| | | *−29* | *−121* | *−219* | *−915* | | |
| | See also: 82HUB/LIC. | | | | | | |
| $C_6N_4{}^+$ | | | | | | | |
| $(NC)_2CC(CN)_2$ | 11.77±0.01 | 440 | 1842 | 169±1 | 706±6 | 77PED/RYL | 670-54-2 |
| $C_6O_6V^+$ | | | | | | | |
| $V(CO)_6$ | 7.52 | −31 | −128 | −204±7 | −854±29 | 67BID/MCI | 20644-87-5 |
| $C_6O_6W^+$ | | | | | | | |
| $W(CO)_6$ | 8.20 | −23 | −96 | −212±1 | −887±4 | 84ALT/CON2 | 14040-11-0 |
| | IP from 82HUB/LIC, 77ROS/DRA. | | | | | | |
| $C_7ClF_5O^+$ | | | | | | | |
|  | (9.8) | (−3) | (−13) | −229 | −959 | *EST | 2251-50-5 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
| $C_7F_3MnO_6{}^+$ | | | | | | | |
| $CF_3COMn(CO)_5$ | (8.5) | (−164) | (−688) | −360±1 | −1508±6 | 82CON/ZAF | 14099-62-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7F_8{}^+$ | | | | | | | |
|  | (9.9) | (−56) | (−232) | −284±2 | −1187±8 | 77PED/RYL | 434-64-0 |
| $C_7HF_5O_2{}^+$ | | | | | | | |
|  | (9.2) | (−62) | (−260) | −274±1 | −1148±4 | 77PED/RYL | 602-94-8 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
| $C_7H_3F_5{}^+$ | | | | | | | |
|  | (9.4) | (15) | (64) | −201.5±0.4 | −842.9±1.8 | 77PED/RYL | 771-56-2 |
| | Value of IP from charge transfer equilibrium constant determinations is 9.63 eV. | | | | | | |

Table 1. Positive Ion Table - Continued

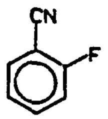
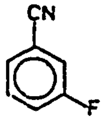
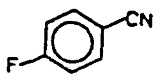
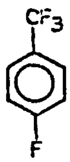
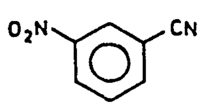
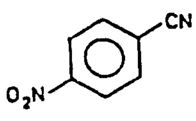
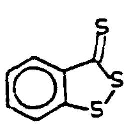
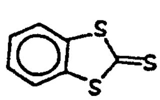
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_4FN^+$ | | | | | | | |
|  | (9.78) | (231) | (965) | 5 | 21 | *EST | 394-47-8 |
|  | (9.79) | (231) | (966) | 5 | 21 | *EST | 403-54-3 |
|  | (9.74) | (229) | (957) | 4 | 17 | *EST | 1194-02-1 |
| $C_7H_4F_4^+$ | | | | | | | |
|  | 9.98<br>IP from 82CAB/COW. | (41) | (171) | −189±0.3 | −792±1 | *EST | 402-44-8 |
| $C_7H_4N_2O_2^+$ | | | | | | | |
|  | (10.29±0.1) | (286) | (1197) | 49 | 204 | *EST | 619-24-9 |
|  | (10.23±0.1) | (284) | (1189) | 48 | 202 | *EST | 619-72-7 |
| $C_7H_4S_3^+$ | | | | | | | |
|  | (7.9)<br>IP is onset of photoelectron band. | (242) | (1013) | 60±1 | 251±5 | 72GEI/RAU | 3354-42-5 |
|  | (8.14) | (246) | (1027) | 57.8±0.4 | 242.0±1.7 | 77PED/RYL | 934-36-1 |

**Table 1. Positive Ion Table - Continued**

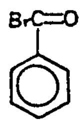
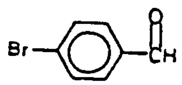
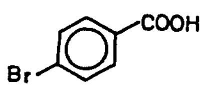
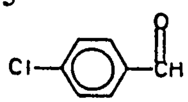
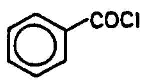
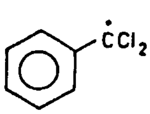
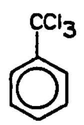
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_5BrO^+$ | | | | | | | |
|  | (9.65) | (211) | (882) | −12 | −49 | 79MCL/TRA | 618-32-6 |
| | IP from 79MCL/TRA. See also: 84GAN/LIV. | | | | | | |
|  | ≤9.22 | (≤209) | (≤874) | −4 | −16 | *EST | 1122-91-4 |
| | IP from 85GAL/GER. | | | | | | |
| $C_7H_5BrO_2^+$ | | | | | | | |
|  | (9.72±0.2) | (155) | (648) | −69±1 | −290±5 | 77PED/RYL | 586-76-5 |
| $C_7H_5ClO^+$ | | | | | | | |
|  | 9.59±0.02 | (205) | (856) | −16 | −69 | *EST | 104-88-1 |
| | IP from 85GAL/GER, 77ROS/DRA. | | | | | | |
|  | 9.54 | 195 | 817 | −25±1 | −103±4 | 75MOS/PRI | 98-88-4 |
| | IP is onset of photoelectron band (84GAN/LIV, 81MEE/WAH). See also: 80GOF/YAR, 79MCL/TRA. | | | | | | |
| $C_7H_5Cl_2^+$ | | | | | | | |
|  | | (197) | (824) | | | | |
| | $\Delta_f H$(Ion) from chloride transfer equilibrium constant determinations (85SHA/SHA). | | | | | | |
| $C_7H_5Cl_3^+$ | | | | | | | |
|  | ≤9.60 | (≤219) | (≤915) | −3 | −11 | *EST | 98-07-7 |
| | IP from 81ZVE/ERM. | | | | | | |

**Table 1. Positive Ion Table - Continued**

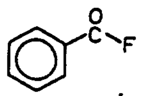
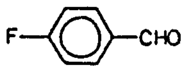
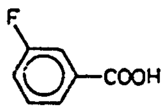
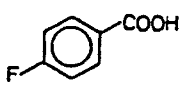
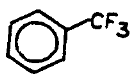
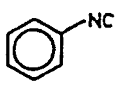
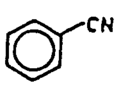
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_5FO^+$ | | | | | | | |
|  | 9.78 | (153) | (639) | −73 | −305 | *EST | 455-32-3 |
| | IP from 79MCL/TRA, 84GAN/LIV. | | | | | | |
|  | ≤9.60 | (≤167) | (≤700) | −54 | −226 | *EST | 459-57-4 |
| | IP from 85GAL/GER. | | | | | | |
| $C_7H_5FO_2^+$ | | | | | | | |
|  | (9.91±0.2) | (111) | (466) | −117 | −490 | *EST | 455-38-9 |
|  | (9.91±0.2) | (111) | (461) | −118±1 | −495±3 | 77PED/RYL | 456-22-4 |
| $C_7H_5F_3^+$ | | | | | | | |
|  | 9.685±0.004 | 80.1 | 335.4 | −143.2±0.2 | −599.0±0.9 | 77PED/RYL | 98-08-8 |
| | See also: 81BER/BOM. | | | | | | |
| $C_7H_5N^+$ | | | | | | | |
|  | (9.4) | (289) | (1208) | 72±2 | 301±7 | *EST | 931-54-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 9.62 | 274 | 1147 | 52 | 219 | 82CHU/NGU | 100-47-0 |
| | See also: 83KLA/KOV, 81KIM/KAT. | | | | | | |

Table 1. Positive Ion Table - Continued

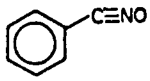
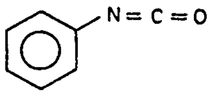
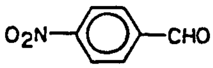
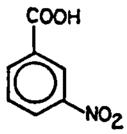
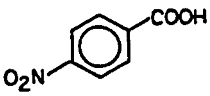
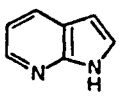
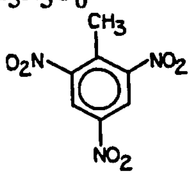
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_5NO^+$ | | | | | | | |
|  | (8.96±0.02) | (275) | (1148) | 68 | 283 | *EST | 873-67-6 |
|  | (8.8)<br>IP is onset of photoelectron band. | (206) | (862) | 3 | 13 | *EST | 103-71-9 |
| $C_7H_5NO_3^+$ | | | | | | | |
|  | 10.27±0.01<br>See also: 85GAL/GER. | (249) | (1043) | 12 | 52 | *EST | 555-16-8 |
| $C_7H_5NO_4^+$ | | | | | | | |
|  | (10.31±0.2) | (143) | (600) | −94.3±0.3 | −394.7±1.3 | 77PED/RYL | 121-92-6 |
|  | 10.18±0.2 | 141 | 589 | −93.7±0.4 | −392.2±1.5 | 77PED/RYL | 62-23-7 |
| $C_7H_5N_2^+$ | | | | | | | |
|  | 8.11±0.01<br>IP from 84FUK/YOS. | (238) | (995) | 51 | 213 | *EST | |
| $C_7H_5N_3O_6^+$ | | | | | | | |
|  | (10.59±0.04) | (252) | (1054) | 8±0.5 | 32±2 | 77PEL | 118-96-7 |

**Table 1. Positive Ion Table - Continued**

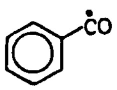
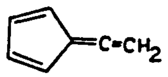
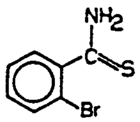
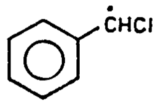
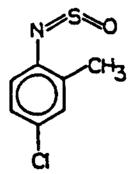
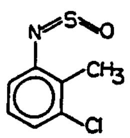
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_5O^+$ | | | | | | | |
|  | | 168±1 | 705±6 | | | | 2652-65-5 |
| | From appearance potential measurements (79MCL/TRA, 82BUR/HOL2. See also: 85TAJ/TOB. | | | | | | |
| $C_7H_6^+$ | | | | | | | |
|  | (8.29) | (275) | (1150) | 84±2 | 350±10 | *EST | 27041-32-3 |
|  | (≤8.82) | (≤292) | (≤1223) | 89±1 | 372±4 | 73BIL/CHO | 4646-69-9 |
| $C_7H_6BrNS^+$ | | | | | | | |
|  | (8.5) | (232) | (972) | 36 | 152 | *EST | 30216-44-5 |
| | IP from 81GRU. | | | | | | |
| $C_7H_6Cl^+$ | | | | | | | |
|  | | (209) | (873) | | | | |
| | $\Delta_f H$(Ion) from chloride transfer equilibrium constant determinations (85SHA/SHA); $\Delta_f H(C_6H_5CCl_2H)$ estimated as 3 kcal/mol, 13 kJ/mol. | | | | | | |
| $C_7H_6ClNOS^+$ | | | | | | | |
|  | (8.5) | (166) | (694) | −30 | −126 | *EST | |
| | IP is onset of photoelectron band (82LOU/VAN). | | | | | | |
|  | (≤9.23) | (≤184) | (≤769) | −29 | −122 | *EST | |
| | IP from 82LOU/VAN. | | | | | | |

**Table 1. Positive Ion Table - Continued**

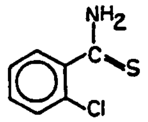
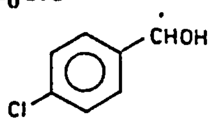
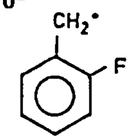
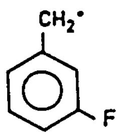
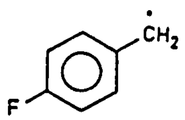
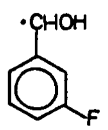
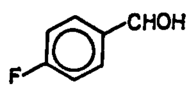
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_6ClNS^+$ | | | | | | | |
|  | 8.8<br>IP from 81GRU. | (226) | (948) | 24 | 99 | *EST | 15717-17-6 |
| $C_7H_6ClO^+$ | | | | | | | |
|  | From proton affinity of 4-$ClC_6H_4CHO$ (RN 104-88-1). PA = 200.2 kcal/mol, 838. kJ/mol. | 149 | 623 | | | | |
| $C_7H_6F^+$ | | | | | | | |
|  | $\Delta_f H$(Ion) from chloride-transfer equilibrium constants (85SHA/SHA); $\Delta_f H$(o-$C_6H_4FCH_2Cl$) estimated as -43.5 kcal/mol, -182 kJ/mol. | (170) | (710) | | | | 40880-01-1 |
|  | $\Delta_f H$(Ion) from chloride-transfer equilibrium constants (85SHA/SHA); $\Delta_f H$(m-$C_6H_4FCH_2Cl$) estimated as -43.5 kcal/mol, -182 kJ/mol. | (173) | (725) | | | | 2599-73-7 |
|  | $\Delta_f H$(Ion) from chloride-transfer equilibrium constants (85SHA/SHA); $\Delta_f H$(o-$C_6H_4FCH_2Cl$) estimated as -43.5 kcal/mol, -182 kJ/mol. | (166) | (696) | | | | 2194-09-4 |
| $C_7H_6FO^+$ | | | | | | | |
|  | From proton affinity of 3-$FC_6H_4CHO$ (RN 456-48-4). PA = 196.4 kcal/mol, 822. kJ/mol. | 113 | 472 | | | | |
|  | From proton affinity of 4-$FC_6H_4CHO$ (RN 459-57-4). PA = 199.2 kcal/mol, 833. kJ/mol. | 110 | 462 | | | | |

**Table 1. Positive Ion Table - Continued**

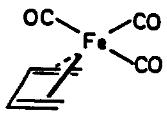
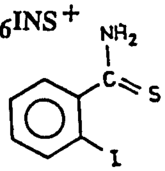
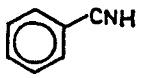
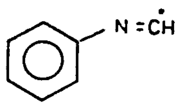
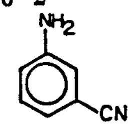
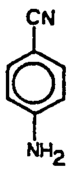
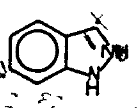
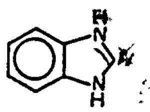
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_6FeO_3^+$ | | | | | | | |
|  | 8.04 | 100 | 417 | −86±2 | −359±9 | 82PIL/SKI | 12078-32-9 |
| | IP is onset of photoelectron band. See also: 82GRE/KEL. | | | | | | |
| $C_7H_6INS^+$ | | | | | | | |
|  | 8.5 | (246) | (1030) | 50 | 210 | *EST | 81568-85-6 |
| | IP from 81GRU. | | | | | | |
| $C_7H_6N^+$ | | | | | | | |
|  | | 222 | 929 | | | | |
| | From proton affinity of $C_6H_5CN$ (RN 100-47-0). PA = 195.9 kcal/mol, 820. kJ/mol. | | | | | | |
|  | | 231 | 965 | | | | |
| | From proton affinity of $C_6H_5NC$ (RN 931-54-4). (86MAU/KAR). PA = 207 kcal/mol, 866 kJ/mol. | | | | | | |
| $C_7H_6N_2^+$ | | | | | | | |
|  | (8.61±0.05) | (252) | (1053) | 53 | 222 | *EST | 2237-30-1 |
|  | (8.17) | (240) | (1004) | 52 | 216 | *EST | 873-74-5 |
| | IP is onset of photoelectron band (81MOD/DIS). | | | | | | |
|  | (8.35) | (253) | (1060) | 60.8±1.1 | 254.2±4.6 | 85FAO/AKA | 271-44-3 |
|  | (8.0) | (228) | (957) | 44±2 | 185±10 | *EST | 51-17-2 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

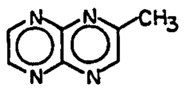
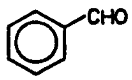
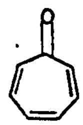
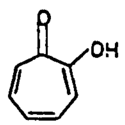
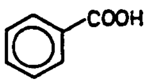
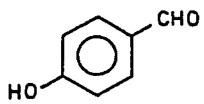
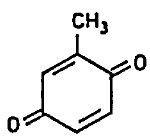
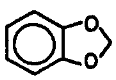
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_6N_4^+$ | | | | | | | |
|  | (8.8) | (283) | (1182) | 80 | 333 | *EST | 6499-38-3 |
| | IP is onset of photoelectron band (84GLE/SPA2). | | | | | | |
| $C_7H_6O^+$ | | | | | | | |
|  | 9.49±0.02 | 210 | 879 | −9±0.5 | −37±2 | 77PED/RYL | 100-52-7 |
| | IP from 79MCL/TRA. See also: 83KLA/KOV, 85GAL/GER. | | | | | | |
|  | 8.90±0.02 | 215 | 903 | 10±0.7 | 44±3 | 77PED/RYL | 539-80-0 |
| $C_7H_6O_2^+$ | | | | | | | |
|  | (9.86±0.02) | (191) | (797) | −36.8±0.2 | −154.0±0.9 | 77PED/RYL | 533-75-5 |
|  | (9.47) | (148) | (620) | −70.3±0.4 | −294.1±1.6 | 77PED/RYL | 65-85-0 |
| | IP from onset of photoelectron band (83KLA/KOV). See also: 81MEE/WAH. | | | | | | |
|  | (9.32±0.02) | (159) | (666) | −56±2 | −233±8 | *EST | |
|  | 9.78±0.02 | 188 | 789 | −37.1±2.0 | −155±9 | *EST | 553-97-9 |
|  | (8.0) | (150) | (629) | −34±0.7 | −143±3 | 77PED/RYL | 274-09-9 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

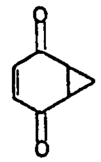
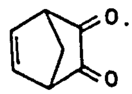
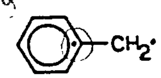
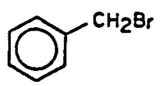
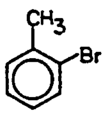
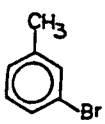
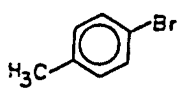
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_6O_2^+$ | | | | | | | |
|  | (9.64) | (232) | (971) | 10 | 41 | *EST | 53735-22-1 |
| | IP from 85GLE/JAH. | | | | | | |
|  | (8.4) | (175) | (731) | −19 | −79 | *EST | 17994-26-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_7^+$ | | | | | | | |
|  | 6.24±0.01 | 203 | 849 | 59 | 247 | 82MCM/GOL | 3551-27-7 |
| | | *208* | *872* | | | | |
| | $\Delta_fH$(Ion) from appearance potential measurements (83BOM/DAN, 83BOM/DAN2); Heat of formation of radical derived from $\Delta_fH(C_7H_7^+)$-IP; 82MCM/GOL cite 65±2 kcal/mol, 271±8 kJ/mol. | | | | | | |
|  | 7.20±0.02 | 215 | 899 | 49 | 204 | 81TSA | 2154-56-5 |
| | | *219* | *917* | *53* | *223* | | |
| | $\Delta_fH$(Ion) from chloride transfer equilibrium constants (81SEN/KEB) is in agreement. | | | | | | |
| $C_7H_7Br^+$ | | | | | | | |
|  | 9.0 | (224) | (935) | 16±0.5 | 67±2 | 76ASH | 100-39-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.58±0.1 | (213) | (890) | 15 | 62 | *EST | 95-46-5 |
| | See also: 85BAI/MIS. | | | | | | |
|  | 8.79±0.02 | (217) | (909) | 15 | 61 | *EST | 591-17-3 |
|  | 8.67±0.01 | (217) | (908) | 17 | 71 | *EST | 106-38-7 |
| | IP from 82LEV/LIA, 78LIA/AUS, 77ROS/DRA. See also: 85BAI/MIS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

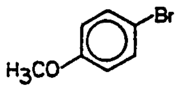
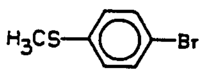
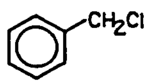
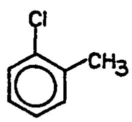
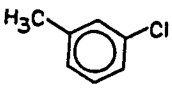
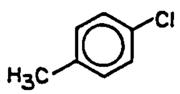
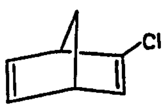
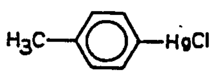
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7BrO^+$ | | | | | | | |
|  | (8.11) | (177) | (739) | −10 | −43 | *EST | 104-92-7 |
| $C_7H_7BrS^+$ | | | | | | | |
|  | (7.5) | (201) | (843) | 28 | 119 | *EST | 104-95-0 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
| $C_7H_7Cl^+$ | | | | | | | |
|  | 9.14±0.01 | 215 | 899 | 4±0.7 | 17±3 | 76ASH | ~~25168-05-2~~ |
| | See also: 81ZVE/ERM, 81KIM/KAT. | | | | | | |
|  | (8.83±0.02) | (208) | (871) | 4 | 18 | *EST | 95-49-8 |
| | See also: 85BAI/MIS. | | | | | | |
|  | (8.83±0.02) | (208) | (870) | 4 | 18 | *EST | 108-41-8 |
|  | 8.69±0.02 | (205) | (856) | 4 | 18 | *EST | 106-43-4 |
| | See also: 85BAI/MIS. | | | | | | |
|  | ≤8.77 | (≤256) | (≤1071) | 54 | 225 | *EST | 2294-41-9 |
| | IP from 83HOU/RON. | | | | | | |
| $C_7H_7ClHg^+$ | | | | | | | |
|  | (8.7) | (223) | (931) | 22 | 92 | *EST | 539-43-5 |
| | IP is onset of photoelectron band (81FUR/PIA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

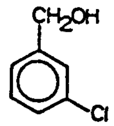
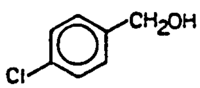
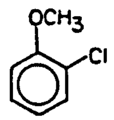
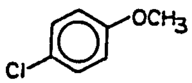
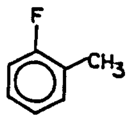
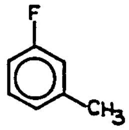
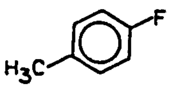
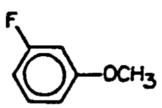
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7ClO^+$ | | | | | | | |
|  | (8.51)<br>IP from 83RUS/FRE. | (166) | (697) | −30 | −124 | 83RUS/FRE | 873-63-2 |
|  | (8.58)<br>IP from 83RUS/FRE. | (167) | (698) | −31 | −130 | 83RUS/FRE | 873-76-7 |
|  | (8.42)<br>IP from 83RUS/FRE. | (169) | (707) | −25 | −105 | 83RUS/FRE | 766-51-8 |
|  | (7.79)<br>IP from 83RUS/FRE. | (153) | (641) | −26 | −111 | 83RUS/FRE | 623-12-1 |
| $C_7H_7F^+$ | | | | | | | |
|  | 8.91±0.01<br>See also: 78LIA/AUS. | (170) | (711) | −36 | −149 | *EST | 95-52-3 |
|  | 8.91±0.01 | (170) | (710) | −36 | −150 | *EST | 352-70-5 |
|  | 8.79±0.01<br>See also: 78LIA/AUS. | 167 | 700 | −35.2±0.3 | −147.5±1.2 | 77PED/RYL | 352-32-9 |
| $C_7H_7FO^+$ | | | | | | | |
|  | 8.41<br>IP from 85OIK/ABE. | (130) | (544) | −64 | −267 | *EST | 456-49-5 |

**Table 1. Positive Ion Table - Continued**

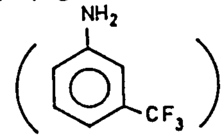
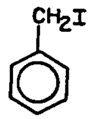
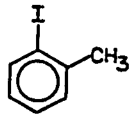
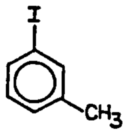
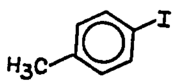
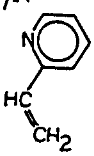
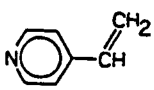
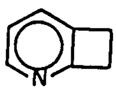
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7F_3N^+$ | | | | | | | |
|  H⁺ | | 19 | 81 | | | | |
| | From proton affinity of 3-$CF_3C_6H_4NH_2$ (RN 98-16-8). PA = 204.2 kcal/mol, 854. kJ/mol. | | | | | | |
| $C_7H_7I^+$ | | | | | | | |
|  | (8.6) | (223) | (933) | 25±1 | 103±4 | 76ASH | 620-05-3 |
|  | (8.62±0.01) | (231) | (965) | 32±1 | 133±6 | 77PED/RYL | 615-37-2 |
| | See also: 85BAI/MIS. | | | | | | |
|  | (8.61±0.03) | (231) | (965) | 32±1 | 134±6 | 77PED/RYL | 625-95-6 |
|  | (8.50±0.01) | (225) | (942) | 29±1 | 122±6 | 77ROS/DRA | 624-31-7 |
| | See also: 85BAI/MIS. | | | | | | |
| $C_7H_7N^+$ | | | | | | | |
|  | (8.6) | (246) | (1030) | 48 | 200 | *EST | 100-69-6 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | (8.9) | (254) | (1061) | 48 | 202 | *EST | 100-43-6 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | (≤9.11) | (≤270) | (≤1129) | 60 | 250 | *EST | 56911-25-2 |
| | IP from 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

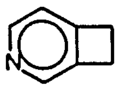
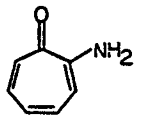
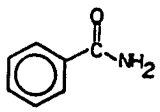
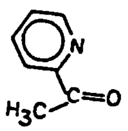
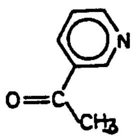
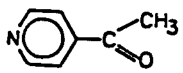
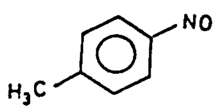
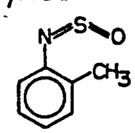
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7N^+$ | | | | | | | |
|  | (≤9.37) | (≤276) | (≤1156) | 60 | 252 | *EST | 56911-27-4 |
| | IP from 79AUE BOW. $\Delta_f H$(Ion) estimated from hydrogen affinities of pyridine ions = 268 kcal/mol, 1121 kJ/mol. Corresponding IP = 9.02 eV. | | | | | | |
| $C_7H_7NO^+$ | | | | | | | |
|  | (9.43±0.02) | (227) | (949) | 9.4±0.6 | 39.5±2.5 | 77PED/RYL | 6264-93-3 |
|  | 9.45 | 194 | 811 | −24±0.2 | −101±1 | 82TOR/SAB2 | 55-21-0 |
|  | (8.9) | (200) | (838) | −5 | −21 | *EST | 1122-62-9 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | (9.1) | (204) | (852) | −6 | −26 | *EST | |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | (9.3) | (208) | (871) | −6 | −26 | *EST | 1122-54-9 |
| | IP is onset of photoelectron band (81MOD/DIS2). | | | | | | |
|  | (8.79±0.1) | (216) | (903) | 13.2±1 | 55±4 | *EST | 623-11-0 |
| $C_7H_7NOS^+$ | | | | | | | |
|  | (8.75) | (187) | (782) | −15 | −62 | *EST | |
| | IP is onset of photoelectron band (82LOU/VAN). | | | | | | |

**Table 1. Positive Ion Table - Continued**

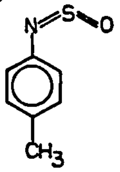
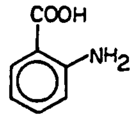
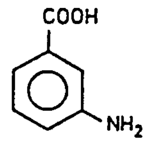
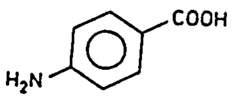
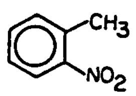
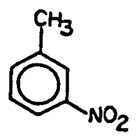
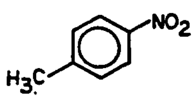
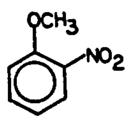
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_7NOS^+$ | | | | | | | |
|  | (≤8.84) | (≤190) | (≤795) | −14 | −58 | *EST | |
| | IP from 82LOU/VAN. | | | | | | |
| $C_7H_7NO_2^+$ | | | | | | | |
|  | (7.6) | (104) | (435) | −71±0.5 | −298±2 | 77NAB/SAB | 118-92-3 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (7.8) | (111) | (463) | −69±1 | −289±4 | 77NAB/SAB | 99-05-8 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (7.8) | (110) | (458) | −70±1 | −294±4 | 77NAB/SAB | 150-13-0 |
| | IP is onset of photoelectron band (81MEE/WAH). See also: 84TOB/TAJ. | | | | | | |
|  | 9.45±0.04 | 231 | 965 | 13 | 53 | 77PED/RYL | 88-72-2 |
| | IP from 82LEV/LIA, 82BAL/CAR. See also: 73GOL/KOR. | | | | | | |
|  | (9.48±0.02) | (226) | (946) | 7 | 31 | 77PED/RYL | 99-08-1 |
|  | (9.4) | (224) | (938) | 7±1 | 31±4 | 77PED/RYL | 99-99-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_7NO_3^+$ | | | | | | | |
|  | (8.8) | (186) | (779) | −17 | −70 | *EST | 91-23-6 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table – Continued**

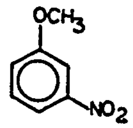
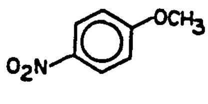
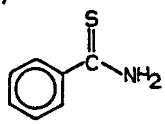
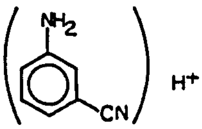
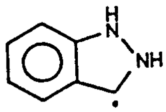
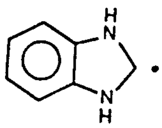
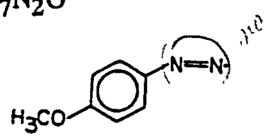
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7NO_3^+$ | | | | | | | |
|  | (8.7)<br>IP is onset of photoelectron band. | (179) | (749) | −22 | −90 | *EST | 555-03-3 |
|  | (8.79) | (182) | (760) | −21 | −88 | *EST | 100-17-4 |
| $C_7H_7NS^+$ | | | | | | | |
|  | (8.8)<br>IP from 81GRU. | (234) | (980) | 31.3±0.3 | 131.0±1.3 | 82TUR/SAB2 | 2227-79-4 |
| $C_7H_7N_2^+$ | | | | | | | |
|  | From proton affinity of 3-cyanobenzenamine (RN 2237-30-1). PA = 200.7 kcal/mol, 840. kJ/mol. | 218 | 912 | | | | |
|  | From proton affinity of indazole (RN 271-44-3) (84FLA/MAQ). PA = 218 kcal/mol, 914 kJ/mol. | 208 | 870 | | | | |
|  | From proton affinity of benzimidazole (RN 51-17-2) (83CAT/ELG, 84FLA/MAQ). PA = 227 kcal/mol, 958 kJ/mol. | 181 | 757 | | | | |
| $C_7H_7N_2O^+$ | | | | | | | |
|  | (7.28)<br>IP from 77NUY/MES. | (178) | (746) | 11 | 44 | *EST | 17333-79-8 |

Table 1. Positive Ion Table - Continued

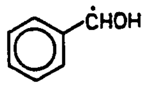
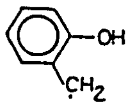
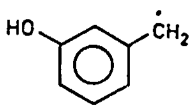
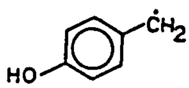
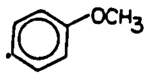
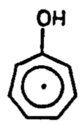
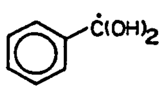
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_7O^+$ | | | | | | | |
|  | | 157 | 655 | | | | |
| | From proton affinity of benzaldehyde (RN 100-52-7). PA = 200.2 kcal/mol, 838. kJ/mol. | | | | | | |
|  | | 176 | 735 | | | | 65108-16-9 |
| | From appearance potential determinations (83RUS/FRE). | | | | | | |
|  | | 174 | 728 | | | | 65108-08-9 |
| | From appearance potential determinations (83RUS/FRE). | | | | | | |
|  | | 175 | 731 | | | | 29180-18-5 |
| | $\Delta_f H$(Ion) from appearance potential determinations (83RUS/FRE). Value derived from proton affinity of 4-methylene-2,5-cyclohexadiene-1-one is (153) kcal/mol, (641) kJ/mol, a serious discrepancy. PA = (222) kcal/mol, (929) kJ/mol. | | | | | | |
|  | (8.32) | (202) | (845) | 10 | 42 | *EST | 2396-03-4 |
| | IP from 77NUY/MES. | | | | | | |
|  | | 157 | 656 | | | | |
| | From proton affinity of 2,4,6-cycloheptatriene-1-one. PA = 219 kcal/mol, 918 kJ/mol (RN 539-80-0) and appearance potential determinations (83RUS/FRE). | | | | | | |
| $C_7H_7O_2^+$ | | | | | | | |
|  | | 97 | 407 | | | | |
| | From proton affinity of benzoic acid (RN 65-85-0). PA = 198.2 kcal/mol, 829. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

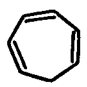
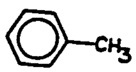
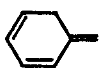
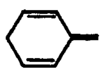
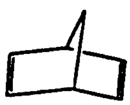
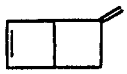
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_8{}^+$ | | | | | | | |
| HC≡C(CH$_2$)$_3$C≡CH | (9.85) | (322) | (1346) | 94.7 | 396 | 58BEN/BUS | 2396-63-6 |
| | IP from 78TRA/MCL. | | | | | | |
|  | 8.29 | 235 | 982 | 43.7±0.2 | 182.8±1 | 77PED/RYL | 544-25-2 |
| | | *240* | *1004* | *48.7* | *203.8* | | |
| | IP from 78TRA/MCL. | | | | | | |
|  | 8.82±0.01 | 215 | 901 | 12.0±0.1 | 50.1±0.3 | 77PED/RYL | 108-88-3 |
| | | *221* | *924* | *17.5* | *73.3* | | |
| | See also: 82SEL/HEL, 81KIM/KAT, 78LIA/AUS, 84HOW/GON. | | | | | | |
|  | 7.9 | 223 | 934 | 41 | 172 | 85BAL/HAS | 20679-59-8 |
| | IP from 85BAL/HAS. See also: 82BUR/TER, 82BAR. | | | | | | |
|  | (8.6) | (233) | (975) | 35±3 | 146±13 | 82BAR | 3217-87-6 |
| | IP from 82BAR. | | | | | | |
|  | 8.35 | 250 | 1046 | 57±1 | 240±4 | 80ROG/CHO | 121-46-0 |
| | IP from 78TRA/MCL. See also: 83HOU/RON, 82BIE/ASB, 85OHN/ISH. | | | | | | |
|  | 8.8 | 288 | 1206 | 85 | 357 | 85BAL/HAS | 67254-49-3 |
| | IP from 85BAL/HAS. | | | | | | |
|  | (7.8) | (260) | (1086) | 80±1 | 333±4 | 80ROG/CHO | 278-06-8 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

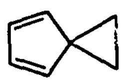
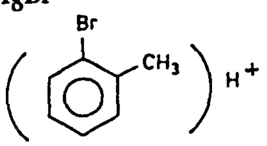
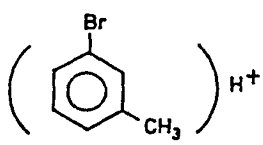
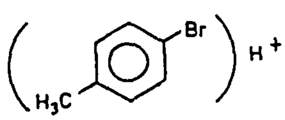
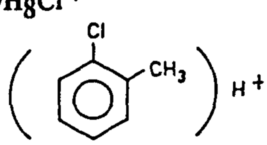
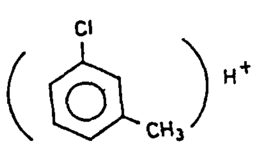
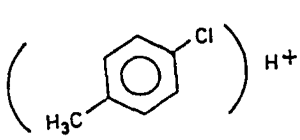
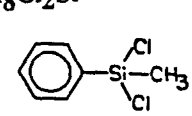
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_7H_8^+$** | | | | | | | |
|  | (8.14) | (250) | (1045) | 62 | 260 | *EST | 765-46-8 |
| **$C_7H_8Br^+$** | | | | | | | |
|  | | 193 | 809 | | | | |
| From proton affinity of 1,2-$C_6H_4(CH_3)Br$ (RN 95-46-5) (82MAS/BOH). PA = 187.2 kcal/mol, 783. kJ/mol. | | | | | | | |
|  | | 191 | 801 | | | | |
| From proton affinity of 1,3-$C_6H_4(CH_3)Br$ (RN 591-17-3) (82MAS/BOH). PA = 188.8 kcal/mol, 790. kJ/mol. | | | | | | | |
|  | | 196 | 818 | | | | |
| From proton affinity of 1,4-$C_6H_4(CH_3)Br$ (RN 106-38-7) (82MAS/BOH). PA = 187.2 kcal/mol, 783. kJ/mol. | | | | | | | |
| **$C_7H_8Cl^+$** | | | | | | | |
|  | | 186 | 777 | | | | |
| From proton affinity of 1,2-$C_6H_4(CH_3)Cl$ (RN 95-49-8) (82MAS/BOH). PA = 184.3 kcal/mol, 771. kJ/mol. | | | | | | | |
|  | | 181 | 758 | | | | |
| From proton affinity of 1,3-$C_6H_4(CH_3)Cl$ (RN 108-41-8) (82MAS/BOH). PA = 188.9 kcal/mol, 790. kJ/mol. | | | | | | | |
|  | | 189 | 792 | | | | |
| From proton affinity of 1,4-$C_6H_4(CH_3)Cl$ (RN 106-43-4) (82MAS/BOH). PA = 180.6 kcal/mol, 756. kJ/mol. | | | | | | | |
| **$C_7H_8Cl_2Si^+$** | | | | | | | |
|  | (8.97) | (132) | (551) | -75 | -314 | *EST | 149-74-6 |
| IP from 84VES/HAR. | | | | | | | |

Table 1. Positive Ion Table - Continued

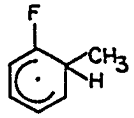
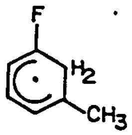
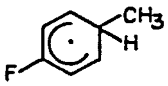
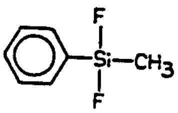
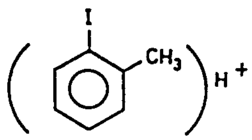
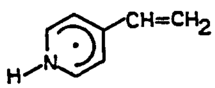
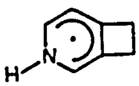
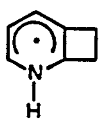
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_8F^+$ | | | | | | | |
|  | | 143 | 599 | | | | |
| From proton affinity of 2-$FC_6H_4CH_3$ (RN 95-52-3) (82MAS/BOH). PA = 187.0 kcal/mol, 782. kJ/mol. | | | | | | | |
|  | | 140 | 587 | | | | |
| From proton affinity of 3-$FC_6H_4CH_3$ (RN 352-70-5) (82MAS/BOH). PA = 189.5 kcal/mol, 793. kJ/mol. | | | | | | | |
|  | | 149 | 625 | | | | |
| From proton affinity of 4-$FC_6H_4CH_3$ (RN 352-32-9) (82MAS/BOH). PA = 180.9 kcal/mol, 757. kJ/mol. | | | | | | | |
| $C_7H_8F_2Si^+$ | | | | | | | |
|  | (8.97) | (29) | (122) | −178 | −743 | *EST | 328-57-4 |
| IP from 84VES/HAR. | | | | | | | |
| $C_7H_8I^+$ | | | | | | | |
|  | | 209 | 875 | | | | |
| From proton affinity of 2-$IC_6H_4CH_3$ (RN 615-37-2) (82MAS/BOH). PA = 188.4 kcal/mol, 788. kJ/mol. | | | | | | | |
| $C_7H_8N^+$ | | | | | | | |
|  | | (191) | (798) | | | | |
| From proton affinity of 4-vinylpyridine (RN 100-43-6). PA = (223.2) kcal/mol, (934) kJ/mol. | | | | | | | |
|  | | (202) | (846) | | | | |
| From proton affinity of 3,4-cyclobutenopyridine (RN 56911-27-4). PA = (225.9) kcal/mol, (945) kJ/mol. | | | | | | | |
|  | | (200) | (838) | | | | |
| From proton affinity of 2,3-cyclobutenopyridine. PA = (223.3) kcal/mol, (934) kJ/mol. | | | | | | | |

**Table 1. Positive Ion Table - Continued**

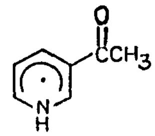
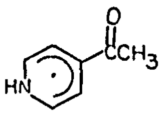
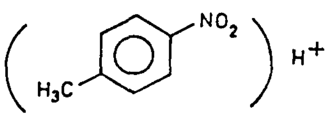
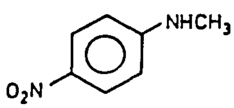
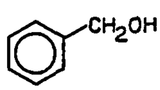
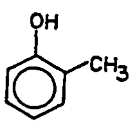
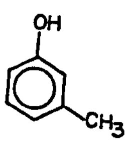
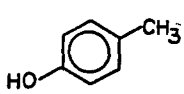
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_8NO^+$ | | | | | | | |
|  | | 142 | 595 | | | | |
| | From proton affinity of 1-(3-pyridinyl)-ethanone (RN 350-03-8).<br>PA = 217.2 kcal/mol, 909 kJ/mol. | | | | | | |
|  | | 142 | 594 | | | | |
| | From proton affinity of 1-(4-pyridinyl)-ethanone (RN 1122-54-9).<br>PA = 217.4 kcal/mol, 910. kJ/mol. | | | | | | |
| $C_7H_8NO_2^+$ | | | | | | | |
|  | | 176 | 738 | | | | |
| | From proton affinity of 4-nitrotoluene (RN 99-99-0) (84ROL/HOU).<br>PA = 196.8 kcal/mol, 823. kJ/mol. | | | | | | |
| $C_7H_8N_2O_2^+$ | | | | | | | |
|  | (8.1) | (201) | (843) | 15 | 61 | *EST | 100-15-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_8O^+$ | | | | | | | |
|  | (8.5) | (172) | (720) | −24.0 | −100.4 | 77PED/RYL | 100-51-6 |
| | See also: 82DES/DUT, 83RUS/FRE. IP is onset of photoelectron band (86BAL/JON). | | | | | | |
|  | 8.14 | 158 | 661 | −30 | −124 | 79KUD/KUD | 95-48-7 |
| | IP from 83RUS/FRE. | | | | | | |
|  | 8.29 | 160 | 668 | −31.6±0.3 | −132.3±1.2 | 79KUD/KUD | 108-39-4 |
| | IP from 85OIK/ABE, 83RUS/FRE. | | | | | | |
|  | 8.13 | 157 | 659 | −29.9 | −125.1 | 79KUD/KUD | 106-44-5 |
| | IP from 83RUS/FRE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

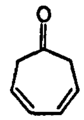
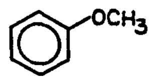
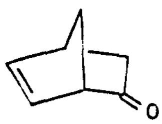
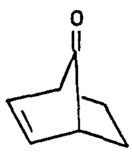
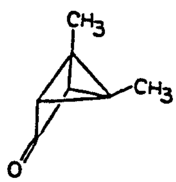
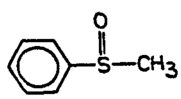
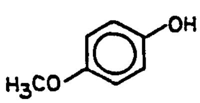
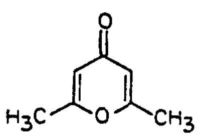
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_8O^+$ | | | | | | | |
|  | (8.24) | (188) | (788) | -1.7 | -7.1 | 83RUS/FRE | 1121-65-9 |
| | IP from 83RUS/FRE. | | | | | | |
|  | 8.21±0.02 | 173 | 724 | -16.2±0.3 | -68.0±1.1 | 77PED/RYL | 100-66-3 |
| | See also: 83KLA/KOV. | | | | | | |
|  | (≤8.86) | (≤197) | (≤826) | -7 | -29 | *EST | 694-98-4 |
|  | (≤9.25) | (≤210) | (≤877) | -4 | -15 | *EST | 694-71-3 |
|  | (8.9) | (251) | (1049) | 45 | 190 | *EST | 3350-02-5 |
| | IP is onset of photoelectron band (84GLE/HAI). | | | | | | |
| $C_7H_8OS^+$ | | | | | | | |
|  | (8.5) | (191) | (800) | -5 | -20 | *EST | 1193-82-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_8O_2^+$ | | | | | | | |
|  | (7.50) | (115) | (482) | -58 | -242 | *EST | 150-76-5 |
|  | (9.03) | (152) | (636) | -56 | -235 | *EST | 1004-36-0 |
| | IP from 85GRU/SPI | | | | | | |

**Table 1. Positive Ion Table - Continued**

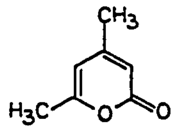
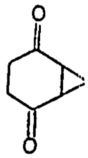
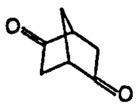
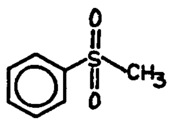
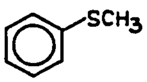
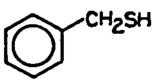
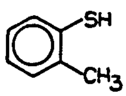
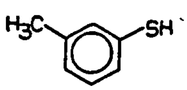
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_8O_2^+$ | | | | | | | |
|  | (8.51) | (135) | (564) | −61 | −257 | *EST | 675-09-2 |
| | IP from 85GRU/SPI | | | | | | |
|  | (9.4) | (168) | (702) | −49 | −205 | *EST | 60582-65-2 |
| | IP is onset of photoelectron band (85GLE/JAH). | | | | | | |
|  | (9.26) | (161) | (674) | −52 | −219 | *EST | 27943-47-1 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
| $C_7H_8O_2S^+$ | | | | | | | |
|  | (9.5) | (159) | (663) | −60.6±0.7 | −253.4±3.0 | 77PED/RYL | 3112-85-4 |
| | IP is onset of photoelectron band (81MOH/JIA). | | | | | | |
| $C_7H_8S^+$ | | | | | | | |
|  | 7.94±0.02 | 206 | 864 | 23.4±0.3 | 97.8±1.2 | 77PED/RYL | 100-68-5 |
|  | (8.5) | (218) | (914) | 22±0.7 | 94±3 | 77PED/RYL | 100-53-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.31) | (≤211) | (≤881) | 19 | 79 | *EST | 137-06-4 |
|  | (≤8.44) | (≤214) | (≤893) | 19 | 79 | *EST | 108-40-7 |

**Table 1. Positive Ion Table - Continued**

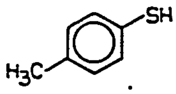
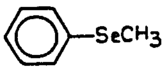
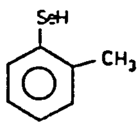
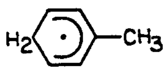
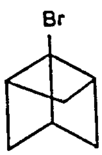
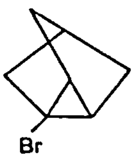
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_8S^+$ | | | | | | | |
|  | (8.0) | (203) | (851) | 19 | 79 | *EST | 106-45-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_8Se^+$ | | | | | | | |
|  | (7.4) | (207) | (867) | 36 | 153 | *EST | 4346-64-9 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
|  | ≤8.4 | (≤225) | (≤940) | 31 | 130 | *EST | 37773-21-0 |
| | IP from 81BAK/ARM. | | | | | | |
| $C_7H_9^+$ | | | | | | | |
|  | | 188 | 786 | | | | |
| | From proton affinity of $C_6H_5CH_3$ (RN 108-88-3). PA = 189.8 kcal/mol, 794. kJ/mol. | | | | | | |
|  | | 220 | 919 | | | | |
| | From proton affinity of 2,5-norbornadiene (RN 121-46-0) (86HOU/SCH). PA = 203.4 kcal/mol, 851. kJ/mol. | | | | | | |
| $C_7H_9Br^+$ | | | | | | | |
|  | (8.7) | (261) | (1091) | 60 | 252 | *EST | 78995-60-5 ~~59346-69-9~~ duplicated by $C_8H_7Br$ p338 |
| | IP is onset of photoelectron band (84ABE/DEL). | | | | | | |
|  | (8.55) | (218) | (912) | 21 | 87 | *EST | 31991-53-4 |
| | IP is onset of photoelectron band (85DEL/PIG). | | | | | | |

Table 1. Positive Ion Table - Continued

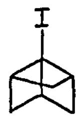
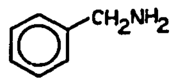
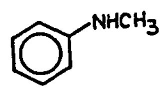
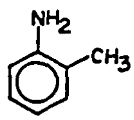
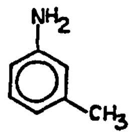
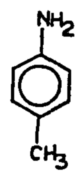
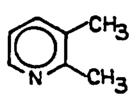
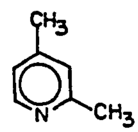
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_9I^+$ | | | | | | | |
|  | (8.6) | (273) | (1143) | 75 | 313 | *EST | 74725-76-1 |
| | IP is onset of photoelectron band (84ABE/DEL). | | | | | | |
| $C_7H_9N^+$ | | | | | | | |
|  | 8.64±0.05 | 219 | 918 | 20±0.7 | 84±3 | 77CAR/LAY | 100-46-9 |
| | See also: 79AUE/BOW. | | | | | | |
|  | 7.33±0.02 | 189 | 792 | 20 | 85 | 78COL/BEN | 100-61-8 |
| | See also: 84MAU/NEL, 83KLA/KOV. | | | | | | |
|  | 7.44±0.02 | (185) | (773) | 13±0.2 | 55±1 | *EST | 95-53-4 |
|  | 7.50±0.02 | (186) | (778) | 13±0.4 | 54±2 | *EST | 108-44-1 |
|  | (7.24±0.02) | (180) | (753) | 13 | 54 | *EST | 106-49-0 |
|  | (8.85±0.02) | (220) | (922) | 16.3 | 68.3 | 77PED/RYL | 583-61-9 |
| | $\Delta_fH$(Ion) predicted from hydrogen affinities of pyridines: 224 kcal/mol, 937 kJ/mol. Corresponding IP = 9.01 eV. See also: 79AUE/BOW. | | | | | | |
|  | (8.85±0.03) | (219) | (918) | 15.3 | 63.9 | 77PED/RYL | 108-47-4 |

**Table 1. Positive Ion Table - Continued**

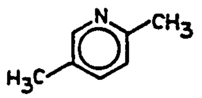
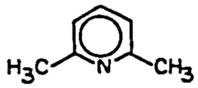
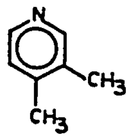
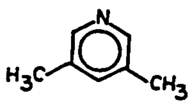
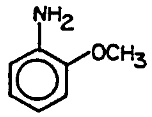
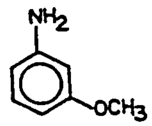
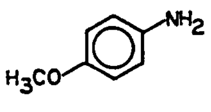
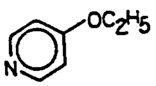
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_9N^+$ | | | | | | | |
|  | (≤8.80±0.05) | (≤219) | (≤916) | 15.9±0.2 | 66.5±1.0 | 77PED/RYL | 589-93-5 |
| | $\Delta_f H$(Ion) predicted from hydrogen affinities of pyridines: 223 kcal/mol, 933 kJ/mol. Corresponding IP = 8.98eV. See also: 79AUE/BOW. | | | | | | |
|  | 8.86±0.03 | 218 | 913 | 14.0±0.4 | 58.7±1.6 | 77PED/RYL | 108-48-5 |
| | See also: 81KIM/KAT. | | | | | | |
|  | (≤9.15) | (≤228) | (≤953) | 16.7±0.2 | 70.1±1.1 | 77PED/RYL | 583-58-4 |
| | $\Delta_f H$(Ion) predicted from hydrogen affinities of pyridines: 224 kcal/mol, 937 kJ/mol. Corresponding IP = 8.98eV. See also: 79AUE/BOW. | | | | | | |
|  | (≤9.25) | (≤231) | (≤965) | 17.4±0.2 | 72.8±0.9 | 77PED/RYL | 591-22-0 |
| | $\Delta_f H$(Ion) predicted from hydrogen affinities of pyridines: 226 kcal/mol, 946 kJ/mol. Corresponding IP = 9.05 eV. | | | | | | |
| $C_7H_9NO^+$ | | | | | | | |
|  | (7.46±0.1) | (158) | (663) | −14 | −57 | *EST | 90-04-0 |
|  | (7.76±0.1) | (163) | (682) | −16 | −67 | *EST | 536-90-3 |
|  | (7.44) | (158) | (660) | −14 | −58 | *EST | 104-94-9 |
|  | (≤9.25±0.03) | (≤202) | (≤845) | −11 | −47 | *EST | 33399-46-1 |

**Table 1. Positive Ion Table - Continued**

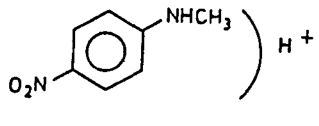
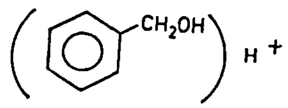
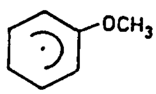
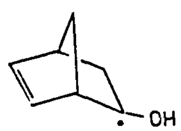
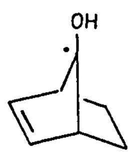
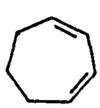
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_9N_2O_2^+$ | | | | | | | |
|  | | 167 | 700 | | | | |
| | From proton affinity of N-methyl-4-nitroaniline (RN 100-23-2) (84ROL/HOU). PA = 212.9 kcal/mol, 891. kJ/mol. | | | | | | |
| $C_7H_9O^+$ | | | | | | | |
|  | | 153 | 641 | | | | |
| | From proton affinity of $C_6H_5CH_2OH$ (RN 100-51-6) (78TAF/TAA). PA = 188.5 kcal/mol, 789. kJ/mol. | | | | | | |
|  | | 149 | 624 | | | | |
| | From proton affinity of $C_6H_5OCH_3$ (RN 100-66-3). PA = 200.3 kcal/mol, 838. kJ/mol. | | | | | | |
|  | | 157 | 655 | | | | |
| | From proton affinity of bicyclo[2.2.1]hept-2-ene-5-one (RN 694-98-4). (86HOU/SCH). PA = 202.1 kcal/mol, 846. kJ/mol. | | | | | | |
|  | | 164 | 686 | | | | |
| | From proton affinity of bicyclo[2.2.1]hept-2-ene-7-one (RN 694-71-3). (86HOU/SCH). PA = 198.1 kcal/mol, 829. kJ/mol. | | | | | | |
| $C_7H_{10}^+$ | | | | | | | |
| $(CH_2=CH)_3CH$ | (≤9.5) | (≤265) | (≤1108) | 46 | 191 | *EST | 26456-63-3 |
| | IP from 83GLE/HAI. | | | | | | |
| (E,E)-$CH_2=CHCH=CHCH=CHCH_3$ | 7.96±0.02 | (215) | (901) | 32±1 | 133±4 | *EST | 17679-93-5 |
| $C_2H_5C{\equiv}CC(CH_3)=CH_2$ | (8.66±0.01) | (247) | (1033) | 47 | 197 | *EST | 23056-94-2 |
| (E)-$HC{\equiv}CC(C_2H_5)=CHCH_3$ | (8.70±0.01) | (247) | (1031) | 46 | 192 | *EST | 14272-82-3 |
|  | ≤8.31±0.03 | ≤214 | ≤896 | 22.5±0.2 | 94.2±0.9 | 77PED/RYL | 4054-38-0 |

Table 1. Positive Ion Table - Continued

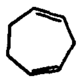
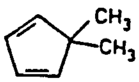
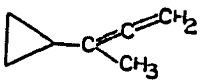
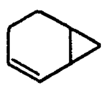
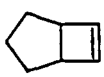
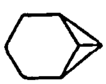
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_{10}^+$ | | | | | | | |
|  | (8.85±0.03) | (232) | (970) | 28 | 116 | 76JEN | 7161-35-5 |
|  | 8.2 | (206) | (860) | 16 | 69 | *EST | 4125-18-2 |
| | IP is onset of photoelectron band (85GUI/PFI3). | | | | | | |
|  | (8.83) | (257) | (1075) | 53 | 223 | 82KOZ/MAS | 51549-86-1 |
|  | (≤8.69) | (≤227) | (≤951) | 27 | 113 | *EST | 2566-57-6 |
|  | (9.37) | (250) | (1046) | 34 | 142 | *EST | 4927-03-1 |
|  | 8.82±0.03 | 225 | 941 | 21±1 | 90±4 | 80ROG/CHO | 498-66-8 |
| | See also: 83HOU/RON. | | | | | | |
|  | 8.72 | 245.5 | 1027.1 | 44.4 | 185.8 | 85SVY/IOF | 287-13-8 |
| | IP is onset of photoelectron band (85DEL/PIG). | | | | | | |
|  | (8.7) | (260) | (1089) | 60 | 250 | *EST | 51273-50-8 |
| | IP is onset of photoelectron band (84ABE/DEL). | | | | | | |

Table 1. Positive Ion Table - Continued

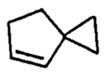
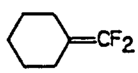
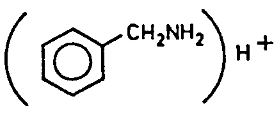
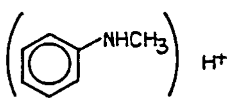
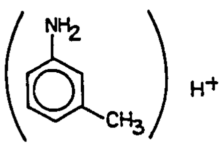
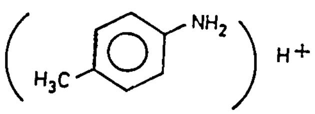
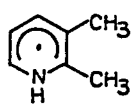
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{10}{}^+$ | | | | | | | |
|  | (8.72) | (221) | (926) | 20±1 | 85±4 | 80ROG/CHO | 279-19-6 |
| | IP is onset of photoelectron band (85DEL/PIG). | | | | | | |
|  | (≤8.48) | (≤236) | (≤986) | 40 | 168 | *EST | 52708-23-3 |
| $C_7H_{10}F_2{}^+$ | | | | | | | |
|  | 8.84 | (103) | (433) | −100 | −420 | *EST | 696-32-2 |
| | IP from 80SAR/WOR. | | | | | | |
| $C_7H_{10}N^+$ | | | | | | | |
|  | | 169 | 707 | | | | |
| | From proton affinity of $C_6H_5CH_2NH_2$ (RN 100-46-9). PA = 216.8 kcal/mol, 907. kJ/mol. | | | | | | |
|  | | 168 | 703 | | | | |
| | From proton affinity of $C_6H_5NHCH_3$ (RN 100-61-8). PA = 218.1 kcal/mol, 912.5 kJ/mol. | | | | | | |
|  | | 165 | 690 | | | | |
| | From proton affinity of 3-$CH_3C_6H_4NH_2$ (RN 108-44-1). PA = 213.4 kcal/mol, 893. kJ/mol. | | | | | | |
|  | | 165 | 690 | | | | |
| | From proton affinity of 4-$CH_3C_6H_4NH_2$ (RN 106-49-0). PA = 213.7 kcal/mol, 894. kJ/mol. | | | | | | |
|  | | 156 | 652 | | | | |
| | From proton affinity of 2,3-dimethylpyridine (RN 583-61-9). PA = 226.2 kcal/mol, 946. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

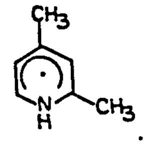
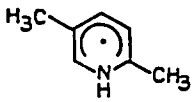
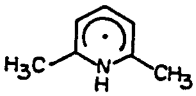
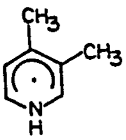
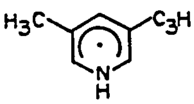
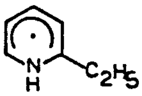
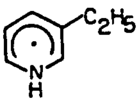
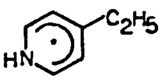
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{10}N^+$ | | | | | | | |
|  | | 153 | 643 | | | | |
| From proton affinity of 2,4-dimethylpyridine (RN 108-47-4). PA = 227.3 kcal/mol, 951. kJ/mol. | | | | | | | |
|  | | 156 | 651 | | | | |
| From proton affinity of 2,5-dimethylpyridine (RN 589-93-5). PA = 226.2 kcal/mol, 946. kJ/mol. | | | | | | | |
|  | | 152 | 634 | | | | |
| From proton affinity of 2,6-dimethylpyridine (RN 108-48-5). PA = 228.2 kcal/mol, 955. kJ/mol. | | | | | | | |
|  | | 157 | 654 | | | | |
| From proton affinity of 3,4-dimethylpyridine (RN 583-58-4). PA = 226.0 kcal/mol, 946. kJ/mol. | | | | | | | |
|  | | 158 | 661 | | | | |
| From proton affinity of 3,5-dimethylpyridine (RN 591-22-0). PA = 225.5 kcal/mol, 943. kJ/mol. | | | | | | | |
|  | | 159 | 665 | | | | |
| From proton affinity of 2-ethylpyridine (RN 100-71-0). PA = 226.2 kcal/mol, 946. kJ/mol. | | | | | | | |
|  | | 162 | 679 | | | | |
| From proton affinity of 3-ethylpyridine (RN 536-78-7). PA = 223.9 kcal/mol, 937. kJ/mol. | | | | | | | |
|  | | (161) | (672) | | | | |
| From proton affinity of 4-ethylpyridine (RN 536-75-4). PA = (224.6) kcal/mol, (940) kJ/mol. | | | | | | | |

**Table 1. Positive Ion Table - Continued**

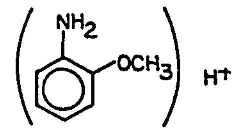
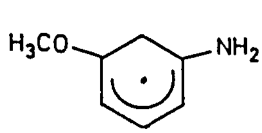
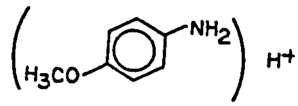
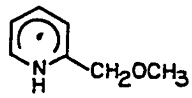
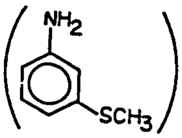
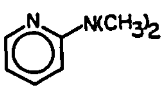
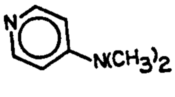
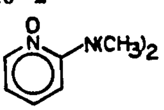
| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_7H_{10}NO^+$** | | | | | | | |
|  | | 137 | 575 | | | | |
| | From proton affinity of 2-$CH_3OC_6H_4NH_2$ (RN 90-04-0). PA = 214.7 kcal/mol, 898. kJ/mol. | | | | | | |
|  | | 132 | 553 | | | | |
| | From proton affinity of 3-$CH_3OC_6H_4NH_2$ (RN 536-90-3). PA = 217.6 kcal/mol, 910. kJ/mol. | | | | | | |
|  | | 137 | 575 | | | | |
| | From proton affinity of 4-$CH_3OC_6H_4NH_2$ (RN 104-94-9). PA = 214.3 kcal/mol, 897. kJ/mol. | | | | | | |
|  | | (134) | (563) | | | | |
| | From proton affinity of pyridine,2-methoxymethyl (RN 23579-92-2). PA = (226.0) kcal/mol, (945.) kJ/mol. | | | | | | |
| **$C_7H_{10}NS^+$** | | | | | | | |
|  | | 176 | 735 | | | | |
| | From proton affinity of 3-methylthiobenzenamine (RN 1783-81-9). PA = 214.5 kcal/mol, 897. kJ/mol. | | | | | | |
| **$C_7H_{10}N_2^+$** | | | | | | | |
|  | 7.75±0.15 | (211) | (880) | 32 | 132 | *EST | 5683-33-0 |
|  | (≤7.82) | (≤214) | (≤898) | 34 | 144 | 84BIC/PIL | 1122-58-3 |
| **$C_7H_{10}N_2O^+$** | | | | | | | |
|  | (7.62±0.05) | (191) | (798) | 15 | 63 | *EST | 3618-79-9 |

**Table 1. Positive Ion Table - Continued**

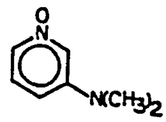
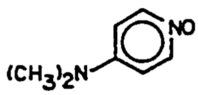
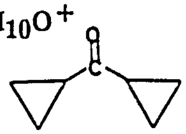
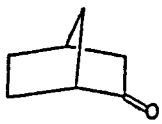
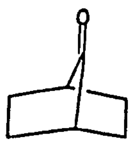
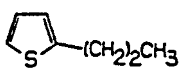
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{10}N_2O^+$ | | | | | | | |
|  | (7.85±0.05) | (197) | (824) | 16 | 67 | *EST | 36100-40-0 |
|  | (7.0) | (178) | (746) | 17 | 71 | *EST | 1005-31-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_{10}O^+$ | | | | | | | |
|  | (9.1) | (249) | (1041) | 39 | 163 | *EST | 1121-37-5 |
|  | 8.94±0.02 | 166 | 695 | −40±0.7 | −168±3 | 78STE2 | 497-38-1 |
| | See also: 80FRO/WES. | | | | | | |
|  | ≤9.01±0.02 | ≤176 | ≤735 | −32±0.7 | −134±3 | 78STE2 | 10218-02-7 |
| $C_7H_{10}S^+$ | | | | | | | |
|  | (≤8.6±0.2) | (≤208) | (≤870) | 10 | 40 | *EST | 1551-27-5 |
| $C_7H_{11}^+$ | | | | | | | |
|  | 6.84 | 186 | 777 | 28 | 117 | DERIVED | 30967-37-4 |
| | IP from 79HOU. $\Delta_fH$ of $C_7H_{11}^+$ from PA of norbornene, 187 kcal/mol, 784 kJ/mol; PA = 199.9 kcal/mol, 836. kJ/mol. From hydride transfer equilibria relative to $\Delta_fH(t\text{-}C_4H_9^+)$, 185 kcal/mol, 773 kJ/mol (76SOL/FIE, 85SHA/SHA); from chloride transfer equilibria 185.8 kcal/mol, 777.4 kJ/mol (85SHA/SHA). Cited $\Delta_fH$ of radical = $\Delta_fH(C_7H_{11}^+)$ - IP. | | | | | | |

Table 1. Positive Ion Table - Continued

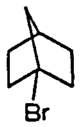
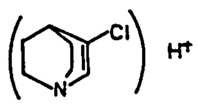
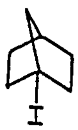
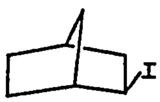
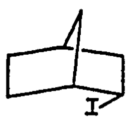
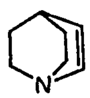
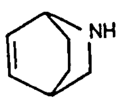
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{11}Br^+$ | | | | | | | |
|  | 9.55 | (209) | (874) | −11 | −47 | *EST | 13474-70-9 |
| | IP is onset of photoelectron band (84DEL/ABE, 85HON/HEI2). | | | | | | |
| $C_7H_{11}Cl^+$ | | | | | | | |
| $(CH_3)_3CCH=C=CHCl$ | 9.05 | (228) | (954) | 19 | 81 | *EST | 65388-53-6 |
| | IP is onset of photoelectron band (85ELS/VER). | | | | | | |
| $C_7H_{11}ClN^+$ | | | | | | | |
|  | | (167) | (697) | | | | |
| | From proton affinity of 3-chloro-1-azabicyclo[2.2.2]oct-2-ene PA = (224.0) kcal/mol, (937.) kJ/mol. | | | | | | |
| $C_7H_{11}I^+$ | | | | | | | |
|  | (8.8) | (206) | (863) | 3 | 14 | *EST | 930-80-3 |
| | IP is onset of photoelectron band (84DEL/ABE). | | | | | | |
|  | (9.00) | (210) | (878) | 2 | 10 | *EST | 57173-48-5 |
| | IP from 84HON/HEI. | | | | | | |
|  | 9.00 | (211) | (882) | 3 | 14 | *EST | 30983-85-8 |
| | IP from 84HON/HEI. | | | | | | |
| $C_7H_{11}N^+$ | | | | | | | |
|  | (8.02) | (222) | (930) | 37 | 156 | *EST | 13929-94-7 |
|  | (≤8.35±0.05) | (≤218) | (≤913) | 26 | 107 | *EST | 3693-58-1 |

**Table 1. Positive Ion Table - Continued**

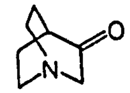
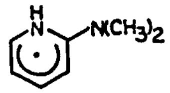
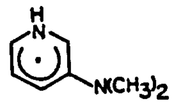
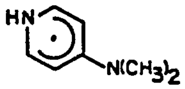
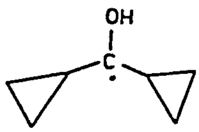
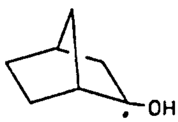
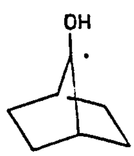
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{11}NO^+$ | | | | | | | |
|  | (≤8.2) | (≤161) | (≤675) | −28 | −116 | *EST | 3731-38-2 |
| | IP from 79AUE/BOW. | | | | | | |
| $C_7H_{11}N_2^+$ | | | | | | | |
|  | | 168 | 703 | | | | |
| | From proton affinity of N,N-dimethyl-2-pyridinamine (RN 5683-33-0). PA = 229.2 kcal/mol, 959. kJ/mol. | | | | | | |
|  | | (174) | (726) | | | | |
| | From proton affinity of N,N-dimethyl-3-pyridinamine (RN 18437-57-5). PA = (229.9) kcal/mol, (962) kJ/mol. | | | | | | |
|  | | 163 | 684 | | | | |
| | From proton affinity of N,N-dimethyl-4-pyridinamine (RN 1122-58-3). (86TAF/GAL, 77ARN/CHA). PA = 236.6 kcal/mol, 990. kJ/mol. | | | | | | |
| $C_7H_{11}O^+$ | | | | | | | |
|  | | 194 | 812 | | | | |
| | From proton affinity of dicyclopropylmethanone (RN 1121-37-5). PA = 210.7 kcal/mol, 881.5 kJ/mol. | | | | | | |
|  | | 123 | 514 | | | | |
| | From proton affinity of bicyclo[2.2.1]heptan-2-one (RN 497-38-1) (86HOU/SCH). PA = 202.6 kcal/mol, 848. kJ/mol. | | | | | | |
|  | | 134 | 561 | | | | |
| | From proton affinity of bicyclo[2.2.1]heptan-7-one (RN 10218-02-7) (86HOU/SCH). PA = 199.5 kcal/mol, 835. kJ/mol. | | | | | | |
| $C_7H_{12}^+$ | | | | | | | |
| (E)-$CH_3CH_2CH_2CH=CHCH=CH_2$ | (8.47) | (204) | (852) | 8 | 35 | *EST | 2384-92-1 |
| | IP from 81MAS/MOU. | | | | | | |

Table 1. Positive Ion Table - Continued

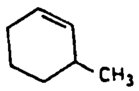
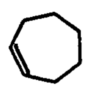
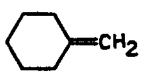
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{12}^+$ | | | | | | | |
| (E),(E)-$CH_3CH_2CH=CHCH=CHCH_3$ | | | | | | | |
| | ≤8.17 | (≤194) | (≤812) | 6 | 24 | *EST | 2384-94-3 |
| | IP from 81MAS/MOU. | | | | | | |
|  | 8.89±0.01 | (196) | (822) | −9 | −36 | *EST | 591-48-0 |
| | See also: 83BRO/BUS. | | | | | | |
| (E)-$(CH_3)_2CHCH=CHCH=CH_2$ | | | | | | | |
| | ≤8.47 | (≤202) | (≤847) | 7 | 30 | *EST | 32763-70-5 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$C_2H_5C(CH_3)=CHCH=CH_2$ | | | | | | | |
| | (8.19) | (195) | (814) | 6 | 24 | *EST | 4842-93-7 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_3CH=C(CH_3)C(CH_3)=CH_2$ | | | | | | | |
| | (8.28) | (194) | (813) | 3 | 14 | *EST | 1625-49-6 |
| | IP from 81MAS/MOU. | | | | | | |
| $CH_2=C(CH_3)C(C_2H_5)=CH_2$ | | | | | | | |
| | (8.65) | (205) | (860) | 6 | 25 | *EST | 14145-44-9 |
| | IP from 81MAS/MOU. | | | | | | |
| n-$C_5H_{11}C{\equiv}CH$ | (10.04) | (256) | (1073) | 25±0.7 | 104±3 | 79ROG/DAG | 628-71-7 |
| | From plot of trends in IP's of 1-alkynes, an IP of ~9.95 eV would be predicted. | | | | | | |
| n-$C_4H_9C{\equiv}CCH_3$ | (9.33±0.01) | (235) | (985) | 20±0.5 | 85±2 | 79ROG/DAG | 1119-65-9 |
| n-$C_3H_7C{\equiv}CC_2H_5$ | (9.26±0.01) | (233) | (976) | 20 | 83±2 | 79ROG/DAG | 2586-89-2 |
| (tert-$C_4H_9$)$C{\equiv}CCH_3$ | | | | | | | |
| | (9.276±0.10) | (235) | (984) | 21 | 89 | *EST | 999-78-0 |
| | See also: 85ORL/BOG. | | | | | | |
|  | (8.91±0.04) | (203) | (850) | −2.2±0.2 | −9.4±0.9 | 77PED/RYL | 628-92-2 |
|  | 8.93±0.01 | 200 | 837 | −6±1 | −25±4 | 79FUC/PEA | 1192-37-6 |
| | IP from 80SAR/WOR. See also: 86SPA/RAD. | | | | | | |

**Table 1. Positive Ion Table - Continued**

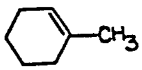
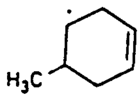
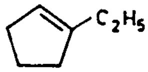
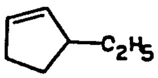
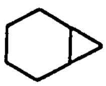
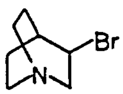
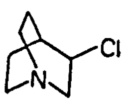
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{12}^+$ | | | | | | | |
|  | 8.67±0.02 | 189.6 | 793.3 | −10.3±0.2 | −43.2±0.7 | 77PED/RYL | 591-49-1 |
|  | (8.91±0.01) | (197) | (824) | −9 | −36 | *EST | 591-47-9 |
|  | (8.53±0.01) | (192) | (801) | −5±0.7 | −22±3 | 82ALL/DOD | 2146-38-5 |
|  | 8.88±0.01 | 202 | 843 | −3 | −14 | 82ALL/DOD | 694-35-9 |
|  | (9.03±0.02) | (209) | (873) | 0.5±0.5 | 2±2 | 77PED/RYL | 286-08-8 |
|  | 9.77±0.03 | 213 | 894 | −12±1 | −49±4 | 80ROG/CHO | 279-23-2 |
| $C_7H_{12}BrN^+$ | | | | | | | |
|  | (≤8.5)<br>IP from 79AUE/BOW. | (≤197) | (≤823) | 1 | 3 | *EST | |
| $C_7H_{12}ClN^+$ | | | | | | | |
|  | (≤8.8)<br>IP from 79AUE/BOW. | (≤192) | (≤805) | −11 | −44 | *EST | 42332-45-6 |

Table 1. Positive Ion Table - Continued

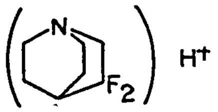
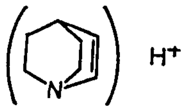
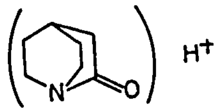
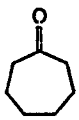
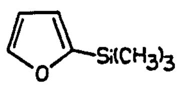
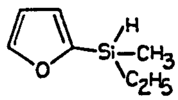
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_{12}F_2N^+$ | | | | | | | |
|  | | (43) | (179) | | | | |
| | From proton affinity of 3,3-difluoro-1-azabicyclo[2.2.2]octane. PA = (221.8) kcal/mol, (928.) kJ/mol. | | | | | | |
| $C_7H_{12}N^+$ | | | | | | | |
|  | | (175) | (730) | | | | |
| | From proton affinity of 1-azabicyclo[2.2.2]oct-2-ene (RN 13929-94-7). PA = (228.5) kcal/mol, (956.) kJ/mol. | | | | | | |
| $C_7H_{12}NO^+$ | | | | | | | |
|  | | (116) | (486) | | | | |
| | From proton affinity of 1-azabicyclo[2.2.2]octan-3-one (RN 3731-38-2). PA = (221.9) kcal/mol, (928) kJ/mol. | | | | | | |
| $C_7H_{12}O^+$ | | | | | | | |
|  | ≤9.14 | ≤152 | ≤634 | −59.1±0.4 | −247.5±1.8 | 77PED/RYL | 502-42-1 |
|  | (9.6±0.1) | (165) | (691) | −56.2 | −235.1 | 82SPL/CAL | 2043-61-0 |
| | IP from 82SPL/CAL. | | | | | | |
| $C_7H_{12}OSi^+$ | | | | | | | |
|  | (8.1) | (134) | (563) | −52 | −219 | *EST | 1578-33-2 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
|  | ≤8.53 | (≤151) | (≤630) | −46 | −193 | *EST | 13271-69-7 |
| | IP from 83ZYK/ERC. | | | | | | |

**Table 1. Positive Ion Table - Continued**

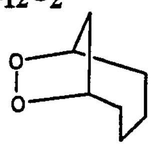
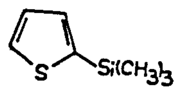
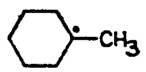
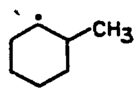
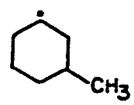
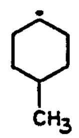
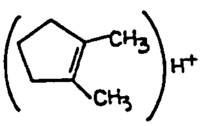
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{12}O_2{}^+$ | | | | | | | |
|  | (8.5) | (161) | (673) | −35 | −147 | *EST | 68525-35-9 |
| | IP is onset of photoelectron band (84GLE/DOB). | | | | | | |
| $C_7H_{12}SSi^+$ | | | | | | | |
|  | (8.1) | (173) | (726) | −13 | −56 | *EST | 18245-28-8 |
| | IP is onset of photoelectron band (83VES/HAR). | | | | | | |
| $C_7H_{13}{}^+$ | | | | | | | |
| $(CH_3)_2CCHC(CH_3)_2$ | | (157) | (655) | | | | 60602-30-4 |
| | From proton affinity of $(CH_3)_2C=CHC(CH_3)=CH_2$. (RN 1000-86-8). PA = (213.1) kcal/mol, (892.) kJ/mol. | | | | | | |
|  | | 157 | 655 | | | | 16998-65-5 |
| | From proton affinity of 1-methylcyclohexene. (RN 591-49-1). PA = 198.8 kcal/mol, 832. kJ/mol. | | | | | | |
|  | | (169) | (708) | | | | 41771-02-2 |
| | From appearance potential measurements (81HER/SIC). | | | | | | |
|  | | (173) | (722) | | | | 61838-22-0 |
| | From appearance potential measurements (81HER/SIC). | | | | | | |
|  | | (172) | (720) | | | | 21029-96-9 |
| | From appearance potential measurements (81HER/SIC). | | | | | | |
|  | | 158 | 660 | | | | |
| | From proton affinity of 1,2-dimethylcyclopentene. (RN 765-47-9). PA = 198.1 kcal/mol, 829. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

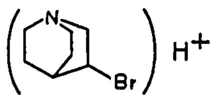
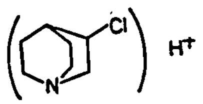
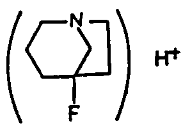
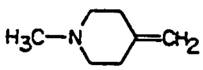
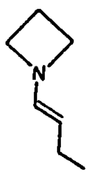
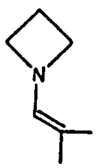
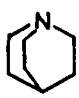
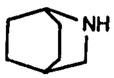
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_7H_{13}BrN^+$** | | | | | | | |
|  | | 139 | 583 | | | | |
| | From proton affinity of 3-bromo-1-azabicyclo[2.2.2]octane. PA = (227.1) kcal/mol, (950.) kJ/mol. | | | | | | |
| **$C_7H_{13}ClN^+$** | | | | | | | |
|  | | (129) | (541) | | | | |
| | From proton affinity of 3-chloro-1-azabicyclo[2.2.2]octane (RN 42332-45-6). PA = (225.8) kcal/mol, (945.) kJ/mol. | | | | | | |
| **$C_7H_{13}FN^+$** | | | | | | | |
|  | | (160) | (670) | | | | |
| | From proton affinity of 3-fluoro-1-azabicyclo[3.2.1]octane. PA = (228.1) kcal/mol, (954.) kJ/mol. | | | | | | |
| **$C_7H_{13}N^+$** | | | | | | | |
|  | (≤8.36) | (≤204) | (≤855) | 11 | 48 | *EST | 13669-28-8 |
| | IP from 80SAR/WOR. | | | | | | |
|  | (7.1) | (197) | (823) | 33 | 138 | *EST | 81156-87-8 |
| | IP is onset of photoelectron band (81MUL/PRE2). | | | | | | |
|  | (6.9) | (192) | (803) | 33 | 137 | *EST | 81156-88-9 |
| | IP is onset of photoelectron band (81MUL/PRE2). | | | | | | |
|  | (7.4) | (170) | (710) | −1.0±0.3 | −4.2±1.2 | 77PED/RYL | 100-76-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.22±0.05) | (≤187) | (≤782) | −3 | −11 | *EST | 280-38-6 |

Table 1. Positive Ion Table - Continued

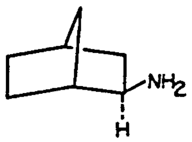
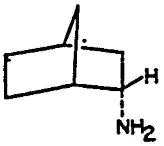
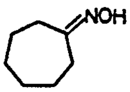
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_7H_{13}N^+$** | | | | | | | |
|  | (8.33) | (185) | (776) | −7±0.2 | −28±1 | *EST | 31002-73-0 |
| | IP from 79AUE/BOW. | | | | | | |
|  | (8.41) | (186) | (779) | −8±0.2 | −32±1 | *EST | 7242-92-4 |
| | IP from 79AUE/BOW. | | | | | | |
| **$C_7H_{13}NO^+$** | | | | | | | |
|  | (8.88±0.03) | (179) | (749) | −26 | −108 | *EST | 2158-31-8 |
| | IP from 79GOL/KUL. | | | | | | |
| **$C_7H_{14}^+$** | | | | | | | |
| 1-$C_7H_{14}$ | (9.44) | (202.8) | (848.9) | −14.8 | −61.9 | 84WIB/WAS | 592-76-7 |
| 2-$C_7H_{14}$ | (8.84±0.02) | (187) | (782) | −17 | −71 | 84WIB/WAS | 592-77-8 |
| | IP from 77ASH/BUR. | | | | | | |
| 3-$C_7H_{14}$ | (8.92) | (189) | (790) | −17 | −71 | 84WIB/WAS | 14686-14-7 |
| | IP from 81HOL/FIN. | | | | | | |
| $(CH_3)_3CCH_2CH=CH_2$ | 9.40±0.01 | 197 | 823 | −20.0±0.2 | −83.8±0.8 | 77PED/RYL | 762-62-9 |
| n-$C_4H_9C(CH_3)=CH_2$ | (9.04±0.01) | (190) | (796) | −18 | −76 | *EST | 6094-02-6 |
| $(CH_3)_2CHCH_2C(CH_3)=CH_2$ | (9.03±0.01) | (188) | (787) | −20.0±0.3 | −83.8±1.4 | 77PED/RYL | 2213-32-3 |
| $(CH_3)_3CC(CH_3)=CH_2$ | (9.02±0.01) | (187.5) | (784.4) | −20.4±0.3 | −85.5±1.4 | 77PED/RYL | 594-56-9 |
| (Z)-$(CH_3)_2CHCH_2CH=CHCH_3$ | (8.92±0.01) | (187) | (782) | −19 | −78 | *EST | 13151-17-2 |
| (E)-$(CH_3)_2CHCH_2CH=CHCH_3$ | (8.92±0.01) | (186) | (779) | −20 | −82 | *EST | 7385-82-2 |
| (E)-$C_2H_5CH(CH_3)CH=CHCH_3$ | (8.91±0.01) | (186) | (778) | −20 | −82 | *EST | 3683-22-5 |
| $C_3H_7CH=C(CH_3)_2$ | (8.62) | (179) | (748) | −20 | −84 | *EST | 2738-19-4 |
| | IP from 81HOL/FIN. | | | | | | |

**Table 1. Positive Ion Table - Continued**

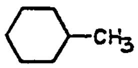
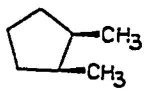
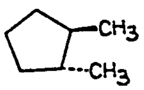
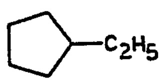
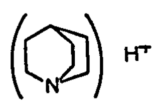
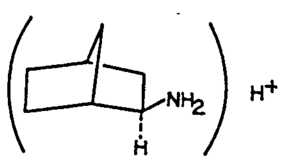
| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_{14}^+$ | | | | | | | |
| $C_2H_5C(CH_3)=C(CH_3)_2$ | (8.21±0.01) | (168) | (702) | −21 | −90 | •EST | 10574-37-5 |
| (Z)-$(CH_3)_3CCH=CHCH_3$ | (8.92±0.01) | (188) | (788) | −17.4±0.3 | −72.6±1.4 | 77PED/RYL | 762-63-0 |
| (E)-$(CH_3)_3CCH=CHCH_3$ | (8.91±0.01) | (184) | (771) | −21.3±0.3 | −88.8±1.1 | 77PED/RYL | 690-08-4 |
|  | 9.97 | 202 | 844 | −28.3±0.1 | −118.2±0.6 | 77PED/RYL | 291-64-5 |
| | 300 K ionization energy from charge transfer equilibrium constants relative to cyclohexane and cyclohexane-$d_{12}$ = 9.99 eV. (82SIE/MAU). | | | | | | |
|  | 9.64 | 185 | 775 | −37.0±0.2 | −154.7±1.0 | 77PED/RYL | 108-87-2 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU; 82LIA). Reference IP's, fluorobenzenes. Threshold determination gives IP = 9.76±0.03 eV. | | | | | | |
|  | (9.92±0.05) | (198) | (828) | −30.9±0.3 | −129.5±1.3 | 77PED/RYL | 1192-18-3 |
| | IP from 81HER/SIC. | | | | | | |
|  | (9.95±0.05) | (197) | (823) | −32.7±0.3 | −136.7±1.1 | 77PED/RYL | 822-50-4 |
| | IP from 81HER/SIC. | | | | | | |
|  | (10.12±0.02) | (203) | (850) | −30.3±0.2 | −126.7±0.9 | 77PED/RYL | 1640-89-7 |
| $C_7H_{14}N^+$ | | | | | | | |
|  | | 132 | 551 | | | | |
| | From proton affinity of 1-azabicyclo[2.2.2]octane (RN 100-76-5). (86TAF/GAL). PA = 233.1 kcal/mol, 975. kJ/mol. | | | | | | |
|  | | 137 | 574 | | | | |
| | From proton affinity of bicyclo[2.2.1]heptan-2-amine,endo (RN 31002-73-0). PA = (221.7) kcal/mol, (927.) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

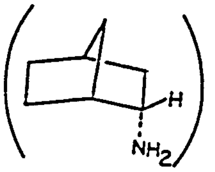
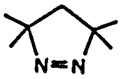
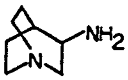
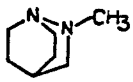
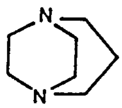
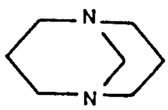
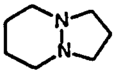
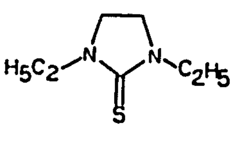
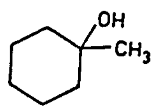
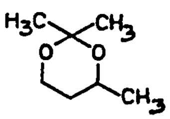
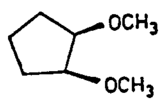
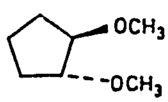
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_7H_{14}N^+$ | | | | | | | |
|  H+ | | 136 | 570 | | | | |
| | From proton affinity of bicyclo[2.2.1]heptan-2-amine,exo (RN 7242-92-4). PA = (221.7) kcal/mol, (927.) kJ/mol. | | | | | | |
| $C_7H_{14}N_2^{+\cdot}$ | | | | | | | |
|  | (≤8.63) | (≤208) | (≤872) | 9.4±0.8 | 39.3±3.6 | 80ENG | 2721-31-5 |
|  | (≤8.0) | (≤188) | (≤785) | 4 | 17 | *EST | 6238-14-8 |
| | IP from 79AUE/BOW. | | | | | | |
|  | ≤8.02 | (≤215) | (≤898) | 30 | 124 | *EST | 6523-29-1 |
| | IP from 82LEV/LIA. See also: 84NEL. | | | | | | |
|  | ≤7.43 | (≤192) | (≤802) | 20 | 85 | *EST | 283-47-6 |
|  | ≤7.75 | (≤191) | (≤800) | 12 | 52 | *EST | 281-17-4 |
|  | (7.63) | (204) | (853) | 28 | 117 | *EST | 5721-43-7 |
| | IP from 82LEV/LIA. See also: 84NEL. | | | | | | |
| $C_7H_{14}N_2S^+$ | | | | | | | |
|  | (7.5) | (177) | (742) | 4 | 18 | *EST | 30826-80-3 |
| | IP is onset of photoelectron band (80AND/DEV). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{14}O^+$ | | | | | | | |
| n-$C_6H_{13}$CHO | (9.65±0.02) | (159) | (667) | −63±1 | −264±4 | 77PED/RYL | 111-71-7 |
| $(CH_3)_2CHCH(C_2H_5)CHO$ | (9.44) | (149) | (624) | −69 | −287 | *EST | 26254-92-2 |
| | IP from 81HOL/FIN. | | | | | | |
| n-$C_5H_{11}COCH_3$ | 9.30±0.01 | 142 | 596 | −72 | −301 | 75TRC | 110-43-0 |
| n-$C_4H_9COC_2H_5$ | (9.22±0.04) | (141) | (590) | −71 | −299 | 75TRC | 106-35-4 |
| | IP is average of values from 81HOL/FIN, 86TRA/MCA. | | | | | | |
| (n-$C_3H_7)_2$CO | 9.10±0.04 | 138 | 578 | −72 | −300 | 75TRC | 123-19-3 |
| $(CH_3)_2CHCH_2CH_2COCH_3$ | (9.28±0.01) | (140) | (587) | −74 | −308 | *EST | 110-12-3 |
| $CH_3(CH_2)_2CH(CH_3)COCH_3$ | (9.20±0.02) | (139) | (581) | −73 | −307 | *EST | 2550-21-2 |
| | IP is average of values from 81HOL/FIN, 86TRA/MCA. | | | | | | |
| neo-$C_5H_{11}COCH_3$ | (9.23±0.01) | (137) | (571) | −76 | −319 | *EST | 590-50-1 |
| $C_2H_5C(CH_3)_2COCH_3$ | (9.02±0.01) | (133) | (555) | −75 | −315 | *EST | 20669-04-9 |
| (iso-$C_3H_7)_2$CO | 8.95±0.01 | 132 | 552 | −74.4±0.3 | −311.3±1.1 | 77PED/RYL | 565-80-0 |
|  | (9.8±0.2) | (140) | (588) | −86 | −358 | 85WIB/WAS | 590-67-0 |
| $C_7H_{14}O_2^+$ | | | | | | | |
|  | ≤9.63 | ≤111 | ≤463 | −111 | −466 | 77PED/RYL | 696-79-7 |
| | IP from 84ASF/ZYK. | | | | | | |
|  | (8.6) | (113) | (472) | −86 | −358 | *EST | 61011-51-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.7) | (115) | (481) | −86 | −358 | *EST | 29887-56-7 |
| | IP is onset of photoelectron band. | | | | | | |

## Table 1. Positive Ion Table - Continued

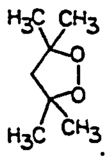
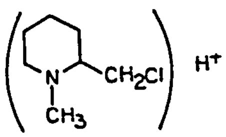
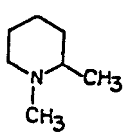
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{14}O_2{}^+$ | | | | | | | |
|  | 8.9 | (139) | (583) | −66 | −276 | *EST | 22431-90-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_{15}{}^+$ | | | | | | | |
| 1-$C_7H_{15}$ | | (183) | (766) | 4 | 15 | *EST | |
| | From appearance potential measurements (82MAC). $\Delta_f H$(Neutral) based on D[C-H] = 100.5 kcal/mol. | | | | | | |
| 2-$C_7H_{15}$ | (6.95) | (162) | (678) | 2 | 8 | *EST | |
| | From appearance potential measurements (82MAC). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). $\Delta_f H$(Neutral) based on D[C-H] = 99 kcal/mol. | | | | | | |
| $(CH_3)_2CCH_2CH_2CH_2CH_3$ | | 147 | 615 | | | | 40626-78-6 |
| | From appearance potential measurement (84LOS/HOL). | | | | | | |
| $(CH_3)_2CCH_2CH(CH_3)_2$ | | 148.4 | 620.9 | | | | 35443-14-2 |
| | From hydride transfer equilibrium constant determinations relative to $\Delta_f H$(tert-$C_4H_9{}^+$) (76MAU/SOL). | | | | | | |
| $(C_2H_5)_3C$ | | 150.6 | 630.1 | | | | 28013-53-8 |
| | From hydride transfer equilibrium constant determinations relative to $\Delta_f H$(tert-$C_4H_9{}^+$) (76MAU/SOL). | | | | | | |
| $(CH_3)_3CC(CH_3)_2$ | | 144.5 | 604.5 | | | | 24436-96-2 |
| | From hydride transfer equilibrium constant determinations relative to $\Delta_f H$(tert-$C_4H_9{}^+$) (76MAU/SOL). | | | | | | |
| $C_7H_{15}ClN^+$ | | | | | | | |
|  | | (115) | (481) | | | | |
| | From proton affinity of Pyrrolidine, 2-chloromethyl-1-methyl- (RN 49665-74-9). PA = (227.6) kcal/mol, (952.) kJ/mol. | | | | | | |
| $C_7H_{15}N^+$ | | | | | | | |
| (E)-$C_2H_5C(N(CH_3)_2)=CHCH_3$ | (≤7.61) | (≤173) | (≤724) | −2 | −10 | *EST | 32317-47-8 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | (7.63) | (157) | (658) | −19 | −78 | *EST | 671-36-3 |
| | IP from 82ROZ/HOU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

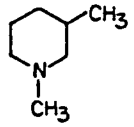
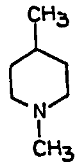
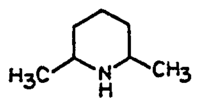
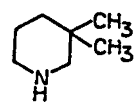
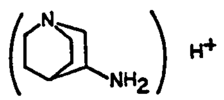
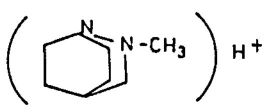
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{15}N^+$ | | | | | | | |
|  | (7.76) | (160) | (669) | −19 | −80 | *EST | 695-35-2 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (7.79) | (161) | (672) | −19 | −80 | *EST | 695-15-8 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (7.93) | (155) | (648) | −28 | −117 | *EST | 766-17-6 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (8.05) | (160) | (670) | −26 | −107 | *EST | 1193-12-0 |
| | IP from 82ROZ/HOU. | | | | | | |
| $C_7H_{15}N_2^+$ | | | | | | | |
|  | | 138 | 577 | | | | |
| | From proton affinity of 3-amino-1-azabicyclo[2.2.2]octane (RN 6238-14-8). PA = (231.8) kcal/mol, (970) kJ/mol. | | | | | | |
|  | | 165 | 690 | | | | |
| | From proton affinity of 2-methyl-1,2-diazabicyclo[2.2.2]octane (RN 6523-29-1). (84MAU/NEL). PA = 230.4 kcal/mol, 964. kJ/mol. | | | | | | |
| $C_7H_{15}O^+$ | | | | | | | |
| $(i\text{-}C_3H_7)_2COH$ | | 87 | 363 | | | | |
| | From proton affinity of $(i\text{-}C_3H_7)_2CO$ (RN 565-80-0). PA = 204.9 kcal/mol, 857. kJ/mol. | | | | | | |
| $C_7H_{16}^+$ | | | | | | | |
| $n\text{-}C_7H_{16}$ | 9.92±0.05 | 184 | 770 | −44.8±0.1 | −187.5±0.5 | 74SCO | 142-82-5 |
| | | *194* | *811* | *−34.8±0.1* | *−145.7±0.5* | | |
| | This value of IP from charge transfer equilibrium constant determinations (76LIA/AUS, 82LIA). | | | | | | |

Table 1. Positive Ion Table - Continued

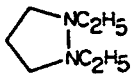
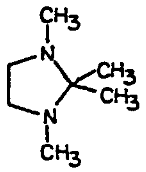
| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_7H_{16}N^+$** | | | | | | | |
| $(CH_3)_2NC(C_2H_5)_2$ | | 127 | 531 | | | | |
| | From proton affinity of (E)-$(CH_3)_2NC(C_2H_5)=CHCH_3$ (RN 78733-73-0). PA = 236.4 kcal/mol, 989. kJ/mol. | | | | | | |
| **$C_7H_{16}N_2^{+\cdot}$** | | | | | | | |
|  | (6.83) | (170) | (710) | 12 | 51 | *EST | 49840-60-0 |
| | IP from 86RUM. See also: 84NEL. | | | | | | |
|  | (≤8.06) | (≤198) | (≤828) | 12 | 50 | *EST | 22825-58-7 |
| | See also: 84NEL. | | | | | | |
|  | (7.2) | (196) | (822) | 30 | 127 | *EST | 33709-65-8 |
| | IP is onset of photoelectron band (82WOR/HAR). | | | | | | |
| **$C_7H_{16}O^+$** | | | | | | | |
| $n-C_7H_{15}OH$ | (9.84±0.03) | (147) | (614) | −80.2±0.4 | −335.5±1.5 | 77PED/RYL | 111-70-6 |
| | IP from 77ASH/BUR. | | | | | | |
| $CH_3(CH_2)_4CHOHCH_3$ | (9.70±0.03) | (139) | (582) | −85 | −354 | 84WIB/WAS | 543-49-7 |
| | IP from 77ASH/BUR. | | | | | | |
| $CH_3(CH_2)_3CHOHCH_2CH_3$ | 9.68±0.03 | 139 | 580 | −85 | −354 | 84WIB/WAS | 589-82-2 |
| | IP from 77ASH/BUR. | | | | | | |
| $CH_3(CH_2)_2CHOH(CH_2)_2CH_3$ | (9.61±0.03) | (137) | (573) | −85 | −354 | 84WIB/WAS | 589-55-9 |
| | IP from 77ASH/BUR. | | | | | | |
| $n-C_5H_{11}OC_2H_5$ | (≤9.49) | (≤144) | (≤602) | −75 | −314 | *EST | 17952-11-3 |
| | IP from 80BAC/MOU. | | | | | | |
| $(i-C_3H_7)O(t-C_4H_9)$ | (≤9.20) | (≤131) | (≤548) | −81 | −339 | *EST | 17348-59-3 |
| | IP from 79AUE/BOW. Authors suggest that adiabatic IP is lower than cited vertical value by 25-29 kJ/mol, 6-7 kcal/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_7H_{16}O_2^+$** | | | | | | | |
| n-$C_7H_{15}$OOH | (9.48±0.03) | (150) | (626) | −69 | −289 | *EST | 764-81-8 |
| | IP from 77ASH/BUR. | | | | | | |
| n-$C_5H_{11}$CH($CH_3$)OOH | (9.30±0.03) | (148) | (621) | −66 | −276 | *EST | 762-46-9 |
| | IP from 77ASH/BUR. | | | | | | |
| **$C_7H_{17}N^+$** | | | | | | | |
| ($C_2H_5$)$_2$(n-$C_3H_7$)N | (7.67) | (150) | (626) | −27 | −114 | *EST | 4458-31-5 |
| | IP from 79AUE/BOW. Ion heat of formation predicted from hydrogen affinities of tertiary amine ions: 146 kcal/mol, 611 kJ/mol, corresponding to IP of 7.50 eV. | | | | | | |
| **$C_7H_{17}O^+$** | | | | | | | |
| (i-$C_3H_7$)OH(t-$C_4H_9$) | | (76) | (317) | | | | |
| | From proton affinity of (i-$C_3H_7$)O(t-$C_4H_9$) (RN 17348-59-3). PA = (208.8) kcal/mol, (874.) kJ/mol. | | | | | | |
| **$C_7H_{17}O_2^+$** | | | | | | | |
| $CH_3$OH($CH_2$)$_5$O$CH_3$ | | 40 | 167 | | | | |
| | From proton affinity of $CH_3$O($CH_2$)$_5$O$CH_3$ (RN 111-89-7). PA = 221.8 kcal/mol, 928. kJ/mol. | | | | | | |
| **$C_7H_{18}N^+$** | | | | | | | |
| n-$C_7H_{15}NH_3$ | | 111 | 463 | | | | |
| | From proton affinity of n-$C_7H_{15}NH_2$ (RN 111-68-2). PA = 219.0 kcal/mol, 916. kJ/mol. | | | | | | |
| ($CH_3$)$_2$(neo-$C_5H_{11}$)NH | | 108 | 450 | | | | |
| | From proton affinity of ($CH_3$)$_2$(neo-$C_5H_{11}$)N (RN 10076-31-0). PA = 229.9 kcal/mol, 962. kJ/mol. | | | | | | |
| ($C_2H_5$)$_2$(n-$C_3H_7$)NH | | (106) | (445) | | | | |
| | From proton affinity of ($C_2H_5$)$_2$(n-$C_3H_7$)N (RN 4458-31-5). PA = (232.0) kcal/mol, (971.) kJ/mol. | | | | | | |
| **$C_7H_{18}N_2^+$** | | | | | | | |
| ($CH_3$)$_2$N($CH_2$)$_3$N($CH_3$)$_2$ | (7.6) | (168) | (704) | −7 | −29 | *EST | 110-95-2 |
| | IP is onset of photoelectron spectrum (81LIV/ROB). | | | | | | |
| ($C_2H_5$)$_2$NN($CH_3$)($C_2H_5$) | (8.02) | (189) | (791) | 4 | 17 | *EST | 50599-43-4 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL, 79NEL/KES. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{18}N_2^+$ | | | | | | | |
| $(n\text{-}C_4H_9)(CH_3)NN(CH_3)_2$ | (6.63) | (156) | (652) | 3 | 12 | *EST | 52598-10-4 |
| | IP from charge transfer equilibrium constant determination (84MAU/NEL). See also: 80NEL/KES, 84NEL. | | | | | | |
| $(t\text{-}C_4H_9)(CH_3)NN(CH_3)_2$ | (6.80) | (159) | (667) | 3 | 11 | *EST | 60678-73-1 |
| | IP from charge transfer equilibrium constant determination (84MAU/NEL). | | | | | | |
| $C_7H_{18}Si^+$ | | | | | | | |
| $(CH_3)_3CSi(CH_3)_3$ | (9.34±0.06) | (170) | (713) | −45 | −188 | 72TRI/ALL | 5037-65-0 |
| $C_7H_{18}Si_2^+$ | | | | | | | |
| $CH_2{=}CHSi(CH_3)_2Si(CH_3)_3$ | (≤8.56) | (≤138) | (≤577) | −60 | −249 | *EST | 1112-06-7 |
| | IP from 81KHV/ZYK. | | | | | | |
| $C_7H_{18}Sn^+$ | | | | | | | |
| $(C_2H_5)_3(CH_3)Sn$ | (≤8.95) | (≤152) | (≤638) | −54±1 | −226±4 | 80TEL/RAB | 2097-60-1 |
| $(CH_3)_3(tert\text{-}C_4H_9)Sn$ | (8.0) | (168) | (705) | −16±1 | −67±6 | 77PED/RYL | 3531-47-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_7H_{19}NSi^+$ | | | | | | | |
| $(CH_3)_3SiN(C_2H_5)_2$ | (7.68) | (97) | (406) | −80±2 | −335±8 | 80TEL/RAB | 996-50-9 |
| | IP from 83MOL/PIK3. | | | | | | |
| $C_7H_{19}N_2^+$ | | | | | | | |
| $H_3N(CH_2)_7NH_2$ | | 100 | 419 | | | | |
| | From proton affinity of $H_2N(CH_2)_7NH_2$ (RN 646-19-5). PA = 238. kcal/mol, 996. kJ/mol. | | | | | | |
| $(CH_3)_2NH(CH_2)_3N(CH_3)_2$ | | 116 | 484 | | | | |
| | From proton affinity of $(CH_3)_2N(CH_2)_3N(CH_3)_2$ (RN 110-95-2). PA = 243. kcal/mol, 1017. kJ/mol. | | | | | | |
| $(n\text{-}C_4H_9)(CH_3)NHN(CH_3)_2$ | | 139 | 580 | | | | |
| | From proton affinity of $(n\text{-}C_4H_9)(CH_3)NN(CH_3)_2$ (RN 52598-10-4). (84MAU/NEL). PA = 230.0 kcal/mol, 962. kJ/mol. | | | | | | |
| $(t\text{-}C_4H_9(CH_3)NHN(CH_3)_2$ | | 139 | 582 | | | | |
| | From proton affinity of $(t\text{-}C_4H_9)(CH_3)NN(CH_3)_2$ (RN 60678-73-1). (84MAU/NEL). PA = 229.3 kcal/mol, 959. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

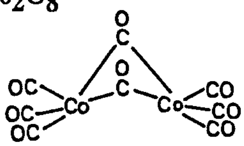
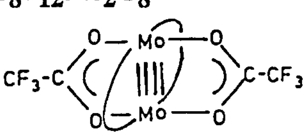
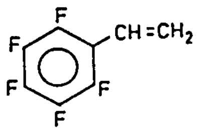
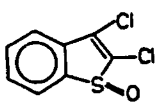
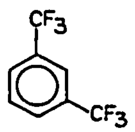
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_7H_{20}NSi^+$ | | | | | | | |
| $(CH_3)_3Si(CH_2)_2NH(CH_3)_2$ | | 79 | 332 | | | | |
| | From proton affinity of $(CH_3)_3Si(CH_2)_2N(CH_3)_2$ (RN 23138-94-5). (84MAU/NEL).<br>PA = 231.8 kcal/mol, 970. kJ/mol. | | | | | | |
| $C_8Co_2O_8^+$ | | | | | | | |
|  | (8.12±0.22) | (−96) | (−402) | −283±2 | −1185±8 | 82PIL/SKI | 10210-68-1 |
| $C_8F_{12}Mo_2O_8^+$ | | | | | | | |
|  | 8.07 | (−818) | (−3421) | −1004 | −4200 | *EST | 36608-07-8 |
| | IP is onset of photoelectron band (82BAN/PEL). | | | | | | |
| $C_8F_{18}O^+$ | | | | | | | |
| $(n\text{-}C_4F_9)_2O$ | 12.68 | −658.5 | −2755.2 | −950.9±1 | −3978.6±3 | 77PED/RYL | 308-48-5 |
| | IP from 83MOL/PIK. | | | | | | |
| $C_8H_2^+$ | | | | | | | |
| CH≡CC≡CC≡CC≡CH | (9.09±0.02) | (416) | (1741) | 207 | 864 | *EST | 6165-96-4 |
| $C_8H_3F_5^+$ | | | | | | | |
|  | (9.18±0.02) | (35) | (145) | −177 | −741 | *EST | 653-34-9 |
| $C_8H_4Cl_2OS^+$ | | | | | | | |
|  | ≤9.00 | (≤205) | (≤857) | −3 | −11 | *EST | 30834-33-4 |
| | IP from 82BEN/DUR. | | | | | | |
| $C_8H_4F_6^+$ | | | | | | | |
|  | 10.57 | (−61) | (−255) | −305 | −1275 | *EST | 402-31-3 |
| | IP from 82CAB/COW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

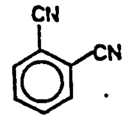
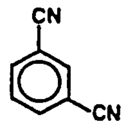
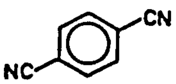
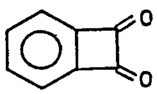
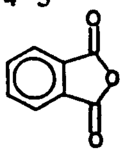
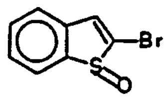
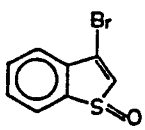
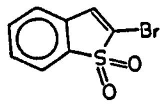
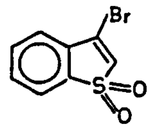
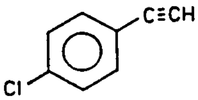
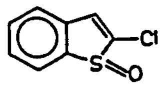
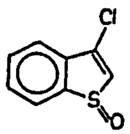
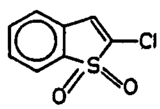
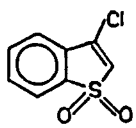
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_4N_2{}^+$ | | | | | | | |
|  | 9.9<br>IP is onset of photoelectron band. | (316) | (1323) | 88±0.5 | 368±2 | 80SAT/SAK | 91-15-6 |
|  | 10.2<br>IP is onset of photoelectron band. | (322) | (1347) | 87±0.5 | 363±2 | 80SAT/SAK | 626-17-5 |
|  | 10.10 | 318 | 1331 | 85±0.5 | 357±2 | 80SAT/SAK | 623-26-7 |
| $C_8H_4O_2{}^+$ | | | | | | | |
|  | ≤9.23 | (≤237) | (≤992) | 24 | 101 | *EST | 6383-11-5 |
| $C_8H_4O_3{}^+$ | | | | | | | |
|  | (10.0)<br>IP is onset of photoelectron band. | (142) | (594) | −89±0.5 | −371±2 | 77PED/RYL | 85-44-9 |
| $C_8H_5BrOS^+$ | | | | | | | |
|  | ≤9.10<br>IP from 82BEN/DUR. | (≤225) | (≤941) | 15 | 63 | *EST | 57147-27-0 |
|  | ≤8.95<br>IP from 82BEN/DUR. | (≤221) | (≤927) | 15 | 63 | *EST | 57147-26-9 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_5BrO_2S^+$ | | | | | | | |
|  | ≤9.10<br>IP from 82BEN/DUR. | (≤171) | (≤715) | −39 | −163 | *EST | 5350-05-0 |
|  | ≤9.40<br>IP from 82BEN/DUR. | (≤178) | (≤744) | −39 | −163 | *EST | 16957-97-4 |
| $C_8H_5Cl^+$ | | | | | | | |
|  | (8.6)<br>IP is onset of photoelectron band. | (264) | (1104) | 65 | 274 | *EST | 873-73-4 |
| $C_8H_5ClOS^+$ | | | | | | | |
|  | ≤9.10<br>IP from 82BEN/DUR. | (≤212) | (≤888) | 2 | 10 | *EST | 57147-28-1 |
|  | ≤8.95<br>IP from 82BEN/DUR. | (≤209) | (≤874) | 2 | 10 | *EST | 63724-95-8 |
| $C_8H_5ClO_2S^+$ | | | | | | | |
|  | ≤9.25<br>IP from 82BEN/DUR. | (≤162) | (≤676) | −52 | −216 | *EST | 10133-41-2 |
|  | ≤9.45<br>IP from 82BEN/DUR. | (≤166) | (≤696) | −52 | −216 | *EST | 21211-29-0 |

## Table 1. Positive Ion Table - Continued

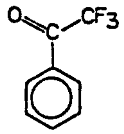
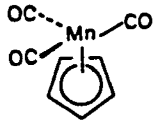
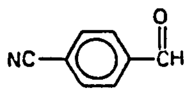
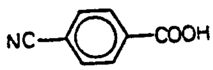
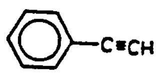
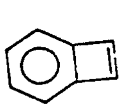
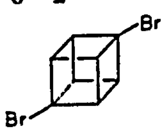
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_5F_3O^+$ | | | | | | | |
|  | (9.72) | (61) | (256) | −163 | −682 | *EST | 434-45-7 |
| | IP from 79MCL/TRA. | | | | | | |
| $C_8H_5MnO_3^{+\cdot}$ | | | | | | | |
|  | (7.6) | (61) | (257) | −114±2 | −476±8 | 77PED/RYL | 12079-65-1 |
| | IP is onset of photoelectron band (81CAL/HUB). See also: 86LIC/KEL. | | | | | | |
| $C_8H_5NO^+$ | | | | | | | |
|  | ≤10.10 | (≤258) | (≤1081) | 25 | 107 | *EST | 105-07-7 |
| | IP from 85GAL/GER. | | | | | | |
| $C_8H_5NO_2^+$ | | | | | | | |
|  | (10.0) | (193) | (807) | −38 | −158 | *EST | 619-65-8 |
| | IP from 84TOB/TAJ. | | | | | | |
| $C_8H_6^+$ | | | | | | | |
| (E),(E)-HC≡CCH=CHCH=CHC≡CH | (7.8) | (278) | (1161) | 98 | 409 | *EST | 53477-04-6 |
| | IP from 74KOP/SCH. | | | | | | |
|  | 8.81±0.04 | 276 | 1156 | 73±0.5 | 306±2 | 85DAV/ALL | 536-74-3 |
| | See also: 80BOC/AYG, 74KOP/SCH, 81ELB/LIE. | | | | | | |
|  | (≤7.5) | (≤291) | (≤1218) | 118 | 494 | 85DEW/MER | 4026-23-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_6Br_2^+$ | | | | | | | |
|  | (9.0) | (358) | (1496) | 150 | 628 | *EST | 59346-70-2 |
| | IP is onset of photoelectron band (85HON/HEI). | | | | | | |

Table 1. Positive Ion Table - Continued

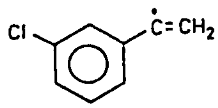
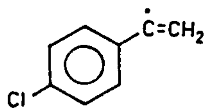
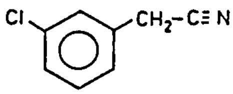
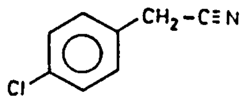
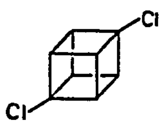
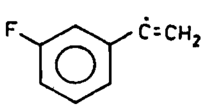
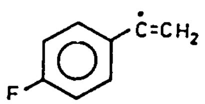
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_6Cl^+$ | | | | | | | |
|  | | 235 | 984 | | | | |
| | From proton affinity of 3-$ClC_6H_4C{\equiv}CH$ (RN 766-83-6). (85MAR/MOD).<br>PA = 196.1 kcal/mol, 820. kJ/mol. | | | | | | |
|  | | 232 | 970 | | | | |
| | From proton affinity of 4-$ClC_6H_4C{\equiv}CH$ (RN 873-73-4). (85MAR/MOD).<br>PA = 199.4 kcal/mol, 834. kJ/mol. | | | | | | |
| $C_8H_6ClN^+$ | | | | | | | |
|  | (9.48±0.05) | (256) | (1071) | 37 | 156 | *EST | |
|  | (9.43±0.05) | (255) | (1066) | 37 | 156 | *EST | |
| $C_8H_6Cl_2^+$ | | | | | | | |
|  | (9.15) | (337) | (1411) | 126 | 528 | *EST | |
| | IP is onset of photoelectron band (85HON/HEI). | | | | | | |
| $C_8H_6F^+$ | | | | | | | |
|  | | 196 | 819 | | | | |
| | From proton affinity of 3-$FC_6H_4C{\equiv}CH$ (RN 2561-17-3). (85MAR/MOD).<br>PA = 195.4 kcal/mol, 818. kJ/mol. | | | | | | |
|  | | 190 | 797 | | | | |
| | From proton affinity of 4-$FC_6H_4C{\equiv}CH$ (RN 766-98-3). (85MAR/MOD).<br>PA = 200.8 kcal/mol, 840. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

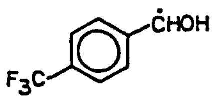
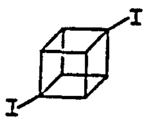
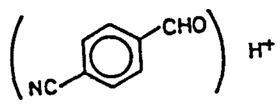
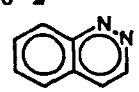
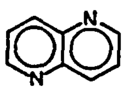
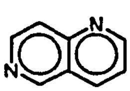
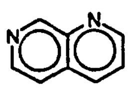
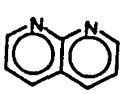
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_6F_3O^+$ | | | | | | | |
|  | | 2 | 10 | | | | |
| | From proton affinity of 4-$CF_3C_6H_4$CHO (RN 455-19-6). PA = 191.9 kcal/mol, 799. kJ/mol. | | | | | | |
| $C_8H_6I_2^+$ | | | | | | | |
|  | (8.7) | (379) | (1587) | 179 | 748 | *EST | |
| | IP is onset of photoelectron band (85HON/HEI). | | | | | | |
| $C_8H_6NO^+$ | | | | | | | |
|  | | 204 | 855 | | | | |
| | From proton affinity of 4-(CN)$C_6H_4$CHO (RN 105-07-7). PA = 187.0 kcal/mol, 782. kJ/mol. | | | | | | |
| $C_8H_6N_2^+$ | | | | | | | |
|  | (8.2) | (270) | (1129) | 81±2 | 338±10 | *EST | 253-66-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.8) | (267) | (1116) | 64 | 267 | *EST | 254-79-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.0) | (271) | (1135) | 64 | 267 | *EST | 253-72-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.99) | (271) | (1134) | 64 | 267 | *EST | 253-69-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.8) | (267) | (1116) | 64 | 267 | *EST | 254-60-4 |

**Table 1. Positive Ion Table - Continued**

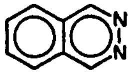
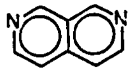
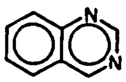
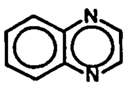
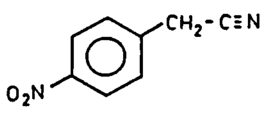
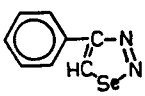
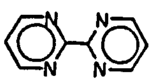
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_6N_2^+$ | | | | | | | |
|  | (8.4) | (274) | (1148) | 81 | 338 | *EST | 253-52-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.8) | (267) | (1116) | 64 | 267 | *EST | 253-50-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.8) | (267) | (1116) | 64 | 267 | *EST | 253-45-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 9.00±0.02 | (269) | (1125) | 61 | 257 | *EST | 253-82-7 |
|  | 9.01±0.02 | 271 | 1131 | 63±1 | 262±4 | 81STE/BAR | 91-19-0 |
| $C_8H_6N_2O_2^+$ | | | | | | | |
|  | (10.11±0.04) | (274) | (1146) | 41±1 | 171±4 | *EST | 555-21-5 |
| $C_8H_6N_2Se^+$ | | | | | | | |
|  | (8.1) | (295) | (1234) | 108.1±2 | 452.3±8 | 73ARS/SHA | 25660-64-4 |
| | IP is onset of photoelectron band (80BOC/AYG). | | | | | | |
| $C_8H_6N_4^+$ | | | | | | | |
|  | (8.3) | (293) | (1227) | 102 | 426 | *EST | 34671-83-5 |
| | IP is onset of photoelectron band (82BAR/CAU). | | | | | | |

Table 1. Positive Ion Table - Continued

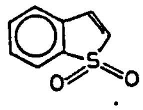
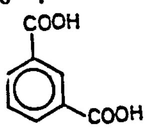
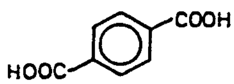
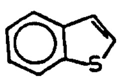
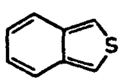
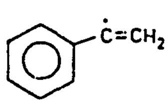
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_6O_2S^+$ | | | | | | | |
|  | (9.1) | (166) | (694) | −44 | −184 | *EST | 825-44-5 |
| | IP is onset of photoelectron band (82BEN/DUR). | | | | | | |
| $C_8H_6O_4^+$ | | | | | | | |
|  | (9.98±0.2) | (64) | (267) | −166±0.5 | −696±2 | 77PED/RYL | 121-91-5 |
|  | (9.86±0.2) | (55) | (233) | −172±0.7 | −718±3 | 77PED/RYL | 100-21-0 |
| $C_8H_6S^+$ | | | | | | | |
|  | 8.13±0.015 | 227 | 950 | 40±0.2 | 166±1 | 79SAB | 95-15-8 |
|  | (7.75) | (228) | (954) | 49 | 206 | *EST | 270-82-6 |
| $C_8H_6S_2^+$ | | | | | | | |
|  | (7.99) | (243) | (1017) | 59 | 246 | *EST | 3172-56-3 |
| $C_8H_7^+$ | | | | | | | |
|  | | 239 | 998 | | | | |
| | From proton affinity of $C_6H_5C{\equiv}CH$ (RN 536-74-3). (85MAR/MOD).<br>PA = 200.2 kcal/mol, 838. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

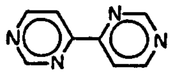
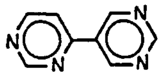
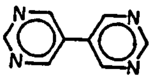
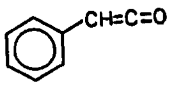
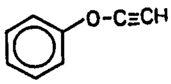
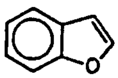
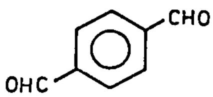
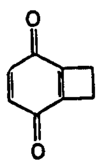
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_6N_4^+$ | | | | | | | |
|  | (9.0) | (309) | (1294) | 102 | 426 | *EST | 2426-94-0 |
| | IP is onset of photoelectron band (82BAR/CAU). | | | | | | |
|  | (9.0) | (306) | (1278) | 98 | 410 | *EST | 28648-89-7 |
| | IP is onset of photoelectron band (82BAR/CAU). | | | | | | |
|  | (9.0) | (306) | (1278) | 98 | 410 | *EST | 56598-46-0 |
| | IP is onset of photoelectron band (82BAR/CAU). | | | | | | |
| $C_8H_6O^+$ | | | | | | | |
|  | (≤8.17) | (≤194) | (≤813) | 6 | 25 | 80DEM/WUL | 3496-32-0 |
|  | (8.7) | (266) | (1113) | 65 | 274 | *EST | 4279-76-9 |
|  | 8.37±0.015 | 199 | 833 | 6±2 | 26±10 | 77PED/RYL | 271-89-6 |
| $C_8H_6O_2^+$ | | | | | | | |
|  | (10.13±0.01) | (196) | (820) | −37.6±2 | −157±8 | *EST | 623-27-8 |
|  | (9.64) | (222) | (927) | −1 | −3 | *EST | 77627-49-7 |
| | IP is onset of photoelectron band (85GLE/JAH). | | | | | | |

**Table 1. Positive Ion Table - Continued**

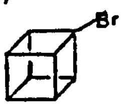
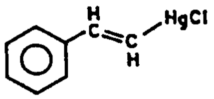
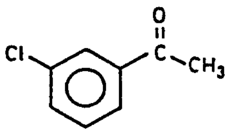
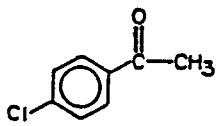
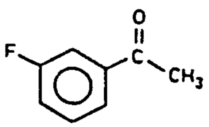
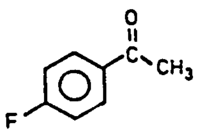
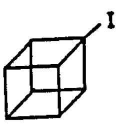
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_7Br^+$ | | | | | | | |
|  | (8.76) | (351) | (1470) | 149 | 625 | *EST | 59346-69-9<br>Duplicated see p 334 |
| | IP is onset of photoelectron band (85HON/HEI, 84ABE/DEL). | | | | | | |
| $C_8H_7ClHg^+$ | | | | | | | |
|  | 8.3 | (232) | (971) | 41 | 170 | *EST | 36525-03-8 |
| | IP is onset of photoelectron band (81BAI/CHI). | | | | | | |
| $C_8H_7ClO^+$ | | | | | | | |
|  | (9.51±0.1) | (191) | (801) | −28±2 | −117±8 | *EST | 99-02-5 |
|  | (8.9) | (177) | (742) | −28±2 | −117±8 | *EST | 99-91-2 |
| | IP is onset of photoelectron band. See also: 85GAL/GER, 82PFI/GER, 77ROS/DRA. | | | | | | |
| $C_8H_7FO^+$ | | | | | | | |
|  | (9.76±0.1) | (158) | (662) | −67±2 | −280±8 | *EST | 455-36-7 |
|  | (9.57±0.2) | (154) | (643) | −67±2 | −280±8 | *EST | 403-42-9 |
| $C_8H_7I^+$ | | | | | | | |
|  | (8.6) | (362) | (1515) | 164 | 685 | *EST | 74725-77-2 |
| | IP is onset of photoelectron band (84ABE/DEL). | | | | | | |

**Table 1. Positive Ion Table - Continued**

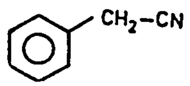
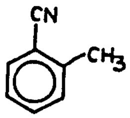
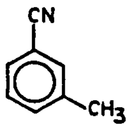
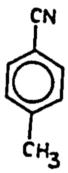
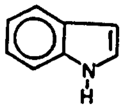
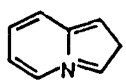
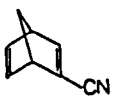
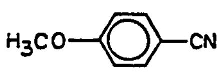
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_7N^+$ | | | | | | | |
|  | (9.34) | (260) | (1087) | 44.5 | 186 | •EST | 140-29-4 |
|  | 9.38 | (259) | (1083) | 43 | 178 | •EST | 529-19-1 |
|  | 9.34 | (259) | (1084) | 44 | 183 | •EST | 620-22-4 |
|  | 9.32 | (258) | (1081) | 44 | 182 | •EST | 104-85-8 |
|  | 7.761±0.001 | 216 | 906 | 38±1 | 157±5 | 77PED/RYL | 120-72-9 |
| | IP from 85HAG/IVA. See also: 79COR. | | | | | | |
|  | 7.26 | 243 | 1015 | 75.2 | 314.6 | 79COR | 274-40-8 |
|  | (≤9.26) | (≤302) | (≤1265) | 89 | 372 | •EST | 39863-20-2 |
| | IP from 83HOU/RON. | | | | | | |
| $C_8H_7NO^+$ | | | | | | | |
|  | (8.6) | (213) | (892) | 15 | 62 | •EST | 874-90-8 |
| | IP is onset of photoelectron band (81MOD/DIS). | | | | | | |

Table 1. Positive Ion Table - Continued

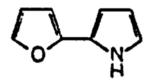
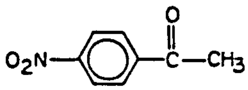
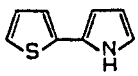
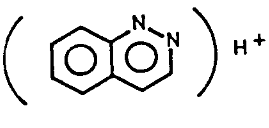
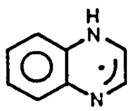
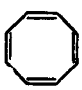
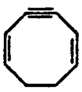
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_7NO^+$ | | | | | | | |
|  | (6.95) | (182) | (760) | 21 | 89 | *EST | 63122-43-0 |
| | IP is onset of photoelectron band (81GAL/KLA). | | | | | | |
| $C_8H_7NO_3^+$ | | | | | | | |
|  | ≤9.98 | (≤206) | (≤861) | -24 | -102 | *EST | 100-19-6 |
| | IP from 85GAL/GER. | | | | | | |
| $C_8H_7NS^+$ | | | | | | | |
|  | (7.1) | (221) | (924) | 57 | 239 | *EST | 52707-46-7 |
| | IP is onset of photoelectron band (81GAL/KLA). | | | | | | |
| $C_8H_7N_2^+$ | | | | | | | |
|  | | (223) | (934) | | | | |
| | From proton affinity of cinnoline (RN 253-66-7). PA = 223.2 kcal/mol, 934. kJ/mol. | | | | | | |
|  | | (214) | (895) | | | | |
| | From proton affinity of quinoxaline (RN 91-19-0). PA = 214.4 kcal/mol, 897. kJ/mol. | | | | | | |
| $C_8H_8^+$ | | | | | | | |
|  | 8.01±0.04 | 256 | 1070 | 71.1±0.3 | 297.6±1.3 | 77PED/RYL | 629-20-9 |
| | See also: 78FU/DUN. | | | | | | |
|  | (8.5) | (287) | (1201) | 91 | 381 | 85KOL/MEI | |
| | IP is onset of photoelectron band (85MEI/KON). | | | | | | |
|  | (8.2) | (281) | (1176) | 92 | 385 | 85KOL/MEI | 68344-46-7 |
| | IP is onset of photoelectron band (85MEI/KON). | | | | | | |

Table 1. Positive Ion Table - Continued

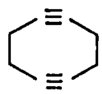
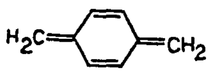
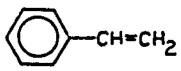
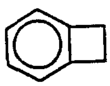
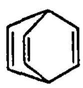
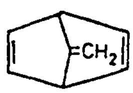
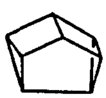
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_8^+$ | | | | | | | |
|  | (8.9) | (321) | (1346) | 116 | 487 | 78LEU/WIR | 49852-40-6 |
|  | (7.5) | (221) | (927) | 48±4 | 203±17 | 81POL/RAI | 502-86-3 |
| | IP is onset of photoelectron band. See also: 82DEW. | | | | | | |
|  | 8.43±0.06 | 230 | 961 | 35.3±0.2 | 147.7±0.7 | 77PED/RYL | 100-42-5 |
| | IP from 78FU/DUN, 81KIM/KAT. | | | | | | |
|  | (≤8.66±0.03) | (≤248) | (≤1037) | 48±1 | 201±4 | 81ROT/SCH | 694-87-1 |
|  | 8.23 | 263 | 1100 | 73 | 306 | 76ALL | 500-24-3 |
| | See also: 82HAS/NEU, 83GLE/BOH. | | | | | | |
|  | (8.5) | (274) | (1145) | 78 | 325 | *EST | 37846-63-2 |
| | IP is onset of photoelectron band. See also: 85MAR/MAY. | | | | | | |
|  | (8.5) | (345) | (1444) | 149±1 | 622±4 | 77PED/RYL | 277-10-1 |
| | Values for this IP of 8.74, 8.64 (77ROS/DRA), 8.46 (82LEV/LIA) and 8.56 eV (83LIF/EAT) have been reported. | | | | | | |
|  | (8.18) | (285) | (1189) | 96 | 400 | 81GOD/SCH | 20656-23-9 |

Table 1. Positive Ion Table - Continued

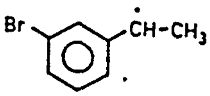
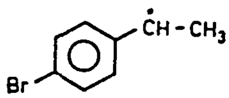
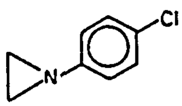
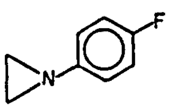
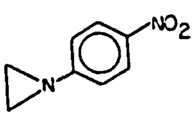
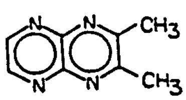
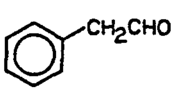
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_8Br^+$ | | | | | | | |
|  | | 199 | 831 | | | | |
| | From proton affinity of 3-$BrC_6H_4CH=CH_2$ (RN 2039-86-3) (84HAR/HOU).<br>PA = 197.4 kcal/mol, 826. kJ/mol. | | | | | | |
|  | | 195 | 815 | | | | |
| | From proton affinity of 4-$BrC_6H_4CH=CH_2$ (RN 2039-82-9) (84HAR/HOU).<br>PA = 201.3 kcal/mol, 842. kJ/mol. | | | | | | |
| $C_8H_8ClN^+$ | | | | | | | |
|  | ≤8.3 | (≤255) | (≤1067) | 64 | 266 | *EST | 28192-05-4 |
| | IP from 82CRI/LIC. | | | | | | |
| $C_8H_8FN^+$ | | | | | | | |
|  | (≤8.2) | (≤213) | (≤890) | 24 | 99 | *EST | 698-53-3 |
| | IP from 82CRI/LIC. | | | | | | |
| $C_8H_8N_2O_2^+$ | | | | | | | |
|  | (≤8.9) | (≤273) | (≤1142) | 68 | 283 | *EST | 30855-79-9 |
| | IP from 82CRI/LIC. | | | | | | |
| $C_8H_8N_4^+$ | | | | | | | |
|  | (≤8.9) | (≤275) | (≤1151) | 70 | 292 | *EST | 6499-39-4 |
| | IP from 84GLE/SPA2. | | | | | | |
| $C_8H_8O^+$ | | | | | | | |
|  | (8.80) | (190) | (796) | −13 | −53 | *EST | 122-78-1 |
| | See also: 81DAL/NIB. | | | | | | |

**Table 1. Positive Ion Table - Continued**

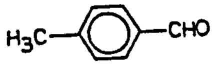
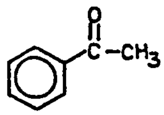
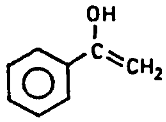
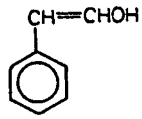
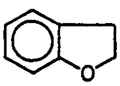
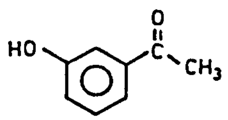
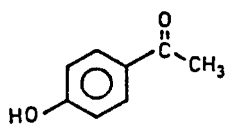
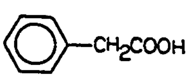
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_8O^+$ | | | | | | | |
|  | 9.33±0.05 | (197) | (825) | −18 | −75 | *EST | 104-87-0 |
| | See also: 85GAL/GER. | | | | | | |
|  | 9.29±0.03 | 194 | 810 | −20.7±0.4 | −86.6±1.5 | 77PED/RYL | 98-86-2 |
| | See also: 81DAL/NIB, 79MCL/TRA, 85GAL/GER, 78CEN/FRA, 82PFI/GER. | | | | | | |
|  | | (175) | (731) | | | | 4383-15-7 |
| | $\Delta_f H$(Ion) from appearance potential determination (81DAL/NIB). | | | | | | |
|  | (8.71±0.1) | (194) | (812) | −7 | −28 | *EST | 4365-04-2 |
| | IP from 81DAL/NIB. | | | | | | |
|  | (7.65) | (163) | (683) | −13 | −55 | *EST | 496-16-2 |
| | IP is onset of photoelectron band (81BAK/ARM). See also: 82LEV/LIA. | | | | | | |
| $C_8H_8O_2^+$ | | | | | | | |
|  | (8.67±0.05) | (137) | (573) | −63±2 | −264±8 | *EST | |
|  | (8.70±0.03) | (138) | (575) | −63±2 | −264±8 | *EST | |
|  | (8.26) | (114) | (478) | −76 | −319 | *EST | 103-82-2 |
| | IP is onset of photoelectron band (83KLA/KOV). See also: 81MEE/WAH. | | | | | | |

**Table 1. Positive Ion Table - Continued**

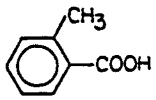
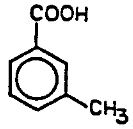
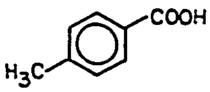
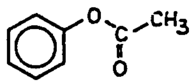
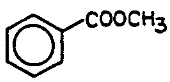
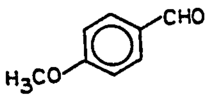
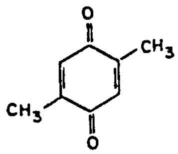
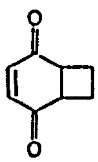
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_8O_2^+$ | | | | | | | |
|  | (9.1) | (133) | (558) | −76.5±0.2 | −320±1 | 76COL/JIM | 118-90-1 |
| | IP from 81MEE/WAH. | | | | | | |
|  | (9.43±0.2) | (139) | (581) | −79±0.2 | −329±1 | 76COL/JIM | 99-04-7 |
| | See also: 81MEE/WAH. | | | | | | |
|  | (9.23±0.2) | (134) | (558) | −79±0.2 | −332±1 | 76COL/JIM | 99-94-5 |
| | See also: 81MEE/WAH. | | | | | | |
|  | (8.6±0.05) | (131) | (550) | −66.8±0.3 | −279.7±1.1 | 77PED/RYL | 122-79-2 |
|  | 9.32±0.03 | 146 | 611 | −69±2 | −288±7 | 77PED/RYL | 93-58-3 |
| | IP from 79MCL/TRA. See also: 81MEE/WAH, 82CAB/COW. | | | | | | |
|  | (8.43) | (145) | (610) | −49±1 | −203±5 | 77PED/RYL | 123-11-5 |
| | See also: 85GAL/GER. | | | | | | |
|  | 9.58 | (176) | (737) | −45 | −187 | *EST | 137-18-8 |
|  | (9.3) | (218) | (910) | 3 | 13 | *EST | 77627-56-6 |
| | IP is onset of photoelectron band 85GLE/JAH. | | | | | | |

**Table 1. Positive Ion Table - Continued**

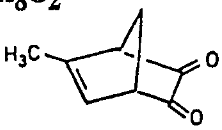
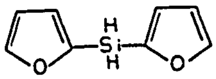
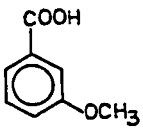
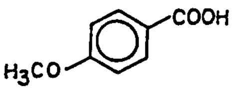
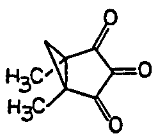
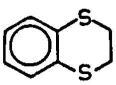
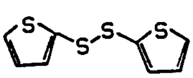
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_8O_2^+$ | | | | | | | |
|  | (8.1) | (160) | (669) | −27 | −113 | *EST | 60526-48-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_8O_2Si^+$ | | | | | | | |
|  | (8.2) | (178) | (743) | −11 | −48 | *EST | 87027-12-1 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
| $C_8H_8O_3^+$ | | | | | | | |
|  | (9.06±0.2) | (102) | (428) | −107±0.2 | −446±1 | 78COL/JIM | 586-38-9 |
|  | (9.04±0.2) | (100) | (420) | −108±0.2 | −452±1 | 78COL/JIM | 100-09-4 |
|  | (8.4) | (80) | (334) | −114 | −476 | *EST | 81640-32-6 |
| | IP is onset of photoelectron band (81BEC/HOF). | | | | | | |
| $C_8H_8S_2^+$ | | | | | | | |
|  | (≤7.91) | (≤219) | (≤916) | 37 | 153 | *EST | 6247-55-8 |
| | IP from 82BRE/SCH. | | | | | | |
| $C_8H_8S_4^+$ | | | | | | | |
|  | (7.5) | (246) | (1032) | 74 | 308 | *EST | |
| | IP is onset of photoelectron band (83BOC/ROT). | | | | | | |

**Table 1. Positive Ion Table - Continued**

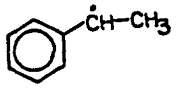
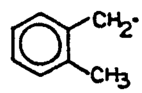
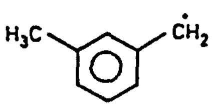
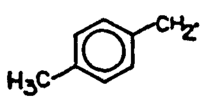
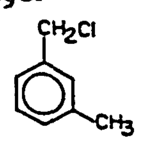
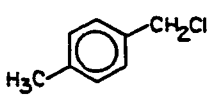
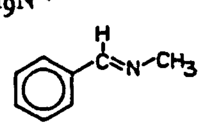
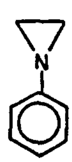
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_9^+$ | | | | | | | |
|  | (6.9) | (199) | (831) | 39.6±1.5 | 165.7±6.3 | 81ROB/STE | 2348-51-8 |
| | $\Delta_fH$(Ion) from proton affinity of $C_6H_5CH=CH_2$ PA = 202.0 kcal/mol, 845. kJ/mol, and from hydride transfer equilibrium constant determinations (85SHA/SHA). IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). | | | | | | |
|  | 7.07 | (203) | (849) | 40 | 167 | 86HAY/KRU | 2348-48-3 |
| | IP from 86HAY/KRU. $\Delta_fH$(Ion) from chloride transfer equilibrium constants (85SHA/SHA). $\Delta_fH(2\text{-}CH_3C_6H_4CH_2Cl)$ estimated as -3.6 kcal/mol, -15.0 KJ/mol. | | | | | | |
|  | 7.12 | (204) | (855) | 40 | 167 | 86HAY/KRU | 2348-47-2 |
| | IP from 86HAY/KRU. $\Delta_fH$(Ion) from chloride transfer equilibrium constants (85SHA/SHA); $\Delta_fH(3\text{-}CH_3C_6H_4CH_2Cl)$ estimated as -3.8 kcal/mol, -15.9 kJ/mol. | | | | | | |
|  | 6.96 | (200) | (837) | 40 | 167 | 86HAY/KRU | 2348-52-9 |
| | IP from 86HAY/KRU. $\Delta_fH$(Ion) from chloride transfer equilibrium constants (85SHA/SHA); $\Delta_fH(4\text{-}CH_3C_6H_4CH_2Cl)$ estimated as -3.8 kcal/mol, -15.0 KJ/mol. | | | | | | |
| $C_8H_9Cl^+$ | | | | | | | |
|  | (8.82±0.03) | (200) | (835) | −4 | −16 | *EST | 620-19-9 |
|  | (8.79±0.03) | (199) | (832) | −4 | −16 | *EST | 104-82-5 |
| $C_8H_9N^+$ | | | | | | | |
|  | 8.77 | (246) | (1031) | 44±2 | 185±10 | *EST | 622-29-7 |
|  | (8.0) | (256) | (1070) | 71 | 298 | *EST | 696-18-4 |
| | IP from 82ROZ/HOU2, 82CRI/LIC. | | | | | | |

Table 1. Positive Ion Table - Continued

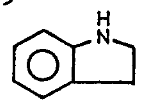
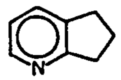
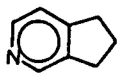
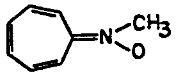
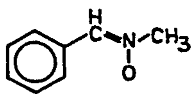
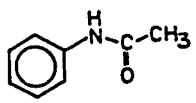
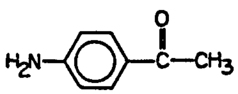
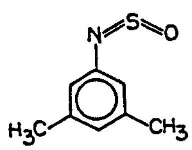
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_9N^+$ | | | | | | | |
|  | (7.15±0.02) | (212) | (888) | 47 | 198 | *EST | 496-15-1 |
|  | ≤9.15 | (≤238) | (≤994) | 27 | 111 | *EST | |
| | IP from 79AUE/BOW. Ion heat of formation predicted from hydrogen affinities of pyridines: 234 kcal/mol, 979 kJ/mol, corresponding to IP of 9.0 eV. | | | | | | |
|  | ≤9.19 | (≤239) | (≤1000) | 27 | 113 | *EST | |
| | IP from (79AUE/BOW). Ion heat of formation predicted from hydrogen affinities of pyridines: 234 kcal/mol, 979 kJ/mol, corresponding to IP of 9.0 eV. | | | | | | |
| $C_8H_9NO^+$ | | | | | | | |
|  | (7.28) | (212) | (888) | 44 | 186 | *EST | 65194-06-1 |
|  | 7.89 | (207) | (866) | 25 | 105 | *EST | 3376-23-6 |
|  | (8.30) | (161) | (672) | −31±0.2 | −129±1 | 77PED/RYL | 103-84-4 |
| | Values reported for this ionization potential range from 8.18 eV to 8.60 eV. | | | | | | |
|  | (7.8±0.1) | (159) | (666) | −21 | −87 | *EST | 99-92-3 |
| | See also: 85GAL/GER. | | | | | | |
| $C_8H_9NOS^+$ | | | | | | | |
|  | (8.2) | (166) | (695) | −23 | −96 | *EST | |
| | IP is onset of photoelectron band (82LOU/VAN). | | | | | | |

**Table 1. Positive Ion Table - Continued**

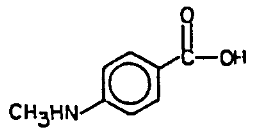
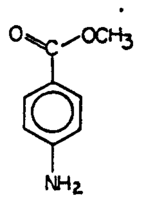
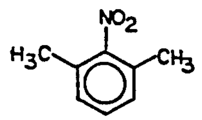
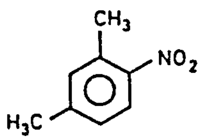
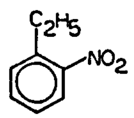
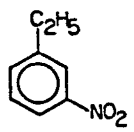
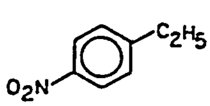
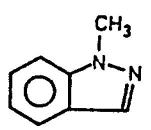
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_9NO_2^+$ | | | | | | | |
|  | (7.3) | (99) | (412) | −70 | −292 | *EST | 10541-83-0 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (7.7) | (109) | (455) | −69 | −288 | *EST | 619-45-4 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | 9.17±0.015 | (221) | (925) | 10 | 40 | *EST | 81-20-9 |
|  | (9.1) | (215) | (898) | 5 | 20 | *EST | 89-87-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.39) | (219) | (917) | 3±2 | 11±7 | 77PED/RYL | 612-22-6 |
| | IP from 82BAL/CAR. | | | | | | |
|  | (9.64) | (224) | (937) | 2 | 7 | *EST | 7369-50-8 |
| | IP from 82BAL/CAR. | | | | | | |
|  | (9.71) | (225) | (943) | 2±2 | 7±7 | 77PED/RYL | 100-12-9 |
| | IP from 82BAL/CAR. | | | | | | |
| $C_8H_9N_2^+$ | | | | | | | |
|  | | 204 | 852 | | | | |
| | From proton affinity of 1-methyl-1H-indazole (RN 13436-48-1) (84FLA/MAQ). PA = (221) kcal/mol, (925) kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

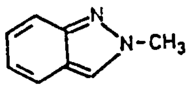
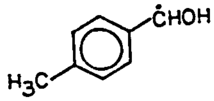
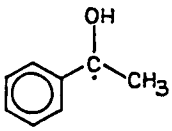
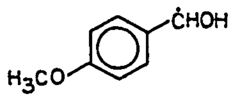
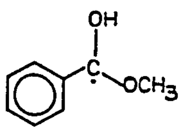
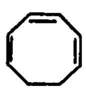
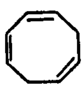
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_9N_2{}^+$ | | | | | | | |
|  | | 218 | 913 | | | | |
| From proton affinity of 2-methyl-2H-indazole (RN 4838-00-0) (84FLA/MAQ). PA = (224) kcal/mol, (939) kJ/mol. | | | | | | | |
| $C_8H_9O^+$ | | | | | | | |
|  | | 144 | 603 | | | | |
| From proton affinity of 4-$(CH_3)C_6H_4CHO$ (RN 104-87-0). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | | |
|  | | 140 | 584 | | | | |
| From proton affinity of $C_6H_5COCH_3$ (RN 98-86-2). PA = 205.4 kcal/mol, 859. kJ/mol. | | | | | | | |
| $C_8H_9O_2{}^+$ | | | | | | | |
|  | | 104 | 434 | | | | |
| From proton affinity of 4-$(CH_3O)C_6H_4CHO$ (RN 123-11-5). PA = 213.5 kcal/mol, 893. kJ/mol. | | | | | | | |
|  | | 94 | 395 | | | | |
| From proton affinity of $C_6H_5COOCH_3$ (RN 93-58-3). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | | |
| $C_8H_{10}{}^+$ | | | | | | | |
| (E)-$CH_2$=CHCH=CHCH=CHCH=$CH_2$ | 7.79±0.02 | (235) | (981) | 55 | 229 | *EST | 3725-31-3 |
| IP from 84HOL, 77ROS/DRA. | | | | | | | |
| $CH_2$=$C(CH_3)C$≡$CC(CH_3)$=$CH_2$ | (8.95±0.1) | (324) | (1357) | 118 | 494 | 77LEB/RYA | 3725-05-1 |
|  | (7.9) | (226) | (945) | 44 | 183 | 69BEN/CRU | 1871-52-9 |
|  | (8.5) | (243) | (1017) | 47 | 197 | *EST | 3725-30-2 |

Table 1. Positive Ion Table - Continued

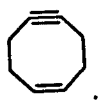
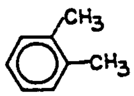
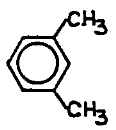
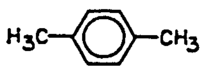
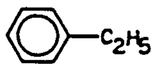
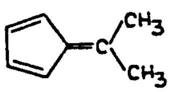
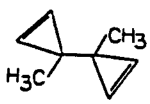
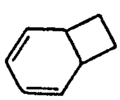
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}^+$ | | | | | | | |
|  | (8.90) | (276) | (1158) | 71 | 299 | 78LEU/WIR | 68177-00-4 |
|  | 8.56±0.01 | 201.7 | 843.9 | 4.3±0.1 | 18.0±0.5 | 77PED/RYL | 95-47-6 |
| | Value derived from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See: 84HOW/GON. | | | | | | |
|  | 8.56±0.01 | 202 | 843 | 4.1±0.1 | 17.3±0.6 | 77PED/RYL | 108-38-3 |
| | Value derived from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See: 84HOW/GON. | | | | | | |
|  | 8.44±0.01 | 199 | 832 | 4.3±0.2 | 18.0±0.9 | 77PED/RYL | 106-42-3 |
| | IP at 298 K from charge transfer equilibrium constant determinations (78LIA/AUS) is 8.52 eV. See: 84HOW/GON. | | | | | | |
|  | 8.77±0.01 | 209 | 875 | 7.0±0.1 | 29.2±0.5 | 77PED/RYL ✓ | 100-41-4 |
| | Value derived from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See also: 83KLA/KOV, 82SEL/HEL, 84HOW/GON. | | | | | | |
|  | (≤8.03) | (≤217) | (≤909) | 32.1±1.3 | 134.4±5.4 | 77PED/RYL | 2175-91-9 |
|  | (8.4) | (320) | (1340) | 127 | 530 | *EST | |
| | IP is onset of photoelectron band (82SPA/KOR). | | | | | | |
|  | (7.6) | (224) | (938) | 49 | 205 | *EST | 3725-28-8 |
| | IP is onset of photoelectron band (81GLE/GUB2). | | | | | | |

**Table 1. Positive Ion Table - Continued**

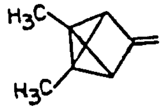
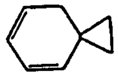
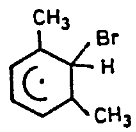
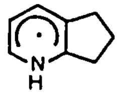
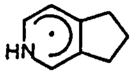
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}^+$ | | | | | | | |
|  | (8.5) | (230) | (964) | 34 | 144 | 76ALL | 657-23-8 |
| | IP is onset of photoelectron band. See also: 82HAS/NEU. | | | | | | |
|  | (8.0) | (273) | (1141) | 88 | 369 | *EST | 63001-13-8 |
| | IP is onset of photoelectron band (84GLE/HAI). | | | | | | |
|  | (8.4) | (242) | (1012) | 48.1 | 201.3 | 81GOD/SCH | 765-72-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤7.89) | (≤242) | (≤1012) | 60 | 251 | *EST | 53143-64-9 |
|  | (8.20) | (246) | (1029) | 57 | 238 | *EST | 15439-15-3 |
| $C_8H_{10}Br^+$ | | | | | | | |
|  | | 178 | 743 | | | | |
| | From proton affinity of 1,3,2-$C_6H_3(CH_3)_2Br$ (RN 576-22-7). PA = (199) kcal/mol, (832) kJ/mol. | | | | | | |
| $C_8H_{10}N^+$ | | | | | | | |
|  | | 166 | 695 | | | | |
| | From proton affinity of 2,3-cyclopentenopyridine. PA = (225.8) kcal/mol, (945.) kJ/mol. | | | | | | |
|  | | 166 | 696 | | | | |
| | From proton affinity of 3,4-cyclopentenopyridine. PA = (226.8) kcal/mol, (949.) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

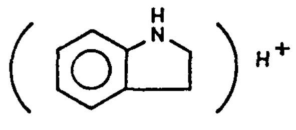
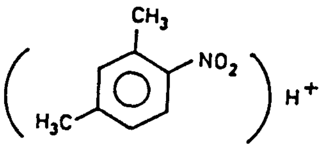
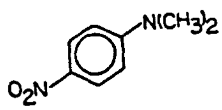
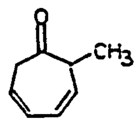
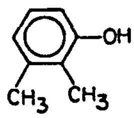
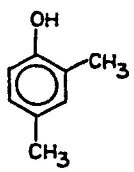
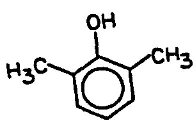
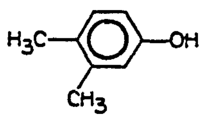
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}N^+$ | | | | | | | |
|  | | 186 | 779 | | | | |
| | From proton affinity of 2,3-dihydroindole (RN 496-15-1) (85BOL/HOU). PA = 226.7 kcal/mol, 949. kJ/mol. | | | | | | |
| $C_8H_{10}NO_2^+$ | | | | | | | |
|  | | 153 | 641 | | | | |
| | From proton affinity of 1,3,4-$C_6H_3(CH_3)_2NO_2$ (RN 89-87-2) (84ROL/HOU). PA = 199.8 kcal/mol, 836. kJ/mol. | | | | | | |
| $C_8H_{10}N_2O_2^+$ | | | | | | | |
|  | (7.6±0.1) | (191) | (801) | 16.1±0.4 | 67.3±1.8 | 84FUR/MUR | 100-23-2 |
| $C_8H_{10}O^+$ | | | | | | | |
|  | 8.23 | (146) | (611) | −44 | −183 | *EST | 42104-03-0 |
| | IP from 83RUS/FRE. | | | | | | |
|  | (8.26) | (153) | (640) | −37.6±0.3 | −157.2±1.4 | 77PED/RYL | 526-75-0 |
| | IP from 83RUS/FRE. | | | | | | |
|  | (8.0) | (146) | (609) | −38.9±0.2 | −162.9±0.9 | 77PED/RYL | 105-67-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.05±0.02 | 147 | 615 | −38.7±0.2 | −161.8±1.0 | 77PED/RYL | 576-26-1 |
|  | (8.09) | (149) | (624) | −37.4±0.3 | −156.6±1.1 | 77PED/RYL | 95-65-8 |
| | IP from 83RUS/FRE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

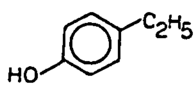
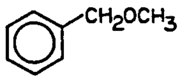
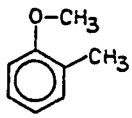
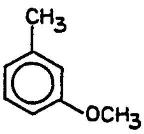
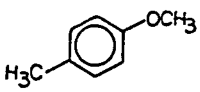
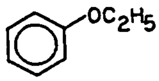
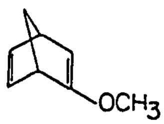
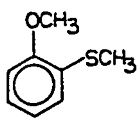
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}O^+$ | | | | | | | |
|  | (7.84) | (146) | (612) | −34.4±0.2 | −144.1±1.0 | 77PED/RYL | 123-07-9 |
| | IP from 83RUS/FRE. | | | | | | |
|  | 8.85±0.03 | 186 | 780 | −18 | −74 | 73BIL/CHO | 538-86-3 |
|  | 7.90 | (157) | (657) | −25 | −105 | *EST | 578-58-5 |
|  | (8.0) | (160) | (668) | −25±1 | −104±5 | 77PED/RYL | 100-84-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 7.9 | (158) | (662) | −24 | −100 | *EST | 104-93-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.13±0.02 | 163 | 683 | −24.3±0.1 | −101.7±0.5 | 77PED/RYL | 103-73-1 |
|  | (≤8.05) | (≤207) | (≤865) | 21 | 88 | *EST | 74437-38-0 |
| | IP from 83HOU/RON. | | | | | | |
| $C_8H_{10}OS^+$ | | | | | | | |
|  | (≤8.05) | (≤172) | (≤720) | −14 | −57 | *EST | 2388-73-0 |

**Table 1. Positive Ion Table - Continued**

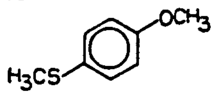
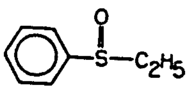
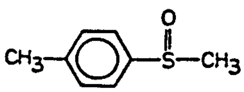
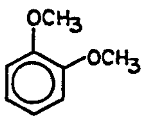
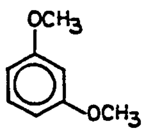
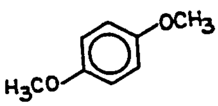
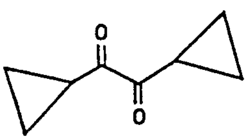
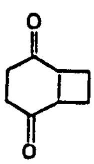
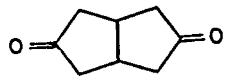
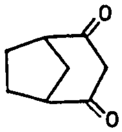
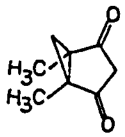
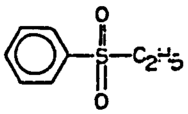
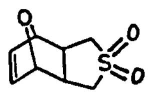
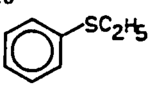
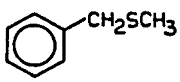
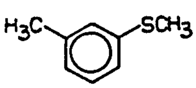
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}OS^+$ | | | | | | | |
|  | ≤7.80 | (≤168) | (≤703) | −12 | −50 | *EST | 1879-16-9 |
|  | (≤8.75) | (≤193) | (≤809) | −8 | −35 | *EST | 4170-80-3 |
| | IP from 81MOH/JIA. | | | | | | |
|  | (≤8.70) | (≤193) | (≤808) | −7.6 | −31.8 | *EST | 934-72-5 |
| | IP from 81MOH/JIA. | | | | | | |
| $C_8H_{10}O_2^+$ | | | | | | | |
|  | (7.8) | (127) | (530) | −53±0.7 | −223±3 | 77PED/RYL | 91-16-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.8) | (122) | (511) | −58 | −242 | *EST | 151-10-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 7.53 | (118) | (493) | −56 | −234 | *EST | 150-78-7 |
| | IP from 85OIK/ABE, 82LEV/LIA. | | | | | | |
|  | (8.8) | (173) | (724) | −30 | −125 | *EST | 15940-88-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.1) | (154) | (645) | −56 | −233 | *EST | 54338-82-8 |
| | IP is onset of photoelectron band (85GLE/JAH). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}O_2^+$ | | | | | | | |
|  | (≤9.33) | (≤138) | (≤576) | −77 | −324 | *EST | |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.7) | (127) | (532) | −73 | −307 | *EST | 74896-14-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.14) | (139) | (582) | −72 | −300 | *EST | 29978-55-0 |
| | IP is onset of photoelectron band (81BEC/HOF). | | | | | | |
| $C_8H_{10}O_2S^+$ | | | | | | | |
|  | (9.4) | (150) | (628) | −67 | −279 | *EST | 599-70-2 |
| | IP from 81MOH/JIA. | | | | | | |
| $C_8H_{10}O_3S^+$ | | | | | | | |
|  | (9.5) | (160) | (668) | −60 | −249 | *EST | |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
| $C_8H_{10}S^+$ | | | | | | | |
|  | 7.88±0.02 | 200 | 837 | 18.4±0.6 | 77.0±2.6 | 77PED/RYL | 622-38-8 |
|  | (8.42) | (213) | (892) | 19.0±0.7 | 79.5±2.9 | 77PED/RYL | 766-92-7 |
|  | (≤8.00) | (≤200) | (≤838) | 16 | 66 | *EST | 4886-77-5 |

## Table 1. Positive Ion Table - Continued

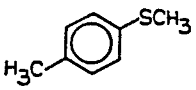
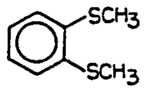
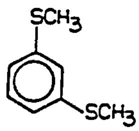
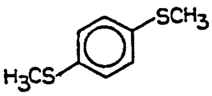
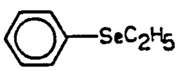
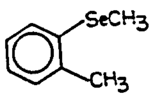
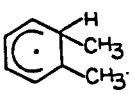
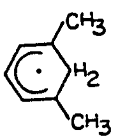
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{10}S^+$ | | | | | | | |
|  | 7.5 | (189) | (790) | 16 | 66 | *EST | 623-13-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{10}S_2^+$ | | | | | | | |
|  | 7.7 | (206) | (864) | 29 | 121 | *EST | 2388-68-3 |
| | IP is onset of photoelectron band (81TRA/RED, 82LEV/LIA). | | | | | | |
|  | (≤8.0) | (≤211) | (≤885) | 27 | 113 | *EST | 2388-69-4 |
|  | (7.3) | (195) | (817) | 27 | 113 | *EST | 699-20-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{10}Se^+$ | | | | | | | |
|  | (7.6) | (207) | (865) | 31 | 132 | *EST | 17774-38-8 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
|  | (7.5) | (200) | (837) | 27 | 113 | *EST | 1528-88-7 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
| $C_8H_{11}^+$ | | | | | | | |
|  | | 177 | 739 | | | | |
| | From proton affinity of 1,2-$C_6H_4(CH_3)_2$ (RN 95-47-6). PA = 193.3 kcal/mol, 809. kJ/mol. | | | | | | |
|  | | 174 | 727 | | | | |
| | From proton affinity of 1,3-$C_6H_4(CH_3)_2$ (RN 108-38-3). PA = 195.9 kcal/mol, 820. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

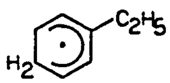
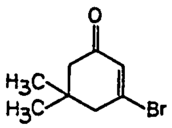
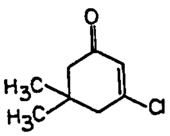
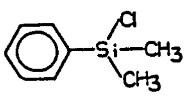
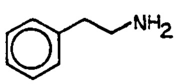
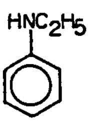
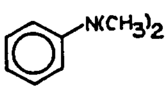
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_{11}^+$ | | | | | | | |
|  | | 178 | 745 | | | | |
| | From proton affinity of 1,4-$C_6H_4(CH_3)_2$ (RN 106-42-3). PA = 192.0 kcal/mol, 803. kJ/mol. | | | | | | |
|  | | 181 | 757 | | | | |
| | From proton affinity of $C_6H_5C_2H_5$ (RN 100-41-4). PA = 191.6 kcal/mol, 802. kJ/mol. | | | | | | |
| $C_8H_{11}BrO^+$ | | | | | | | |
|  | (≤9.35) | (≤180) | (≤755) | −35 | −147 | *EST | 13271-49-3 |
| | IP from 82PFI/GER. | | | | | | |
| $C_8H_{11}ClO^+$ | | | | | | | |
|  | (9.35) | (170) | (713) | −45 | −189 | *EST | 17530-69-7 |
| | IP from 82PFI/GER. | | | | | | |
| $C_8H_{11}ClSi^+$ | | | | | | | |
|  | (8.93) | (156) | (652) | −50 | −210 | *EST | 768-33-2 |
| | IP from 84VES/HAR. | | | | | | |
| $C_8H_{11}N^+$ | | | | | | | |
|  | (8.5) | (212) | (885) | 16 | 65 | *EST | 64-04-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤7.67) | (≤190) | (≤796) | 13±1 | 56±6 | 77PED/RYL | 103-69-5 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | 7.12±0.02 | 188 | 788 | 24±0.7 | 101±3 | 82FUR/SAK | 121-69-7 |

**Table 1. Positive Ion Table - Continued**

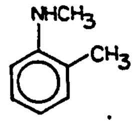
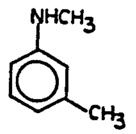
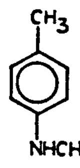
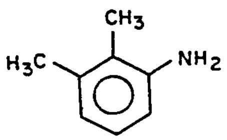
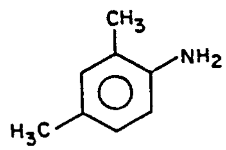
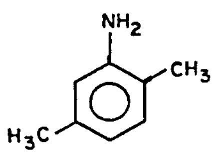
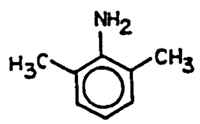
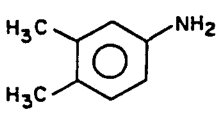
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{11}N^+$ | | | | | | | |
|  | (7.27) | (182) | (759) | 14 | 58 | *EST | 611-21-2 |
|  | (7.26) | (180) | (753) | 13 | 53 | *EST | 696-44-6 |
|  | (7.13) | (177) | (741) | 13 | 53 | *EST | 623-08-5 |
|  | ≤7.77±0.05 | (≤186) | (≤777) | 6 | 27 | *EST | 87-59-2 |
|  | (≤7.65±0.05) | (≤182) | (≤761) | 5 | 23 | *EST | 95-68-1 |
|  | 7.2<br>IP is onset of photoelectron band. | (172) | (718) | 5 | 23 | *EST | 95-78-3 |
|  | 7.33±0.05 | (175) | (734) | 6±0.2 | 27±1 | *EST | 87-62-7 |
|  | (≤7.68±0.05) | (≤183) | (≤764) | 5 | 23 | *EST | 95-64-7 |

**Table 1. Positive Ion Table - Continued**

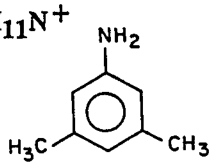
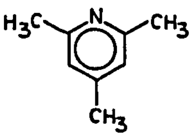
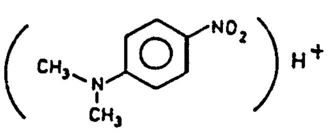
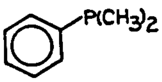
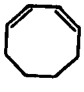
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{11}N^+$ | | | | | | | |
|  | 7.2 | (171) | (716) | 5 | 21 | *EST | 108-69-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.9±0.1) | (≤210) | (≤879) | 5 | 20 | *EST | 108-75-8 |
| $C_8H_{11}N_2O_2^+$ | | | | | | | |
|  | | 167 | 699 | | | | |
| | From proton affinity of N,N-dimethyl-4-nitroaniline (RN 100-23-2) (84ROL/HOU). PA = 214.6 kcal/mol, 898. kJ/mol. | | | | | | |
| $C_8H_{11}P^+$ | | | | | | | |
|  | 7.58±0.05 | (184) | (771) | 10 | 40 | *EST | 672-66-2 |
| $C_8H_{12}^+$ | | | | | | | |
| (E),(E)-$CH_3CH=C(CH_3)CH=CHCH=CH_2$ | (≤8.01) | (≤208) | (≤872) | 24 | 99 | *EST | 58434-77-8 |
| $CH_2=CHCH=CHCH(CH_3)CH=CH_2$ | (8.4±0.1) | (226) | (945) | 32.2 | 134.7 | *EST | 925-52-0 |
| | IP from 84GRO/GRO. | | | | | | |
| n-$C_4H_9C{\equiv}CCH=CH_2$ | (8.83±0.01) | (248) | (1038) | 44±2 | 186±7 | 78SHA | 17679-92-4 |
| (E)-n-$C_4H_9CH=CHC{\equiv}CH$ | (8.87±0.01) | (248) | (1040) | 44 | 184 | *EST | 42104-42-7 |
| n-$C_3H_7C{\equiv}CC(CH_3)=CH_2$ | (8.62±0.01) | (241) | (1008) | 42 | 176 | *EST | 17669-40-8 |
| $(C_2H_5)_2C=CHC{\equiv}CH$ | (8.54±0.01) | (240) | (1004) | 43 | 180 | *EST | 2750-71-2 |
|  | (8.4) | (213) | (891) | 19 | 81 | 82KOZ/MAS | 1700-10-3 |

**Table 1. Positive Ion Table - Continued**

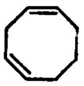
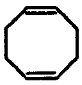
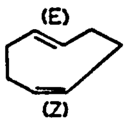
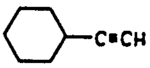
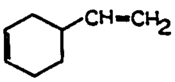
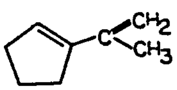
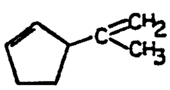
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}^+$ | | | | | | | |
|  | (8.5) | (221) | (925) | 25±2 | 105±8 | *EST | 1073-07-0 |
|  | (8.9) | (219) | (917) | 14.0±0.3 | 58.6±1.2 | 77PED/RYL | 111-78-4 |
|   | (8.2)<br>IP is onset of photoelectron band. | (218) | (912) | 29 | 121 | *EST | 5259-71-2 |
|  | (8.9) | (248) | (1041) | 43±1 | 182±3 | 75ALL/MEY | 1781-78-8 |
|   | (≤9.92) | (≤257) | (≤1076) | 28±1 | 119±3 | 75ALL/MEY | 931-48-6 |
|   | (8.93±0.02)<br>See also: 84GRO/GRO. | (221) | (927) | 15.6±0.3 | 65.1±1.2 | 77PED/RYL | 100-40-3 |
|   | (8.60±0.01) | (219) | (917) | 21 | 87 | *EST | 37689-19-3 |
|   | (8.89±0.02) | (227) | (950) | 22 | 92 | *EST | 14564-97-7 |

**Table 1. Positive Ion Table - Continued**

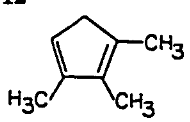
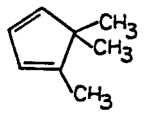
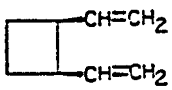
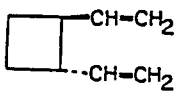
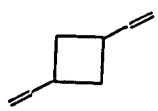
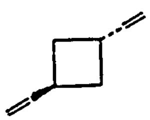
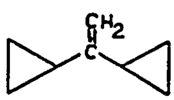
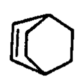
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}^+$ | | | | | | | |
|  | (7.96±0.05) | (192) | (804) | 9 | 36 | *EST | 3853-27-8 |
|  | (8.0±0.1) | (195) | (818) | 11 | 46 | *EST | 4249-09-6 |
|  | (≤9.22) | (≤252) | (≤1056) | 39.8±0.8 | 166.5±3.5 | 77PED/RYL | 16177-46-1 |
| | IP from 81BIS/GLE. | | | | | | |
|  | (≤9.20) | (≤246) | (≤1031) | 34.3±0.8 | 143.5±3.4 | 77PED/RYL | 6553-48-6 |
| | IP from 81BIS/GLE. | | | | | | |
|  | (8.9) | (247) | (1035) | 42 | 176 | *EST | 77614-53-0 |
| | IP is onset of photoelectron band (81BIS/GLE). | | | | | | |
|  | (8.9) | (247) | (1035) | 42 | 176 | *EST | 77614-67-6 |
| | IP is onset of photoelectron band (81BIS/GLE). | | | | | | |
|  | 8.08 | (237) | (993) | 51 | 213 | *EST | 822-93-5 |
|  | (8.92) | (211) | (881) | 4.9±0.2 | 20.5±0.8 | 77PED/RYL | 931-64-6 |
| | See also: 82HAS/NEU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

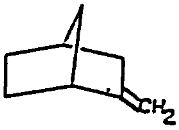
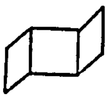
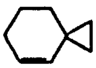
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}{}^+$ | | | | | | | |
|  | ≤9.02 | ≤220 | ≤920 | 12 | 50 | 79AUE/BOW | 497-35-8 |
|  | (≤9.40) | (≤231.2) | (≤967.2) | 14±1 | 60±3 | 77KOZ/BYC | 31463-35-1 |
| | See also: 85MAR/MAY. | | | | | | |
|  | (≤8.95) | (≤234) | (≤980) | 28 | 116 | *EST | 50695-42-6 |
|  | (≤9.39) | (≤244) | (≤1022) | 28 | 116 | *EST | 50895-58-4 |
|  | (≤9.18) | (≤264) | (≤1102) | 52±2 | 216±8 | 73ENG/AND2 | 28636-10-4 |
|  | (≤9.23) | (≤259) | (≤1084) | 46±2 | 193±7 | 73ENG/AND2 | 13027-75-3 |
|  | (9.4) | (238) | (997) | 21±3 | 90±14 | 81GOD/SCH2 | 250-21-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.44) | (≤228) | (≤954) | 33 | 140 | *EST | 7647-57-6 |

Table 1. Positive Ion Table - Continued

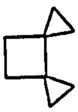
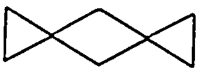
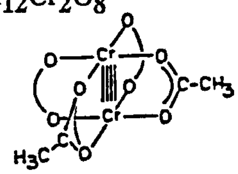
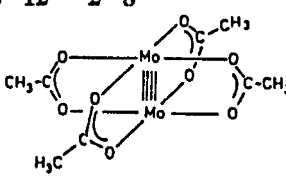
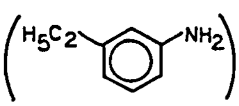
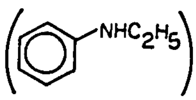
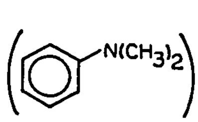
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}^+$ | | | | | | | |
|  | (8.65) | (233) | (975) | 33 | 140 | *EST | 14783-50-7 |
|  | (8.4)<br>IP is onset of photoelectron band. | (266) | (1112) | 72 | 302 | *EST | 21426-37-9 |
|  | (8.8)<br>IP is onset of photoelectron band. | (275) | (1151) | 72 | 302 | *EST | 25399-32-0 |
| $C_8H_{12}Cr_2O_8^+$ | | | | | | | |
|  | (8.0)<br>IP is onset of photoelectron band. | (−290) | (−1212) | −474±7 | −1984±28 | 82PIL/SKI | 15020-15-2 |
| $C_8H_{12}Mo_2O_8^+$ | | | | | | | |
|  | 6.54<br>IP from 84LIC/BLE. | (−280) | (−1175) | −432±2 | −1806±10 | 81CAV/CON | 14221-06-8 |
| $C_8H_{12}N^+$ | | | | | | | |
|  $H^+$ | From proton affinity of 3-$C_2H_5C_6H_4NH_2$ (RN 587-02-0). PA = 214.0 kcal/mol, 895. kJ/mol. | 158 | 662 | | | | |
|  $H^+$ | From proton affinity of $C_6H_5NHC_2H_5$ (RN 103-69-5). PA = 221.8 kcal/mol, 928. kJ/mol. | 157 | 658 | | | | |
|  $H^+$ | From proton affinity of $C_6H_5N(CH_3)_2$ (RN 121-69-7). PA = 223.4 kcal/mol, 935. kJ/mol. | 166 | 696 | | | | |

Table 1. Positive Ion Table - Continued

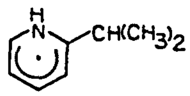
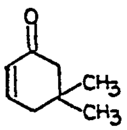
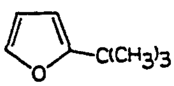
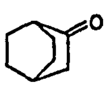
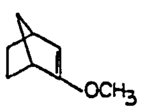
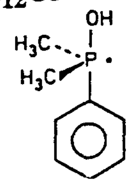
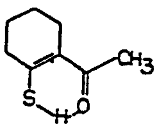
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}N^+$ | | | | | | | |
|  | | 152 | 635 | | | | |
| | From proton affinity of 2-isopropylpyridine (RN 75981-47-4). PA = 227.2 kcal/mol, 951. kJ/mol. | | | | | | |
| $C_8H_{12}N_4^+$ | | | | | | | |
| (E)-$(NCC(CH_3)_2)_2N_2$ | (9.2) | (271) | (1134) | 59±0.4 | 246±1.8 | 84LEB/GUT | 34241-39-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{12}O^+$ | | | | | | | |
|  | (≤9.24) | (≤171) | (≤718) | −42 | −174 | *EST | 4694-17-1 |
| | IP from 82PFI/GER. | | | | | | |
|  | (8.38) | (157) | (656) | −37 | −153 | *EST | 7040-43-9 |
| | IP from 83ZYK/ERC. | | | | | | |
|  | (8.8) | (148) | (619) | −55±1 | −230±5 | 77PED/RYL | 2716-23-6 |
| | IP is onset of photoelectron band (81CAR/GAN). | | | | | | |
|  | (≤8.15) | (≤173) | (≤724) | −15 | −62 | *EST | 17190-90-8 |
| | IP from 83HOU/RON. | | | | | | |
| $C_8H_{12}OP^+$ | | | | | | | |
|  | | 82 | 341 | | | | |
| | From proton affinity of $(CH_3)_2(C_6H_5)PO$ (RN 10311-08-7) (86TRA/MUN). PA = 216 kcal/mol, 904 kJ/mol. | | | | | | |
| $C_8H_{12}OS^+$ | | | | | | | |
|  | (8.0) | (125) | (523) | −60 | −249 | *EST | 76698-82-3 |
| | IP is onset of photoelectron band (81JOR/CAR). | | | | | | |

Table 1. Positive Ion Table - Continued

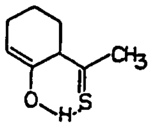
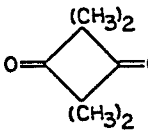
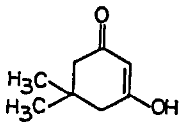
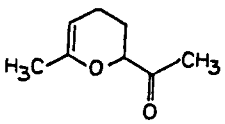
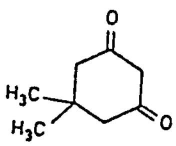
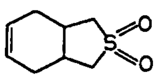
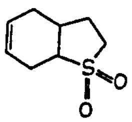
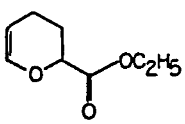
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}OS^+$ | | | | | | | |
|  | (7.8) | (120) | (504) | −60 | −249 | *EST | |
| | IP is onset of photoelectron band (81JOR/CAR). | | | | | | |
| $C_8H_{12}O_2^+$ | | | | | | | |
|  | ≤8.80 | ≤129 | ≤541 | −74±0.5 | −308±2 | 77PED/RYL | 933-52-8 |
| | See also: 84OLI/FLE. | | | | | | |
|  | (≤9.45) | (≤149) | (≤625) | −68±3 | −287±13 | *EST | 3471-13-4 |
| | IP from 82PFI/GER. | | | | | | |
|  | (8.62) | (120) | (502) | −79 | −330 | 82MOR/MER | |
| | IP from 82MOR/MER. | | | | | | |
|  | (9.28±0.05) | (145) | (608) | −68.5±3 | −287±12 | *EST | 126-81-8 |
| $C_8H_{12}O_2S^+$ | | | | | | | |
|  | (≤9.2) | (≤139) | (≤584) | −73 | −304 | *EST | |
| | IP from 84AIT/GOS. | | | | | | |
|  | (9.05) | (136) | (569) | −73 | −304 | *EST | |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
| $C_8H_{12}O_3^+$ | | | | | | | |
|  | (8.6) | (69) | (288) | −129 | −542 | *EST | |
| | IP from 82MOR/MER. | | | | | | |

**Table 1. Positive Ion Table - Continued**

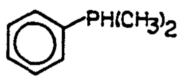
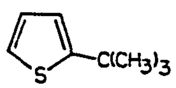
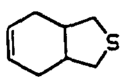
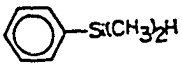
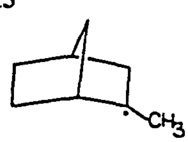
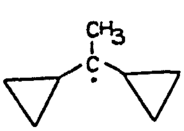
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{12}P^+$ | | | | | | | |
|   | | 156 | 651 | | | | |
| | From proton affinity of $C_6H_5P(CH_3)_2$ (RN 672-66-2). PA = 229.6 kcal/mol, 961. kJ/mol. | | | | | | |
| $C_8H_{12}S^+$ | | | | | | | |
|   | (8.32) | (194) | (812) | 2 | 9 | *EST | 1689-78-7 |
| | IP is onset of photoelectron band (83VES/HAR). | | | | | | |
|   | (8.0) | (192) | (804) | 8 | 32 | *EST | |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
| $C_8H_{12}Si^+$ | | | | | | | |
| $(CH_2{=}CH)_4Si$ | (9.3) | (229) | (958) | 15 | 61 | 85GAD/GUB | 1112-55-6 |
| | IP is onset of photoelectron band. | | | | | | |
|   | (8.92±0.15) | (203) | (848) | −3 | −13 | *EST | 766-77-8 |
| $C_8H_{12}Sn^+$ | | | | | | | |
| $Sn(CH{=}CH_2)_4$ | (8.4) | (277) | (1162) | 84 | 352 | *EST | 1112-56-7 |
| | IP is onset of photoelectron band (81NOV/CVI). | | | | | | |
| $C_8H_{13}^+$ | | | | | | | |
|   | | 171 | 717 | | | | 3197-78-2 |
| | From proton affinities of 2-methylenebicyclo[2.2.1]heptane PA = (207) kcal/mol, (866) kJ/mol, (RN 497-35-8), 2-methylbicyclo[2.2.1]hept-2-ene PA = 206 kcal/mol, 862 kJ/mol, (RN 694-92-8) and hydride and chloride transfer equilibrium constants. (76SOL/FIE, 85SHA/SHA). | | | | | | |
|   | | 200 | 837 | | | | 50555-45-8 |
| | From proton affinity of 1,1-dicyclopropylethylene (RN 822-93-5). PA = 216.5 kcal/mol, 906. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

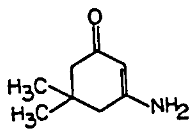
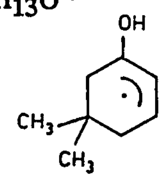
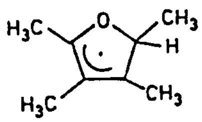
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{13}Br^+$ | | | | | | | |
|  | (9.4±0.1) | (194) | (812) | −23 | −95 | *EST | 7697-09-8 |
| | IP is onset of photoelectron band (84DEL/ABE). | | | | | | |
| $C_8H_{13}I^+$ | | | | | | | |
|  | (8.7) | (192) | (805) | −8 | −34 | *EST | 931-98-6 |
| | IP is onset of photoelectron band (84DEL/ABE). | | | | | | |
| $C_8H_{13}NO^+$ | | | | | | | |
|  | (≤8.55) | (≤150) | (≤628) | −47 | −197 | *EST | 873-95-0 |
| | IP from 82PFI/GER. | | | | | | |
| $C_8H_{13}O^+$ | | | | | | | |
|  | | 116 | 487 | | | | |
| | From proton affinity of 5,5-dimethylcyclohex-2-ene-1-one PA = 207.6 kcal/mol, 869. kJ/mol (86TAF/GAL). | | | | | | |
|  | | 106 | 444 | | | | |
| | From proton affinity of 2,3,4,5-tetramethylfuran (RN 10599-58-3) (85HOU/ROL). PA = 217.6 kcal/mol, 910. kJ/mol. | | | | | | |
| $C_8H_{14}^+$ | | | | | | | |
| (E)-$CH_3CH_2CH_2CH_2CH=CHCH=CH_2$ | (8.45) | (198) | (830) | 4 | 15 | *EST | 39491-65-1 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_2=CHCH_2CH=CH(CH_2)_2CH_3$ | (8.96) | (215) | (897) | 8 | 32 | *EST | 53793-31-0 |
| | IP from 84HOL. | | | | | | |
| (E),(E)-$CH_3CH_2CH_2CH=CHCH=CHCH_3$ | (8.13) | (188) | (786) | 0.5 | 2 | *EST | 60919-80-4 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$CH_3CH_2CH_2C(CH_3)=CHCH=CH_2$ | (8.02) | (185) | (776) | 0.5 | 2 | *EST | 40095-05-4 |
| | IP from 81MAS/MOU. | | | | | | |

Table 1. Positive Ion Table - Continued

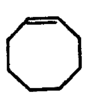
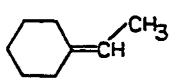
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{14}^+$ | | | | | | | |
| (Z)-$(CH_3)_3CCH=CHCH=CH_2$ | | | | | | | |
| | (8.46) | (199) | (833) | 4 | 17 | *EST | 59697-92-6 |
| | IP from 81MAS/MOU. | | | | | | |
| (E)-$(CH_3)_3CCH=CHCH=CH_2$ | | | | | | | |
| | (8.43) | (197) | (823) | 2 | 10 | *EST | 36320-14-6 |
| | IP from 81MAS/MOU. | | | | | | |
| $(CH_3)_2C=CHCH=C(CH_3)_2$ | | | | | | | |
| | (7.67) | (171) | (716) | −6 | −24 | *EST | 764-13-6 |
| | IP from 81MAS/MOU. | | | | | | |
| (Z),(Z)-$(CH_3CH=C(CH_3))_2$ | | | | | | | |
| | (8.1) | (182) | (761) | −5 | −20 | *EST | 21293-01-6 |
| | IP is onset of photoelectron band (84HON/ZHO). | | | | | | |
| (E),(E)-$(CH_3CH=C(CH_3))_2$ | | | | | | | |
| | (7.8) | (177) | (740) | −3 | −12 | *EST | 18265-39-9 |
| | IP is onset of photoelectron band (84HON/ZHO). | | | | | | |
| (E),(Z)-$(CH_3CH=C(CH_3))_2$ | | | | | | | |
| | (8.0) | (181) | (756) | −4 | −16 | *EST | 2417-88-1 |
| | IP is onset of photoelectron band (84HON/ZHO). | | | | | | |
| $C_2H_5C(=CH_2)C(=CH_2)C_2H_5$ | | | | | | | |
| | (8.58) | (199) | (834) | 1 | 6 | *EST | 16356-05-1 |
| | IP from 81MAS/MOU. | | | | | | |
| 1-$C_8H_{14}$ | (9.95±0.02) | (248) | (1041) | 19±1 | 81±4 | 79ROG/DAG | 629-05-0 |
| n-$C_5H_{11}C{\equiv}CCH_3$ | 9.31±0.01 | 230 | 962 | 15±0.2 | 64±2 | 79ROG/DAG | 2809-67-8 |
| $C_4H_9C{\equiv}CC_2H_5$ | 9.22±0.01 | 228 | 953 | 15±0.5 | 63±2 | 79ROG/DAG | 15232-76-5 |
| n-$C_3H_7C{\equiv}CC_3H_7$ | 9.20±0.01 | 226 | 948 | 14±0.5 | 60±2 | 79ROG/DAG | 1942-45-6 |
|  | 8.82 | 196.9 | 824.0 | −6.5±0.3 | −27.0±1.1 | 77PED/RYL | 931-88-4 |
| <br> | 8.44±0.05 | 174 | 726 | −21 | −88 | 76JEN | 1003-64-1 |

Table 1. Positive Ion Table - Continued

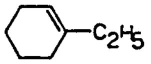
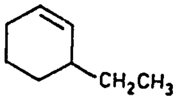
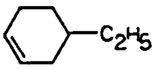
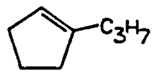
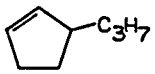
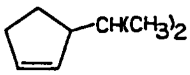
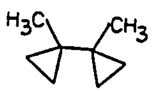
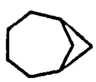
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{14}^+$ | | | | | | | |
|  | (8.48±0.01) | (180) | (755) | −15.2±0.2 | −63.4±1 | 77PED/RYL | 1453-24-3 |
|  | (8.83±0.01) | (191) | (799) | −13 | −53 | *EST | 2808-71-1 |
|  | (8.88±0.01) | (192) | (804) | −13 | −53 | *EST | 3742-42-5 |
|  | (8.48±0.01) | (186) | (779) | −9 | −39 | *EST | 3074-61-1 |
|  | (8.84±0.02) | (196) | (819) | −8 | −34 | *EST | 34067-75-9 |
|  | 8.81<br>IP from 84HOL. | (193) | (807) | −10 | −43 | *EST | 4276-45-3 |
|  | (8.8)<br>IP is onset of photoelectron band (82SPA/GLE). | (222) | (931) | 20 | 82 | *EST | 59020-33-6 |
|  | (9.6)<br>IP is onset of photoelectron band. | (220) | (921) | −1.2 | −5 | 81MAI/SCH | 7078-34-4 |

Table 1. Positive Ion Table - Continued

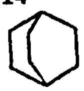
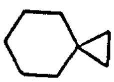
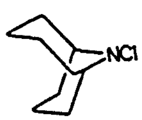
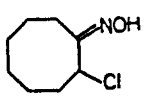
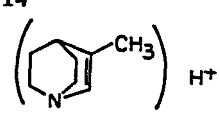
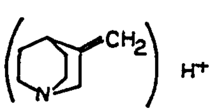
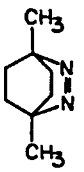
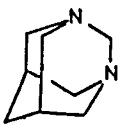
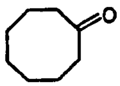
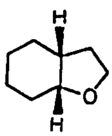
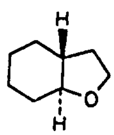
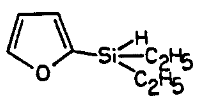
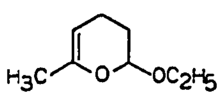
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{14}^+$ | | | | | | | |
|  | 9.43±0.02 | 194 | 813 | −23±1 | −97±4 | 81GOD/SCH | 280-33-1 |
|  | (≤9.46) | (≤221) | (≤925) | 3 | 12 | *EST | 185-65-9 |
|  | (9.45) | (225) | (941) | 7 | 29 | *EST | 175-56-4 |
| $C_8H_{14}ClN^+$ | | | | | | | |
|  | (≤8.55) | (≤190) | (≤795) | −7 | −30 | *EST | |
| | IP from 82NEL/GAN. | | | | | | |
| $C_8H_{14}ClNO^+$ | | | | | | | |
|  | (9.19±0.03) | (178) | (747) | −33 | −140 | *EST | 10499-33-9 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_8H_{14}N^+$ | | | | | | | |
|  | | (164) | (687) | | | | |
| | From proton affinity of 1-azabicyclo[2.2.2]oct-2-ene,3-methyl-. PA = (231.0) kcal/mol, (966.5) kJ/mol. | | | | | | |
|  | | (156) | (651) | | | | |
| | From proton affinity of 1-azabicyclo[2.2.2]octane, 3-methylene-. PA = (230.1) kcal/mol, (963.) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{14}N_2{}^+$ | | | | | | | |
|  | (7.8) | (202) | (846) | 22±1 | 93±5 | 80ENG | 49570-30-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | ≤7.75 | (≤190) | (≤795) | 11 | 47 | *EST | 281-29-8 |
| $C_8H_{14}O^+$ | | | | | | | |
| n-$C_3H_7CH=C(CH_3)C(=O)CH_3$ | (9.22) | (159) | (666) | -54 | -224 | *EST | 39899-08-6 |
|  | 9.08 | 144 | 604 | -65±1 | -272±5 | 77PED/RYL | 502-49-8 |
| | See also: 86SPA/RAD. | | | | | | |
|  | (9.0) | (149) | (624) | -58 | -244 | *EST | |
| | IP is onset of photoelectron band (83TUR/HAN). | | | | | | |
|  | (9.0) | (148) | (620) | -59 | -248 | *EST | |
| | IP is onset of photoelectron band (83TUR/HAN). | | | | | | |
| $C_8H_{14}OSi^+$ | | | | | | | |
|  | (8.1) | (129) | (540) | -58 | -241 | *EST | 13271-67-5 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
| $C_8H_{14}O_2{}^+$ | | | | | | | |
|  | (≤8.6) | (≤86) | (≤358) | -113 | -471 | 82MOR/MER | |
| | IP from 82MOR/MER. | | | | | | |

## Table 1. Positive Ion Table - Continued

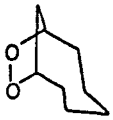
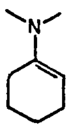
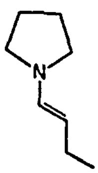
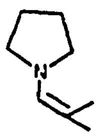
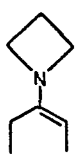
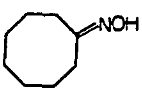
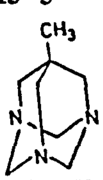
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{14}O_2{}^+$ | | | | | | | |
|  | (≤9.2) | (≤177) | (≤741) | −35 | −147 | *EST | 69492-24-6 |
| | IP from 84GLE/DOB. | | | | | | |
| $C_8H_{15}{}^+$ | | | | | | | |
| $(CH_3)_2C=C(CH_3)C(CH_3)_2$ | | (152) | (636) | | | | |
| | From proton affinity of $(CH_3)_2C=C(CH_3)C(CH_3)=CH_2$ PA = (210.6) kcal/mol, (881.) kJ/mol. | | | | | | |
| $C_8H_{15}N^+$ | | | | | | | |
|  | ≤7.50 | (≤170) | (≤711) | −3 | −12 | *EST | 13815-46-8 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | (6.7) | (153) | (642) | −1 | −4 | *EST | 13937-89-8 |
| | IP is onset of photoelectron band (81MUL/PRE2). | | | | | | |
|  | (6.8) | (160) | (671) | 4 | 15 | *EST | 2403-57-8 |
| | IP is onset of photoelectron band (81MUL/PRE2). | | | | | | |
|  | (≤7.48) | (≤193) | (≤809) | 21 | 87 | *EST | |
| | IP from 81MUL/PRE2. | | | | | | |
| $C_8H_{15}NO^+$ | | | | | | | |
|  | (8.80±0.03) | (171) | (717) | −32 | −132 | *EST | 1074-51-7 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_8H_{15}N_3{}^+$ | | | | | | | |
|  | (≤8.08) | (≤212) | (≤889) | 26 | 109 | *EST | 38705-10-1 |

Table 1. Positive Ion Table - Continued

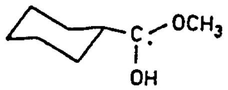
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{15}O^+$ | | | | | | | |
|  | | 98 | 410 | | | | |
| From proton affinity of cyclohexylethanone (RN 823-76-7). PA = 202.4 kcal/mol, 847. kJ/mol. | | | | | | | |
| $C_8H_{15}O_2^+$ | | | | | | | |
|  | | 51 | 212 | | | | |
| From proton affinity of methylcyclohexane carboxylate (RN 4630-82-4). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | | |
| $C_8H_{16}^+$ | | | | | | | |
| 1-$C_8H_{16}$ | 9.43±0.01 | 198 | 829 | −19.4±0.2 | −81.2±1 | 77PED/RYL | 111-66-0 |
| (Z)-2-$C_8H_{16}$ | 8.91±0.01 | (184) | (767) | −22 | −91 | *EST | 7642-04-8 |
| (E)-2-$C_8H_{16}$ | 8.91±0.01 | (183) | (765) | −23 | −95 | *EST | 13389-42-9 |
| (Z)-3-$C_8H_{16}$ | 8.85±0.01 | (183) | (764) | −21 | −90 | *EST | 14850-22-7 |
| (E)-3-$C_8H_{16}$ | 8.85±0.01 | (181) | (759) | −23 | −95 | *EST | 14919-01-8 |
| (Z)-4-$C_8H_{16}$ | 8.84±0.01 | (182) | (763) | −21 | −90 | *EST | 7642-15-1 |
| (E)-4-$C_8H_{16}$ | 8.83±0.01 | (181) | (758) | −22 | −94 | *EST | 14850-23-8 |
| $(C_2H_5)_2C=CHC_2H_5$ | (8.48±0.01) | (171) | (715) | −25 | −103 | *EST | 16789-51-8 |
| $C_2H_5CH_2C(CH_3)=C(CH_3)_2$ | (8.19±0.01) | (162) | (680) | −26 | −110 | *EST | 7145-20-2 |
| (Z)-$(CH_3)_2CHCH=CHCH(CH_3)_2$ | (8.85±0.01) | (179) | (749) | −25 | −105 | *EST | 10557-44-5 |
| (E)-$(CH_3)_2CHCH=CHCH(CH_3)_2$ | (8.84±0.01) | (178) | (743) | −26 | −110 | *EST | 692-70-6 |
| (Z)-$C_2H_5C(CH_3)=C(CH_3)C_2H_5$ | (8.17±0.01) | (162) | (678) | −26 | −110 | *EST | 19550-87-9 |
| (E)-$C_2H_5C(CH_3)=C(CH_3)C_2H_5$ | (8.16±0.01) | (162) | (677) | −26 | −110 | *EST | 19550-88-0 |
| (tert-$C_4H_9$)$CH_2C(CH_3)=CH_2$ | (8.91±0.01) | (179) | (749) | −26.4±0.2 | −110.4±1 | 77PED/RYL | 107-39-1 |
| $(C_2H_5)_2C=C(CH_3)_2$ | 8.17±0.01 | (162) | (678) | −26 | −110 | *EST | 19780-67-7 |

**Table 1. Positive Ion Table - Continued**

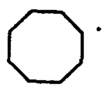
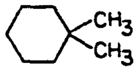
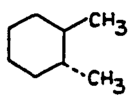
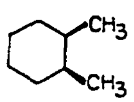
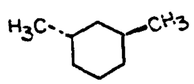
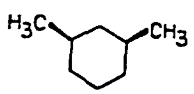
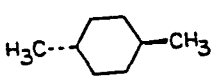
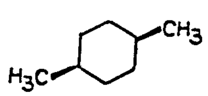
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_{16}^+$ | | | | | | | |
| $(CH_3)_2CHC(CH_3)=C(CH_3)_2$ | (8.17±0.01) | (160) | (670) | −28 | −118 | *EST | 565-77-5 |
|  | 9.76 | 195 | 817 | −29.7±0.2 | −124.4±0.9 | 77PED/RYL | 292-64-8 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenzenes. Photoelectron spectroscopy IP = 9.74±0.05 (79GOL/KUL). | | | | | | |
|  | 9.42 | 174 | 728 | −43.2±0.5 | −180.9±1.9 | 77PED/RYL | 590-66-9 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenzenes. | | | | | | |
|  | 9.41 | 174 | 728 | −43.0±0.4 | −179.9±1.8 | 77PED/RYL | 6876-23-9 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenzenes. Electron impact IP = 9.89 eV (81HER/SIC). | | | | | | |
|  | (<9.78) | (<184) | (<771) | −41.1±0.4 | −172.3±1.8 | 77PED/RYL | 2207-01-4 |
| | IP from 81HER/SIC. | | | | | | |
|  | 9.53 | 178 | 743 | −42.2±0.4 | −176.5±1.7 | 77PED/RYL | 2207-03-6 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenzenes. Electron impact IP = 9.89 eV (81HER/SIC). | | | | | | |
|  | (<9.98) | (<186) | (<778) | −44.1±0.4 | −184.6±1.7 | 77PED/RYL | 638-04-0 |
| | IP from 81HER/SIC. | | | | | | |
|  | 9.56 | 176 | 738 | −44.1±0.4 | −184.5±1.7 | 77PED/RYL | 2207-04-7 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenenes. Threshold photoionization value of IP = 9.67 eV. | | | | | | |
|  | (<9.93) | (<187) | (<781) | −42.2±0.4 | −176.6±1.7 | 77PED/RYL | 624-29-3 |
| | IP from 81HER/SIC. | | | | | | |

**Table 1. Positive Ion Table - Continued**

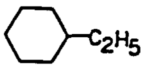
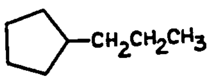
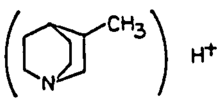
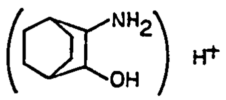
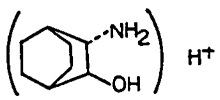
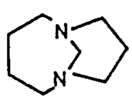
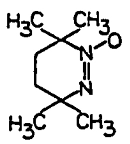
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{16}^+$ | | | | | | | |
|  | 9.54 | 178.8 | 748.1 | −41.2±0.1 | −172.4±0.6 | 77PED/RYL | 1678-91-7 |
| | IP from charge transfer equilibrium constant determinations (82SIE/MAU, 82LIA). Reference IP's, fluorobenzenes. | | | | | | |
|  | (10.00±0.04) | (195) | (817) | −35.3±0.2 | −147.8±0.6 | 77PED/RYL | 2040-96-2 |
| $C_8H_{16}N^+$ | | | | | | | |
|  | | (126) | (528) | | | | |
| | From proton affinity of 3-methyl-1-azabicyclo[2.2.2]octane (RN 695-88-5). PA = (231.7) kcal/mol, (969.) kJ/mol. | | | | | | |
| $C_8H_{16}NO^+$ | | | | | | | |
|  | | 84 | 353 | | | | |
| | From proton affinity of cis-3-aminobicyclo[2.2.2]octan-2-ol (RN 17997-65-8). PA = 223.9 kcal/mol, 937. kJ/mol. | | | | | | |
|  | | 86 | 359 | | | | |
| | From proton affinity of trans-3-aminobicyclo[2.2.2]octan-2-ol (RN 40335-14-6). PA = 220.6 kcal/mol, 923. kJ/mol. | | | | | | |
| $C_8H_{16}N_2^+$ | | | | | | | |
|  | 7.0 | (174) | (729) | 13 | 54 | *EST | |
| | IP is onset of photoelectron band (85HON/YAN). | | | | | | |
| $C_8H_{16}N_2O^+$ | | | | | | | |
|  | (≤9.13±0.03) | (≤204) | (≤854) | −6.33±0.55 | −26.48±0.3 | 83BYS | 54143-34-9 |
| $C_8H_{16}O^+$ | | | | | | | |
| n-$C_6H_{13}COCH_3$ | 9.40±0.03 | 140 | 586 | −77 | −321 | 75TRC | 111-13-7 |
| n-$C_4H_9COCH_2CH_2CH_3$ | (9.10±0.05) | (133) | (558) | −76 | −320 | 75TRC | 589-63-9 |

**Table 1. Positive Ion Table - Continued**

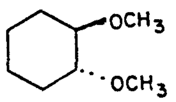
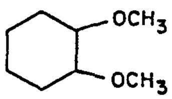
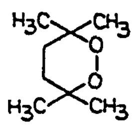
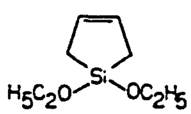
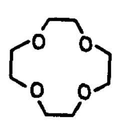
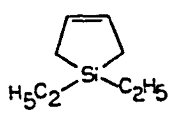
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{16}O^+$ | | | | | | | |
| tert-$C_4H_9CO$(iso-$C_3H_7$) | (8.80±0.01) | (122) | (510) | −80.8±0.3 | −338.3±1.2 | 77PED/RYL | 5857-36-3 |
| $C_8H_{16}O_2{}^+$ | | | | | | | |
|  | (8.7)<br>IP is onset of photoelectron band. | (104) | (435) | −97 | −404 | *EST | 29887-60-3 |
|  | (8.6)<br>IP is onset of photoelectron band. | (102) | (426) | −97 | −404 | *EST | 30363-80-5 |
|  | 9.2<br>IP is onset of photoelectron band. | (135) | (567) | −77 | −321 | *EST | 22431-89-6 |
| $C_8H_{16}O_2Si^+$ | | | | | | | |
|  | ≤9.44<br>IP from 81KHV/ZYK. | (≤52) | (≤216) | −166 | −695 | *EST | 67059-49-8 |
| $C_8H_{16}O_4{}^+$ | | | | | | | |
|  | (8.8)<br>IP is onset of photoelectron band (83BAK/ARM, 82LEV/LIA). | (52) | (218) | −151±0.5 | −631±2 | 82BYS/MAN | 294-93-9 |
| $C_8H_{16}Si^+$ | | | | | | | |
|  | (≤8.89)<br>IP from 81KHV/ZYK. | (≤175) | (≤734) | −30 | −124 | *EST | 69657-20-1 |
| $C_8H_{17}{}^+$ | | | | | | | |
| $(CH_3)_2CCH_2CH_2CH_2CH_2CH_3$ | From appearance potential measurement (84LOS/HOL). | 139 | 582 | | | | 40626-79-7 |

Table 1. Positive Ion Table - Continued

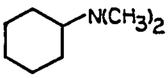
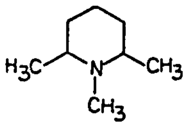
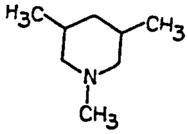
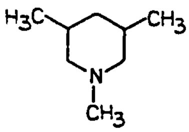
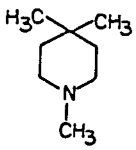
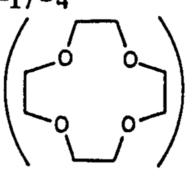
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{17}N^+$ | | | | | | | |
|  | (7.5) | (148) | (618) | −25 | −106 | *EST | 98-94-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.77) | (148) | (620) | −31 | −130 | *EST | 2439-13-6 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (7.66) | (152) | (637) | −24 | −102 | *EST | 16544-52-8 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (7.63) | (149) | (625) | −27 | −111 | *EST | 14446-76-5 |
| | IP from 82ROZ/HOU. | | | | | | |
|  | (7.77) | (148) | (621) | −31 | −129 | *EST | 1003-84-5 |
| | IP from 82ROZ/HOU. | | | | | | |
| $C_8H_{17}O_4{}^+$ | | | | | | | |
|  $H^+$ | | −7 | −29 | | | | |
| | From proton affinity of 1,4,7,10-tetraoxacyclododecane (12-Crown-4) (RN 294-93-9). PA = 221.6 kcal/mol, 927. kJ/mol. | | | | | | |
| $C_8H_{18}{}^+$ | | | | | | | |
| n-$C_8H_{18}$ | (9.82) | (177) | (739) | −49.8 | −208.5 | 74SCO | 111-65-9 |
| | | *(188)* | *(786)* | *−38.6* | *−161.4* | | |
| | IP from charge transfer equilibrium constant determinations (81MAU/SIE, 82LIA). Reference IP's, fluorobenzenes. | | | | | | |
| $(CH_3)_2CH(CH_2)_4CH_3$ | 9.84 | 176 | 734 | −51.4±0.3 | −215.1±1.4 | 74SCO | 592-27-8 |
| | | *187* | *784* | *−39.6±0.3* | *−165.9±1.4* | | |
| | IP from charge transfer equilibrium constant determinations (81MAU/SIE, 82LIA). Reference IP's, fluorobenzenes. | | | | | | |
| $(CH_3)_3CC(CH_3)_3$ | 9.8 | (172) | (720) | −53.9±0.3 | −225.7±1.1 | 77PED/RYL | 594-82-1 |
| | IP is onset of photoelectron band (81SZE/KOR, 81KIM/KAT). | | | | | | |

**Table 1. Positive Ion Table - Continued**

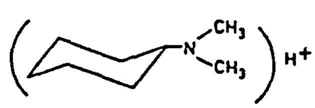
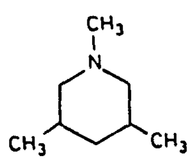
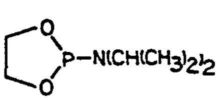
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{18}^+$ | | | | | | | |
| $(CH_3)_2CHCH_2C(CH_3)_3$ | 9.86 | (171) | (714) | -57 | -238 | *EST | 540-84-1 |
| $C_8H_{18}ClP^+$ | | | | | | | |
| $(tert\text{-}C_4H_9)_2PCl$ | (8.0) | (112) | (469) | -72 | -303 | *EST | 13716-10-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{18}FP^+$ | | | | | | | |
| $(tert\text{-}C_4H_9)_2PF$ | (8.2) | (63) | (265) | -126 | -526 | *EST | 29146-24-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{18}Hg^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_2Hg$ | (≤8.35) | (≤185) | (≤774) | -8±2 | -32±8 | 77PED/RYL | 629-35-6 |
| $(iso\text{-}C_4H_9)_2Hg$ | (≤8.30) | (≤182) | (≤763) | -9±2 | -38±8 | 77PED/RYL | 24470-76-6 |
| $C_8H_{18}N^+$ | | | | | | | |
|  | | 108 | 450 | | | | |
| | From proton affinity of N,N-dimethylcyclohexanamine (RN 98-94-2) (86TAF/GAL). PA = 232.7 kcal/mol, 974. kJ/mol. | | | | | | |
|  | | (109) | (457) | | | | |
| | From proton affinity of N,3,5-trimethylpiperidine PA = (230) kcal/mol, (962) kJ/mol, (RN 14446-76-5) (84HOP/JAH). | | | | | | |
| $C_8H_{18}NO^+$ | | | | | | | |
| $(tert\text{-}C_4H_9)_2NO$ | (6.77) | (126) | (527) | -30±3 | -126±13 | *EST | 2406-25-9 |
| $C_8H_{18}NO_2P^+$ | | | | | | | |
|  | (≤8.52) | (≤71) | (≤295) | -126 | -527 | *EST | |
| | IP from 82WOR/HAR. | | | | | | |
| $C_8H_{18}N_2^+$ | | | | | | | |
| $(E)\text{-}(tert\text{-}C_4H_9N)_2$ | (7.7) | (169) | (707) | -9±0.7 | -36±3 | 80ENG | 927-83-3 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

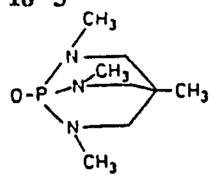
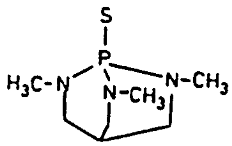
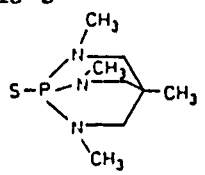
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{18}N_3OP^+$ | | | | | | | |
|  | (≤8.14±0.10) | (≤88) | (≤367) | −100 | −418 | *EST | 15199-21-0 |
| | IP from 82COW/LAT. | | | | | | |
| $C_8H_{18}N_3P^+$ | | | | | | | |
|  | (≤7.71±0.10) | (≤177) | (≤739) | −1 | −5 | *EST | 14418-26-9 |
| | IP from 82COW/LAT. | | | | | | |
| $C_8H_{18}N_3PS^+$ | | | | | | | |
|  | (≤8.14±0.10) | (≤164) | (≤688) | −23 | −97 | *EST | 15199-22-1 |
| | IP from 82COW/LAT. | | | | | | |
| $C_8H_{18}O^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_2O$ | ≤9.43 | ≤138 | ≤577 | −80 | −333 | 77PED/RYL | 142-96-1 |
| | IP from 80BAC/MOU. Value derived from hydrogen affinity considerations: 9.37 eV. | | | | | | |
| $(sec\text{-}C_4H_9)_2O$ | (9.11) | (122) | (509) | −88±0.5 | −370±2 | 77PED/RYL | 6863-58-7 |
| | IP from 81HOL/FIN. | | | | | | |
| $(tert\text{-}C_4H_9)_2O$ | 8.81 | 117 | 488 | −87±0.2 | −362±1 | 77PED/RYL | 6163-66-2 |
| | See also: 80BAC/MOU. | | | | | | |
| $C_8H_{18}OS^+$ | | | | | | | |
| $[(CH_3)_3C]_2SO$ | 8.0 | (113) | (471) | −72 | −301 | *EST | 2211-92-9 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{18}O_2^+$ | | | | | | | |
| $(tert\text{-}C_4H_9O)_2$ | (8.4) | (111) | (461) | −83±0.7 | −349±3 | 77PED/RYL | 110-05-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{18}O_2S^+$ | | | | | | | |
| $(iso\text{-}C_4H_9)_2SO_2$ | (9.54±0.05) | (92) | (384) | −128±0.7 | −536±3 | 77PED/RYL | 10495-45-1 |
| $C_8H_{18}O_4^+$ | | | | | | | |
| $(CH_3O(CH_2)_2OCH_2)_2$ | (≤9.8) | (≤69) | (≤289) | −157 | −656 | *EST | 112-49-2 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_8H_{18}S^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_2S$ | (8.2) | (149) | (624) | −40.0±0.3 | −167.3±1.1 | 77PED/RYL | 544-40-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $(iso\text{-}C_4H_9)_2S$ | 8.36±0.05 | 150 | 628 | −43±0.5 | −179±2 | 77PED/RYL | 592-65-4 |

**Table 1. Positive Ion Table - Continued**

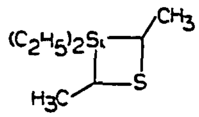
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_8H_{18}S^+$** | | | | | | | |
| (tert-$C_4H_9$)$_2$S | (8.0) | (139) | (582) | −45.1±0.2 | −188.9±0.7 | 77PED/RYL | 107-47-1 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_8H_{18}SSi^{+\cdot}$** | | | | | | | |
|  | (7.92±0.03) | (165) | (691) | (−17) | (−73) | 81GUS/VOL | |
| | IP from 81GUS/VOL. | | | | | | |
| **$C_8H_{18}S_2^+$** | | | | | | | |
| (n-$C_4H_9$S)$_2$ | (≤8.51) | (≤158) | (≤663) | −38±0.7 | −158±3 | 77PED/RYL | 629-45-8 |
| | Dialkyl disulfides undergo a change in the CSSC bond angle from 90° to 180° upon ionization; adiabatic ionization potentials are probably well below the the experimentally observed ionization onset. | | | | | | |
| (tert-$C_4H_9$S)$_2$ | (7.7) | (130) | (542) | −48±0.7 | −200±3 | 77PED/RYL | 110-06-5 |
| | IP is onset of photoelectron band. Dialkyl disulfides undergo a change in the CSSC bond angle from 90° to 180° upon ionization; adiabatic ionization potentials are probably well below the experimentally observed ionization onset. | | | | | | |
| **$C_8H_{18}Si_2^+$** | | | | | | | |
| $CH_2$=CH[Si($CH_3$)$_2$]$_2$CH=$CH_2$ | (≤8.63) | (≤166) | (≤694) | −33 | −139 | *EST | |
| | IP from 81KHV/ZYK. | | | | | | |
| **$C_8H_{19}ClNP^+$** | | | | | | | |
| ($CH_3$)$_3$CP(Cl)NHC($CH_3$)$_3$ | (≤8.75) | (≤145) | (≤606) | −57 | −238 | *EST | |
| | IP from 85ELB/ELL. | | | | | | |
| **$C_8H_{19}N^+$** | | | | | | | |
| n-$C_8H_{17}NH_2$ | (8.5) | (155) | (648) | −41 | −172 | *EST | 111-86-4 |
| | IP from 79AUE/BOW. | | | | | | |
| (n-$C_4H_9$)$_2$NH | (7.69±0.03) | (140) | (585) | −37.4±0.3 | −156.6±1.3 | 77PED/RYL | 111-92-2 |
| | Ion heat of formation predicted from hydrogen affinities of secondary amines: 143 kcal/mol, 598 kJ/mol, corresponding to IP of 7.8 eV. | | | | | | |
| (sec-$C_4H_9$)$_2$NH | (7.63) | (138) | (579) | −38 | −157 | *EST | 626-23-3 |
| | IP from 79AUE/BOW. | | | | | | |
| (i-$C_4H_9$)$_2$NH | (7.81) | (137) | (574) | −43±2 | −179±8 | 73PEP/GAF | 110-96-3 |
| | IP from 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

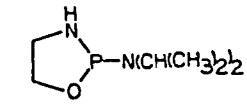
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_8H_{19}N_2OP^+$ | | | | | | | |
|  | (≤7.74) | (≤79) | (≤330) | −100 | −417 | *EST | |
| | IP from 82WOR/HAR. | | | | | | |
| $C_8H_{19}O^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_2OH$ | | 82 | 345 | | | | |
| | From proton affinity of $(n\text{-}C_4H_9)_2O$ (RN 142-96-1). PA = 203.7 kcal/mol, 852. kJ/mol. | | | | | | |
| $(sec\text{-}C_4H_9)_2OH$ | | 68 | 286 | | | | |
| | From proton affinity of $(sec\text{-}C_4H_9)_2O$ (RN 6863-58-7). PA = 209.0 kcal/mol, 874. kJ/mol. | | | | | | |
| $C_8H_{19}O_4^+$ | | | | | | | |
| $CH_3(OCH_2CH_2)_2O(H)CH_2CH_2OCH_3$ | | −15 | −64 | | | | |
| | From proton affinity of $CH_3(OCH_2CH_2)_3OCH_3$ (RN 112-49-2). PA = 224.1 kcal/mol, 938. kJ/mol. | | | | | | |
| $C_8H_{19}P^+$ | | | | | | | |
| $(tert\text{-}C_4H_9)_2PH$ | (7.9) | (132) | (551) | −50 | −211 | *EST | 819-19-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{19}S^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_2SH$ | | 117 | 490 | | | | |
| | From proton affinity of $(n\text{-}C_4H_9)_2S$ (RN 544-40-1). PA = 208.7 kcal/mol, 873. kJ/mol. | | | | | | |
| $(t\text{-}C_4H_9)_2SH$ | | 108 | 451 | | | | |
| | From proton affinity of $(t\text{-}C_4H_9)_2S$ (RN 107-47-1). PA = 212.8 kcal/mol, 890. kJ/mol. | | | | | | |
| $C_8H_{20}Ge^+$ | | | | | | | |
| $(C_2H_5)_4Ge$ | 8.9 | (167) | (698) | −38±2 | −161±8 | 77PED/RYL | 597-63-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_8H_{20}N^+$ | | | | | | | |
| $n\text{-}C_8H_{17}NH_3$ | | (104) | (436) | | | | |
| | From proton affinity of $n\text{-}C_8H_{17}NH_2$ (RN 111-86-4). PA = 220.4 kcal/mol, 922. kJ/mol. | | | | | | |
| $(n\text{-}C_4H_9)_2NH_2$ | | 100 | 417 | | | | |
| | From proton affinity of $(n\text{-}C_4H_9)_2NH$ (RN 111-92-2). PA = 228.4 kcal/mol, 956. kJ/mol. | | | | | | |
| $(sec\text{-}C_4H_9)_2NH_2$ | | (97) | (407) | | | | |
| | From proton affinity of $(sec\text{-}C_4H_9)_2NH$ (RN 626-23-3), re-evaluated (84HOP/JAH). PA = (230.9) kcal/mol, (966) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

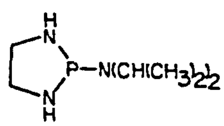
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_8H_{20}N^+$ | | | | | | | |
| (iso-$C_4H_9)_2NH_2$ | | 94 | 395 | | | | |
| | From proton affinity of (iso-$C_4H_9)_2NH$ (RN 110-96-3). PA = 228.6 kcal/mol, 956. kJ/mol. | | | | | | |
| (tert-$C_4H_9)_2NH_2$ | | 91 | 382 | | | | |
| | From proton affinity of (tert-$C_4H_9)_2NH$ (RN 21981-37-3). PA = 233.2 kcal/mol, 976. kJ/mol. | | | | | | |
| (i-$C_3H_7)_2(C_2H_5)NH$ | | (97) | (406) | | | | |
| | From proton affinity of (i-$C_3H_7)_2(C_2H_5)N$ (RN 7087-68-5). PA = 235.3 kcal/mol, 984. kJ/mol. | | | | | | |
| $(CH_3)_3C(CH_2)_2NH(CH_3)_2$ | | (100) | (417) | | | | |
| | From proton affinity of $(CH_3)_3C(CH_2)_2N(CH_3)_2$ (RN 15673-04-8). PA = 230.4 kcal/mol, 964. kJ/mol. | | | | | | |
| $C_8H_{20}N_2^+$ | | | | | | | |
| $(C_2H_5)_2NN(C_2H_5)_2$ | (6.50) | (149) | (625) | −0.5 | −2 | *EST | 4267-00-9 |
| | IP from charge transfer equilibrium constant determination (84MAU/NEL). Reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV). See also: 84NEL. | | | | | | |
| (i-$C_3H_7)_2NN(CH_3)_2$ | (6.53) | (153) | (639) | 2 | 9 | *EST | 60678-72-0 |
| | IP from charge transfer equilibrium constant determination (86RUM). | | | | | | |
| (i-$C_3H_7)(CH_3)NN(CH_3)$(i-$C_3H_7$) | (6.58) | (154) | (645) | 2 | 10 | *EST | 60678-71-9 |
| | IP from charge transfer equilibrium constant determination (86RUM). See also: 84NEL. | | | | | | |
| $C_8H_{20}N_3P^+$ | | | | | | | |
|  | (≤7.40) | (≤136) | (≤568) | −35 | −146 | *EST | |
| | IP from 82WOR/HAR. | | | | | | |
| $C_8H_{20}N_4^+$ | | | | | | | |
| $(N_2(C_2H_5)_2)_2$ | (≤7.1) | (≤213) | (≤890) | 49 | 205 | 70BEN/O'N | 13304-29-5 |
| $C_8H_{20}O_4Si^+$ | | | | | | | |
| $(C_2H_5O)_4Si$ | (≤9.77) | (≤−93) | (≤−388) | −318±5 | −1331±21 | 80TEL/RAB | 78-10-4 |
| $C_8H_{20}Pb^+$ | | | | | | | |
| $(C_2H_5)_4Pb$ | (11.1) | (282) | (1180) | 26±1 | 109±5 | 77PED/RYL | 78-00-2 |

**Table 1. Positive Ion Table - Continued**

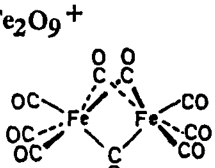
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_8H_{20}Si^+$** | | | | | | | |
| $(C_2H_5)_4Si$ | (8.9) | (142) | (594) | −63±4 | −265±15 | 77PED/RYL | 631-36-7 |
| **$C_8H_{20}Sn^+$** | | | | | | | |
| $(C_2H_5)_4Sn$ | (8.1) | (176) | (737) | −11±0.7 | −45±3 | 77PED/RYL | 597-64-8 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_8H_{21}N_2^+$** | | | | | | | |
| $(CH_3)_2NH(CH_2)_4N(CH_3)_2$ | | 108 | 450 | | | | |
| | From proton affinity of $(CH_3)_2N(CH_2)_4N(CH_3)_2$ (RN 111-51-3). PA = 246. kcal/mol, 1029. kJ/mol. | | | | | | |
| $(C_2H_5)_2NHN(C_2H_5)_2$ | | 135 | 564 | | | | |
| | From proton affinity of $(C_2H_5)_2NN(C_2H_5)_2$ (RN 4267-00-9) (84MAU/NEL). PA = 230.4 kcal/mol, 964. kJ/mol. | | | | | | |
| **$C_8H_{22}NSi^+$** | | | | | | | |
| $(CH_3)_3Si(CH_2)_3NH(CH_3)_2$ | | 75 | 312 | | | | |
| | From proton affinity of $(CH_3)_3Si(CH_2)_3N(CH_3)_2$ (RN 28247-29-2). 231.8 kcal/mol, 970. kJ/mol. | | | | | | |
| $(CH_3)_2$(tert-$C_4H_9$)$SiNH(CH_3)_2$ | | 68 | 283 | | | | |
| | From proton affinity of $(CH_3)_2$(tert-$C_4H_9$)$SiN(CH_3)_2$ (RN 66365-05-7). PA = 229.7 kcal/mol, 961. kJ/mol. | | | | | | |
| **$C_8H_{24}N_4Mo^+$** | | | | | | | |
| $((CH_3)_2N)_4Mo$ | (≤5.30) | (≤153) | (≤642) | 31±2 | 131±8 | 81CAV/CON | |
| **$C_8H_{24}O_2Si_3^+$** | | | | | | | |
| $[(CH_3)_3SiO]_2Si(CH_3)_2$ | (≤10.04) | (≤−99) | (≤−412) | −330±3 | −1381±12 | 77PED/RYL | 107-51-7 |
| | IP from 82ERM/KIR. | | | | | | |
| **$C_8H_{24}Si_3^+$** | | | | | | | |
| $Si_3(CH_3)_8$ | (7.7) | (65) | (273) | −112±4 | −470±17 | 77PED/RYL | 3704-44-7 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_9Fe_2O_9^+$** | | | | | | | |
|  | (7.91±0.01) | (−136) | (−571) | −319±6 | −1334±23 | 77PED/RYL | 15321-51-4 |

**Table 1. Positive Ion Table - Continued**

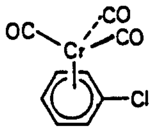
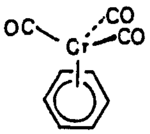
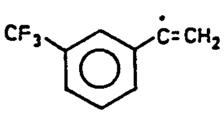
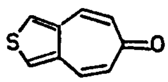
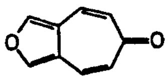
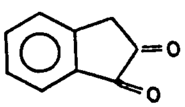
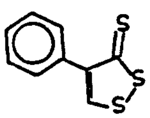
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_5ClCrO_3{}^+$ | | | | | | | |
|  | (7.00±0.1) | (74) | (311) | −87±1 | −364±6 | 77PED/RYL | 12082-03-0 |
| $C_9H_6CrO_3{}^+$ | | | | | | | |
|  | 7.0 | (78) | (325) | −84±2 | −350±9 | 77PED/RYL | 12082-08-5 |
| | IP is onset of photoelectron band. See also: 82GUI/PFI. | | | | | | |
| $C_9H_6F_3{}^+$ | | | | | | | |
|  | | 83 | 347 | | | | |
| | From proton affinity of 3-$CF_3C_6H_4C\equiv CH$ (RN 705-28-2) (85MAR/MOD). PA = 192.9 kcal/mol, 807. kJ/mol. | | | | | | |
| $C_9H_6OS^+$ | | | | | | | |
|  | (8.5) | (222) | (930) | 26 | 110 | *EST | 10095-83-7 |
| | IP is onset of photoelectron band (84GLE/BIS). | | | | | | |
| $C_9H_6O_2{}^+$ | | | | | | | |
|  | (8.65) | (190) | (795) | −10 | −40 | *EST | 18895-06-2 |
| | IP is onset of photoelectron band (84GLE/BIS). | | | | | | |
|  | (8.8) | (167) | (699) | −36 | −150 | *EST | 16214-27-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_9H_6S_3{}^+$ | | | | | | | |
|  | (7.8) | (253) | (1060) | 74±2 | 311±10 | 72GEI/RAU | 3445-76-9 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

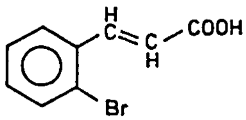
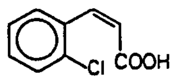
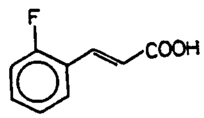
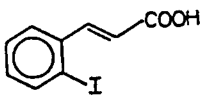
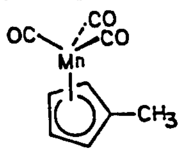
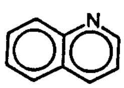
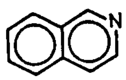
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_7BrO_2{}^+$ | | | | | | | |
|  | (8.80) IP from 84SCH. | (152) | (638) | -50 | -211 | *EST | |
| $C_9H_7ClO_2{}^+$ | | | | | | | |
|  | (8.85) IP from 84SCH. | (147) | (615) | -57 | -239 | *EST | 4513-41-1 |
| $C_9H_7FO_2{}^+$ | | | | | | | |
|  | (9.00) IP from 84SCH. | (103) | (430) | -105 | -438 | *EST | 451-69-4 |
| $C_9H_7IO_2{}^+$ | | | | | | | |
|  | (8.55) IP from 84SCH. | (160) | (668) | (-37) | (-156) | *EST | 90276-19-0 |
| $C_9H_7MnO_3{}^+$ | | | | | | | |
|  | (7.4) IP is onset of photoelectron band (81CAL/HUB, 81CAL/LIC). | (47) | (196) | -124 | -518 | *EST | 12108-13-3 |
| $C_9H_7N^+$ | | | | | | | |
|  | 8.62±0.01 | 249 | 1043 | 50±0.2 | 211±1 | 79VIS | 91-22-5 |
|  | 8.53±0.03 | 247 | 1031 | 50±0.2 | 208±1 | 79VIS/WIL | 119-65-3 |

**Table 1. Positive Ion Table - Continued**

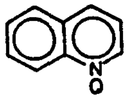
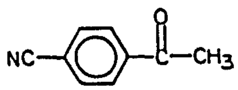
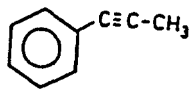
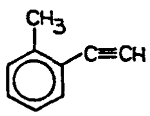
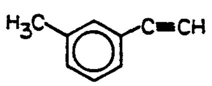
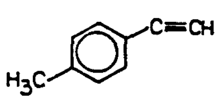
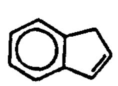
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_7NO^+$ | | | | | | | |
|  | 8.00±0.02 | (215) | (903) | 31 | 131 | *EST | 1613-37-2 |
|  | (≤9.82)<br>IP from 85GAL/GER. | (≤237) | (≤991) | 11 | 44 | *EST | 1443-80-7 |
|  | (7.9)<br>IP is onset of photoelectron band. | (213) | (890) | 31 | 128 | *EST | 1532-72-5 |
| $C_9H_8^+$ | | | | | | | |
|  | 8.41<br>See also: 81ELB/LIE. | (258) | (1079) | 64 | 268 | 85DAV/ALL | 673-32-5 |
|  | (≤8.61±0.02) | (≤264) | (≤1105) | 65 | 274 | *EST | 766-47-2 |
|  | (≤8.63±0.02) | (≤264) | (≤1106) | 65 | 273 | *EST | 766-82-5 |
|  | 8.3<br>IP is onset of photoelectron band. | (257) | (1075) | 65 | 274 | *EST | 766-97-2 |
|  | 8.14±0.01 | 227 | 948 | 39±0.2 | 163±1 | 80KUD/KUD | 95-13-6 |

**Table 1. Positive Ion Table - Continued**

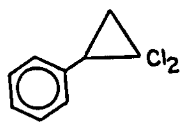
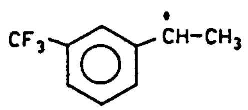
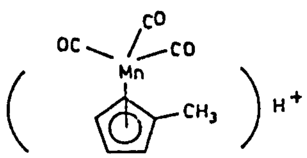
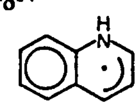
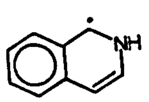
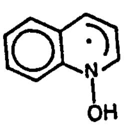
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_8^+$ | | | | | | | |
|  | (7.99) | (271) | (1134) | 87 | 363 | *EST | 14867-83-5 |
| $C_9H_8Cl_2^+$ | | | | | | | |
|  | (8.7) | (234) | (979) | 33 | 140 | *EST | 2415-80-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_9H_8F_3^+$ | | | | | | | |
|  | | 43 | 182 | | | | |
| | From proton affinity of 3-$CF_3C_6H_4CH=CH_2$ (RN 402-24-4) (84HAR/HOU). PA = 194.6 kcal/mol, 814. kJ/mol. | | | | | | |
| $C_9H_8MnO_3^+$ | | | | | | | |
|  | | (44) | (183) | | | | |
| | From proton affinity of $\eta^5$-methylcyclopentadienyl-(RN 12108-13-3). PA = (200.6) kcal/mol, (839.) kJ/mol. | | | | | | |
| $C_9H_8N^+$ | | | | | | | |
|  | | 190 | 793 | | | | |
| | From proton affinity of quinoline (RN 91-22-5). PA = (226.5) kcal/mol, 948. kJ/mol. | | | | | | |
|  | | 190 | 793 | | | | |
| | From proton affinity of isoquinoline (RN 119-65-3). PA = 225.9 kcal/mol, 945. kJ/mol. | | | | | | |
| $C_9H_8NO^+$ | | | | | | | |
|  | | 172 | 721 | | | | |
| | From proton affinity of quinoline-1-oxide (RN 1613-37-2). PA = 224.6 kcal/mol, 940. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

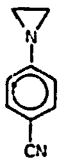
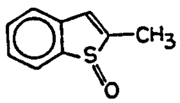
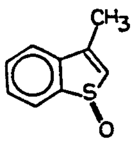
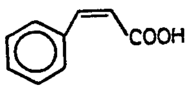
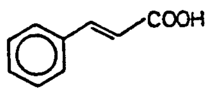
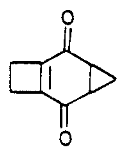
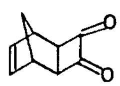
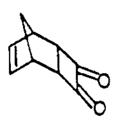
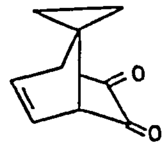
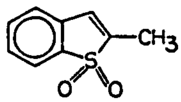
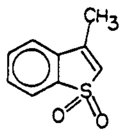
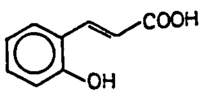
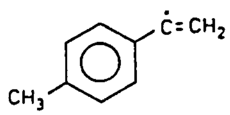
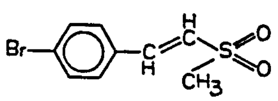
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_8N_2{}^+$ | | | | | | | |
|  | (≤8.5)<br>IP from 82CRI/LIC. | (≤299) | (≤1251) | 103 | 431 | *EST | 30855-80-2 |
| $C_9H_8OS^+$ | | | | | | | |
|  | (≤8.75)<br>IP from 82BEN/DUR. | (≤203) | (≤848) | 1 | 4 | *EST | 33945-86-7 |
|  | (8.2)<br>IP is onset of photoelectron band (82BEN/DUR). | (190) | (795) | 1 | 4 | *EST | 51500-43-7 |
| $C_9H_8O_2{}^+$ | | | | | | | |
|  | (8.90±0.05)<br>IP from 84SCH. | (155) | (649) | −50 | −210 | *EST | 102-94-3 |
|  | (9.00±0.05)<br>IP from 84SCH. | (153) | (641) | −54 | −227 | 77PED/RYL | 140-10-3 |
|  | (≤9.38)<br>IP from 85GLE/JAH. | (≤249) | (≤1043) | 33 | 138 | *EST | 94499-50-0 |
|  | (≤8.65)<br>IP from 78MAR/SCH. | (≤193) | (≤809) | −6 | −26 | *EST | |
|  | (≤8.90)<br>IP from 78MAR/SCH. | (≤204) | (≤854) | −1 | −5 | *EST | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_8O_2^+$ | | | | | | | |
|  | (8.1) | (199) | (834) | 12 | 52 | *EST | 60526-40-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_9H_8O_2S^+$ | | | | | | | |
|  | (≤9.10) | (≤158) | (≤662) | -52 | -216 | *EST | 6224-55-1 |
| | IP from 82BEN/DUR. | | | | | | |
|  | (≤9.20) | (≤160) | (≤672) | -52 | -216 | *EST | 6406-91-3 |
| | IP from 82BEN/DUR. | | | | | | |
| $C_9H_8O_3^+$ | | | | | | | |
|  | (8.50±0.05) | (93) | (389) | -103 | -431 | 84SCH | 614-60-8 |
| | IP from 84SCH. | | | | | | |
| $C_9H_9^+$ | | | | | | | |
|  | | 227 | 951 | | | | |
| | From proton affinity of 4-$CH_3C_6H_4C{\equiv}CH$ (RN 766-97-2) (85MAR/MOD). PA = 203.8 kcal/mol, 853. kJ/mol. | | | | | | |
| | | (217) | (907) | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination in $C_6H_5C(CH_3) = CH_2$ (85HON/SEG); structure may be indanyl or vinyltropylium. | | | | | | |
| $C_9H_9BrO_2S^+$ | | | | | | | |
|  | ≤8.92 | (≤174) | (≤727) | -32 | -134 | *EST | |
| | IP from 84CAU/FUR. | | | | | | |

## Table 1. Positive Ion Table - Continued

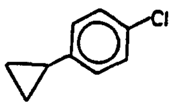
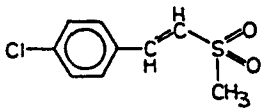
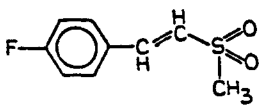
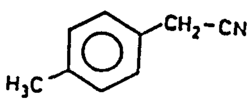
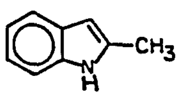
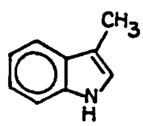
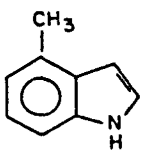
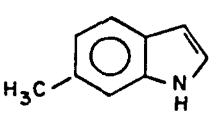
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_9Cl^+$ | | | | | | | |
|  | (≤8.64) | (≤228) | (≤953) | 28 | 119 | *EST | 1798-84-1 |
| $C_9H_9ClO_2S^+$ | | | | | | | |
|  | ≤8.94<br>IP from 84CAU/FUR. | (≤162) | (≤679) | −44 | −184 | *EST | |
| $C_9H_9FO_2S^+$ | | | | | | | |
|  | (≤9.05)<br>IP from 84CAU/FUR. | (≤145) | (≤607) | −64 | −266 | *EST | |
| $C_9H_9N^+$ | | | | | | | |
|  | (9.16±0.06) | (248) | (1037) | 36.6 | 153 | *EST | |
|  | (7.44±0.015) | (203) | (850) | 32 | 132 | *EST | 95-20-5 |
|  | (7.54±0.01) | (205) | (859) | 32 | 132 | *EST | 83-34-1 |
|  | (7.60±0.015) | (207) | (865) | 32 | 132 | *EST | 16096-32-5 |
|  | (7.54±0.015) | (205) | (859) | 32 | 132 | *EST | 3420-02-8 |

Table 1. Positive Ion Table - Continued

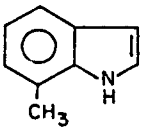
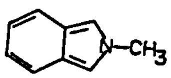
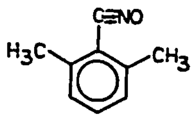
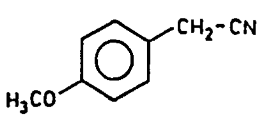
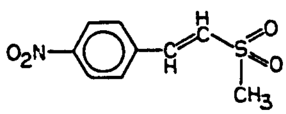
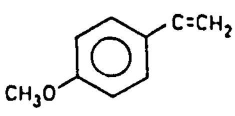
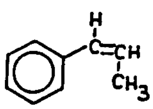
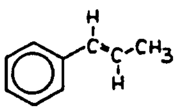
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_9N^+$ | | | | | | | |
|  | (7.53±0.015) | (205) | (859) | 32 | 132 | *EST | 933-67-5 |
|  | (≤7.12) | (≤214) | (≤895) | 50 | 208 | *EST | 33804-84-1 |
| $C_9H_9NO^+$ | | | | | | | |
|  | (8.4) | (249) | (1042) | 55 | 232 | *EST | 19111-74-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.77±0.05) | (209) | (876) | 7.1 | 30 | *EST | 104-47-2 |
| $C_9H_9NO_4S^+$ | | | | | | | |
|  | (≤9.62) | (≤181) | (≤758) | −41 | −170 | *EST | |
| | IP from 84CAU/FUR. | | | | | | |
| $C_9H_9O^+$ | | | | | | | |
|  | | 193 | 806 | | | | |
| | From proton affinity of 4-$CH_3OC_6H_4C{\equiv}CH$ (RN 768-60-5) (85MAR/MOD). PA = 210.1 kcal/mol, 879. kJ/mol. | | | | | | |
| $C_9H_{10}^+$ | | | | | | | |
|  | 8.15 | 217 | 907 | 29 | 121 | 69BEN/CRU | 766-90-5 |
| | IP from 78FU/DUN and onset of photoelectron band (81KOB/ARA). | | | | | | |
|  | (8.08) | (214) | (897) | 28 | 117 | 69BEN/CRU | 873-66-5 |
| | IP is onset of photoelectron band (81KOB/ARA). | | | | | | |

Table 1. Positive Ion Table - Continued

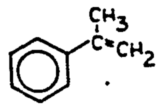
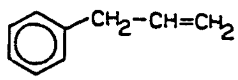
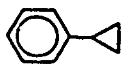
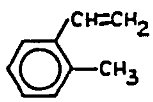
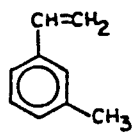
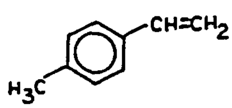
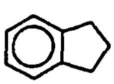
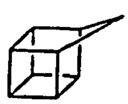
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}^+$ | | | | | | | |
|  | 8.19±0.02 | 216 | 903 | 27 | 113 | 69BEN/CRU | 98-83-9 |
|  | 8.60 | (236) | (986) | 37±2 | 156±8 | 81CHI/HYM | 300-57-2 |
| | See also: 78FU/DUN. | | | | | | |
|  | 8.35 | 229 | 957 | 36±0.2 | 151±1 | 82FUC/HAL | 873-49-4 |
| | IP from 78FU/DUN. | | | | | | |
|  | 8.20±0.02 | 217 | 909 | 28 | 118 | 69BEN/CRU | 611-15-4 |
|  | 8.15±0.02 | 215 | 901 | 27 | 115 | 69BEN/CRU | 100-80-1 |
|  | 8.1±0.1 | (214) | (896) | 27 | 115 | 69BEN/CRU | 622-97-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.3) | (206) | (862) | 15±0.2 | 61±1 | 80KUD/KUD | 496-11-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.47) | (293) | (1225) | 97±2 | 408±8 | 73ENG/AND2 | 452-61-9 |

**Table 1. Positive Ion Table - Continued**

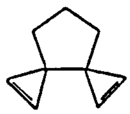
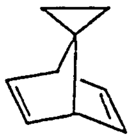
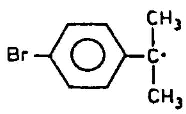
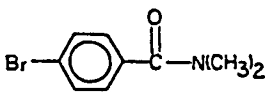
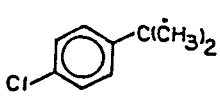
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}^+$ | | | | | | | |
|  | (8.2) | (246) | (1030) | 57 | 239 | •EST | 766-30-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.2) | (246) | (1030) | 57 | 239 | •EST | 24430-29-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.3) | (344) | (1441) | 153 | 640 | •EST | 55980-70-6 |
| | IP is onset of photoelectron band (82SPA/KOR). | | | | | | |
|  | (7.9) | (271) | (1133) | 89 | 371 | •EST | 7092-57-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_9H_{10}Br^+$ | | | | | | | |
|  | | 186 | 777 | | | | |
| | Value from appearance energy determinations (86ORL/MIS). | | | | | | |
| $C_9H_{10}BrNO^+$ | | | | | | | |
|  | (≤9.09) | (≤192) | (≤803) | −18 | −74 | •EST | 18469-37-9 |
| | IP from 85GAL/GER. | | | | | | |
| $C_9H_{10}Cl^+$ | | | | | | | |
|  | | 180 | 753 | | | | |
| | From proton affinity of 4-$ClC_6H_4C(CH_3)=CH_2$ (RN 1712-70-5). PA = 205.0 kcal/mol, 858. kJ/mol. Value from appearance energy determination (86ORL/MIS) = 171 kcal/mol, 716 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

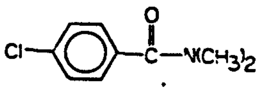
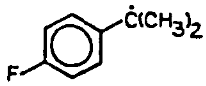
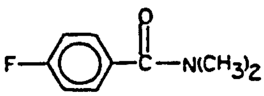
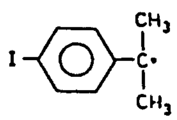
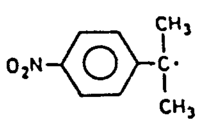
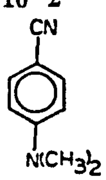
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}ClNO^+$ | | | | | | | |
|  | (≤9.16) | (≤182) | (≤760) | −30 | −124 | *EST | 14062-80-7 |
| | IP from 85GAL/GER. | | | | | | |
| $C_9H_{10}F^+$ | | | | | | | |
|  | | 138 | 579 | | | | |
| | From proton affinity of 4-$FC_6H_4C(CH_3)=CH_2$ (RN 350-40-3). PA = 206.7 kcal/mol, 865. kJ/mol. Value from appearance energy determinations (86ORL/MIS). | | | | | | |
| $C_9H_{10}FNO^+$ | | | | | | | |
|  | (≤9.13) | (≤140) | (≤587) | −70 | −294 | *EST | 24167-56-4 |
| | IP from 85GAL/GER. | | | | | | |
| $C_9H_{10}I^+$ | | | | | | | |
|  | | 199 | 833 | | | | |
| | Value from appearance energy determinations (86ORL/MIS). | | | | | | |
| $C_9H_{10}N^+$ | | | | | | | |
| $(HC{\equiv}CCH_2)_3NH$ | | (319) | (1336) | | | | |
| | From proton affinity of $(HC{\equiv}CCH_2)_3N$ (RN 6921-29-5). PA = 220.2 kcal/mol, 921. kJ/mol. | | | | | | |
| $C_9H_{10}NO_2^+$ | | | | | | | |
|  | | 189 | 789 | | | | |
| | Value from appearance energy determinations (86ORL/MIS). | | | | | | |
| $C_9H_{10}N_2^+$ | | | | | | | |
|  | (7.60) | (230) | (963) | 55 | 230 | *EST | 1197-19-9 |
| | IP is onset of photoelectron band (81MOD/DIS). | | | | | | |

**Table 1. Positive Ion Table - Continued**

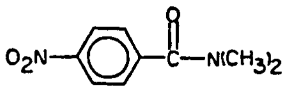
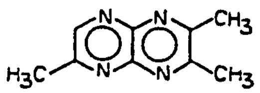
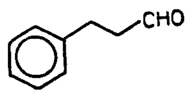
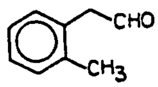
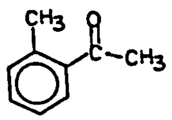
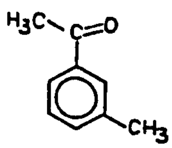
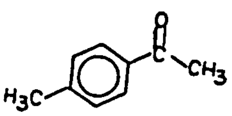
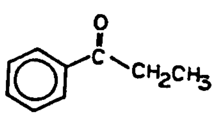
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}N_2O_3^+$ | | | | | | | |
|  | (≤9.46) | (≤192) | (≤803) | −26 | −110 | *EST | 7291-01-2 |
| | IP from 85GAL/GER. | | | | | | |
| $C_9H_{10}N_4^+$ | | | | | | | |
|  | (≤8.7) | (≤261) | (≤1090) | 60 | 251 | *EST | 6479-02-3 |
| | IP from 84GLE/SPA2 | | | | | | |
| $C_9H_{10}O^+$ | | | | | | | |
|  | (8.7±0.2) | (182) | (763) | −17 | −73 | 84DEN/AUD | 1335-10-0 |
| | IP from 84DEN/AUD. | | | | | | |
|  | (8.5) | (176) | (735) | −20 | −85 | 83AUD/MIL | 69380-02-5 |
| | IP from 83AUD/MIL. | | | | | | |
|  | (8.92) | (180) | (754) | −26 | −107 | *EST | 577-16-2 |
| | IP is onset of photoelectron band. See also: 81RAB/HEL. | | | | | | |
|  | (8.85) | (175) | (734) | −29 | −120 | *EST | 585-74-0 |
| | IP is onset of photoelectron band. See also: 81RAB/HEL. | | | | | | |
|  | (8.85) | (176) | (735) | −28 | −119 | *EST | 122-00-9 |
| | IP is onset of photoelectron band. See also: 81RAB/HEL, 85GAL/GER. | | | | | | |
|  | (9.16) | (185) | (775) | −26±0.5 | −109±2 | 77PED/RYL | 93-55-0 |
| | IP from 79MCA/TRA. | | | | | | |

**Table 1. Positive Ion Table - Continued**

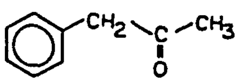
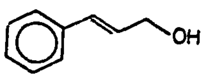
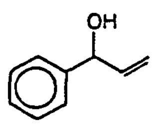
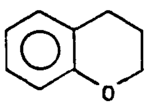
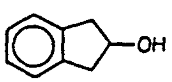
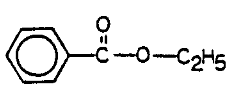
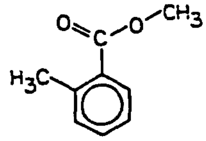
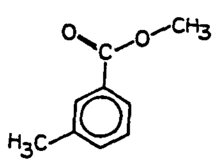
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}O^+$ | | | | | | | |
|  | (8.7) | (177) | (741) | −23.6±0.3 | −98.6±1.4 | 77PED/RYL | 103-79-7 |
| | IP is onset of photoelectron band (78CEN/FRA). | | | | | | |
|  | (8.4±0.2) | (186) | (779) | −7 | −29 | 84DEN/AUD | 104-54-1 |
| | IP from 84DEN/AUD. | | | | | | |
|  | (8.6±0.2) | (192) | (802) | −6 | −25 | 84DEN/AUD | |
| | IP from 84DEN/AUD. | | | | | | |
|  | (7.93) | (161) | (673) | −22±1 | −92±5 | 77SHA/GOL | 493-08-3 |
|  | (8.6) | (167) | (697) | −32 | −133 | 83AUD/MIL | 4254-29-9 |
| | IP from 83AUD/MIL. | | | | | | |
| $C_9H_{10}O_2^+$ | | | | | | | |
|  | (8.9) | (128) | (537) | −77 | −322 | *EST | 93-89-0 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (8.6) | (123) | (514) | −75 | −316 | *EST | 89-71-4 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (8.5) | (119) | (499) | −77 | −321 | *EST | 99-36-5 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |

Table 1. Positive Ion Table - Continued

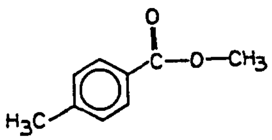
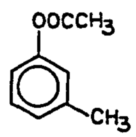
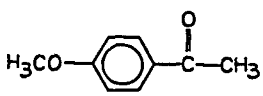
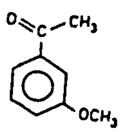
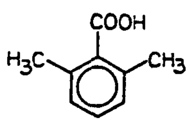
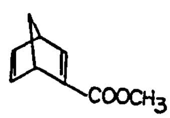
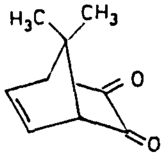
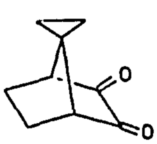
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}O_2^+$ | | | | | | | |
|  | (8.4) | (117) | (489) | −77 | −321 | *EST | 99-75-2 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | (8.98±0.2) | (132) | (553) | −75±0.5 | −313±2 | 77PED/RYL | 122-46-3 |
|  | 8.2±0.1 | (132) | (552) | −57 | −239 | *EST | 100-06-1 |
| | See also: 85GAL/GER. | | | | | | |
|  | (8.53±0.05) | (137) | (573) | −59.8±1 | −250±4 | *EST | 586-37-8 |
|  | (8.9) | (124) | (517) | −81.6±0.4 | −341.6±1.7 | 84COL/JIM | 632-46-2 |
| | IP from 81MEE/WAH. | | | | | | |
|  | (≤8.92) | (≤176) | (≤737) | −30 | −124 | *EST | 3604-36-2 |
| | IP from 83HOU/RON. | | | | | | |
|  | (8.2) | (155) | (649) | −34 | −142 | *EST | 60526-42-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.3) | (≤191) | (≤799) | −23 | −98 | *EST | 94499-48-6 |
| | IP from 85GLE/JAH. | | | | | | |

Table 1. Positive Ion Table - Continued

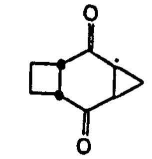
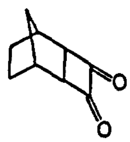
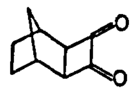
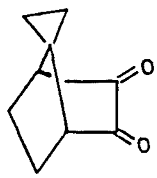
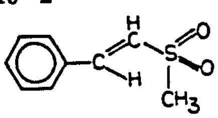
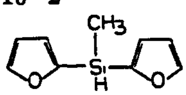
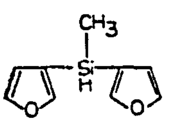
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{10}O_2^+$ | | | | | | | |
|  | (9.14)<br>IP is onset of photoelectron band (85GLE/JAH). | (187) | (784) | −23 | −98 | *EST | 94595-48-9 |
|  | (≤8.85)<br>IP from 78MAR/SCH. | (≤167) | (≤699) | −37 | −155 | *EST | 67843-62-3 |
|  | (≤8.85)<br>IP from 78MAR/SCH. | (≤160) | (≤668) | −44 | −186 | *EST | 67843-61-2 |
|  | (8.4)<br>IP is onset of photoelectron band. | (243) | (1017) | 49 | 207 | *EST | 70705-73-6 |
| $C_9H_{10}O_2S^+$ | | | | | | | |
|  | (8.7)<br>IP from 84CAU/FUR. | (164) | (684) | −37 | −155 | *EST | |
| $C_9H_{10}O_2Si^+$ | | | | | | | |
|  | (8.0)<br>IP is onset of photoelectron band (83ZYK/ERC). | (156) | (651) | −29 | −121 | *EST | 1911-24-6 |
|  | (8.1)<br>IP is onset of photoelectron band (83ZYK/ERC). | (157) | (661) | −29 | −121 | *EST | 73357-16-1 |

**Table 1. Positive Ion Table - Continued**

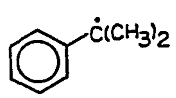
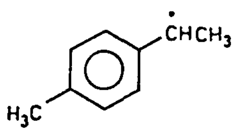
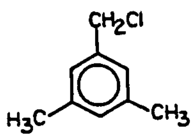
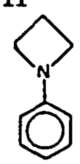
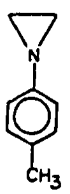
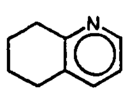
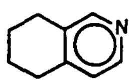
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{11}{}^+$ | | | | | | | |
|  | (6.6) | (186)<br>*(196)* | (777)<br>*(821)* | 32.4±1.5 | 135.5±6.3 | 81ROB/STE | 16804-70-9 |
| | Value at 298 K from proton affinity of $C_6H_5C(CH_3)=CH_2$ (RN 98-83-9). PA = 207.0 kcal/mol, 866. kJ/mol Value at 0 K from appearance potential measurements (83BRA/BAE, 85BUT/LER). See also: 85DOM/LAK. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
|  | | 186 | 780 | | | | |
| | From proton affinity of $4\text{-}CH_3C_6H_4CH=CH_2$ (RN 622-97-9) (84HAR/HOU). PA = 206.8 kcal/mol, 865. kJ/mol. | | | | | | |
| $C_9H_{11}Cl^+$ | | | | | | | |
|  | (8.63±0.03) | (187) | (784) | -12 | -49 | *EST | 2745-54-2 |
| $C_9H_{11}N^+$ | | | | | | | |
|  | (7.1) | (222) | (929) | 58 | 244 | *EST | 3334-89-2 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (≤8.0) | (≤248) | (≤1037) | 63 | 265 | *EST | 38201-24-0 |
| | IP from 82CRI/LIC. | | | | | | |
|  | (≤9.15) | (≤229) | (≤957) | 18 | 74 | *EST | 10500-57-9 |
| | IP from 79AUE/BOW. | | | | | | |
|  | (≤9.19) | (≤230) | (≤963) | 18 | 76 | *EST | 36556-06-6 |
| | IP from 79AUE/BOW. | | | | | | |

**Table 1. Positive Ion Table - Continued**

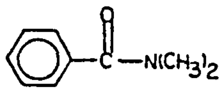
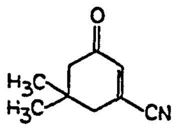
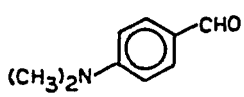
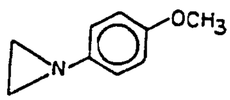
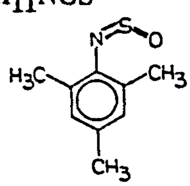
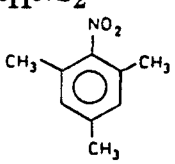
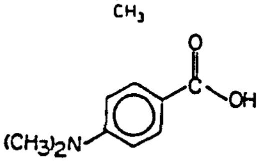
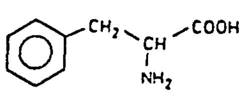
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{11}NO^+$ | | | | | | | |
|  | (≤9.04) | (≤186) | (≤777) | −23 | −95 | *EST | 611-74-5 |
| | IP from 85GAL/GER. | | | | | | |
|  | (≤9.72) | (≤214) | (≤896) | −10 | −42 | *EST | 65115-71-1 |
| | IP from 82PFI/GER. | | | | | | |
|  | 7.36±0.02 | (160) | (670) | −10 | −40 | *EST | 100-10-7 |
| | See also: 85GAL/GER. | | | | | | |
|  | (≤7.6) | (≤210) | (≤880) | 35 | 147 | *EST | 27347-09-7 |
| | IP from 82CRI/LIC. | | | | | | |
| $C_9H_{11}NOS^+$ | | | | | | | |
|  | (8.2) | (160) | (670) | −29 | −121 | *EST | |
| | IP is onset of photoelectron band (82LOU/VAN). | | | | | | |
| $C_9H_{11}NO_2^+$ | | | | | | | |
|  | (8.8) | (200) | (836) | −3 | −13 | *EST | 603-71-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.1) | (97) | (405) | −67 | −280 | *EST | 619-84-1 |
| | IP is onset of photoelectron band (81MEE/WAH). | | | | | | |
|  | 8.4 | 119 | 497 | −74.8±0.3 | −312.9±1.2 | 77PED/RYL | 150-30-1 |
| | See also: 83CAN/HAM. | | | | | | |

**Table 1. Positive Ion Table - Continued**

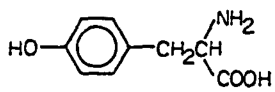
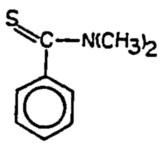
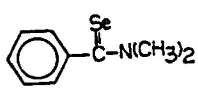
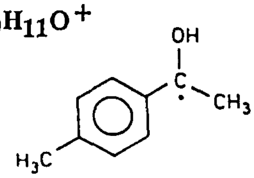
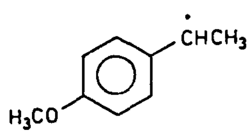
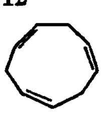
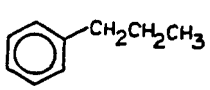
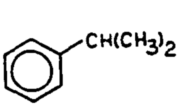
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{11}NO_3^+$ | | | | | | | |
|  | (8.0) | (68) | (286) | −116 | −486 | *EST | 556-03-6 |
| | IP is onset of photoelectron band(83CAN/HAM). | | | | | | |
| $C_9H_{11}NS^+$ | | | | | | | |
|  | (≤7.70) | (≤212) | (≤885) | 34 | 142 | *EST | 15482-60-7 |
| | IP from 82BER/HEN. | | | | | | |
| $C_9H_{11}NSe^+$ | | | | | | | |
|  | (≤7.33) | (≤220) | (≤919) | 51 | 212 | *EST | 13120-03-1 |
| | IP from 82BER/HEN. | | | | | | |
| $C_9H_{11}O^+$ | | | | | | | |
|  | | 128 | 535 | | | | |
| | From proton affinity of $(4\text{-}CH_3)C_6H_4COCH_3$ (RN 122-00-9). PA = 208.7 kcal/mol, 873. kJ/mol. | | | | | | |
|  | | 150 | 628 | | | | |
| | From proton affinity of $(4\text{-}CH_3O)C_6H_4CH=CH_2$ (RN 637-69-4) (84HAR/HOU). PA = 214.4 kcal/mol, 897. kJ/mol. | | | | | | |
| $C_9H_{12}^+$ | | | | | | | |
|  | 8.43±0.02 | 228 | 954 | 34 | 141 | 76JEN | 696-86-6 |
|  | 8.72±0.01 | 203 | 849 | 1.9±0.2 | 7.9±0.7 | 77PED/RYL | 103-65-1 |
| | Value from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See also: 82SEL/HEL. | | | | | | |
|  | 8.73±0.01 | 202 | 846 | 1.0±0.2 | 4.0±1.0 | 77PED/RYL | 98-82-8 |
| | Value from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See also: 84HOW/GON. | | | | | | |

**Table 1. Positive Ion Table - Continued**

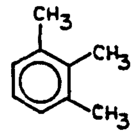
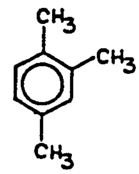
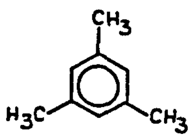
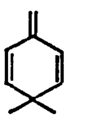
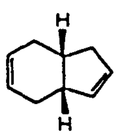
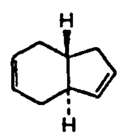
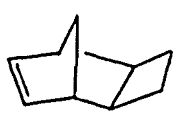
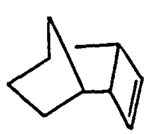
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}{}^+$ | | | | | | | |
|  | 8.42±0.02 | 192 | 803 | −2.3±0.2 | −9.5±1.1 | 77PED/RYL | 526-73-8 |
| | From charge transfer equilibrium constant determinations (78LIA/AUS). See: 84HOW/GON. | | | | | | |
|  | 8.27±0.01 | 187 | 784 | −3.3±0.2 | −13.8±1.0 | 77PED/RYL | 95-63-6 |
| | IP from 77ROS/DRA, 84HOW/GON. | | | | | | |
|  | 8.41±0.01 | 190 | 795 | −3.8±0.3 | −15.9±1.3 | 77PED/RYL | 108-67-8 |
| | Value from charge transfer equilibrium constant determinations (78LIA/AUS) is in agreement. See also: 83CET/LAP, 84HOW/GON. | | | | | | |
|  | (8.07) | (207) | (868) | 21 | 89 | *EST | 29304-70-9 |
| | IP from 83BAL/NEU. | | | | | | |
|  | 8.81±0.03 | 229 | 959 | 26.1±0.3 | 109±1 | 72KOZ/TIM | |
| | IP from 85TUR/PAN. | | | | | | |
|  | (8.89) | (236) | (988) | 31 | 130 | *EST | |
| | IP from 85TUR/PAN. | | | | | | |
|  | (8.3) | (231) | (965) | 39 | 164 | *EST | 16529-82-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.92±0.03) | (≤252) | (≤1056) | 47 | 195 | *EST | 16529-83-2 |

Table 1. Positive Ion Table - Continued

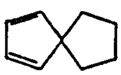
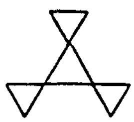
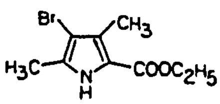
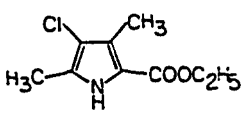
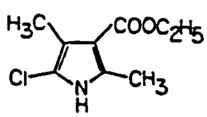
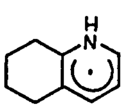
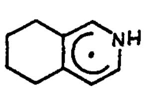
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}^+$ | | | | | | | |
|  | (8.2) | (283) | (1185) | 94.1 | 393.7 | 81GOD/SCH | 3105-29-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | ≤8.10 | (≤217) | (≤910) | 31 | 128 | *EST | 766-29-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.12) | (≤317) | (≤1325) | 106 | 445 | *EST | 31561-59-8 |
| $C_9H_{12}BrO_2^+$ | | | | | | | |
|  | (7.75) | (88) | (369) | −91 | −379 | *EST | 5408-07-1 |
| | IP is onset of photoelectron band (81CAU/GIA). | | | | | | |
| $C_9H_{12}ClNO_2^+$ | | | | | | | |
|  | (≤8.03) | (≤83) | (≤346) | −103 | −429 | *EST | 58921-31-6 |
| | IP from 81CAU/GIA. | | | | | | |
|  | (≤7.94) | (≤81) | (≤337) | −103 | −429 | *EST | 56453-93-1 |
| | IP from 81CAU/GIA. | | | | | | |
| $C_9H_{12}N^+$ | | | | | | | |
|  | | (156) | (651) | | | | |
| | From proton affinity of 2,3-cyclohexenopyridine (RN 10500-57-9).<br>PA = (227.7) kcal/mol, (953.) kJ/mol. | | | | | | |
|  | | (156) | (653) | | | | |
| | From proton affinity of 3,4-cyclohexenopyridine (RN 36566-06-6).<br>PA = (227.7) kcal/mol, (953.) kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

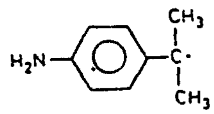
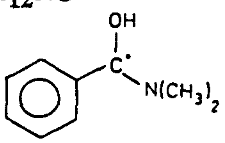
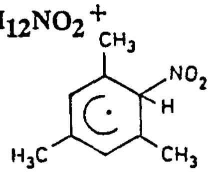
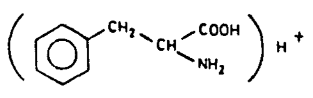
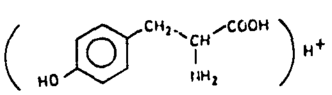
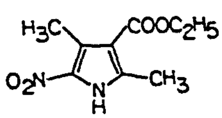
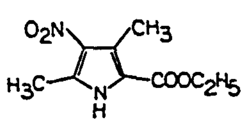
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}N^+$ | | | | | | | |
|  | | 179 | 750 | | | | |
| | From appearance energy determination (86ORL/MIS). | | | | | | |
| $C_9H_{12}NO^+$ | | | | | | | |
|  | | (122) | (510) | | | | |
| | From proton affinity of $C_6H_5CON(CH_3)_2$ (RN 611-74-5) (86TAF). PA = (221) kcal/mol, (925) kJ/mol. | | | | | | |
| $C_9H_{12}NO_2^+$ | | | | | | | |
|  | | 164 | 687 | | | | |
| | From proton affinity of 2,4,6-$(CH_3)_3C_6H_2NO_2$ (RN 603-71-4) (84ROL/HOU). PA = 198.4 kcal/mol, 830. kJ/mol. | | | | | | |
|  | | 74 | 311 | | | | |
| | From proton affinity of L-$C_6H_5CH_2CH(NH_2)COOH$ (RN 150-30-1). PA = 216.5 kcal/mol, 906. kJ/mol. | | | | | | |
| $C_9H_{12}NO_3^+$ | | | | | | | |
|  | | 27 | 114 | | | | |
| | From proton affinity of L-tyrosine. PA = 222.3 kcal/mol, 930. kJ/mol. | | | | | | |
| $C_9H_{12}N_2O_4^+$ | | | | | | | |
|  | (≤8.78) | (≤103) | (≤432) | -99 | -415 | *EST | |
| | IP from 81CAU/GIA. | | | | | | |
|  | (≤8.76) | (≤103) | (≤430) | -99 | -415 | *EST | |
| | IP from 81CAU/GIA. | | | | | | |

Table 1. Positive Ion Table - Continued

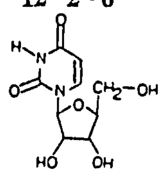
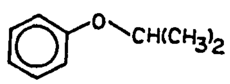
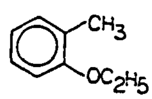
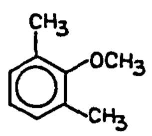
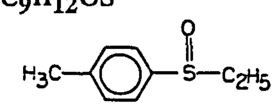
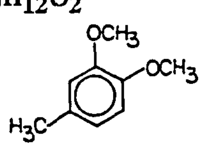
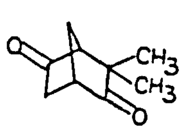
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}N_2O_6{}^+$ | | | | | | | |
|  | (9.0) | (142) | (593) | −66 | −275 | *EST | 58-96-8 |
| $C_9H_{12}O^+$ | | | | | | | |
|  | (≤8.32) | (≤159) | (≤665) | −33 | −138 | *EST | 2741-16-4 |
|  | (8.0)<br>IP from 81BAK/ARM. | (152) | (637) | −32 | −135 | *EST | 614-71-1 |
|  | 8.10±0.02 | (161) | (674) | −26 | −108 | *EST | 1004-66-6 |
| $C_9H_{12}OS^+$ | | | | | | | |
|  | (≤8.56)<br>IP from 81MOH/JIA. | (≤180) | (≤752) | −18 | −74 | *EST | 6378-07-0 |
| $C_9H_{12}O_2{}^+$ | | | | | | | |
|  | (≤7.95) | (≤122) | (≤511) | −61 | −256 | *EST | 494-99-5 |
|  | (9.0)<br>IP is onset of photoelectron band (80FRO/WES). | (143) | (599) | −64 | −269 | *EST | 38476-46-9 |

**Table 1. Positive Ion Table - Continued**

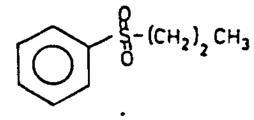
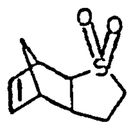
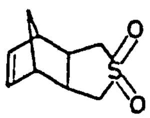
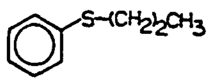
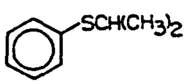
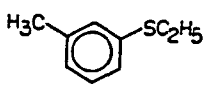
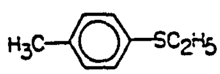
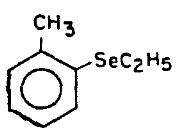
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}O_2S^+$ | | | | | | | |
|  | (9.21±0.03) | (136) | (570) | −76.3±0.5 | −319±2 | *EST | 13596-75-3 |
|  | (9.1) IP is onset of photoelectron band (84AIT/GOS). | (176) | (735) | −34 | −143 | *EST | |
|  | (9.4) IP is onset of photoelectron band (84AIT/GOS). | (183) | (764) | −34 | −143 | *EST | |
| $C_9H_{12}S^+$ | | | | | | | |
|  | (7.81±0.03) | (194) | (811) | 14 | 57 | *EST | 874-79-3 |
|  | (7.9) IP is onset of photoelectron band. | (195) | (814) | 12 | 52 | *EST | 3019-20-3 |
|  | (≤7.92) | (≤193) | (≤808) | 11 | 44 | *EST | 34786-24-8 |
|  | (8.0) IP is onset of photoelectron band. | (195) | (816) | 11 | 44 | *EST | 622-63-9 |
| $C_9H_{12}Se^+$ | | | | | | | |
|  | (7.3) IP is onset of photoelectron band (81BAK/ARM). | (193) | (806) | 24 | 102 | *EST | 37773-42-5 |

Table 1. Positive Ion Table - Continued

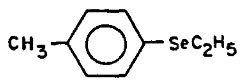
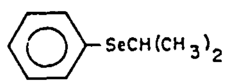
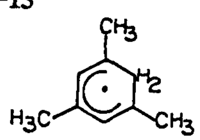
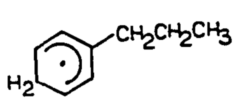
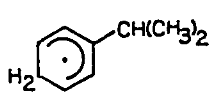
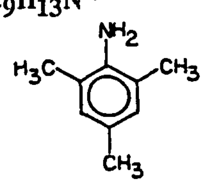
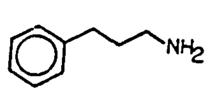
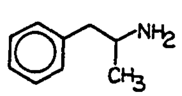
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}Se^+$ | | | | | | | |
|  | (7.1) | (187) | (784) | 24 | 99 | *EST | 37773-43-6 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
|  | (≤8.3) | (≤217) | (≤908) | 26 | 107 | *EST | 22233-89-2 |
| | IP from 81BAK/ARM. | | | | | | |
| $C_9H_{13}^+$ | | | | | | | |
|  | | 161 | 674 | | | | |
| | From proton affinity of 1,3,5-$(CH_3)_3C_6H_3$ (RN 108-67-8). PA = 200.7 kcal/mol, 840. kJ/mol. | | | | | | |
|  | | 175 | 733 | | | | |
| | From proton affinity of n-$C_3H_7C_6H_5$ (RN 103-65-1). PA = 192.4 kcal/mol, 805. kJ/mol. | | | | | | |
|  | | 175 | 730 | | | | |
| | From proton affinity of i-$C_3H_7C_6H_5$ (RN 98-82-8). PA = 192.1 kcal/mol, 804. kJ/mol. | | | | | | |
| $C_9H_{13}N^+$ | | | | | | | |
|  | (7.15) | (164) | (686) | -1 | -4 | *EST | 88-05-1 |
| | See also: 83CET/LAP | | | | | | |
|  | (≤8.89±0.12) | (≤216) | (≤902) | 11 | 44 | *EST | 2038-57-5 |
|  | (8.5) | (203) | (849) | 7 | 29 | *EST | 300-62-9 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

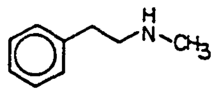
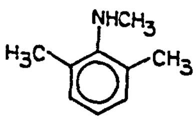
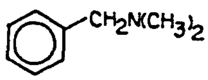
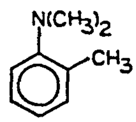
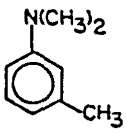
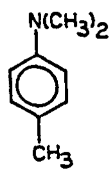
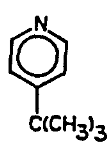
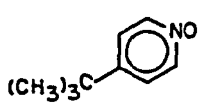
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{13}N^+$ | | | | | | | |
|  | (8.4) | (205) | (857) | 11 | 47 | *EST | 589-08-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.34) | (182) | (763) | 13 | 55 | *EST | 767-71-5 |
|  | 7.69 | (197) | (826) | 20 | 84 | *EST | 103-83-3 |
| | See also: 81LOG/TAK, 79AUE/BOW. | | | | | | |
|  | 7.40±0.02 | (195) | (813) | 24 | 99 | *EST | 609-72-3 |
|  | 7.02 | (178) | (744) | 16 | 67 | *EST | 121-72-2 |
| | IP from charge transfer equilibrium constant determinations (85LIA/JAC). Reference standard: IP ($C_6H_5N(CH_3)_2$) = 7.12 eV. | | | | | | |
|  | 6.93 | (177) | (739) | 17 | 70 | *EST | 99-97-8 |
| | IP from charge transfer equilibrium constant determinations (85LIA/JAC, 84MAU/NEL); Reference standard: IP($C_6H_5N(CH_3)_2$) = 7.12 eV. | | | | | | |
|  | (≤9.30±0.05) | (≤222) | (≤929) | 8 | 32 | *EST | 3978-81-2 |
| $C_9H_{13}NO^+$ | | | | | | | |
|  | (7.8) | (169) | (705) | −11 | −48 | *EST | 23569-17-7 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

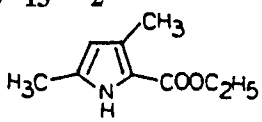
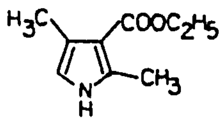
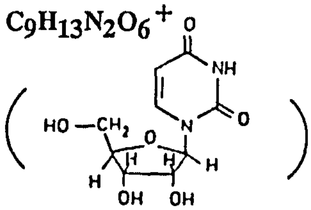
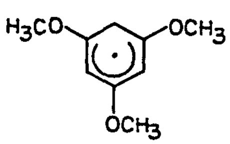
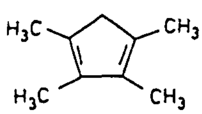
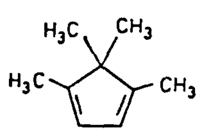
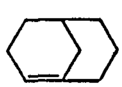
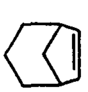
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{13}NO_2{}^+$ | | | | | | | |
|  | (≤7.91) | (≤87) | (≤363) | −96 | −400 | *EST | |
| | IP from 81CAU/GIA. | | | | | | |
|  | (≤7.95) | (≤88) | (≤367) | −96 | −400 | *EST | |
| | IP from 81CAU/GIA. | | | | | | |
| $C_9H_{13}N_2O_6{}^+$ | | | | | | | |
|  $H^+$ | | −66 | −275 | | | | |
| | From proton affinity of uridine (RN 58-96-8) PA = (208) kcal/mol, (870) kJ/mol. | | | | | | |
| $C_9H_{13}O_3{}^+$ | | | | | | | |
|  | | 55 | 228 | | | | |
| | From proton affinity of 1,3,5-$C_6H_3(OCH_3)_3$ (RN 621-23-8) PA = 220.6 kcal/mol, 923. kJ/mol. | | | | | | |
| $C_9H_{14}{}^+$ | | | | | | | |
|  | 7.8±0.1 | (183) | (768) | 4 | 15 | *EST | 4249-10-9 |
|  | 7.84±0.05 | (183) | (765) | 2 | 9 | *EST | 4249-11-0 |
|  | (8.0) | (195) | (817) | 11 | 45 | 81MAI/SCH | 17530-61-9 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.7) | (200) | (835) | −1±0.7 | −4±3 | 83JOC/DEK | 7124-86-9 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

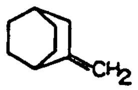
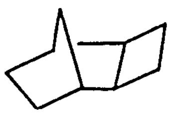
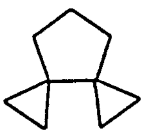
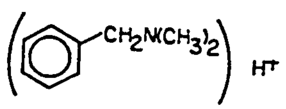
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{14}{}^+$ | | | | | | | |
|  | (≤8.87) | (≤202) | (≤847) | −2±0.7 | −9±3 | 77PED/RYL | 2972-20-5 |
|  | (8.3) | (210) | (879) | 19 | 78 | *EST | 81969-71-3 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |
|  | (8.2) | (208) | (869) | 19 | 78 | *EST | 81969-72-4 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |
|  | (≤9.65±0.03) | (≤236) | (≤987) | 13 | 56 | 73ENG/AND | 16526-28-6 |
|  | (8.8) | (211) | (884) | 8 | 35 | 73ENG/AND | 16526-27-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.73) | (208) | (872) | 7 | 30 | *EST | 873-12-1 |
|  | (8.3) | (237) | (993) | 46 | 192 | *EST | 24973-90-8 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |
| $C_9H_{14}N^+$ | | | | | | | |
|  | | (158) | (660) | | | | |
| | From proton affinity of $C_6H_5CH_2N(CH_3)_2$ (RN 103-83-3). PA = 228.1 kcal/mol, 954. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

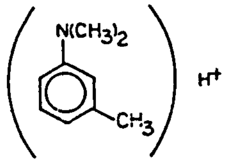
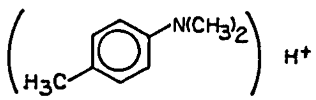
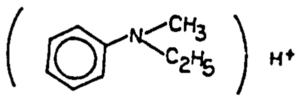
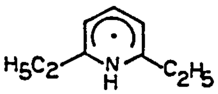
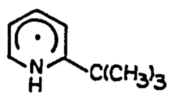
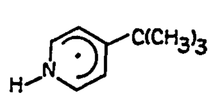
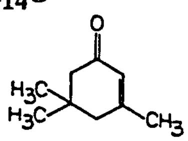
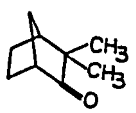
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{14}N^+$ | | | | | | | |
|  | | 157 | 658 | | | | |
| | From proton affinity of $3\text{-}CH_3C_6H_4N(CH_3)_2$ (RN 121-72-2). PA = 224.5 kcal/mol, 939. kJ/mol. | | | | | | |
|  | | 157 | 656 | | | | |
| | From proton affinity of $4\text{-}CH_3C_6H_4N(CH_3)_2$ (RN 99-97-8). PA = 225.6 kcal/mol, 944. kJ/mol. | | | | | | |
|  | | (156) | (651) | | | | |
| | From proton affinity of $C_6H_5N(CH_3)(C_2H_5)$ (RN 613-97-8). PA = 227.1 kcal/mol, 950. kJ/mol. | | | | | | |
|  | | (139) | (582) | | | | |
| | From proton affinity of 2,6-diethylpyridine (RN 935-28-4). PA = 231.1 kcal/mol, 967. kJ/mol. | | | | | | |
|  | | (145) | (607) | | | | |
| | From proton affinity of 2-tert-butylpyridine (RN 5944-41-2). PA = (227.4) kcal/mol, (951.) kJ/mol. | | | | | | |
|  | | (147) | (616) | | | | |
| | From proton affinity of 4-tert-butylpyridine (RN 3978-81-2). PA = 225.9 kcal/mol, 945. kJ/mol. | | | | | | |
| $C_9H_{14}O^+$ | | | | | | | |
|  | (≤9.07) | (≤160) | (≤669) | −49 | −206 | *EST | 78-59-1 |
| | IP from 82PFI/GER. | | | | | | |
|  | (8.6) | (144) | (603) | −54 | −227 | *EST | 13211-15-9 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |

**Table 1. Positive Ion Table - Continued**

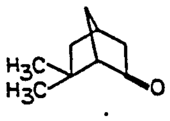
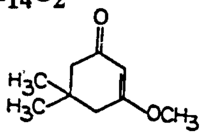
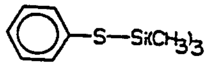
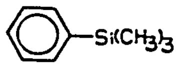
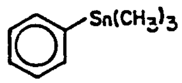
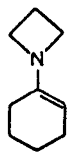
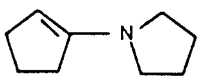
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{14}O^+$ | | | | | | | |
|  | (8.75) | (148) | (617) | −54 | −227 | *EST | 38476-45-8 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
| $C_9H_{14}O_2^+$ | | | | | | | |
|  | (≤9.35) | (≤138) | (≤576) | −78 | −326 | *EST | 4683-45-8 |
| | IP from 82PFI/GER. | | | | | | |
| $C_9H_{14}SSi^+$ | | | | | | | |
|  | (8.67±0.05) | (166) | (696) | −34 | −141 | *EST | 4551-15-9 |
| $C_9H_{14}Si^+$ | | | | | | | |
|  | 8.22 | (168) | (704) | −21 | −89 | *EST | 768-32-1 |
| | IP is onset of photoelectron band (82TRA/RED). | | | | | | |
| $C_9H_{14}Sn^+$ | | | | | | | |
|  | 8.83±0.05 | 231 | 965 | 27±1 | 113±5 | 77PED/RYL | 934-56-5 |
| $C_9H_{15}N^+$ | | | | | | | |
| $(CH_2{=}CHCH_2)_3N$ | (7.5) | (226) | (948) | 54 | 224 | *EST | 102-70-5 |
| | IP is onset of photoelectron band. See also: 79AUE/BOW. | | | | | | |
|  | (≤7.46) | (≤197) | (≤826) | 25 | 106 | *EST | 7326-44-5 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | 7.1 | (164) | (686) | 0.2 | 1 | *EST | 7148-07-4 |
| | IP from 79AUE/BOW. | | | | | | |

Table 1. Positive Ion Table - Continued

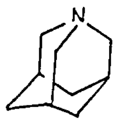
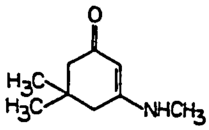
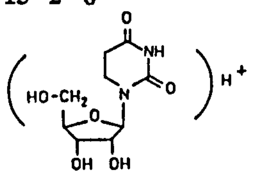
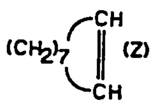
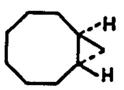
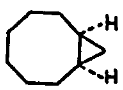
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{15}N^+$ | | | | | | | |
|  | (7.57±0.02) | (165) | (692) | −9 | −38 | *EST | 281-27-6 |
| $C_9H_{15}NO^+$ | | | | | | | |
|  | (≤8.11)<br>IP from 82PFI/GER. | (≤144) | (≤602) | −43 | −180 | *EST | 701-58-6 |
| $C_9H_{15}N_2O_6^+$ | | | | | | | |
|  | | −76 | −317 | | | | |
| | From proton affinity of 5,6-dihydrouridine (RN 5627-05-4). PA = (208) kcal/mol, (870) kJ/mol. | | | | | | |
| $C_9H_{16}^+$ | | | | | | | |
| (E)-n-$C_5H_{11}CH=CHCH=CH_2$ | (8.44)<br>IP from 81MAS/MOU. | (193) | (809) | −1 | −5 | *EST | 56700-77-7 |
| 1-$C_9H_{16}$ | (9.93±0.02) | (244) | (1020) | 15±0.7 | 62±3 | 79ROG/DAG | 3452-09-3 |
| 2-$C_9H_{16}$ | 9.30±0.02 | 225 | 941 | 11±1 | 44±3 | 79ROG/DAG | 19447-29-1 |
| 3-$C_9H_{16}$ | 9.20±0.01 | 222 | 930 | 10±0.7 | 42±3 | 79ROG/DAG | 20184-89-8 |
| 4-$C_9H_{16}$ | (9.17±0.03) | (221) | (927) | 10±0.7 | 42±3 | 79ROG/DAG | 20184-91-2 |
|  | (8.81±0.15) | (190) | (795) | −13 | −55 | 78GRE/LIE | 933-21-1 |
|  | ≤9.36 | ≤210 | ≤878 | −6.0±0.3 | −25.2±1.4 | 84WIB/LUP | 39124-79-3 |
|  | (≤9.4) | (≤211) | (≤884) | −5.5±0.2 | −23±1 | 77PED/RYL | 286-60-2 |

**Table 1. Positive Ion Table - Continued**

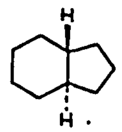
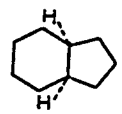
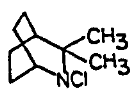
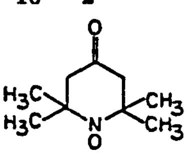
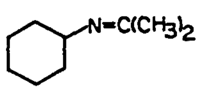
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{16}^+$ | | | | | | | |
|  | (9.46±0.06) | (187) | (782) | −31±0.5 | −131±2 | 77PED/RYL | 3296-50-2 |
| | IP from 80MIK/ZAI. | | | | | | |
|  | (9.46±0.06) | (188) | (786) | −30±0.5 | −127±2 | 77PED/RYL | 4551-51-3 |
| | IP from 80MIK/ZAI. | | | | | | |
|  | (9.35) | (185) | (774) | −31±1 | −128±3 | 77PAR/STE | 280-65-9 |
|  | (9.0) | (183) | (765) | −25 | −103 | 81MAI/SCH | 283-19-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_9H_{16}ClN^+$ | | | | | | | |
|  | (≤8.34) | (≤179) | (≤748) | −14 | −57 | *EST | 82666-06-6 |
| | IP from 82NEL/GAN. | | | | | | |
| $C_9H_{16}N^+$ | | | | | | | |
| $(CH_2=CHCH_2)_3NH$ | | (189) | (792) | | | | |
| | From proton affinity of $(CH_2=CHCH_2)_3N$ (RN 102-70-5). PA = 230.0 kcal/mol, 962. kJ/mol. | | | | | | |
| $C_9H_{16}NO_2^+$ | | | | | | | |
|  | 7.40±0.05 | 120 | 499 | −51±2 | −215±7 | 77PED/RYL | 2896-70-0 |
| $C_9H_{17}N^+$ | | | | | | | |
|  | (8.23) | (183) | (763) | −7 | −31 | *EST | 6407-36-9 |

Table 1. Positive Ion Table - Continued

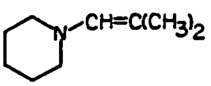
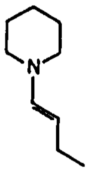
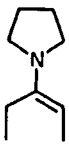
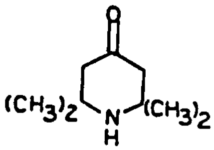
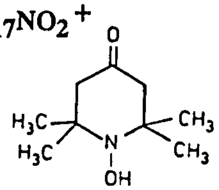
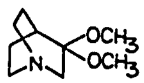
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{17}N^+$ | | | | | | | |
|  | (≤7.93±0.03) | (≤172) | (≤717) | −11 | −48 | *EST | 673-33-6 |
| | See also: 81MUL/PRE2. | | | | | | |
|  | ≤7.46 | (≤160) | (≤670) | −12 | −50 | *EST | 7182-10-7 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | (≤7.29) | (≤164) | (≤688) | −4 | −15 | *EST | 13750-57-7 |
| | IP from 81MUL/PRE2. | | | | | | |
| $C_9H_{17}NO^+$ | | | | | | | |
|  | (7.74) | (113) | (474) | −65±1 | −273±4 | 77PED/RYL | 826-36-8 |
| $C_9H_{17}NO_2^+$ | | | | | | | |
|  | (8.51±0.05) | (125) | (523) | −71±1 | −298±5 | 77PED/RYL | 3637-11-4 |
|  | (≤7.9) | (≤104) | (≤436) | −78 | −326 | *EST | |
| | IP from 79AUE/BOW. | | | | | | |
| $C_9H_{18}^+$ | | | | | | | |
| 1-$C_9H_{18}$ | (9.42±0.01) | (192) | (805) | −25±0.2 | −104±1 | 74ROG/KAN | 124-11-8 |
| n-$C_4H_9C(CH_3)=C(CH_3)_2$ | (8.14±0.01) | (157) | (655) | −31 | −131 | *EST | 3074-64-4 |
| (E)-$C_3H_7C(CH_3)=C(CH_3)C_2H_5$ | (8.08±0.01) | (155) | (649) | −31 | −130 | *EST | 3074-67-7 |
| (Z)-2-$C_9H_{18}$ | (8.90±0.01) | (179) | (748) | −26 | −111 | *EST | 6434-77-1 |
| (E)-2-$C_9H_{18}$ | (8.90±0.01) | (178) | (745) | −27 | −114 | *EST | 6434-78-2 |

Table 1. Positive Ion Table - Continued

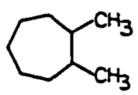
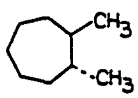
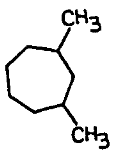
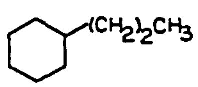
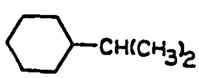
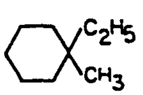
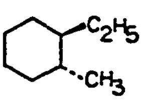
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | kJ/mol | $\Delta_fH$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_9H_{18}^+$ | | | | | | | |
| (Z)-3-$C_9H_{18}$ | (8.84±0.01) | (178) | (743) | −26 | −110 | *EST | 20237-46-1 |
| (E)-3-$C_9H_{18}$ | 8.84±0.01 | (177) | (739) | −27 | −114 | *EST | 20063-92-7 |
| (Z)-4-$C_9H_{18}$ | (8.80±0.01) | (177) | (739) | −26 | −110 | *EST | 10405-84-2 |
| (E)-4-$C_9H_{18}$ | (8.81±0.01) | (176) | (736) | −27 | −114 | *EST | 10405-85-3 |
|  | (10.21) | (196) | (818) | −40 | −167 | *EST | 13151-51-4 |
| | IP from 81HER/SIC. | | | | | | |
|  | (10.31) | (196) | (820) | −42 | −175 | *EST | 13151-50-3 |
| | IP from 81HER/SIC. | | | | | | |
|  | (10.41) | (197) | (824) | −43 | −180 | *EST | 13151-53-6 |
| | IP from 81HER/SIC. | | | | | | |
|  | (9.46) | (172) | (720) | −46.0±0.2 | −192.7±0.7 | 77PED/RYL | 1678-92-8 |
| | From charge transfer equilibrium constants (82SIE/MAU). Reference standards, IP's of fluorobenzenes. | | | | | | |
|  | (9.33) | (168) | (703) | −47 | −197 | *EST | 696-29-7 |
| | From charge transfer equilibrium constants (82SIE/MAU). Reference standards, IP's of fluorobenzenes. IP from photoionization threshold:9.55 eV. | | | | | | |
|  | (9.34) | (169) | (706) | −47±0.5 | −195±2 | 77PED/RYL | 4926-90-3 |
| | From charge transfer equilibrium constants (82SIE/MAU). Reference standards, IP's of fluorobenzenes. | | | | | | |
|  | (9.32) | (168) | (704) | −47±0.5 | −195±2 | 77PED/RYL | 4923-78-8 |
| | From charge transfer equilibrium constants (82SIE/MAU). Reference standards, IP's of fluorobenzenes. | | | | | | |

**Table 1. Positive Ion Table - Continued**

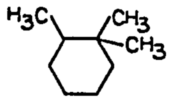
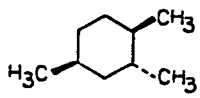
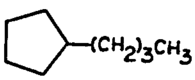
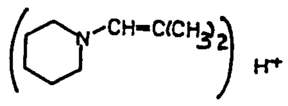
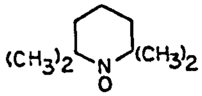
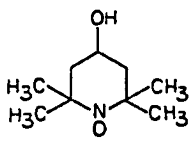
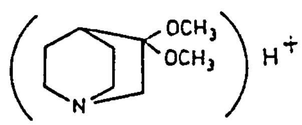
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{18}^+$ | | | | | | | |
|  | 9.39 | 160 | 671 | −56.2 | −235.1 | 69STU/WES | 3073-66-3 |
| | IP from charge transfer equilibrium constants (82SIE/MAU). Reference standards, IP's of fluorobenzenes. | | | | | | |
|  | (9.38) | (166) | (695) | −50 | −210 | *EST | 2234-75-5 |
| | IP from 82SIE/MAU. | | | | | | |
|  | (9.95±0.03) | (189) | (792) | −40 | −168 | 71ASTM | 2040-95-1 |
| $C_9H_{18}N^+$ | | | | | | | |
|  | | (128) | (534) | | | | |
| | From proton affinity of 1-(N-piperidino)isobutene (RN 673-33-6). PA = (230.7) kcal/mol, (965.) kJ/mol. | | | | | | |
| $C_9H_{18}NO^+$ | | | | | | | |
|  | (6.73) | (181) | (757) | 26±2 | 108±10 | *EST | 2564-83-2 |
| $C_9H_{18}NO_2^+$ | | | | | | | |
|  | (7.4±0.1) | (101) | (423) | −70±2 | −291±9 | 77PED/RYL | 2226-96-2 |
|  | | (56) | (233) | | | | |
| | From proton affinity of 3,3-dimethoxy-1-azabicyclo[2.2.2]octane. PA = (232) kcal/mol, (971) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

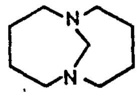
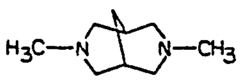
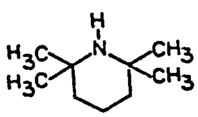
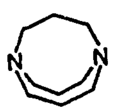
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{18}N_2^+$ | | | | | | | |
|  | 7.0 | (166) | (694) | 5 | 19 | •EST | |
| | IP is onset of photoelectron band (85HON/YAN). | | | | | | |
|  | 7.0 | (157) | (656) | −5 | −19 | •EST | |
| | IP is onset of photoelectron band (85HON/YAN). | | | | | | |
|  | (6.8) | (164) | (685) | 7 | 29 | •EST | 14789-33-4 |
| | IP is onset of photoelectron band (81LIV/ROB). | | | | | | |
| $C_9H_{18}O^+$ | | | | | | | |
| n-$C_7H_{15}COCH_3$ | (9.16) | (130) | (542) | −81±0.5 | −340±2 | 78SEL/STR2 | 821-55-6 |
| | IP from 81HOL/FIN. | | | | | | |
| (n-$C_4H_9$)$_2$CO | (9.07) | (127) | (530) | −82.4±0.3 | −344.9±1.2 | 77PED/RYL | 502-56-7 |
| | IP from 81HOL/FIN. | | | | | | |
| (iso-$C_4H_9$)$_2$CO | 9.04±0.03 | 123 | 515 | −85.5±0.3 | −357.6±1.1 | 77PED/RYL | 108-83-8 |
| (t-$C_4H_9$)$_2$CO | 8.67±0.02 | 117 | 491 | −82.6±0.3 | −345.8±1.1 | 77PED/RYL | 815-24-7 |
| $C_9H_{19}^+$ | | | | | | | |
| (n-$C_4H_9$)(n-$C_3H_7$)($CH_3$)C | | 133 | 556 | | | 84LOS/HOL | 92056-65-0 |
| | From appearance potential measurement (84LOS/HOL). | | | | | | |
| $C_9H_{19}N^+$ | | | | | | | |
|  | 7.59 | 137 | 572 | −38±0.7 | −160±3 | 81SUR/HAC | 768-66-1 |
| | IP from 82ROZ/HOU, 79AUE/BOW. | | | | | | |
| $C_9H_{19}N_2^+$ | | | | | | | |
|  | | 166 | 696 | | | | |
| | From proton affinity of 1,5-diazabicyclo[3.3.3]undecane. PA = 232.4 kcal/mol, 972. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

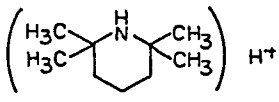
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{19}O^+$ | | | | | | | |
| (tert-$C_4H_9)_2$COH | | | | | | | |
| | | 77 | 320 | | | | |
| | From proton affinity of (tert-$C_4H_9)_2$CO (RN 815-24-7). PA = 206.5 kcal/mol, 864. kJ/mol. | | | | | | |
| $C_9H_{20}^+$ | | | | | | | |
| n-$C_9H_{20}$ | (9.72) | (170) | (709) | −54.5±0.1 | −228.4±0.6 | 74SCO | 111-84-2 |
| | | *(182)* | *(761)* | *−42.3±0.1* | *−177.1±0.6* | | |
| | IP from charge transfer equilibrium constants (81MAU/SIE, 82LIA). Reference standards, fluorobenzenes. | | | | | | |
| $C_9H_{20}N^+$ | | | | | | | |
|  | | (96) | (401) | | | | |
| | From proton affinity of 2,2,6,6-tetramethylpiperidine (RN 768-66-1). PA = (231.7) kcal/mol, (969.) kJ/mol. | | | | | | |
| $C_9H_{21}BO_3^+$ | | | | | | | |
| (n-$C_3H_7O)_3$B | (10.02) | (−26) | (−109) | −257±1 | −1076±5 | 77PED/RYL | 688-71-1 |
| $C_9H_{21}N^+$ | | | | | | | |
| (n-$C_3H_7)_3$N | (7.4) | (132) | (552) | −38±0.2 | −161±1 | *EST | 102-69-2 |
| | IP is onset of photoelectron band. | | | | | | |
| tert-$C_5H_{11}$(tert-$C_4H_9$)NH | | | | | | | |
| | (7.81±0.1) | (134) | (563) | −46±1 | −191±4 | *EST | 58471-09-3 |
| | $\Delta_f H$(Ion) predicted from hydrogen affinities of secondary amines: 131 kcal/mol, 548 kJ/mol. Corresponding IP = 7.7 eV. | | | | | | |
| $C_9H_{22}N^+$ | | | | | | | |
| (n-$C_3H_7)_3$NH | | (93) | (390) | | | | |
| | From proton affinity of (n-$C_3H_7)_3$N (RN 102-69-2). PA = 234.0 kcal/mol, 979. kJ/mol. | | | | | | |
| (tert-$C_4H_9$)C$(CH_3)_2$NH$(CH_3)_2$ | | | | | | | |
| | | (97) | (404) | | | | |
| | From proton affinity of (tert-$C_4H_9$)C$(CH_3)_2$N$(CH_3)_2$ (RN 3733-36-6). PA = 235.1 kcal/mol, 984. kJ/mol. | | | | | | |
| (tert-$C_5H_{11}$)(tert-$C_4H_9$)$NH_2$ | | | | | | | |
| | | (88) | (366) | | | | |
| | From proton affinity of (tert-$C_5H_{11}$)(tert-$C_4H_9$)NH (RN 58471-09-3). PA = 232.5 kcal/mol, 973. kJ/mol. | | | | | | |
| $C_9H_{22}OP^+$ | | | | | | | |
| (i-$C_3H_7)_3$POH | | 17 | 73 | | | | |
| | From proton affinity of (i-$C_3H_7)_3$PO (RN 17513-58-5) (85BOL/HOU). PA = 227.5 kcal/mol, 952. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

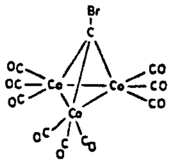
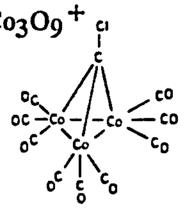
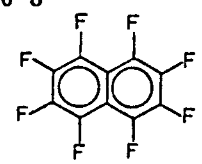
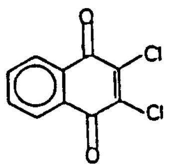
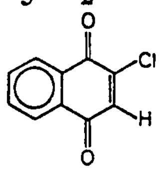
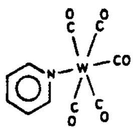
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_9H_{25}N_3OP^+$ | | | | | | | |
| $HOP(CH_2N(CH_3)_2)_3$ | | | | | | | |
| | | 51 | 214 | | | | |
| | From proton affinity of $OP(CH_2N(CH_3)_2)_3$ (RN 2327-88-0) (85BOL/HOU).<br>PA = 235. kcal/mol, 983. kJ/mol. | | | | | | |
| $C_9H_{27}NSi_3^+$ | | | | | | | |
| $((CH_3)_3Si)_3N$ | (≤8.60) | (≤38) | (≤160) | −160±3 | −670±12 | 77PED/RYL | 1586-73-8 |
| $C_{10}BrCo_3O_9^+$ | | | | | | | |
|  | 7.8 | −81 | −337 | −261±2 | −1090±9 | 82PIL/SKI | 19439-14-6 |
| | IP is onset of photoelectron band (81CHE/HAL, 82COS/LLO). See also: 82GRA/TON. | | | | | | |
| $C_{10}ClCo_3O_9^+$ | | | | | | | |
|  | 7.8 | −76 | −316 | −255±2 | −1069±10 | 82PIL/SKI | 13682-02-5 |
| | IP is onset of photoelectron band (81CHE/HAL, 82GRA/TON, 82COS/LLO). | | | | | | |
| $C_{10}F_8^+$ | | | | | | | |
|  | 8.85 | (−88) | (−368) | −292 | −1222 | *EST | 313-72-4 |
| | IP from 84HOH/DIS, 82LEV/LIA. | | | | | | |
| $C_{10}H_4Cl_2O_2^+$ | | | | | | | |
|  | (9.5) | (180) | (754) | −39±2 | −162±10 | *EST | 117-80-6 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{10}H_5ClO_2^+$ | | | | | | | |
|  | (9.6) | (189) | (789) | −33 | −137 | *EST | 1010-60-2 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{10}H_5NO_5W^+$ | | | | | | | |
|  | 7.53±0.05 | 29 | 121 | −145 | −606 | 84ALT/CON2 | 14586-49-3 |

Table 1. Positive Ion Table - Continued

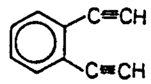
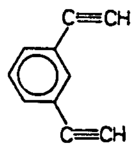
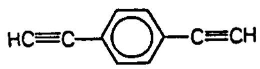
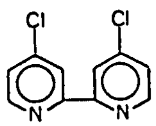
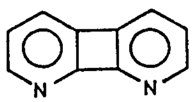
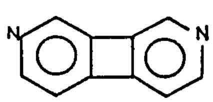
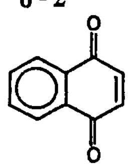
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_6^+$ | | | | | | | |
|  | (8.69±0.02) | (329) | (1378) | 129 | 540 | *EST | 21792-52-9 |
|  | (8.82±0.02) | (332) | (1390) | 129 | 539 | *EST | 1785-61-1 |
|  | (8.58±±0.02) | (327) | (1368) | 129 | 540 | *EST | 935-14-8 |
| $C_{10}H_6Cl_2N_2^+$ | | | | | | | |
|  | (8.8) | (257) | (1074) | 54 | 225 | *EST | 1762-41-0 |
| | IP is onset of photoelectron band (83DOB/HIL). | | | | | | |
| $C_{10}H_6N_2^+$ | | | | | | | |
|  | 7.7 | (309) | (1294) | 132 | 551 | *EST | |
| | IP is onset of photoelectron band (85YAM/HIG). | | | | | | |
|  | 8.3 | (323) | (1352) | 132 | 551 | *EST | |
| | IP is onset of photoelectron band (85YAM/HIG). | | | | | | |
| $C_{10}H_6O_2^+$ | | | | | | | |
|  | 9.56±0.01 | 194 | 811 | -27±1 | -111±4 | 77PED/RYL | 130-15-4 |
| | See also: 80RED/FRE. | | | | | | |

**Table 1. Positive Ion Table - Continued**

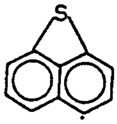
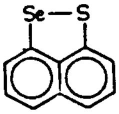
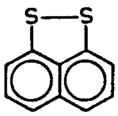
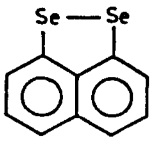
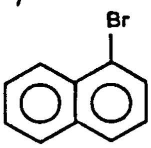
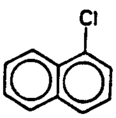
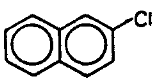
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_6S^+$ | | | | | | | |
|  | (8.0) | (262) | (1096) | 77 | 324 | *EST | 3968-63-6 |
| | IP is onset of photoelectron band (81BOC/BRA). | | | | | | |
| $C_{10}H_6SSe^+$ | | | | | | | |
|  | (≤7.14) | (≤236) | (≤986) | 71 | 297 | *EST | 64869-35-8 |
| | IP from 81BOC/BRA. | | | | | | |
| $C_{10}H_6S_2^+$ | | | | | | | |
|  | 7.14 | (222) | (931) | 58 | 242 | *EST | 209-22-3 |
| | IP from 81BOC/BRA, 82LEV/LIA. | | | | | | |
| $C_{10}H_6Se_2^+$ | | | | | | | |
|  | (7.06) | (247) | (1033) | 84 | 352 | *EST | 36579-71-2 |
| | IP from 81BOC/BRA. | | | | | | |
| $C_{10}H_7Br^+$ | | | | | | | |
|  | (8.09) | (228) | (954) | 42 | 174 | *EST | 90-11-9 |
| | IP from 83KLA/KOV. | | | | | | |
| $C_{10}H_7Cl^+$ | | | | | | | |
|  | (8.13) | (216) | (904) | 29±2 | 120±10 | 77PED/RYL | 90-13-1 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.11) | (220) | (920) | 33±2 | 137±10 | 77PED/RYL | 91-58-7 |
| | IP from 83KLA/KOV. | | | | | | |

Table 1. Positive Ion Table - Continued

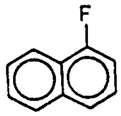
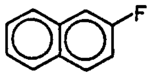
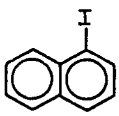
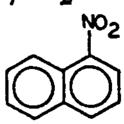
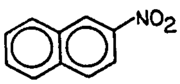
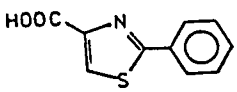
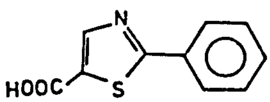
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_7F^+$ | | | | | | | |
|  | (8.15) | (200) | (835) | 12 | 49 | *EST | 321-38-0 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.23) | (201) | (843) | 12 | 49 | *EST | 323-09-1 |
| | IP from 83KLA/KOV. | | | | | | |
| $C_{10}H_7I^+$ | | | | | | | |
|  | (8.03) | (241) | (1009) | 56±2 | 234±9 | 77PED/RYL | 76279-71-5 |
| | IP from 83KLA/KOV. | | | | | | |
| $C_{10}H_7NO_2^+$ | | | | | | | |
|  | 8.60±0.01 | 234 | 980 | 36±1 | 150±5 | 77PED/RYL | 86-57-7 |
| | See also: 83KLA/KOV. | | | | | | |
|  | 8.65±0.02 | (232) | (970) | 32 | 135 | *EST | 581-89-5 |
| | IP from 83KLA/KOV, 82LEV/LIA. | | | | | | |
| $C_{10}H_7NO_2S^+$ | | | | | | | |
|  | (8.6) | (168) | (705) | -30 | -125 | *EST | 7113-10-2 |
| | IP from 84DEM/SIM. | | | | | | |
|  | (8.7) | (171) | (714) | -30 | -125 | *EST | 10058-38-5 |
| | IP from 84DEM/SIM. | | | | | | |

**Table 1. Positive Ion Table - Continued**

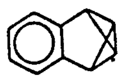
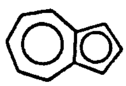
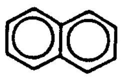
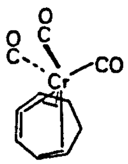
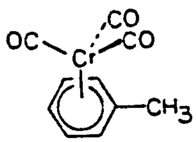
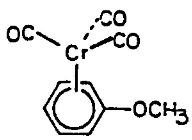
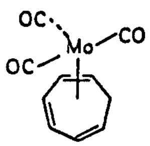
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_8^+$ | | | | | | | |
|  | (8.0) | (238) | (997) | 54 | 225 | *EST | 34305-47-0 |
| | IP is onset of photoelectron band (81GLE/GUB). | | | | | | |
|  | 7.41±0.02 | 240 | 1004 | 69±0.7 | 289±3 | 77PED/RYL | 275-51-4 |
|  | 8.14±0.01 | 223.6 | 935.8 | 35.9±0.3 | 150.4±1 | 82COL/JIM | 91-20-3 |
| $C_{10}H_8CrO_3^+$ | | | | | | | |
|  | 6.9±0.2 | (108) | (452) | −51±2 | −214±9 | 77PED/RYL | 12125-72-3 |
|  | (6.6±0.2) | (61) | (257) | −91±1 | −380±5 | 84ALT/CON | 12083-24-8 |
| $C_{10}H_8CrO_4^+$ | | | | | | | |
|  | (6.75±0.1) | (39) | (162) | −117 | −489 | 84ALT/CON | 12116-44-8 |
| $C_{10}H_8MoO_3^+$ | | | | | | | |
|  | (7.0) | (111) | (466) | −50±1 | −209±7 | 82PIL/SKI | 12125-77-8 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

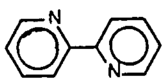
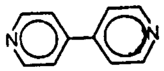
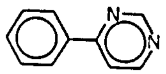
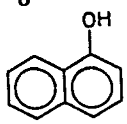
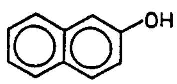
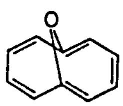
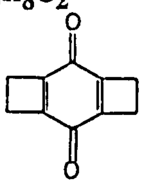
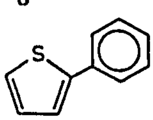
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_8N_2{}^+$ | | | | | | | |
|  | 8.35±0.02 | (262) | (1095) | 69.1±1.2 | 289.0±5.2 | 85FAO/AKA | 366-18-7 |
| | See also: 83DOB/HIL. | | | | | | |
|  | (9.10±0.02) | (283) | (1182) | 73 | 304 | *EST | 553-26-4 |
|  | (8.65) | (270) | (1131) | 71 | 296 | *EST | 3438-48-0 |
| | IP is onset of photoelectron band (84BAR/CAU). | | | | | | |
| $C_{10}H_8O^+$ | | | | | | | |
|  | 7.76±0.03 | 172 | 719 | −7.1±0.2 | −29.9±1 | 77PED/RYL | 90-15-3 |
|  | 7.85±0.05 | 174 | 727 | −7.2±0.3 | −30.3±1.2 | 77PED/RYL | 135-19-3 |
| | IP from 85OIK/ABE, 82LEV/LIA. | | | | | | |
|  | (7.9) | (230) | (962) | 48±2 | 200±10 | 77PED/RYL | 4759-11-9 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |
| $C_{10}H_8O_2{}^+$ | | | | | | | |
|  | (9.3) | (241) | (1009) | 27 | 112 | *EST | 87258-06-8 |
| | IP is onset of photoelectron band (85GLE/JAH). | | | | | | |
| $C_{10}H_8S^+$ | | | | | | | |
|  | (8.06) | (235) | (981) | 49 | 203 | *EST | 825-55-8 |

**Table 1. Positive Ion Table - Continued**

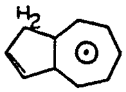
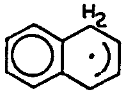
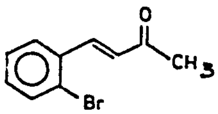
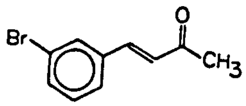
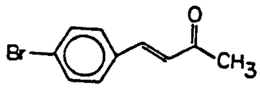
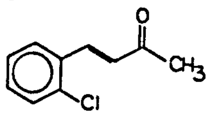
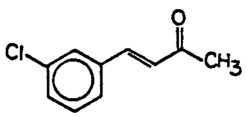
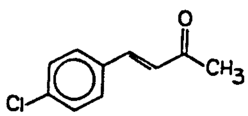
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{10}H_9{}^+$** | | | | | | | |
|  | | 215 | 898 | | | | |
| | From proton affinity of azulene (RN 275-51-4). PA = 220. kcal/mol, 921. kJ/mol. | | | | | | |
|  | | 207 | 865 | | | | |
| | From proton affinity of naphthalene (RN 91-20-3). PA = 194.7 kcal/mol, 815. kJ/mol. | | | | | | |
| **$C_{10}H_9BrO^+$** | | | | | | | |
|  | (8.7±0.05) | (202) | (843) | 1 | 4 | 79SCH/GRU | |
| | IP from 79SCH/GRU, 80GRU/SCH, 81SCH/GRO. | | | | | | |
|  | (8.9) | (206) | (862) | 1 | 4 | *EST | 65300-30-3 |
| | IP from 81SCH/GRO. | | | | | | |
|  | (8.9) | (206) | (863) | 1 | 4 | *EST | 3815-31-4 |
| | IP from 81SCH/GRO. | | | | | | |
| **$C_{10}H_9ClO^+$** | | | | | | | |
|  | (8.8) | (190) | (795) | -13 | -54 | *EST | |
| | IP from 80GRU/SCH, 81SCH/GRO. | | | | | | |
|  | (8.9) | (192) | (805) | -13 | -54 | *EST | 30626-02-9 |
| | IP from 81SCH/GRO. | | | | | | |
|  | (8.7) | (188) | (785) | -13 | -54 | *EST | 30626-03-0 |
| | IP from 81SCH/GRO. | | | | | | |

Table 1. Positive Ion Table - Continued

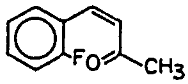
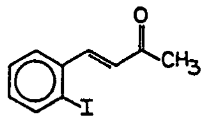
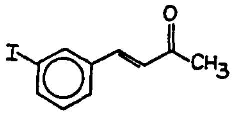
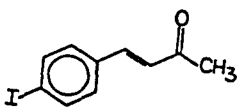
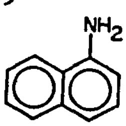
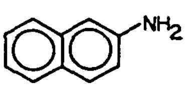
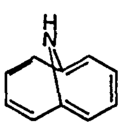
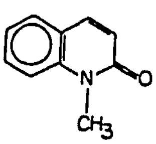
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_9FO^+$ | | | | | | | |
|  | (8.9) | (154) | (646) | −51 | −213 | 79SCH/GRU | 2143-80-8 |
| | IP from 79SCH/GRU, 80GRU/SCH. | | | | | | |
| $C_{10}H_9IO^+$ | | | | | | | |
|  | (8.6±0.05) | (214) | (895) | 16 | 65 | *EST | |
| | IP from 81SCH/GRO. See also: 80GRU/SCH. | | | | | | |
|  | (8.7±0.05) | (214) | (893) | 13 | 54 | *EST | |
| | IP from 81SCH/GRO. | | | | | | |
|  | (8.4±0.05) | (207) | (864) | 13 | 54 | *EST | |
| | IP from 81SCH/GRO. | | | | | | |
| $C_{10}H_9N^+$ | | | | | | | |
|  | (7.1) | (201) | (843) | 38±2 | 158±7 | 77PED/RYL | 134-32-7 |
| | IP is onset of photoelectron band (83KLA/KOV). | | | | | | |
|  | 7.10±0.02 | 196 | 821 | 32±3 | 136±12 | 77PED/RYL | 91-59-8 |
| | See also: 83KLA/KOV. | | | | | | |
|  | 7.75 | (266) | (1115) | 88±2 | 367±7 | 77PED/RYL | 4753-55-3 |
| | IP from 84AND/CER. | | | | | | |
| $C_{10}H_9NO^+$ | | | | | | | |
|  | (8.0) | (174) | (727) | −11 | −45 | *EST | 606-43-9 |
| | IP is onset of photoelectron band (81PFI/GUI). | | | | | | |

**Table 1. Positive Ion Table - Continued**

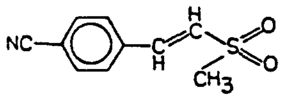
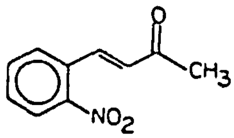
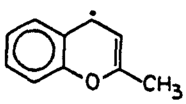
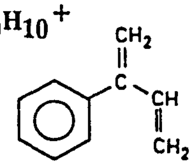
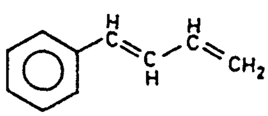
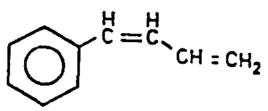
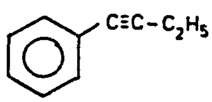
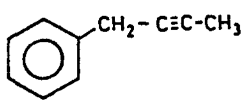
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_9NO_2S^+$ | | | | | | | |
|  | (9.0) | (203) | (849) | -4 | -19 | *EST | 69957-44-4 |
| | IP is onset of photoelectron band (84CAU/FUR). | | | | | | |
| $C_{10}H_9NO_3^+$ | | | | | | | |
|  | (9.0) | (198) | (827) | -10 | -41 | 79SCH/GRU | 20766-40-9 |
| | IP from 80GRU/SCH. | | | | | | |
| $C_{10}H_9O^+$ | | | | | | | |
|  | | (147) | (617) | | | | 45883-76-9 |
| | $\Delta_f H$(Ion) from appearance potential determinations (79SCH/GRU). | | | | | | |
| $C_{10}H_{10}^+$ | | | | | | | |
|  | 8.15±0.04 | (237) | (990) | 49 | 204 | *EST | 2288-18-8 |
| | IP from 75DER/JOC, 83DAS/GRO. | | | | | | |
|  | 8.06±0.07 | (235) | (982) | 49 | 204 | *EST | 16939-57-4 |
| | IP from 74KOP/SCH, 83DAS/GRO. | | | | | | |
|  | (8.39) | (243) | (1017) | 50 | 208 | *EST | 31915-94-3 |
|  | 8.35±0.02 | (259) | (1082) | 66 | 276 | *EST | 622-76-4 |
| | IP from 82LEV/LIA, 81ELB/LIE. See also: 74KOP/SCH. | | | | | | |
|  | (8.6) | (260) | (1089) | 62 | 259 | *EST | 33598-22-0 |
| | IP from 74KOP/SCH. | | | | | | |

Table 1. Positive Ion Table - Continued

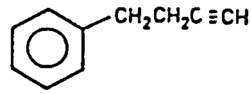
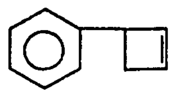
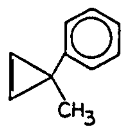
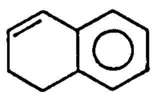
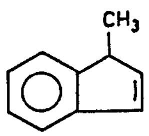
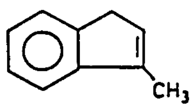
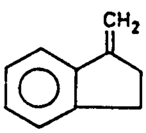
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}{}^{+}$ | | | | | | | |
|  | (8.5) | (263) | (1099) | 67 | 279 | *EST | 16520-62-0 |
| | IP from 74KOP/SCH. | | | | | | |
|  | 8.20±0.02 | (249) | (1041) | 60 | 250 | *EST | 3365-26-2 |
| | IP from 75DER/JOC, 82LEV/LIA. See also: 83DAS/GRO. | | | | | | |
|  | (8.42) | (258) | (1078) | 64 | 266 | *EST | 20211-64-7 |
| | IP from 83DAS/GRO. | | | | | | |
|  | (8.3) | (277) | (1160) | 86 | 359 | *EST | 65051-83-4 |
| | IP from 84BAI/DOM. | | | | | | |
|  | 8.07±0.04 | (214) | (897) | 28 | 119 | 77PED/RYL | 447-53-0 |
| | IP from 83DAS/GRO, 74KOP/SCH. | | | | | | |
|  | (8.27) | (226) | (945) | 35 | 147 | *EST | 767-59-9 |
| | IP from 83DAS/GRO. | | | | | | |
|  | 8.05 | (219) | (916) | 33 | 139 | *EST | 767-60-2 |
| | IP from 83DAS/GRO, 74KOP/SCH. | | | | | | |
|  | (8.00±0.02) | (220) | (921) | 36 | 149 | *EST | 1194-56-5 |
| | See also: 83DAS/GRO. | | | | | | |

Table 1. Positive Ion Table - Continued

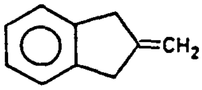
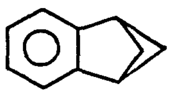
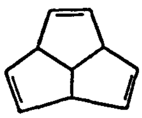
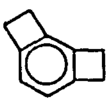
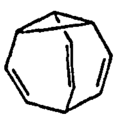
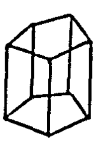
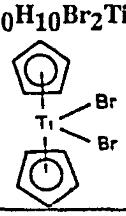
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}^+$ | | | | | | | |
|  | (8.34)<br>See also: 83DAS/GRO. | (230) | (964) | 38 | 159 | *EST | 68846-65-1 |
|  | (8.26)<br>IP from 83DAS/GRO. | (254) | (1065) | 64 | 268 | *EST | |
|  | (8.6)<br>IP is onset of photoelectron band. | (252) | (1054) | 53.5±1 | 224±4 | 86LIE/PAQ | 6053-74-3 |
|  | (8.17) | (265) | (1107) | 76 | 319 | *EST | 1610-51-1 |
|  | (8.18) | (266) | (1114) | 78 | 325 | *EST | 58436-35-4 |
|  | 8.09±0.05 | 266 | 1115 | 80±0.7 | 334±3 | 81MAN/SUN | 1005-51-2 |
|  | (8.3)<br>IP is onset of photoelectron band (82HON/EAT). | (310) | (1298) | 119±5 | 497±20 | 73ENG/AND | 4572-17-2 |
| $C_{10}H_{10}Br_2Ti^+$ | | | | | | | |
|  | ≤8.8<br>IP from 82BOH. See also: 82LEV/LIA. | (≤158) | (≤663) | −44 | −186 | *EST | 1293-73-8 |

**Table 1. Positive Ion Table - Continued**

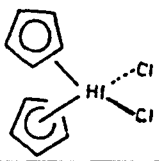
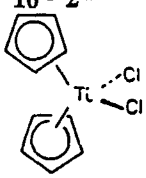
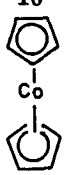
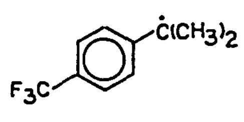
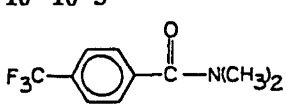
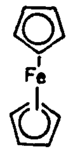
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}Cl_2Hf^+$ | | | | | | | |
|  | (8.5) | (93) | (391) | −103±0.7 | −429±3 | 82PIL/SKI | 12116-66-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{10}Cl_2Ti^+$ | | | | | | | |
|  | (8.2) | (126) | (525) | −64±2 | −266±9 | 82PIL/SKI | 1271-19-8 |
| | IP is onset of photoelectron band. See also: 82BOH. | | | | | | |
| $C_{10}H_{10}Co^+$ | | | | | | | |
|  | (5.2) | (193) | (809) | 73±1 | 307±5 | 77PED/RYL | 1277-43-6 |
| $C_{10}H_{10}Cr^+$ | | | | | | | |
|  | 5.50 | 184 | 772 | 58±1 | 241±5 | 77PED/RYL | 1271-24-5 |
| $C_{10}H_{10}F_3^+$ | | | | | | | |
|  | | 35 | 146 | | | | |
| | From proton affinity of 4-$CF_3C_6H_4C(CH_3)=CH_2$ (RN 55186-75-9). PA = 199.6 kcal/mol, 835. kJ/mol. | | | | | | |
| $C_{10}H_{10}F_3NO^+$ | | | | | | | |
|  | (≤9.38) | (≤31) | (≤128) | −186 | −777 | *EST | 25771-21-5 |
| | IP from 85GAL/GER. | | | | | | |
| $C_{10}H_{10}Fe^+$ | | | | | | | |
|  | 6.747 | 213 | 893 | 58±0.7 | 242±3 | 77PED/RYL | 102-54-5 |
| | IP from 82BAR/HEI. See also: 86VON. | | | | | | |

Table 1. Positive Ion Table - Continued

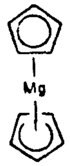
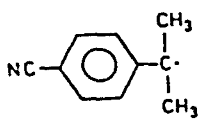
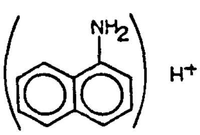
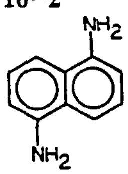
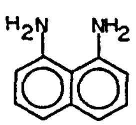
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}Mg^+$ | | | | | | | |
|  | (8.11) | (218) | (913) | 31±2 | 131±8 | 77PED/RYL | 1284-72-6 |
| $C_{10}H_{10}Mn^+$ | | | | | | | |
|  | 6.55 | 217 | 909 | 66 | 277 | 82PIL/SKI | 1271-27-8 |
| $C_{10}H_{10}N^+$ | | | | | | | |
|  | | 219 | 915 | | | | |
| | From appearance energy determinations (86ORL/MIS). | | | | | | |
|  | | 187 | 781 | | | | |
| | From proton affinity of 1-naphthalenamine (RN 134-32-7). PA = 216.9 kcal/mol, 907.5 kJ/mol. | | | | | | |
| $C_{10}H_{10}N_2^+$ | | | | | | | |
|  | (6.74±0.02) | (194) | (815) | 39 | 165 | *EST | 2243-62-1 |
|  | (6.65±0.02) | (199) | (835) | 46 | 193 | *EST | 479-27-6 |
| $C_{10}H_{10}Ni^+$ | | | | | | | |
|  | 6.2 | 228 | 955 | 85±1 | 357±5 | 77PED/RYL | 1271-28-9 |

Table 1. Positive Ion Table - Continued

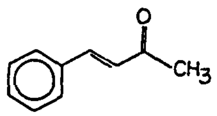
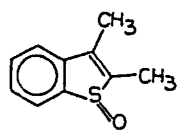
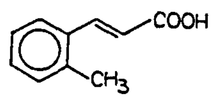
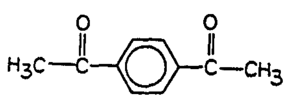
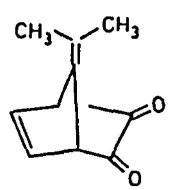
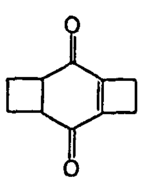
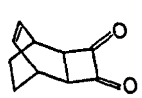
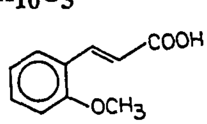
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}O^+$ | | | | | | | |
|  | (8.8±0.05)<br>IP from 79SCH/GRU, 81SCH/GRO, 80GRU/SCH. | (197) | (824) | −6 | −25 | 79SCH/GRU | 122-57-6 |
| $C_{10}H_{10}OS^+$ | | | | | | | |
|  | (≤8.40)<br>IP from 82BEN/DUR. | (≤134) | (≤561) | −60 | −249 | *EST | 70445-88-4 |
| $C_{10}H_{10}O_2^+$ | | | | | | | |
|  | (8.65±0.05)<br>IP from 84SCH. | (134) | (563) | −65 | −272 | 84SCH | 939-57-1 |
|  | (≤9.61)<br>IP from 85GAL/GER. | (≤160) | (≤670) | −61 | −257 | *EST | 1009-61-6 |
|  | (8.0)<br>IP is onset of photoelectron band. | (173) | (726) | −11 | −46 | *EST | 60526-38-7 |
|  | (≤9.25)<br>IP from 85GLE/JAH. | (≤240) | (≤1002) | 26 | 110 | *EST | 94499-49-7 |
|  | (≤9.02)<br>IP from 85ALB/HEL. | (≤157) | (≤656) | −51 | −214 | *EST | 72590-52-4 |
| $C_{10}H_{10}O_3^+$ | | | | | | | |
|  | (8.50±0.05)<br>IP from 84SCH. | (102) | (427) | −94 | −393 | 84SCH | 1011-54-7 |

**Table 1. Positive Ion Table - Continued**

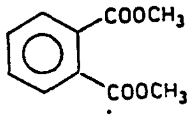
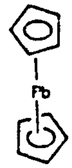
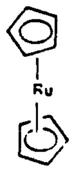
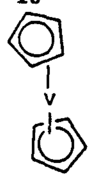
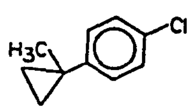
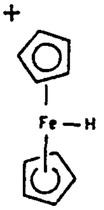
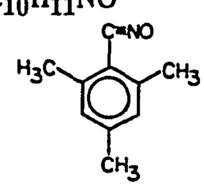
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}O_4^+$  | (9.64±0.07) | (66) | (276) | −156.2±4 | −654±17 | *EST | 131-11-3 |
| $C_{10}H_{10}Pb^+$  | (≤7.55)<br>IP from 82BAX/COW, 82LEV/LIA. | (≤308) | (≤1288) | 134 | 559 | 85DEW/HOL | 1294-74-2 |
| $C_{10}H_{10}Ru^+$  | (7.1)<br>IP is onset of photoelectron band. | (102) | (425) | −62 | −260 | *EST | 1287-13-4 |
| $C_{10}H_{10}V^+$  | (6.4)<br>IP is onset of photoelectron band. | (196) | (822) | 49±2 | 204±10 | 77PED/RYL | 1277-47-0 |
| $C_{10}H_{11}Cl^+$  | (≤8.67) | (≤221) | (≤925) | 21±1 | 88±4 | *EST | 63340-05-6 |
| $C_{10}H_{11}Fe^+$  | From proton affinity of Iron, bis($\eta^5$-cyclopentadienyl) (RN 102-54-5).<br>PA = (210) kcal/mol, (879) kJ/mol. | (214) | (893) | | | | |
| $C_{10}H_{11}NO^+$  | ≤8.37<br>IP is onset of photoelectron band. | (≤238) | (≤998) | 45 | 190 | *EST | 2904-57-6 |

Table 1. Positive Ion Table - Continued

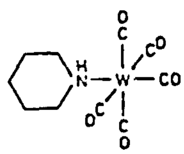
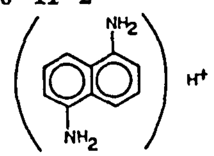
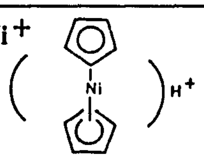
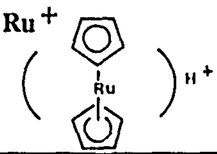
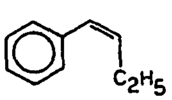
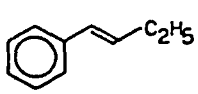
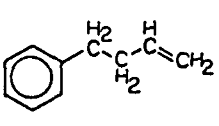
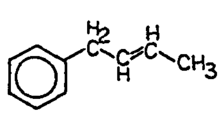
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{11}NO_5W^+$ | | | | | | | |
|  | (7.0) | (−33) | (−140) | −195 | −815 | 84ALT/CON2 | 31082-68-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{11}N_2^+$ | | | | | | | |
|  | | 188 | 787 | | | | |
| | From proton affinity of 1,8-diaminonaphthalene (RN 479-27-6). PA = 223.8 kcal/mol, 936. kJ/mol. | | | | | | |
| $C_{10}H_{11}Ni^+$ | | | | | | | |
|  | | 228 | 954 | | | | |
| | From proton affinity of Nickel, bis($\eta^5$-cyclopentadinyl) (RN 1271-28-9). PA = 223. kcal/mol, 933. kJ/mol. | | | | | | |
| $C_{10}H_{11}Ru^+$ | | | | | | | |
|  | | (86) | (358) | | | | |
| | From proton affinity of Ruthenium, bis($\eta^5$-cyclopentadienyl) (RN 1287-13-4). PA = (218) kcal/mol, (912) kJ/mol. | | | | | | |
| $C_{10}H_{12}^+$ | | | | | | | |
|  | (8.15) | (213) | (892) | 25 | 106 | *EST | 1560-09-4 |
| | IP from onset of photoelectron band (81KOB/ARA). | | | | | | |
|  | (8.0) | (208) | (873) | 24 | 101 | *EST | 1005-64-7 |
| | IP from onset of photoelectron band (81KOB/ARA). | | | | | | |
|  | (8.6) | (225) | (943) | 27 | 113 | *EST | 768-56-9 |
| | IP from 78FU/DUN. | | | | | | |
|  | (8.48) | (220) | (918) | 24 | 100 | *EST | 935-00-2 |
| | IP from 78FU/DUN. | | | | | | |

**Table 1. Positive Ion Table - Continued**

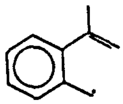
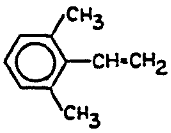
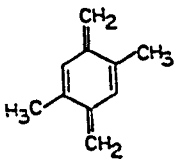
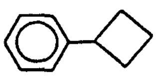
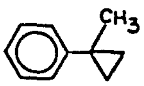
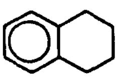
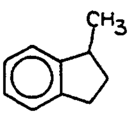
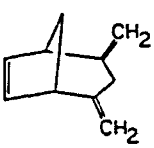
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{12}{}^+$ | | | | | | | |
|  | (7.78±0.04) | (199) | (832) | 19 | 81 | 85DAS/GRO | 1587-04-8 |
| | See also: 78FU/DUN. | | | | | | |
|  | (8.10±0.02) | (212) | (886) | 25 | 104 | *EST | 2039-90-9 |
|  | (7.4) | (205) | (856) | 34 | 142 | *EST | 63238-49-3 |
| | IP from onset of photoelectron band. See also: 82DEW. | | | | | | |
|  | (8.4) | (226) | (946) | 33 | 136 | *EST | 4392-30-7 |
| | IP from onset of photoelectron band. | | | | | | |
|  | (8.4) | (223) | (930) | 29±1 | 120±4 | *EST | 2214-14-4 |
| | IP from onset of photoelectron band. | | | | | | |
|  | 8.47 | 201 | 841 | 6±0.5 | 24±2 | 77PED/RYL | 119-64-2 |
| | See also: 80MAU. | | | | | | |
|  | (8.47) | (205) | (856) | 9 | 39 | 85DAS/GRO | 767-58-8 |
|  | ≤8.98 | ≤268 | ≤1123 | 61 | 257 | 80MAR/HEL | 72569-84-7 |

Table 1. Positive Ion Table - Continued

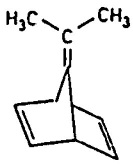
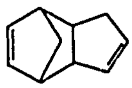
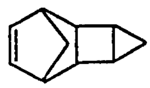
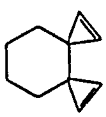
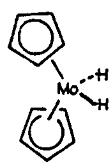
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{12}^+$ | | | | | | | |
|  | (7.97) | (249) | (1042) | 65 | 273 | *EST | 36456-22-1 |
|  | ≤9.00 | (≤238) | (≤996) | 30.5±1 | 128±4 | 86LIE/PAQ | 31678-74-7 |
|  | (8.79±0.05) | (248) | (1038) | 45±2 | 190±9 | 80ROT/KLA | 77-73-6 |
|  | ≤8.83±0.03 | ≤275 | ≤1152 | 72 | 300 | 80ROT/KLA | 6574-77-2 |
|  | 7.33±0.05 | (260) | (1087) | 91 | 380 | *EST | 36262-33-6 |
|  | (8.3)<br>IP is onset of photoelectron band (82SPA/KOR). | (298) | (1246) | 106 | 445 | *EST | 54440-40-3 |
|  | (≤7.74) | (≤269) | (≤1125) | 90 | 378 | *EST | 30353-70-9 |
| $C_{10}H_{12}Mo^+$ | | | | | | | |
|  | (≤6.4±0.1) | (≤220) | (≤920) | 72±1 | 303±6 | 86SIM/BEA | 1291-40-3 |

Table 1. Positive Ion Table - Continued

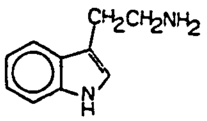
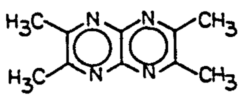
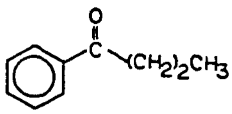
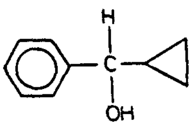
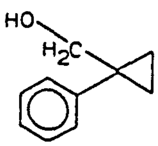
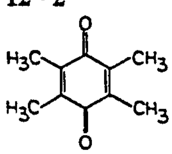
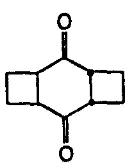
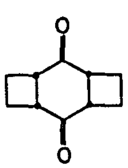
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{12}N_2^+$ | | | | | | | |
|  | (7.7) | (211) | (882) | 33 | 139 | *EST | 61-54-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{12}N_4^+$ | | | | | | | |
|  | (≤8.6) | (≤249) | (≤1040) | 50 | 210 | *EST | 6479-03-4 |
| | IP from 84GLE/SPA2. | | | | | | |
| $C_{10}H_{12}O^+$ | | | | | | | |
|  | 9.06±0.02 | 178 | 746 | −30.6±0.6 | −128.2±2.4 | 77PED/RYL | 495-40-9 |
| | IP is average of values from 79MCL/TRA and 81DAL/NIB. | | | | | | |
|  | (8.31) | (186) | (780) | −5 | −22 | 81DAL/NIB | 1007-03-0 |
| | IP from 81DAL/NIB. | | | | | | |
|  | (8.35) | (189) | (790) | −4 | −16 | 81DAL/NIB | 31729-66-5 |
| | IP from 81DAL/NIB. | | | | | | |
| $C_{10}H_{12}O_2^+$ | | | | | | | |
|  | (9.1) | (150) | (626) | −60 | −252 | *EST | 527-17-3 |
| | IP from 80BOC/KAI, 82LEV/LIA. | | | | | | |
|  | (≤9.0) | (≤180) | (≤752) | −28 | −116 | *EST | 87305-43-9 |
| | IP is onset of photoelectron band (85GLE/JAH). | | | | | | |
|  | (8.8) | (175) | (733) | −28 | −116 | *EST | 87305-42-8 |
| | IP from 85GLE/JAH. | | | | | | |

Table 1. Positive Ion Table - Continued

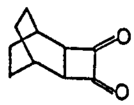
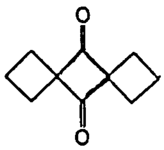
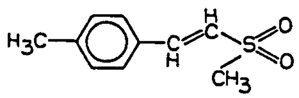
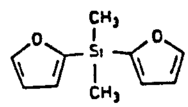
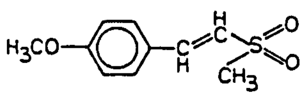
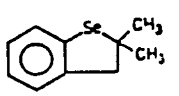
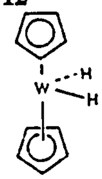
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{12}O_2{}^+$ | | | | | | | |
|  | (≤9.06)<br>IP from 85ALB/HEL. | (≤130) | (≤542) | −79 | −332 | *EST | |
|  | (9.0±0.02)<br>IP from 84OLI/FLE. | (216) | (904) | 9 | 36 | *EST | 4893-00-9 |
| $C_{10}H_{12}O_2S^+$ | | | | | | | |
|  | (8.3)<br>IP is onset of photoelectron band (84CAU/FUR). | (146) | (613) | −45 | −188 | *EST | 77355-29-4 |
| $C_{10}H_{12}O_2Si^+$ | | | | | | | |
|  | (≤8.60)<br>IP from 83ZYK/ERC. | (≤151) | (≤633) | −47 | −197 | *EST | 1578-44-5 |
| $C_{10}H_{12}O_3S^+$ | | | | | | | |
|  | (≤8.52)<br>IP from 84CAU/FUR. | (≤123) | (≤516) | −73 | −306 | *EST | 70784-98-4 |
| $C_{10}H_{12}Se^+$ | | | | | | | |
|  | (7.3)<br>IP is onset of photoelectron band (81BAK/ARM). | (144) | (603) | −24 | −101 | *EST | 60096-27-7 |
| $C_{10}H_{12}W^+$ | | | | | | | |
|  | (6.35±0.2) | (221) | (924) | 74±1 | 311±5 | 82PIL/SKI | 1271-33-6 |

**Table 1. Positive Ion Table - Continued**

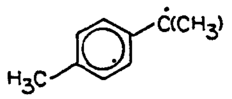
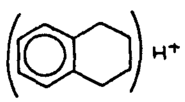
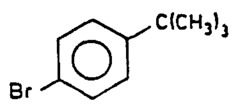
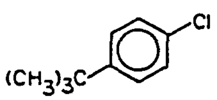
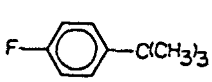
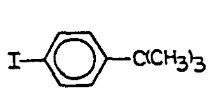
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{13}^+$ | | | | | | | |
|  | | (174) | (727) | | | | |
| | From proton affinity of 4-$CH_3C_6H_4C(CH_3)CH_2$ (RN 1195-32-0). PA = 211.0 kcal/mol, 883. kJ/mol and from appearance energy determination (86ORL/MIS). | | | | | | |
|  | | 177 | 740 | | | | |
| | From proton affinity of 1,2,3,4-tetrahydronaphthalene (RN 119-64-2). PA = 194.7 kcal/mol, 815. kJ/mol. | | | | | | |
| $C_{10}H_{13}Br^+$ | | | | | | | |
|  | 8.50±0.02 | (198) | (828) | 2 | 8 | 86ORL/MIS | 3972-65-4 |
| | IP from 86ORL/MIS, 85BAI/MIS. | | | | | | |
| $C_{10}H_{13}Cl^+$ | | | | | | | |
|  | (8.56±0.02) | (184) | (772) | −13 | −54 | 86ORL/MIS | 3972-56-3 |
| | IP from 86ORL/MIS. See also: 85BAI/MIS. | | | | | | |
| $C_{10}H_{13}F^+$ | | | | | | | |
|  | (8.59) | (146) | (609) | −52 | −219 | 86ORL/MIS | 701-30-4 |
| | IP from 85ORL/MIS. | | | | | | |
| $C_{10}H_{13}I^+$ | | | | | | | |
|  | (8.35±0.02) | (206) | (862) | 14 | 57 | 86ORL/MIS | 35779-04-5 |
| | IP from 86ORL/MIS. See also: 85BAI/MIS. | | | | | | |
| $C_{10}H_{13}N^+$ | | | | | | | |
|  | (6.8) | (185) | (773) | 28 | 117 | *EST | 4096-21-3 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |

Table 1. Positive Ion Table - Continued

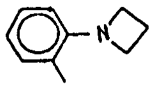
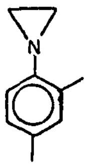
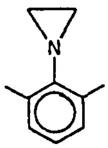
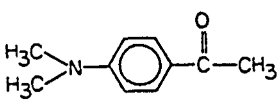
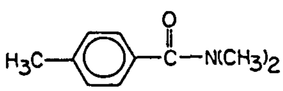
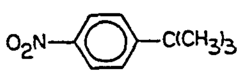
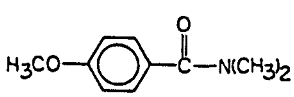
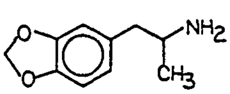
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{13}N^+$ | | | | | | | |
|  | (7.1) | (222) | (927) | 58 | 242 | *EST | 19198-94-8 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (≤7.80) | (≤243) | (≤1017) | 63 | 265 | *EST | 78376-89-3 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (7.6) | (232) | (969) | 56 | 236 | *EST | 78376-90-6 |
| | IP is onset of photoelectron band (82ROZ/HOU2). See also: 82CRI/LIC. | | | | | | |
| $C_{10}H_{13}NO^+$ | | | | | | | |
|  | ≤7.55 | (≤157) | (≤655) | −17 | −73 | *EST | 2124-31-4 |
|  | (≤8.90) | (≤175) | (≤731) | −31 | −128 | *EST | 14062-78-3 |
| | IP from 85GAL/GER. | | | | | | |
| $C_{10}H_{13}NO_2^+$ | | | | | | | |
|  | (9.2) | (203) | (850) | −9 | −38 | 85ORL/MIS | 3282-56-2 |
| | IP is onset of photoelectron band (85BAI/MIS2). See also: 86ORL/MIS. | | | | | | |
|  | ≤8.40 | (≤135) | (≤564) | −59 | −246 | *EST | 7291-00-1 |
| | IP from 85GAL/GER. | | | | | | |
|  | (≤8.01±0.06) | (≤136) | (≤570) | −49 | −203 | *EST | 51497-09-7 |

**Table 1. Positive Ion Table - Continued**

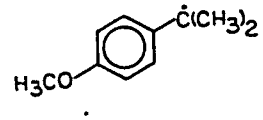
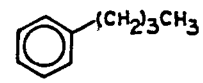
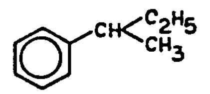
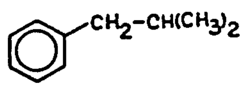
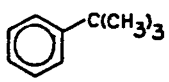
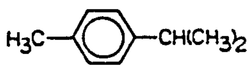
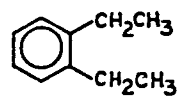
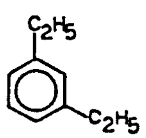
| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{13}O^+$ | | | | | | | |
|  | | 139 | 580 | | | | |
| | From proton affinity of 4-$CH_3OC_6H_4(C(CH_3)=CH_2)$ (RN 1712-69-2). PA = 217.4 kcal/mol, 910. kJ/mol. Value from appearance energy determination (86ORL/MIS) = 143 kcal/mol, 598 kJ/mol. | | | | | | |
| $C_{10}H_{14}^+$ | | | | | | | |
|  | 8.69±0.01 | 198 | 827 | −3.1±0.1 | −13.2±0.6 | 77PED/RYL | 104-51-8 |
| | IP at 298 K from charge transfer equilibrium constant determinations (78LIA/AUS) is 8.71±0.01 eV. | | | | | | |
|  | 8.68±0.01 | 196 | 820 | −4.1±0.2 | −17.3±1 | 77PED/RYL | 135-98-8 |
|  | 8.68±0.01 | 195 | 816 | −5.1±0.3 | −21.5±1 | 77PED/RYL | 538-93-2 |
|  | 8.64±0.02 | 194 | 812 | −5.1±0.3 | −21.5±1.2 | 77PED/RYL | 98-06-6 |
| | IP is average of values from 80VAN (cited in 83BRA/BAE) and from 84HOW/GON. IP at 298 K from charge transfer equilibrium constant determinations (78LIA/AUS) is 8.72±0.01 eV. See also: 85DOM/LAK, 85BAI/MIS. | | | | | | |
|  | (8.29) | (184) | (772) | −7 | −28 | *EST | 99-87-6 |
| | IP from 84HOW/GON. | | | | | | |
|  | ≤8.51 | ≤192 | ≤804 | −4±0.2 | −17±1 | 77PED/RYL | 135-01-3 |
|  | (8.49±0.01) | (191) | (798) | −5 | −21 | 77PED/RYL | 141-93-5 |
| | IP is 298 K value from charge transfer equilibrium constant determinations (78LIA/AUS). | | | | | | |

Table 1. Positive Ion Table - Continued

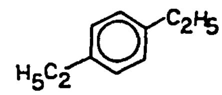
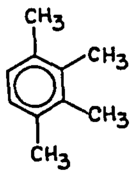
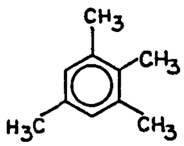
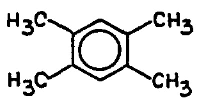
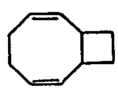
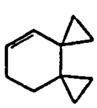
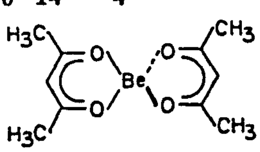
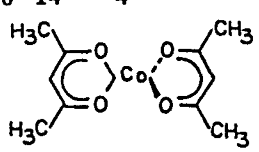
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{14}^+$ | | | | | | | |
|  | 8.40 | 189 | 790 | −5±0.5 | −20±2 | 77PED/RYL | 105-05-5 |
| | See also: 80GLE/HOP. | | | | | | |
|  | 8.16±0.02 | 180 | 754 | −8 | −33 | 75GOO | 488-23-3 |
| | IP from 82LEV/LIA, 84HOW/GON. | | | | | | |
|  | (8.07) | (176) | (738) | −10 | −41 | 75GOO | 527-53-7 |
| | IP from 84HOW/GON. | | | | | | |
|  | 8.04±0.01 | 174 | 731 | −11 | −45 | 75GOO | 95-93-2 |
| | See also: 82CAB/COW, 84HOW/GON. | | | | | | |
|  | (8.7) | (248) | (1036) | 47 | 197 | *EST | 77614-69-8 |
| | IP from 81BIS/GLE. | | | | | | |
|  | (≤8.48) | (≤259) | (≤1085) | 64 | 267 | *EST | 53143-76-3 |
| $C_{10}H_{14}BeO_4^+$ | | | | | | | |
|  | (8.1) | (−90) | (−376) | −277±1 | −1158±4 | 80TEL/RAB | 10210-64-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{14}CoO_4^+$ | | | | | | | |
|  | 7.6 | (−17) | (−70) | −192±0.5 | −803±2 | 83KAK/GIE | 14024-48-7 |
| | IP is onset of photoelectron band (82LEV/LIA, 83KIT/MOR). | | | | | | |

**Table 1. Positive Ion Table - Continued**

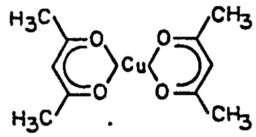
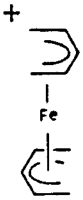
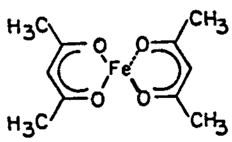
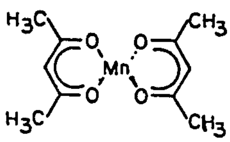
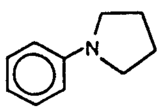
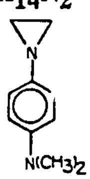
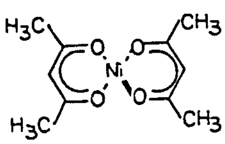
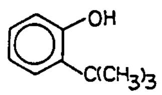
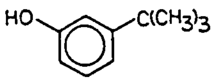
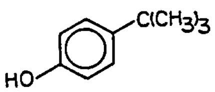
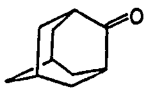
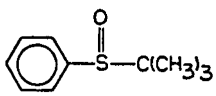
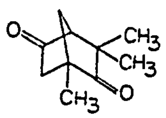
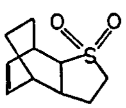
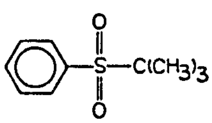
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{14}CuO_4{}^+$  | (7.2) | (5) | (20) | −161±0.5 | −675±2 | 83KAK/GIE | 13395-16-9 |
| | IP is onset of photoelectron band (83KIT/MOR). | | | | | | |
| $C_{10}H_{14}Fe^+$  | (6.6) | (192) | (803) | 40 | 166 | *EST | 74910-62-6 |
| | IP is onset of photoelectron band (84GLE/BOH). | | | | | | |
| $C_{10}H_{14}FeO_4{}^+$  | (7.50±0.04) | (−25) | (−105) | −198±0.5 | −829±2 | 83KAK/GIE | 14024-17-0 |
| $C_{10}H_{14}MnO_4{}^+$  | (8.34±0.05) | (−37) | (−154) | −229±1 | −959±4 | 83KAK/GIE | 14024-58-9 |
| $C_{10}H_{14}N^+$  | | (171) | (716) | | | | |
| | From proton affinity of N-phenylpyrrolidine (RN 4096-21-3). PA = 224.7 kcal/mol, 940. kJ/mol. | | | | | | |
| $C_{10}H_{14}N_2{}^+$  | (≤7.1) | (≤230) | (≤965) | 67 | 280 | *EST | 82027-08-5 |
| | IP from 82CRI/LIC. | | | | | | |
| $C_{10}H_{14}NiO_4{}^+$  | (7.1) | (−31) | (−130) | −195±0.5 | −815±2 | 83KAK/GIE | 3264-82-2 |
| | IP is onset of photoelectron band. See also: 83KIT/MOR. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{14}O^+$ | | | | | | | |
|  | (7.9) | (138) | (576) | −44 | −186 | *EST | 88-18-6 |
| | IP is onset of photoelectron band (85BAI/MIS2). See also: 83CET/LAP. | | | | | | |
|  | (≤8.40) | (≤145) | (≤608) | −48 | −202 | *EST | 585-34-2 |
| | IP from 83CET/LAP. | | | | | | |
|  | (7.8) | (132) | (551) | −48 | −202 | *EST | 98-54-4 |
| | IP is onset of photoelectron band (85BAI/MIS). See also: 83CET/LAP. | | | | | | |
|  | 8.62 | (144) | (601) | −55±1 | −231±5 | 78ARO/STE | 700-58-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{14}OS^+$ | | | | | | | |
|  | (≤8.50) | (≤171) | (≤717) | −25 | −103 | *EST | 4170-71-2 |
| | IP from 81MOH/JIA. | | | | | | |
| $C_{10}H_{14}O_2^+$ | | | | | | | |
|  | (9.11) | (119) | (497) | −91 | −382 | *EST | 31211-08-2 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
| $C_{10}H_{14}O_2S^+$ | | | | | | | |
|  | (9.15) | (165) | (690) | −46 | −192 | *EST | |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
|  | (≤9.7) | (145) | (607) | −78 | −328 | *EST | 4170-72-3 |
| | IP from 81MOH/JIA. | | | | | | |

### Table 1. Positive Ion Table - Continued

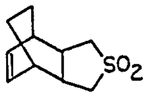
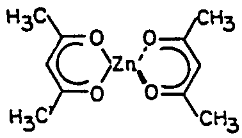
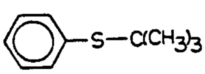
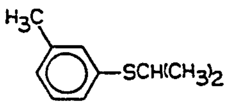
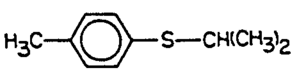
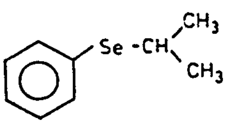
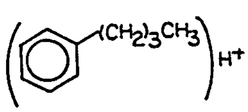
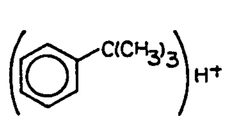
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{10}H_{14}O_2S^+$** | | | | | | | |
|  | (9.2) | (166) | (696) | −46 | −192 | •EST | |
| | IP is onset of photoelectron band (84AIT/GOS). | | | | | | |
| **$C_{10}H_{14}O_4Zn^+$** | | | | | | | |
|  | 7.8 | (−26) | (−107) | −206±2 | −860±10 | 83KAK/GIE | 14024-63-6 |
| | IP is onset of photoelectron band (83KIT/MOR, 82LEV/LIA). | | | | | | |
| **$C_{10}H_{14}S^+$** | | | | | | | |
|  | 8.39±0.05 | (197) | (825) | 4 | 15 | •EST | 3019-19-0 |
|  | (≤8.38) | (≤198) | (≤828) | 5 | 19 | •EST | 14905-80-7 |
|  | (8.5) | (201) | (839) | 5 | 19 | •EST | 14905-81-8 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_{10}H_{14}Se^+$** | | | | | | | |
|  | (7.2) | (184) | (772) | 18 | 77 | •EST | 78805-16-0 |
| | IP is onset of photoelectron band (81BAK/ARM). | | | | | | |
| **$C_{10}H_{15}^+$** | | | | | | | |
|  | | 170 | 713 | | | | |
| | From proton affinity of n-$C_4H_9C_6H_5$ (RN 104-51-8). PA = 192.1 kcal/mol, 804. kJ/mol. | | | | | | |
|  | | 167 | 700 | | | | |
| | From proton affinity of tert-$C_4H_9C_6H_5$ (RN 98-06-6). PA = 193.0 kcal/mol, 807. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

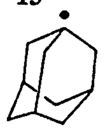
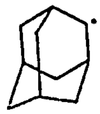
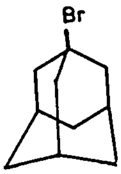
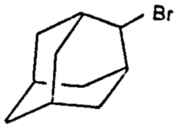
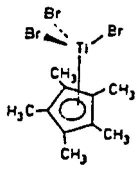
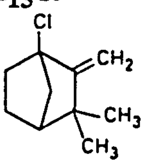
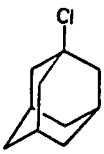
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{15}^+$ | | | | | | | |
|  | (6.21) | (159) | (665) | 16 | 66 | 86KRU/BEA | 19740-18-2 |
| | $\Delta_f H$(Ion) from chloride and hydride transfer equilibrium constant determinations (85SHA/SHA, 86KRU/BEA); $\Delta_f H$ (Adamantyl chloride) estimated as -43 kcal/mol, -180 kJ/mol. | | | | | | |
|  | (6.73) | (168) | (704) | 13 | 54 | 86KRU/BEA | |
| | IP from 86KRU/BEA. | | | | | | |
| $C_{10}H_{15}Br^+$ | | | | | | | |
|  | 9.30±0.06 | (183) | (766) | −31 | −131 | *EST | 768-90-1 |
| | IP from 84ABE/DEL, 82LEV/LIA. | | | | | | |
|  | (9.31±0.05) | (185) | (772) | −30 | −126 | *EST | 7314-85-4 |
| $C_{10}H_{15}Br_3Ti^+$ | | | | | | | |
|  | (8.0) | (30) | (126) | −154 | −646 | *EST | 33151-84-7 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |
| $C_{10}H_{15}Cl^+$ | | | | | | | |
|  | (≤9.11) | (≤193) | (≤809) | −17 | −70 | *EST | 4017-64-5 |
| | IP from 81NES/BAI. | | | | | | |
|  | (9.30) | (171) | (717) | −43 | −180 | *EST | 935-56-8 |

Table 1. Positive Ion Table - Continued

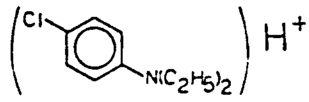
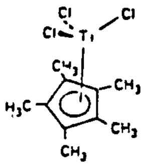
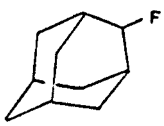
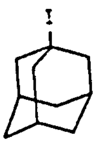
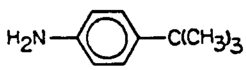
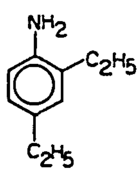
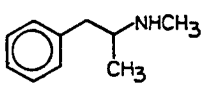
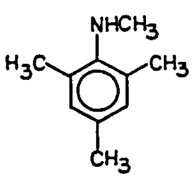
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{15}ClN^+$ | | | | | | | |
|  | | 142 | 594 | | | | |
| | From proton affinity of 4-$ClC_6H_4N(C_2H_5)_2$ (RN 2873-89-4). PA = 225.6 kcal/mol, 944. kJ/mol. | | | | | | |
| $C_{10}H_{15}Cl_3Ti^+$ | | | | | | | |
|  | (8.1) | (7) | (30) | −179 | −751 | *EST | 12129-06-5 |
| | IP is onset of photoelectron band (84TER/LOU). | | | | | | |
| $C_{10}H_{15}F^+$ | | | | | | | |
|  | (9.46) | (141) | (592) | −77 | −321 | *EST | 16668-83-0 |
| $C_{10}H_{15}I^+$ | | | | | | | |
|  | (8.6) | (182) | (760) | −17 | −70 | *EST | 768-93-4 |
| | IP is onset of photoelectron band (84ABE/DEL). | | | | | | |
| $C_{10}H_{15}N^+$ | | | | | | | |
|  | (7.35±0.02) | (165) | (691) | −4.5 | −19 | 85ORL/MIS | 769-92-6 |
| | IP from 85ORL/MIS. See also: 85BAI/MIS2. | | | | | | |
|  | (≤7.77) | (≤176) | (≤736) | −3 | −14 | *EST | 579-66-8 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (≤8.60±0.20) | (≤199) | (≤832) | 0.5 | 2 | *EST | 7632-10-2 |
|  | (7.22) | (171) | (717) | 5 | 20 | *EST | 13021-14-2 |

Table 1. Positive Ion Table - Continued

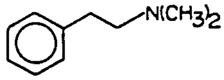
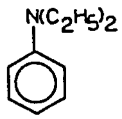
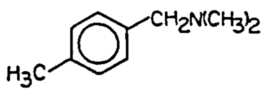
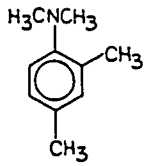
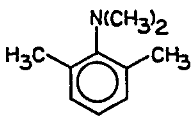
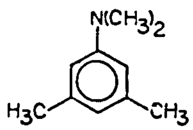
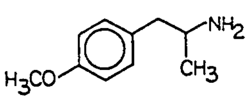
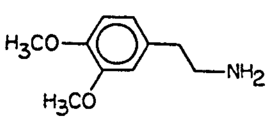
| ION<br>Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{15}N^+$ | | | | | | | |
|  | (7.70±0.05) | (193) | (807) | 15 | 64 | *EST | 1126-71-2 |
| | See also: 81LOG/TAK. | | | | | | |
|  | 6.98±0.02 | (171) | (714) | 9.5 | 40 | 69BEN/CRU | 91-66-7 |
| | IP from charge transfer equilibrium constant determinations; reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12eV) (84MAU/NEL, 85LIA/JAC). | | | | | | |
|  | (7.61) | (187) | (784) | 12 | 49 | *EST | 4052-88-4 |
| | See also: 81LOG/TAK. | | | | | | |
|  | (≤7.79) | (≤196) | (≤820) | 16 | 68 | *EST | 769-53-9 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (7.30±0.02) | (190) | (797) | 22 | 93 | *EST | 769-06-2 |
| | See also: 82ROZ/HOU2. | | | | | | |
|  | (6.95) | (168) | (706) | 8 | 35 | *EST | 4913-13-7 |
| | IP from charge transfer equilibrium constant determinations; reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV) (85LIA/JAC). | | | | | | |
| $C_{10}H_{15}NO^+$ | | | | | | | |
|  | (≤8.16±0.06) | (≤184) | (≤768) | -5 | -19 | *EST | 23239-32-9 |
| $C_{10}H_{15}NO_2{}^+$ | | | | | | | |
|  | 7.4 | (113) | (473) | -58 | -241 | *EST | 120-20-7 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |

Table 1. Positive Ion Table - Continued

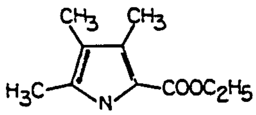
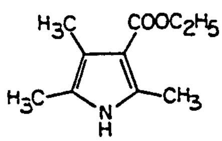
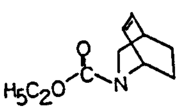
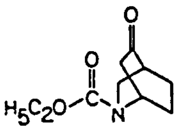
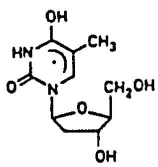
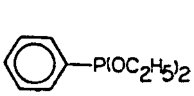
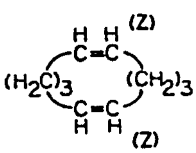
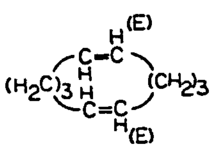
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{15}NO_2^+$ | | | | | | | |
|  | (≤7.71) | (≤74) | (≤311) | −103 | −433 | *EST | 2199-46-4 |
| | IP from 81CAU/GIA. | | | | | | |
|  | (7.5) | (69) | (290) | −103 | −433 | *EST | 55770-78-0 |
| | IP is onset of photoelectron band (81CAU/GIA). | | | | | | |
|  | (8.0) | (114) | (479) | −70 | −293 | *EST | 3693-69-4 |
| | IP is onset of photoelectron band (81CAR/GAN). | | | | | | |
| $C_{10}H_{15}NO_3^+$ | | | | | | | |
|  | (8.5) | (53) | (220) | −143 | −600 | *EST | 37778-51-1 |
| | IP is onset of photoelectron band (81CAR/GAN). | | | | | | |
| $C_{10}H_{15}N_2O_5^+$ | | | | | | | |
|  | | (−72) | (−301) | | | | |
| | From proton affinity of thymidine (RN 50-89-5). PA = (208) kcal/mol, (870) kJ/mol. | | | | | | |
| $C_{10}H_{15}O_2P^+$ | | | | | | | |
|  | (8.2) | (87) | (362) | −103 | −429 | *EST | 1638-86-4 |
| | IP is onset of photoelectron band (81ARS/ZVE, 81ZVE/VIL2). | | | | | | |
| $C_{10}H_{16}^+$ | | | | | | | |
|  | (≤8.68) | (≤194) | (≤813) | −6 | −24 | 76JEN | 1124-79-4 |
|  | (≤8.05) | (≤184) | (≤769) | −2 | −8 | 76JEN | 15840-81-0 |

**Table 1. Positive Ion Table - Continued**

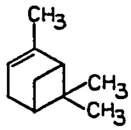
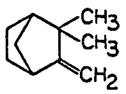
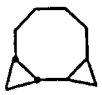
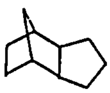
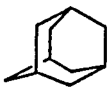
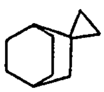
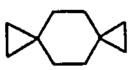
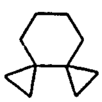
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{16}^+$ | | | | | | | |
|  | (8.07) | (193) | (807) | 7±0.5 | 28±2 | 77PED/RYL | 80-56-8 |
|  | (≤8.86) | (≤198) | (≤827) | −7 | −28 | 77KOZ/BYC | 79-92-5 |
| | IP from 81NES/BAI. | | | | | | |
|  | (8.5) | (219) | (915) | 23 | 95 | *EST | 81969-73-5 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |
|  | 9.35±0.05 | 201.2 | 841.9 | −14.4±1 | −60.2±3 | 71BOY/SAN | 6004-38-2 |
|  | 9.24±0.06 | 181 | 759 | −31.8±0.3 | −132.7±1.3 | 75CLA/KNO | 281-23-2 |
|  | (8.7) | (209) | (875) | 9 | 36 | *EST | 53764-10-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤9.17) | (≤211) | (≤882) | −0.7 | −3 | *EST | 24518-94-3 |
|  | (8.5) | (231) | (967) | 35 | 147 | *EST | 24029-74-1 |
| | IP is onset of photoelectron band (82SPA/GLE, 82LEV/LIA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

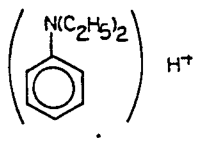
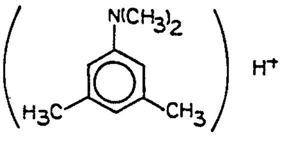
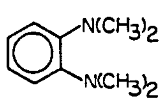
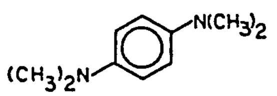
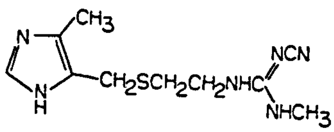
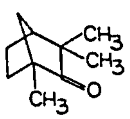
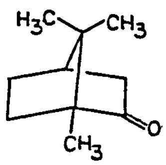
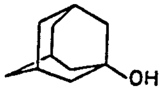
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{16}N^+$ | | | | | | | |
|  | | 148 | 617 | | | | |
| | From proton affinity of $C_6H_5N(C_2H_5)_2$ (RN 91-66-7). PA = 227.6 kcal/mol, 952. kJ/mol. | | | | | | |
|  | | 147 | 615 | | | | |
| | From proton affinity of 3,5-$(CH_3)_2C_6H_3N(CH_3)_2$ (RN 4913-13-7). PA = 227.0 kcal/mol, 950. kJ/mol. | | | | | | |
| $C_{10}H_{16}N_2^+$ | | | | | | | |
|  | (7.1) | (200) | (836) | 36 | 151 | *EST | 704-01-8 |
| | IP is onset of photoelectron band (81NEL/GRE). | | | | | | |
|  | 6.20±0.05 | 164 | 686 | 21 | 88 | 83MET/ARA | 100-22-1 |
| $C_{10}H_{16}N_6S^+$ | | | | | | | |
|  | (7.7) | (249) | (1042) | 72 | 300 | *EST | 51481-61-9 |
| | IP is onset of photoelectron band (80KLA/BUT). | | | | | | |
| $C_{10}H_{16}O^+$ | | | | | | | |
|  | (8.5) | (125) | (523) | −71 | −297 | *EST | 1195-79-5 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
|  | (8.76±0.03) | (138) | (578) | −64±0.7 | −267±3 | 77STE | 76-22-2 |
|  | (9.09±0.05) | (136) | (566) | −74±0.7 | −311±3 | 78ARO/STE | 768-95-6 |

**Table 1. Positive Ion Table - Continued**

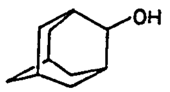
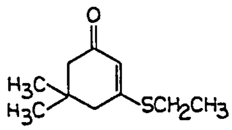
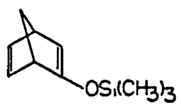
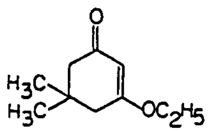
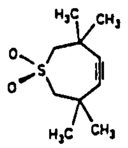
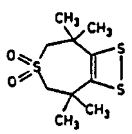
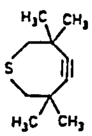
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{16}O^+$ | | | | | | | |
|  | (9.09±0.07) | (139) | (578) | −71±1 | −299±5 | 78ARO/STE | 700-57-2 |
| $C_{10}H_{16}OS^+$ | | | | | | | |
|  | (8.2)<br>IP is onset of photoelectron band (82PFI/GER). | (147) | (613) | −43 | −178 | *EST | 52735-49-6 |
| $C_{10}H_{16}OSi^+$ | | | | | | | |
|  | (≤8.06)<br>IP from 83HOU/RON. | (≤136) | (≤571) | −49 | −207 | *EST | 68364-22-7 |
| $C_{10}H_{16}O_2^+$ | | | | | | | |
|  | (≤8.87)<br>IP from 82PFI/GER. | (≤117) | (≤489) | −88 | −367 | *EST | 6267-39-6 |
| $C_{10}H_{16}O_2S^+$ | | | | | | | |
|  | ≤9.75<br>IP from 83JIA/MOH. | (≤185) | (≤773) | −40 | −168 | *EST | |
| $C_{10}H_{16}O_2S_3^+$ | | | | | | | |
|  | ≤8.55<br>IP from 83JIA/MOH. | (≤152) | (≤637) | −45 | −188 | *EST | |
| $C_{10}H_{16}S^+$ | | | | | | | |
|  | ≤8.40<br>IP from 83JIA/MOH. | (≤237) | (≤992) | 43 | 182 | *EST | |

**Table 1. Positive Ion Table - Continued**

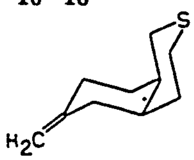
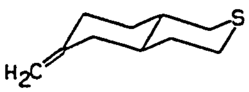
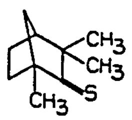
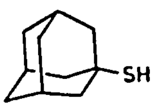
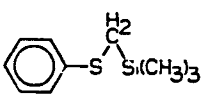
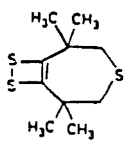
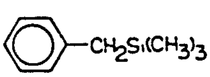
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{10}H_{16}S^+$** | | | | | | | |
|  | (8.22)<br>IP from 80SAR/WOR. | (187) | (782) | −3 | −11 | *EST | 77471-74-0 |
|  | (8.26)<br>IP from 80SAR/WOR. | (185) | (773) | −6 | −24 | *EST | 77471-73-9 |
|  | (8.13)<br>IP from 80FRO/WES. See also: 82LEV/LIA. | (167) | (697) | −21 | −87 | *EST | 875-06-9 |
|  | (8.6)<br>IP is onset of photoelectron band. | (158) | (663) | −40 | −167 | *EST | 34301-54-7 |
| **$C_{10}H_{16}SSi^+$** | | | | | | | |
|  | (≤7.81±0.05) | (≤121) | (≤506) | −59 | −248 | *EST | 17873-08-4 |
| **$C_{10}H_{16}S_3^+$** | | | | | | | |
|  | 7.8<br>IP is onset of photoelectron band (83JIA/MOH). | (219) | (915) | 39 | 162 | *EST | |
| **$C_{10}H_{16}Si^+$** | | | | | | | |
|  | 8.35 | (164) | (685) | −29 | −121 | *EST | 770-09-2 |

**Table 1. Positive Ion Table - Continued**

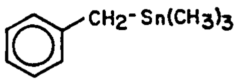
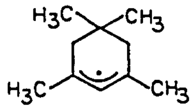
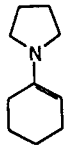
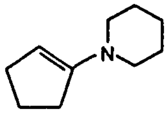
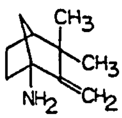
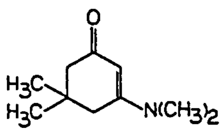
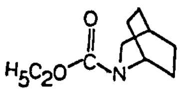
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{16}Sn^+$ | | | | | | | |
|  | 8.08±0.05 | 206 | 863 | 20±1 | 83±6 | 77PED/RYL | 4314-94-7 |
| $C_{10}H_{17}^+$ | | | | | | | |
|  | | (148) | (618) | | | | |
| | From proton affinity of 1,5,5-trimethyl-3-methylenecyclohexene (RN 16609-28-2).<br>PA = (216.1) kcal/mol, (904.) kJ/mol. | | | | | | |
| $C_{10}H_{17}N^+$ | | | | | | | |
|  | 7.10 | (165) | (689) | 1 | 4 | *EST | 1125-99-1 |
| | See also: 81MUL/PRE2. | | | | | | |
|  | (7.0) | (138) | (580) | −23±1 | −95±4 | *EST | 1614-92-2 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.67) | (≤198) | (≤828) | −2 | −9 | *EST | 13487-72-4 |
| | IP from 81NES/BAI. | | | | | | |
| $C_{10}H_{17}NO^+$ | | | | | | | |
|  | (≤7.88) | (≤143) | (≤596) | −39 | −164 | *EST | 31039-88-0 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{10}H_{17}NO_2^+$ | | | | | | | |
|  | (7.9) | (63) | (265) | −119 | −497 | *EST | 39926-11-9 |
| | IP is onset of photoelectron band (81CAR/GAN). | | | | | | |

**Table 1. Positive Ion Table - Continued**

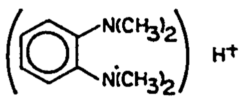
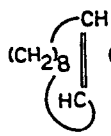
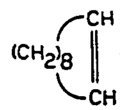
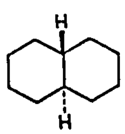
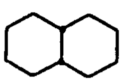
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{10}H_{17}N_2^+$** | | | | | | | |
|  | | 167 | 697 | | | | |
| | From proton affinity of 1,2-$(N(CH_3)_2)_2C_6H_4$ (RN 704-01-8). PA = 235.2 kcal/mol, 984. kJ/mol. | | | | | | |
| **$C_{10}H_{18}^+$** | | | | | | | |
| 1-$C_{10}H_{18}$ | (9.91±0.02) | (239) | (998) | 10±.7 | 42±3 | 79ROG/DAG | 764-93-2 |
| 2-$C_{10}H_{18}$ | (9.30±0.02) | (220) | (921) | 6±0.7 | 24±3 | 79ROG/DAG | 2384-70-5 |
| 3-$C_{10}H_{18}$ | 9.19±0.01 | 217 | 909 | 5±0.7 | 22±3 | 79ROG/DAG | 2384-85-2 |
| 4-$C_{10}H_{18}$ | (9.17±0.02) | (216) | (905) | 5±0.7 | 20±3 | 79ROG/DAG | 2384-86-3 |
| 5-$C_{10}H_{18}$ | 9.13±0.03 | (216) | (905) | 6 | 24 | *EST | 1942-46-7 |
| (tert-$C_4H_9$)C≡C(tert-$C_4H_9$) | (9.05±0.01) | (206) | (861) | −3 | −13 | *EST | 17530-24-4 |
| | See also: 85ORL/BOG. | | | | | | |
|  (E) | (8.80) | (199) | (832) | −4 | −17 | 78GRE/LIE | 2198-20-1 |
|  (Z) | (8.80) | (196) | (820) | −7 | −29 | 78GRE/LIE | 935-31-9 |
|  | 9.24 | 170 | 709 | −43.5±0.5 | −182.1±2.3 | 77PED/RYL | 493-02-7 |
| | From charge transfer equilibrium constant determinations (82SIE/MAU, 85AUS/LIA). Photoionization onset, 9.32 eV (80MIK/ZAI); onset of photoelectron band, 9.26 eV (77BIE/BUR). | | | | | | |
|  | 9.26 | 173 | 724 | −40.4±0.5 | −169.1±2.3 | 77PED/RYL | 493-01-6 |
| | From charge transfer equilibrium constant determination (85AUS/LIA). Photoionization onset, 9.32 eV (80MIK/ZAI); onset of photoelectron band, 9.26 eV. | | | | | | |

Table 1. Positive Ion Table - Continued

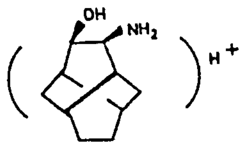
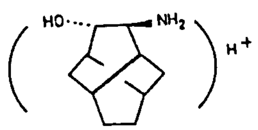
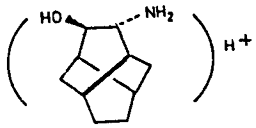
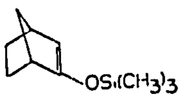
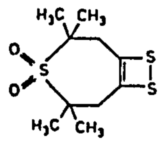
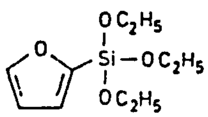
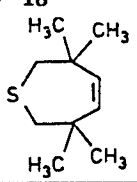
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{10}H_{18}NO^+$** | | | | | | | |
|  | | (95) | (396) | | | | |
| | From proton affinity of cis-3-amino-2-twistanol. PA = 224.0 kcal/mol, 937. kJ/mol. | | | | | | |
|  | | (95) | (398) | | | | |
| | From proton affinity of trans-3-amino-2-twistanol (isomer 1). PA = 221.5 kcal/mol, 927. kJ/mol. | | | | | | |
|  | | (97) | (405) | | | | |
| | From proton affinity of trans-3-amino-2-twistanol (isomer 2). PA = 220.0 kcal/mol, 920. kJ/mol. | | | | | | |
| **$C_{10}H_{18}OSi^+$** | | | | | | | |
|  | (≤8.09) | (≤101) | (≤424) | -85 | -357 | *EST | 57722-40-4 |
| | IP from 83HOU/RON. | | | | | | |
| **$C_{10}H_{18}O_2S_3^+$** | | | | | | | |
|  | (≤9.55) | (≤132) | (≤552) | -88 | -369 | *EST | |
| | IP from 83JIA/MOH. | | | | | | |
| **$C_{10}H_{18}O_4Si^+$** | | | | | | | |
|  | (8.0) | (-26) | (-110) | -211 | -882 | *EST | 55811-52-4 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
| **$C_{10}H_{18}S^+$** | | | | | | | |
|  | ≤8.35 | (≤188) | (≤787) | -5 | -19 | *EST | |
| | IP from 83JIA/MOH. | | | | | | |

Table 1. Positive Ion Table - Continued

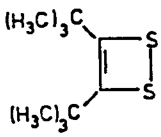
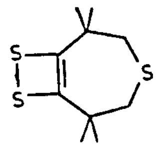
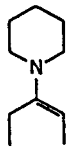
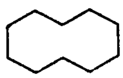
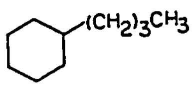
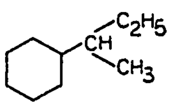
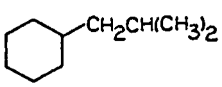
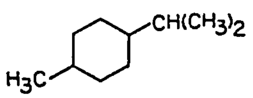
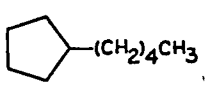
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{18}S_2^+$ | | | | | | | |
|  | 7.65 | (204) | (853) | 27 | 115 | *EST | |
| | IP is onset of photoelectron band (83JIA/MOH). | | | | | | |
| $C_{10}H_{18}S_3^{+\cdot}$ | | | | | | | |
|  | 7.8 | 172 | 719 | −8 | −34 | *EST | |
| | IP is onset of photoelectron band (83JIA/MOH). | | | | | | |
| $C_{10}H_{19}N^+$ | | | | | | | |
|  | (≤7.61) | (≤161) | (≤673) | −14 | −61 | *EST | 21086-43-1 |
| | IP from 81MUL/PRE2. | | | | | | |
|  | (6.94±0.09) | (166) | (695) | 6 | 25 | *EST | 31023-92-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{20}^+$ | | | | | | | |
| 1-$C_{10}H_{20}$ | 9.42±0.01 | 188 | 786 | −29.5±0.5 | −123.3±2 | 77PED/RYL | 872-05-9 |
| | See also: 81HOL/FIN. | | | | | | |
| (Z)-$C_{10}H_{20}$ | 8.90±0.01 | (174) | (727) | −32 | −132 | *EST | 20348-51-0 |
| (E)-2-$C_{10}H_{20}$ | 8.90±0.01 | (173) | (724) | −32 | −135 | *EST | 20063-97-2 |
| (Z)-3-$C_{10}H_{20}$ | 8.83±0.01 | (172) | (721) | −31 | −131 | *EST | 19398-86-8 |
| (E)-3-$C_{10}H_{20}$ | 8.83±0.01 | (171) | (717) | −32 | −135 | *EST | 19150-21-1 |
| (Z)-4-$C_{10}H_{20}$ | 8.78±0.01 | (171) | (716) | −31 | −131 | *EST | 19398-88-0 |
| (E)-4-$C_{10}H_{20}$ | 8.78±0.01 | (170) | (712) | −32 | −135 | *EST | 19398-89-1 |
| (Z)-5-$C_{10}H_{20}$ | 8.77±0.01 | (171) | (715) | −31 | −131 | *EST | 7433-78-5 |
| (E)-5-$C_{10}H_{20}$ | 8.76±0.01 | (170) | (710) | −32 | −135 | *EST | 7433-56-9 |
| (tert-$C_4H_9)_2C=CH_2$ | (8.79±0.01) | (164) | (688) | −38 | −161 | *EST | 5857-68-1 |
| n-$C_5H_{11}C(CH_3)=C(CH_3)_2$ | (8.13±0.01) | (151) | (633) | −36 | −152 | *EST | 19781-18-1 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{20}^+$ | | | | | | | |
| $C_4H_9C(C_2H_5)=C(CH_3)_2$ | | | | | | | |
| | (8.10±0.01) | (151) | (630) | −36 | −151 | *EST | 19780-61-1 |
| (tert-$C_4H_9$)$CH_2C(CH_3)=C(CH_3)_2$ | | | | | | | |
| | (8.10±0.01) | (146) | (610) | −41 | −172 | *EST | 33175-59-6 |
| (Z)-(t-$C_4H_9$)$CH=CH$(t-$C_4H_9$) | | | | | | | |
| | 8.69±0.01 | (171) | (717) | −29±0.7 | −121±3 | *EST | 692-47-7 |
| (E)-(t-$C_4H_9$)$CH=CH$(t-$C_4H_9$) | | | | | | | |
| | 8.74±0.01 | 162 | 677 | −40±0.7 | −166±3 | 79FUC/PEA | 692-48-8 |
|  | (9.5) | (182) | (762) | −36.9±0.4 | −154.3±1.5 | 77PED/RYL | 293-96-9 |
| | IP is onset of photoelectron band (77BIE/BUR). | | | | | | |
|  | 9.41 | 166 | 695 | −50.9±0.2 | −213.0±1 | 77PED/RYL | 1678-93-9 |
| | From charge transfer equilibrium constant determinations (82SIE/MAU); reference standard, fluorobenzenes. Threshold determinations give IP at 0 K of 9.57 eV. | | | | | | |
|  | 9.23 | (164) | (686) | −49 | −205 | *EST | 7058-01-7 |
| | From charge transfer equilibrium constant determinations (82SIE/MAU); reference standard, fluorobenenes. Threshold determinations give IP at 0 K of 9.51 eV. | | | | | | |
|  | (9.54±0.03) | (171) | (716) | −49 | −204 | *EST | 1678-98-4 |
|  | 9.32 | 160 | 668 | −55±0.7 | −231±3 | 77PED/RYL | 99-82-1 |
| | From charge transfer equilibrium constant determinations (82SIE/MAU); reference standard fluorobenzenes. | | | | | | |
|  | (9.91±0.05) | (184) | (767) | −45 | −189 | 71ASTM | 3741-00-2 |

## Table 1. Positive Ion Table - Continued

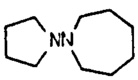
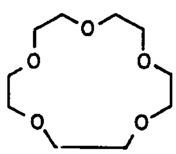
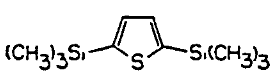
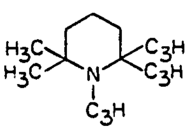
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{20}N^+$ | | | | | | | |
|  $H^+$ | | (142) | (592) | | | | |
| | From proton affinity of 1-azabicyclo[3.3.3]undecane (RN 31023-92-4). PA = 230.1 kcal/mol, 963. kJ/mol. | | | | | | |
| $C_{10}H_{20}NO^+$ | | | | | | | |
|  $H^+$ | | 67 | 280 | | | | |
| | From proton affinity of 4-aminodecahydro-3-naphthalenol. PA = 222.1 kcal/mol, 929. kJ/mol. | | | | | | |
| $C_{10}H_{20}N_2^+$ | | | | | | | |
|  | (7.60) | (195) | (814) | 19 | 81 | *EST | 60678-75-3 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |
|  | (7.89) | (189) | (791) | 7 | 30 | *EST | 6130-94-5 |
| | See also: 84NEL. | | | | | | |
| $C_{10}H_{20}O_5^+$ | | | | | | | |
|  | (8.9) | (14) | (60) | −191±0.5 | −799±2 | 82BYS/MAN | 33100-27-5 |
| | IP is onset of photoelectron band. See also: 83BAK/ARM. | | | | | | |
| $C_{10}H_{20}SSi_2^+$ | | | | | | | |
|  | (7.8) | (126) | (526) | −54 | −227 | *EST | 17906-71-7 |
| | IP is onset of photoelectron band (83VES/HAR). | | | | | | |
| $C_{10}H_{21}N^+$ | | | | | | | |
|  | (7.23) | (127) | (530) | −40 | −167 | *EST | 79-55-0 |
| | IP from 82ROZ/HOU. | | | | | | |

**Table 1. Positive Ion Table - Continued**

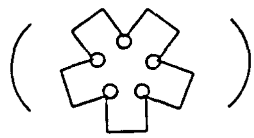
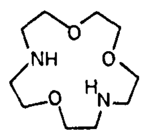
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{21}O_5^+$ | | | | | | | |
|  $H^+$ | | −49 | −205 | | | | |
| | From proton affinity of 1,4,7,10,13-pentaoxacyclopentadecane (15-Crown-5) (RN 33100-27-5). PA = 223.6 kcal/mol, 936. kJ/mol. | | | | | | |
| $C_{10}H_{22}^+$ | | | | | | | |
| n-$C_{10}H_{22}$ | 9.65 | 163 | 682 | −59.6±0.2 | −249.5±0.9 | 77PED/RYL | 124-18-5 |
| | | *176* | *738* | *−46.1±0.2* | *−192.7±0.9* | | |
| | From charge transfer equilibrium constants (81MAU/SIE). Reference standards, fluorobenzenes. | | | | | | |
| $C_{10}H_{22}N_2O_3^+$ | | | | | | | |
|  | (≤8.4) | (≤88) | (≤369) | −105 | −441 | *EST | 31249-95-3 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{10}H_{23}N^+$ | | | | | | | |
| n-$C_{10}H_{21}NH_2$ | (8.63±0.05) | (148) | (619) | −51 | −214 | *EST | 2016-57-1 |
| | See also: 79AUE/BOW. | | | | | | |
| $C_{10}H_{23}O^+$ | | | | | | | |
| (n-$C_5H_{11})_2OH$ | | 72 | 304 | | | | |
| | From proton affinity of (n-$C_5H_{11})_2O$ (RN 693-65-2) (86SAN/BAL, 85HOU/ROL). PA = 203.5 kcal/mol, 851. kJ/mol. | | | | | | |
| $C_{10}H_{24}N^+$ | | | | | | | |
| n-$C_{10}H_{21}NH_3$ | | (94) | (393) | | | | |
| | From proton affinity of n-$C_{10}H_{21}NH_2$. PA = (220.7) kcal/mol, (923.) kJ/mol. | | | | | | |
| $C_{10}H_{24}N_2^+$ | | | | | | | |
| (n-$C_3H_7)_2NN(C_2H_5)_2$ | (≤7.87) | (≤191) | (≤797) | 9 | 38 | *EST | 52598-09-1 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |
| (n-$C_4H_9)_2NN(CH_3)_2$ | (≤7.96) | (≤191) | (≤801) | 8 | 33 | *EST | 60678-67-3 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |

Table 1. Positive Ion Table - Continued

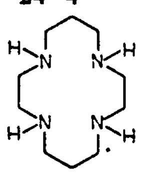
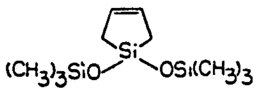
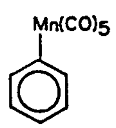
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{24}N_4^+$ | | | | | | | |
|  | (7.7) | (182) | (761) | 4.3±0.8 | 18.0±3.3 | 83CLA/COR | 295-37-4 |
| | IP is onset of photoelectron band (83BAK/ARM). | | | | | | |
| $C_{10}H_{24}O_2Si_3^+$ | | | | | | | |
|  | (≤9.36) | (≤−70) | (≤−293) | −286 | −1196 | *EST | 76795-95-4 |
| | IP from 81KHV/ZYK. | | | | | | |
| $C_{10}H_{25}N_2^+$ | | | | | | | |
| $(CH_3)_2NH(CH_2)_6N(CH_3)_2$ | | 106 | 444 | | | | |
| | From proton affinity of $(CH_3)_2N(CH_2)_6N(CH_3)_2$ (RN 111-18-2). PA = 245. kcal/mol, 1023. kJ/mol. | | | | | | |
| $C_{10}H_{30}N_5Ta^+$ | | | | | | | |
| $Ta(N(CH_3)_2)_5$ | (6.5) | (93) | (390) | −57±4 | −237±15 | 82TN270 | |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{10}H_{30}O_3Si_4^+$ | | | | | | | |
| $[(CH_3)_3SiOSi(CH_3)_2]_2O$ | (≤10.24) | (≤−226) | (≤−947) | −462±5 | −1935±23 | 77PED/RYL | 141-62-8 |
| | IP from 82ERM/KIR. | | | | | | |
| $C_{10}H_{30}Si_4^+$ | | | | | | | |
| n-$Si_4(CH_3)_{10}$ | 7.29±0.01 | 32 | 135 | −136±6 | −568±24 | 77PED/RYL | 865-76-9 |
| $C_{10}MnO_{10}Re^+$ | | | | | | | |
| $MnRe(CO)_{10}$ | 8.22±0.01 | (−184) | (−769) | −373 | −1562 | *EST | 14693-30-2 |
| $C_{10}Mn_2O_{10}^+$ | | | | | | | |
| $Mn_2(CO)_{10}$ | (7.7) | (−201) | (−842) | −379±1 | −1585±5 | 82CON/ZAF | 10170-69-1 |
| | IP is onset of photoelectron band. See also: 81MIC/SVE. | | | | | | |
| $C_{10}O_{10}Re_2^+$ | | | | | | | |
| $Re_2(CO)_{10}$ | (7.8) | (−193) | (−806) | −373±3 | −1559±11 | 83ALT/CON | 14285-68-8 |
| | IP is onset of photoelectron band. See also: 81MIC/SVE. | | | | | | |
| $C_{11}H_5MnO_5^+$ | | | | | | | |
|  | (8.22±0.05) | (49) | (203) | −141±0.2 | −590±1 | 82CON/ZAF | 13985-77-8 |

**Table 1. Positive Ion Table - Continued**

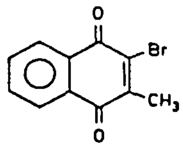
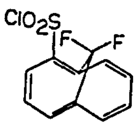
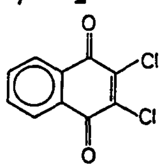
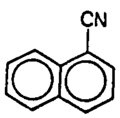
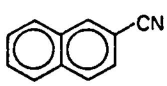
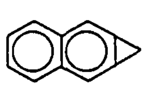
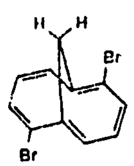
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_7BrO_2^+$ | | | | | | | |
|  | (9.25) | (182) | (760) | −31 | −132 | *EST | 3129-39-3 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{11}H_7ClF_2O_2S^+$ | | | | | | | |
|  | (≤8.90) | (≤35) | (≤146) | −170 | −713 | *EST | |
| | IP from 84AND/CER. | | | | | | |
| $C_{11}H_7ClO_2^+$ | | | | | | | |
|  | (9.4) | (180) | (754) | −37 | −153 | *EST | 17015-99-5 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{11}H_7N^+$ | | | | | | | |
|  | (8.59) | (244) | (1021) | 46 | 192 | *EST | 86-53-3 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.56) | (243) | (1016) | 45 | 190 | *EST | 613-46-7 |
| | IP is onset of photoelectron band (83KLA/KOV). | | | | | | |
| $C_{11}H_8^+$ | | | | | | | |
|  | (8.03) | (289) | (1210) | 104 | 435 | 73BIL/CHO | 286-85-1 |
| | IP from 80SCH/SCH. | | | | | | |
| $C_{11}H_8Br_2^+$ | | | | | | | |
|  | (7.85) | (252) | (1053) | 71 | 296 | *EST | 15825-93-1 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |

Table 1. Positive Ion Table - Continued

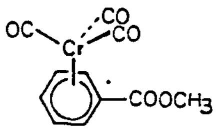
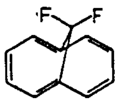
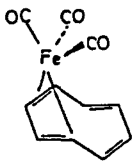
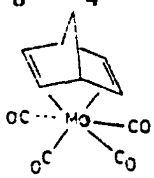
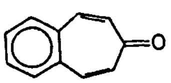
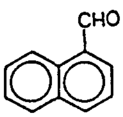
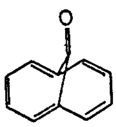
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_8CrO_5^+$ | | | | | | | |
|  | (7.02±0.1) | (4) | (18) | −157 | −659 | 84ALT/CON | 12125-87-0 |
| $C_{11}H_8F_2^+$ | | | | | | | |
|  | (8.19±0.03) | (149) | (625) | −39 | −165 | *EST | 61997-36-2 |
| | IP from 84AND/CER. | | | | | | |
| $C_{11}H_8FeO_3^+$ | | | | | | | |
|  | (7.3) | (132) | (554) | −36±3 | −150±13 | 82PIL/SKI | 12093-05-9 |
| | IP is onset of photoelectron band (82LEV/LIA, 80BOH/GLE). | | | | | | |
| $C_{11}H_8MoO_4^+$ | | | | | | | |
|  | (7.0) | (81) | (339) | −80±3 | −336±11 | 82PIL/SKI | 12146-37-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{11}H_8O^+$ | | | | | | | |
|  | (8.3) | (210) | (879) | 19 | 78 | *EST | 4443-91-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.33) | (199) | (834) | 7 | 30 | *EST | 66-77-3 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.0) | (218) | (914) | 34 | 142 | *EST | 36628-80-5 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |

Table 1. Positive Ion Table - Continued

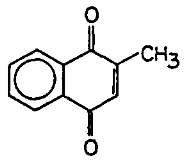
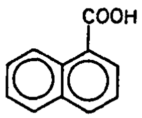
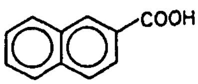
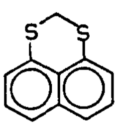
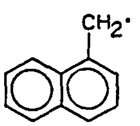
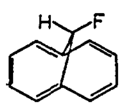
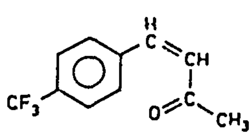
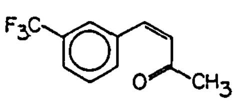
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_8O_2{}^+$ | | | | | | | |
|  | (9.3) | (184) | (770) | −30 | −127 | *EST | 58-27-5 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
|  | (8.29) | (138) | (577) | −53.3±0.2 | −223.1±0.9 | 77PED/RYL | 86-55-5 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.26) | (135) | (564) | −55.6±0.4 | −232.5±1.6 | 77PED/RYL | 93-09-4 |
| | IP from 83KLA/KOV. | | | | | | |
| $C_{11}H_8S_2{}^+$ | | | | | | | |
|  | (7.3) | (237) | (991) | 69 | 287 | *EST | 204-14-8 |
| | IP is onset of photoelectron band (81BOC/BRA). | | | | | | |
| $C_{11}H_9{}^+$ | | | | | | | |
|  | (7.35±0.1) | (229) | (962) | 60 | 253 | 82MCM/GOL | 7419-60-5 |
| | Appearance potential results (see 85HON/SEG and references cited therein) lead to value for $\Delta_f H$(Ion) of ~252 kcal/mol, ~1054 kJ/mol. | | | | | | |
| $C_{11}H_9F^+$ | | | | | | | |
|  | (8.10±0.03) | (203) | (848) | 16 | 66 | *EST | 72791-63-0 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |
| $C_{11}H_9F_3O^+$ | | | | | | | |
|  | (9.0±0.05) | (39) | (164) | −168 | −704 | 79SCH/GRU | 76293-37-3 |
| | IP from 79SCH/GRU, 80GRU/SCH, 81SCH/GRO. | | | | | | |
|  | (9.1±0.05) | (42) | (175) | −168 | −703 | *EST | |
| | IP from 81SCH/GRO. | | | | | | |

**Table 1. Positive Ion Table - Continued**

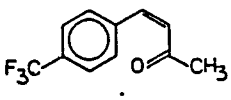
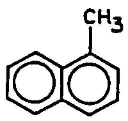
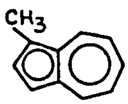
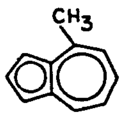
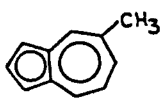
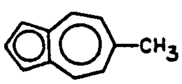
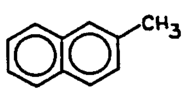
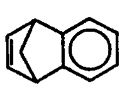
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_9F_3O^+$ | | | | | | | |
|  | (9.1±0.05) | (42) | (175) | −168 | −703 | *EST | |
| | IP from 81SCH/GRO. | | | | | | |
| $C_{11}H_{10}^+$ | | | | | | | |
|  | 7.85 | 208 | 870 | 27±0.5 | 113±2 | 74SAB/CHA | 90-12-0 |
| | IP from 82LEV/LIA, 83KLA/KOV. | | | | | | |
|  | (≤7.26±0.03) | (≤227) | (≤953) | 60 | 253 | *EST | 769-31-3 |
|  | (≤7.33±0.03) | (≤229) | (≤960) | 60 | 253 | *EST | 17647-77-7 |
|  | (≤7.30±0.03) | (≤227) | (≤950) | 59 | 246 | *EST | 1654-55-3 |
|  | (≤7.34±0.03) | (≤228) | (≤954) | 59 | 246 | *EST | 1654-52-0 |
|  | (7.8) | (206) | (864) | 27±0.5 | 111±2 | 74SAB/CHA | 91-57-6 |
| | IP is onset of photoelectron band (82LEV/LIA, 83KLA/KOV). | | | | | | |
|  | (8.1) | (253) | (1057) | 66 | 276 | *EST | 4453-90-1 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

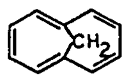
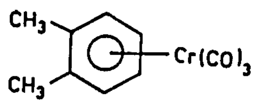
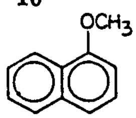
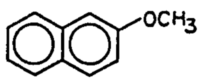
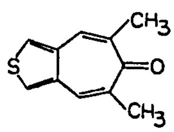
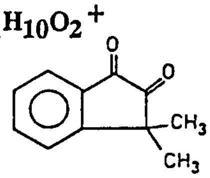
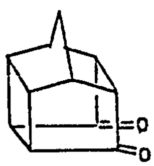
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{10}^+$ | | | | | | | |
|  | (7.7) | (253) | (1058) | 75±1 | 315±6 | 77PED/RYL | 2443-46-1 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |
| $C_{11}H_{10}CrO_3^+$ | | | | | | | |
|  | (6.70±0.1) | (54) | (224) | −101 | −422 | *EST | 12129-29-2 |
| | See also: 82GUI/PFI. | | | | | | |
| $C_{11}H_{10}O^+$ | | | | | | | |
|  | 7.70 | (177) | (742) | −0.2 | −1 | *EST | 2216-69-5 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (7.44) | (171) | (717) | −0.2 | −1 | *EST | 93-04-9 |
| | IP is onset of photoelectron band (83KLA/KOV). | | | | | | |
| $C_{11}H_{10}OS^+$ | | | | | | | |
|  | (≤8.40) | (≤201) | (≤840) | 7 | 30 | *EST | |
| | IP from 84GLE/BIS. | | | | | | |
| $C_{11}H_{10}O_2^+$ | | | | | | | |
|  | (8.5) | (145) | (607) | −51 | −213 | *EST | 20651-88-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | ≤9.1 | ≤195 | ≤814 | −15 | −64 | 64COO/CRU | |
| | IP from 84MAR/KAY. | | | | | | |

Table 1. Positive Ion Table - Continued

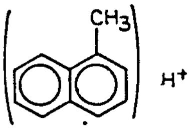
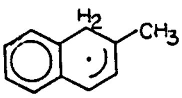
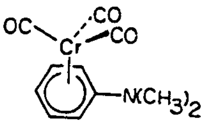
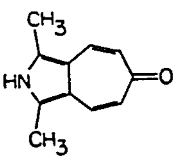
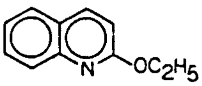
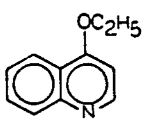
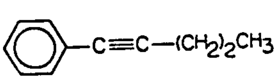
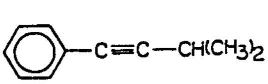
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{11}^+$ | | | | | | | |
|  | | 192 | 803 | | | | |
| | From proton affinity of 1-methylnaphthalene (RN 90-12-0). PA = 200.7 kcal/mol, 840. kJ/mol. | | | | | | |
|  | | 192 | 804 | | | | |
| | From proton affinity of 2-methylnaphthalene (RN 91-57-6). PA = 200.0 kcal/mol, 837. kJ/mol. | | | | | | |
| $C_{11}H_{11}CrNO_3^+$ | | | | | | | |
|  | (6.9) | (63) | (262) | −96±3 | −404±13 | 84ALT/CON | 12109-10-3 |
| $C_{11}H_{11}NO^+$ | | | | | | | |
|  | (7.55) | (182) | (763) | 8 | 35 | *EST | |
| | IP from 84GLE/BIS. | | | | | | |
|  | (8.0) | (181) | (756) | −4 | −16 | *EST | 46185-83-5 |
| | IP is onset of photoelectron band (81PFI/GUI). | | | | | | |
|  | (8.1) | (192) | (804) | 5 | 23 | *EST | 13720-91-7 |
| | IP is onset of photoelectron band (81PFI/GUI). | | | | | | |
| $C_{11}H_{12}^+$ | | | | | | | |
|  | (≤8.29±0.02) | (≤252) | (≤1055) | 61 | 255 | *EST | 4250-81-1 |
|  | (8.35±0.08) | (252) | (1053) | 59 | 247 | *EST | 1612-03-9 |
| | IP is onset of photoelectron band (81ELB/LIE). | | | | | | |

**Table 1. Positive Ion Table - Continued**

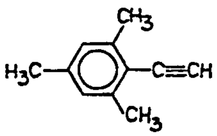
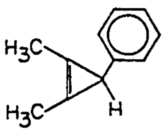
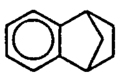
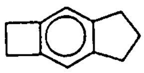
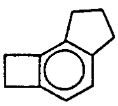
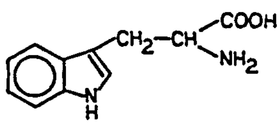
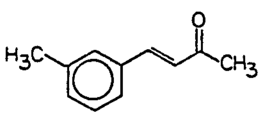
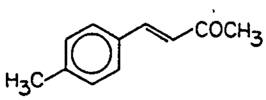
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{12}^+$ | | | | | | | |
|  | (8.16±0.08)<br>IP from 81ELB/LIE. | (263) | (1102) | 75 | 315 | *EST | 769-26-6 |
|  | (≤8.17)<br>IP from 84BAI/DOM. | (≤253) | (≤1058) | 65 | 270 | *EST | 23063-31-2 |
|  | (≤8.42±0.05)<br>IP from 82HAS/NEU, 82LEV/LIA. | (≤224) | (≤938) | 30 | 126 | *EST | 4486-29-7 |
|  | (8.05) | (228) | (956) | 43 | 179 | *EST | 60582-10-7 |
|  | (8.19) | (232) | (969) | 43 | 179 | *EST | 60582-11-8 |
| $C_{11}H_{12}N_2O_2^+$ | | | | | | | |
|  | (≤7.5)<br>See also: 83CAN/HAM. | (≤115) | (≤481) | −58 | −243 | *EST | 54-12-6 |
| $C_{11}H_{12}O^+$ | | | | | | | |
|  | (8.6±0.05)<br>IP from 81SCH/GRO. | (182) | (762) | −16 | −68 | 81SCH/GRO | 15753-84-1 |
|  | (8.5±0.05)<br>IP is onset of photoelectron band (81SCH/GRO). | (180) | (752) | −16 | −68 | *EST | 4023-84-1 |

**Table 1. Positive Ion Table - Continued**

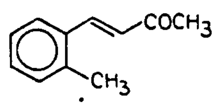
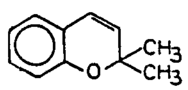
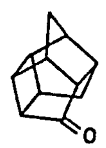
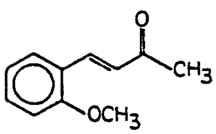
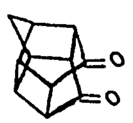
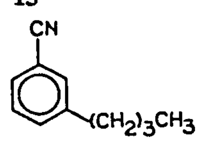
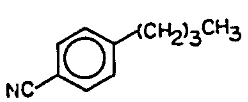
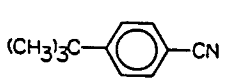
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{12}O^+$ | | | | | | | |
|  | 8.5±0.05 | 183 | 766 | −13 | −54 | 79SCH/GRU | 16927-82-5 |
| | IP from 79SCH/GRU, 80GRU/SCH, 81SCH/GRO. | | | | | | |
|  | (7.8±0.05) | (170) | (711) | −10 | −41 | 79SCH/GRU | 2513-25-9 |
| | IP from 79SCH/GRU. | | | | | | |
|  | ≤8.8 | (≤208) | (≤871) | 5 | 22 | *EST | |
| | IP from 84MAR/KAY. | | | | | | |
| $C_{11}H_{12}O_2^+$ | | | | | | | |
|  | (8.2) | (146) | (612) | −43 | −179 | 79SCH/GRU | 10542-87-7 |
| | IP from 79SCH/GRU, 80GRU/SCH. | | | | | | |
|  | (8.1) | (205) | (860) | 19 | 78 | *EST | 60526-44-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{11}H_{13}N^+$ | | | | | | | |
|  | (9.77±0.1) | (254) | (1064) | 29±0.2 | 121±1 | *EST | 20651-74-5 |
|  | (10.08±0.1) | (261) | (1094) | 29±0.2 | 121±1 | *EST | 20651-73-4 |
|  | (8.8) | (229) | (959) | 26 | 110 | 85ORL/MIS | 4210-32-6 |
| | IP is onset of photoelectron band (85BAI/MIS2). See also: 86ORL/MIS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

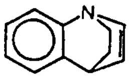
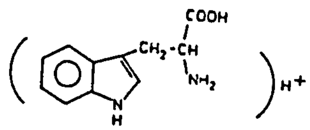
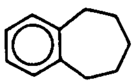
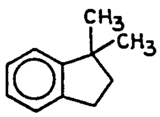
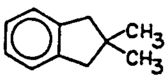
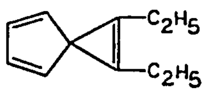
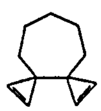
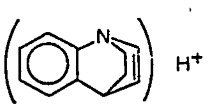
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{13}N^+$ | | | | | | | |
|  | (7.85±0.02) | (222) | (930) | 41 | 173 | *EST | 4363-25-1 |
| $C_{11}H_{13}N_2O_2^+$ | | | | | | | |
|  | | 82 | 344 | | | | |
| | From proton affinity of L-tryptophan (RN 54-12-6). PA = 225.4 kcal/mol, 943. kJ/mol. | | | | | | |
| $C_{11}H_{14}^+$ | | | | | | | |
|  | ≤8.40±0.02 | (≤198) | (≤827) | 4±0.7 | 17±3 | *EST | 1075-16-7 |
|  | (8.47) | (195) | (815) | -0.5±0.2 | -2±1 | 78OSB/SCO | 4912-92-9 |
|  | (8.47) | (195) | (815) | 0.5±0.2 | -2±1 | *EST | 20836-11-7 |
|  | (7.87) | (260) | (1089) | 79 | 330 | *EST | 49542-94-1 |
|  | (8.25) | (286) | (1196) | 96 | 400 | *EST | 58738-49-1 |
| | IP is onset of photoelectron band (82SPA/KOR). | | | | | | |
| $C_{11}H_{14}N^+$ | | | | | | | |
|  | | 175 | 732 | | | | |
| | From proton affinity of 1,4-dihydro-1,4-ethanoquinoline (RN 4363-25-1). PA = 232.0 kcal/mol, 971. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

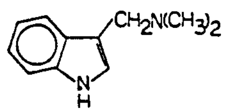
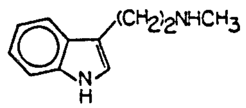
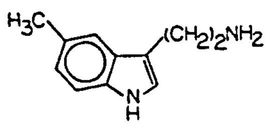
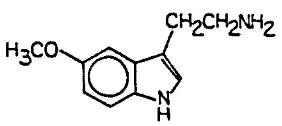
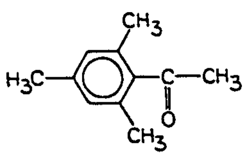
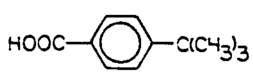
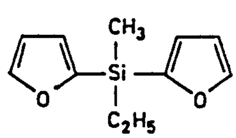
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{14}N_2^+$ | | | | | | | |
|  | (≤7.69±0.16) | (≤215) | (≤900) | 38 | 158 | *EST | 87-52-5 |
|  | (7.7) | (206) | (864) | 29 | 121 | *EST | 61-49-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.6) | (201) | (839) | 25 | 106 | *EST | 1821-47-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{11}H_{14}N_2O^+$ | | | | | | | |
|  | (≤7.68±0.12) | (≤174) | (≤729) | −3 | −12 | *EST | 608-07-1 |
| $C_{11}H_{14}O^+$ | | | | | | | |
|  | (8.2) | (140) | (586) | −49.0±0.9 | −204.9±3.6 | 77PED/RYL | 1667-01-2 |
| | IP is onset of photoelectron band (78CEN/FRA). | | | | | | |
| $C_{11}H_{14}O_2^+$ | | | | | | | |
|  | (8.6) | (103) | (431) | −95 | −399 | 85ORL/MIS | 98-73-7 |
| | IP is onset of photoelectron band (85BAI/MIS2). See also: 86ORL/MIS. | | | | | | |
| $C_{11}H_{14}O_2Si^+$ | | | | | | | |
|  | (8.1) | (138) | (577) | −49 | −205 | *EST | |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |

Table 1. Positive Ion Table - Continued

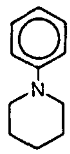
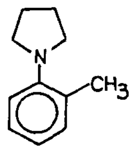
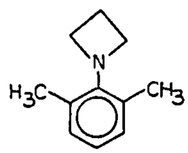
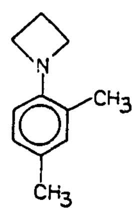
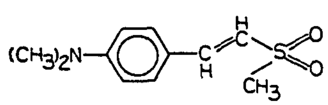
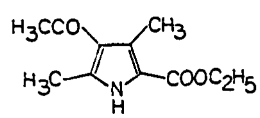
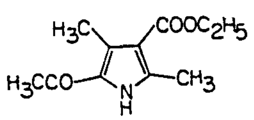
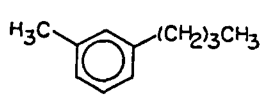
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{15}N^+$ | | | | | | | |
|  | (7.1) | (172) | (718) | 8 | 33 | *EST | 4096-20-2 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (6.8) | (184) | (771) | 27 | 115 | *EST | 41378-30-7 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (7.0) | (230) | (961) | 68 | 286 | *EST | 19199-06-5 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (≤7.48) | (≤223) | (≤933) | 50 | 211 | *EST | 81506-10-7 |
| | IP from 82ROZ/HOU2. | | | | | | |
| $C_{11}H_{15}NO_2S^+$ | | | | | | | |
|  | (7.0) | (129) | (538) | −33 | −137 | *EST | |
| | IP is onset of photoelectron band (84CAU/FUR). | | | | | | |
| $C_{11}H_{15}NO_3^+$ | | | | | | | |
|  | ≤8.26 | (≤54) | (≤227) | −136 | −570 | *EST | |
| | IP from 81CAU/GIA. | | | | | | |
|  | (≤8.23) | (≤54) | (≤224) | −136 | −570 | *EST | 6314-22-3 |
| | IP from 81CAU/GIA. | | | | | | |
| $C_{11}H_{16}^+$ | | | | | | | |
|  | (8.42±0.1) | (184) | (768) | −11 | −44 | *EST | 1595-04-6 |

**Table 1. Positive Ion Table - Continued**

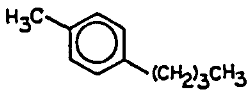
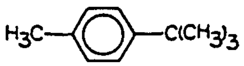
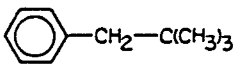
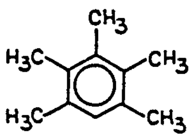
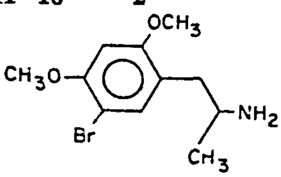
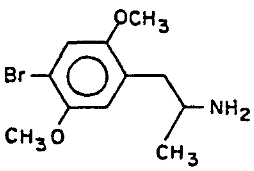
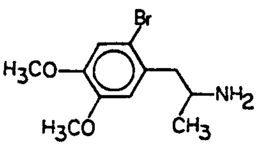
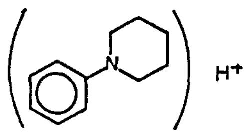
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{16}^+$ | | | | | | | |
|  | (8.35±0.1) | (182) | (761) | −11 | −45 | *EST | 1595-05-7 |
|  | 8.28 | (178) | (744) | −13 | −55 | 85ORL/MIS | 98-51-1 |
| | IP from 86ORL/MIS. See also: 85BAI/MIS. | | | | | | |
|  | ≤8.7 | (≤187) | (≤784) | −13 | −55 | *EST | 1007-26-7 |
|  | 7.92±0.02 | (165) | (690) | −18 | −74 | *EST | 700-12-9 |
| | See: 84HOW/GON. | | | | | | |
| $C_{11}H_{16}BrNO_2^+$ | | | | | | | |
|  | (7.4) | (97) | (406) | −74 | −308 | *EST | 60917-67-1 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
|  | (7.3) | (97) | (404) | −72 | −300 | *EST | 64638-07-9 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |
|  | (7.4) | (102) | (425) | −69 | −289 | *EST | 32156-25-5 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
| $C_{11}H_{16}N^+$ | | | | | | | |
|  | | 154 | 642 | | | | |
| | From proton affinity of 1-phenylpiperidine (RN 4096-20-2). PA = 225.8 kcal/mol, 945. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

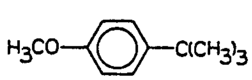
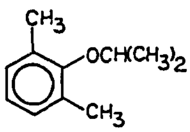
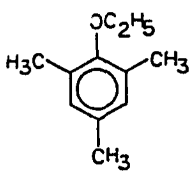
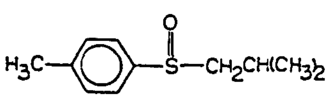
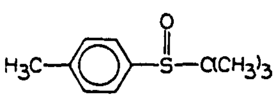
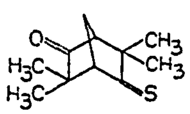
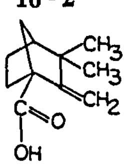
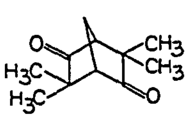
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{16}O^+$ | | | | | | | |
|  | (7.77) | (138) | (576) | −41.5 | −173.8 | 86ORL/MIS | 5396-38-3 |
| | IP from 86ORL/MIS. | | | | | | |
|  | 8.49 | (162) | (676) | −34 | −143 | *EST | 54350-31-1 |
|  | (≤8.28) | (≤165) | (≤692) | −26 | −107 | *EST | 61248-63-3 |
| $C_{11}H_{16}OS^+$ | | | | | | | |
|  | (≤8.50) | (≤163) | (≤681) | −33 | −139 | *EST | 77919-66-5 |
| | IP from 81MOH/JIA. | | | | | | |
|  | (≤8.33) | (≤162) | (≤678) | −30 | −126 | *EST | 49833-45-6 |
| | IP from 81MOH/JIA. | | | | | | |
|  | (8.25) | (144) | (601) | −47 | −195 | *EST | 75503-13-8 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
| $C_{11}H_{16}O_2^+$ | | | | | | | |
|  | (≤9.05) | (≤112) | (≤468) | −97 | −405 | *EST | 10309-20-3 |
| | IP from 81NES/BAI. | | | | | | |
|  | (8.86) | (108) | (450) | −97 | −405 | *EST | 57239-03-9 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |

**Table 1. Positive Ion Table - Continued**

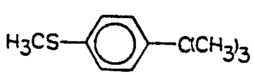
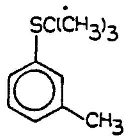
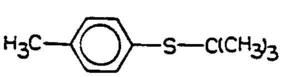
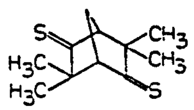
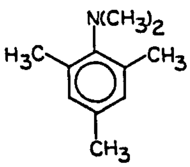
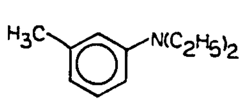
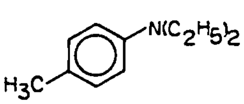
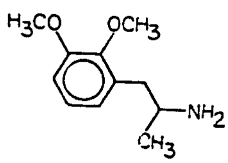
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{16}S^+$ | | | | | | | |
|  | (≤7.83±0.05) | (≤179) | (≤747) | −2 | −8 | *EST | 7252-86-0 |
|  | (≤8.35) | (≤188) | (≤788) | −4 | −18 | *EST | 34786-26-0 |
|  | (≤8.31) | (≤187) | (≤784) | −4 | −18 | *EST | 7439-10-3 |
| $C_{11}H_{16}S_2^+$ | | | | | | | |
|  | (8.2) | (193) | (806) | 4 | 15 | *EST | 75503-14-9 |
| | IP is onset of photoelectron band (80FRO/WES). | | | | | | |
| $C_{11}H_{17}N^+$ | | | | | | | |
|  | (7.24) | (174) | (729) | 7 | 30 | *EST | 13021-15-3 |
|  | (6.90) | (160) | (670) | 1 | 4 | *EST | 91-67-8 |
| | IP from charge transfer equilibrium constant determinations; reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV). (85LIA/JAC). | | | | | | |
|  | (6.83) | (160) | (671) | 3 | 12 | *EST | 613-48-9 |
| | IP from charge transfer equilibrium constant determinations; reference standard: IP ($C_6H_5N(CH_3)_2$ = 7.12 eV). (84MAU/NEL, 85LIA/JAC). | | | | | | |
| $C_{11}H_{17}NO_2^+$ | | | | | | | |
|  | (≤8.30) | (≤130) | (≤544) | −61 | −257 | *EST | 15402-81-0 |
| | IP from 81DOM/EAT. | | | | | | |

Table 1. Positive Ion Table - Continued

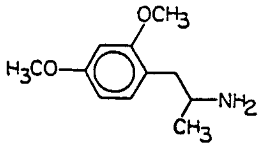
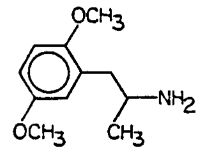
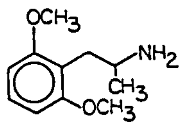
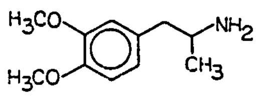
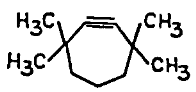
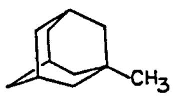
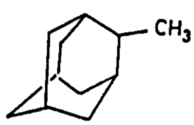
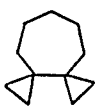
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{17}NO_2^+$ | | | | | | | |
|  | (7.4) | (99) | (416) | −71 | −298 | *EST | 23690-13-3 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |
|  | (7.1) | (94) | (395) | −69 | −290 | *EST | 13641-74-2 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |
|  | (8.18) | (117) | (491) | −71 | −298 | *EST | 23690-14-4 |
| | IP from 81DOM/EAT. | | | | | | |
|  | (≤8.03±0.06) | (≤118) | (≤492) | −68 | −283 | *EST | 120-26-3 |
| | See also: 81DOM/GAP. | | | | | | |
| $C_{11}H_{18}^+$ | | | | | | | |
|  | (8.4) | (225) | (940) | 31 | 130 | *EST | 33470-40-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (9.17±0.02) | (170.9) | (715.0) | −40.6±0.3 | −169.8±1.4 | 79CLA/KNO | 768-91-2 |
|  | 9.24 | 176 | 737 | −36.9 | −154 | 79CLA/KNO | |
|  | (8.5) | (232) | (972) | 36 | 152 | *EST | 52879-54-6 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |

**Table 1. Positive Ion Table - Continued**

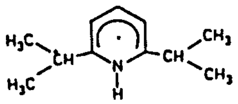
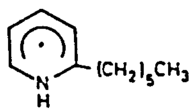
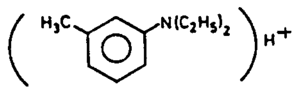
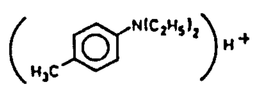
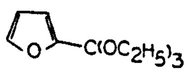
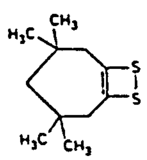
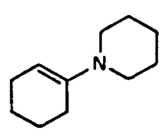
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{18}N^+$ | | | | | | | |
|  | | 125 | 523 | | | | |
| | From proton affinity of 2,6-diisopropylpyridine (RN 6832-21-9). PA = 232.9 kcal/mol, 974. kJ/mol. | | | | | | |
|  | | 137 | 572 | | | | |
| | From proton affinity of 2-n-hexylpyridine (RN 1129-69-7). PA = 228.9 kcal/mol, 958. kJ/mol. | | | | | | |
|  | | 138 | 578 | | | | |
| | From proton affinity of 3-$CH_3C_6H_4N(C_2H_5)_2$ (RN 91-67-8). PA = 228.9 kcal/mol, 956. kJ/mol. | | | | | | |
|  | | 140 | 587 | | | | |
| | From proton affinity of 4-$CH_3C_6H_4N(C_2H_5)_2$ (RN 613-48-9). PA = 228.6 kcal/mol, 956. kJ/mol. | | | | | | |
| $C_{11}H_{18}O_4^+$ | | | | | | | |
|  | (8.7) | (46) | (190) | −155 | −649 | *EST | 75905-10-1 |
| | IP is onset of photoelectron band (83ZYK/ERC). | | | | | | |
| $C_{11}H_{18}S_2^+$ | | | | | | | |
|  | 7.65 | (203) | (848) | 26 | 110 | *EST | |
| | IP is onset of photoelectron band (83JIA/MOH). | | | | | | |
| $C_{11}H_{19}N^+$ | | | | | | | |
|  | (≤7.44±0.03) | (≤162) | (≤676) | −10 | −42 | *EST | 2981-10-4 |

**Table 1. Positive Ion Table - Continued**

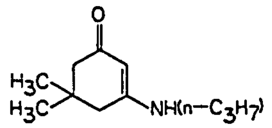
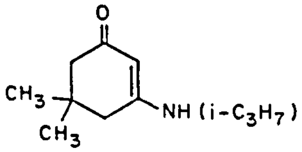
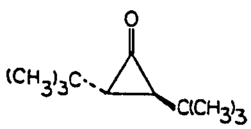
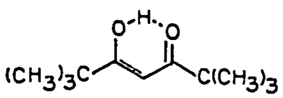
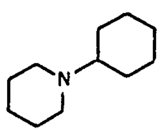
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{11}H_{19}NO^+$** | | | | | | | |
|  | (≤8.03)<br>IP from 82PFI/GER. | (≤131) | (≤548) | −54 | −227 | *EST | 56570-54-8 |
|  | (≤7.94)<br>IP from 82PFI/GER. | (≤125) | (≤525) | −58 | −241 | *EST | 80555-73-3 |
| **$C_{11}H_{20}^+$** | | | | | | | |
| (tert-$C_4H_9)_2C=C=CH_2$ | (≤8.55) | (≤206) | (≤860) | 8 | 35 | *EST | 22585-31-5 |
| $(CH_3)_3CCH=C=CHC(CH_3)_3$ | (8.6)<br>IP is onset of photoelectron band (85ELS/VER). | (193) | (807) | −5 | −23 | *EST | 42066-39-7 |
| 1-$C_{11}H_{20}$ | (9.90±0.02) | (233) | (976) | 5 | 21 | *EST | 2243-98-3 |
| 2-$C_{11}H_{20}$ | (9.28±0.02) | (214) | (897) | 0.5 | 2 | *EST | 60212-29-5 |
| 3-$C_{11}H_{20}$ | (9.17±0.02) | (212) | (888) | 0.8 | 3 | *EST | 60212-30-8 |
| 4-$C_{11}H_{20}$ | (9.13±0.02) | (211) | (884) | 0.8 | 3 | *EST | 60212-31-9 |
| 5-$C_{11}H_{20}$ | (9.11±0.02) | (211) | (882) | 0.8 | 3 | *EST | 2294-72-6 |
| **$C_{11}H_{20}O^+$** | | | | | | | |
|  | (≤8.45) | (≤147) | (≤613) | −48 | −202 | *EST | 14743-58-9 |
| **$C_{11}H_{20}O_2^+$** | | | | | | | |
|  | (7.9)<br>Heat of formation of neutral molecule refers to enol form.<br>IP is onset of photoelectron band. | (56) | (234) | −126±1 | −528±4 | 81FER/RIB | 1118-71-4 |
| **$C_{11}H_{21}N^+$** | | | | | | | |
|  | (≤7.93±0.03) | (≤146) | (≤609) | −37 | −156 | *EST | 3319-01-5 |

**Table 1. Positive Ion Table - Continued**

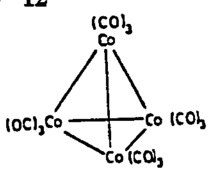
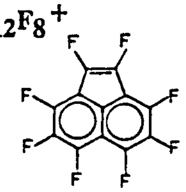
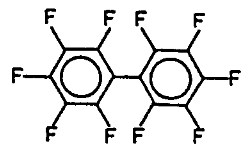
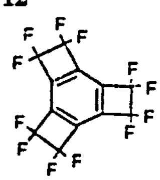
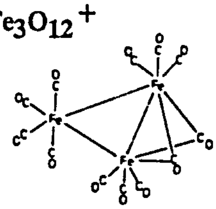
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{11}H_{22}^+$ | | | | | | | |
| $C_2H_5CH_2C(C_2H_5)=C(C_2H_5)_2$ | (8.04±0.02)' | (145) | (606) | −41 | −170 | *EST | 50787-14-9 |
| $C_{11}H_{24}^+$ | | | | | | | |
| n-$C_{11}H_{24}$ | (9.56) | (156) | (651) | −65±0.6 | −271±3 | 77PED/RYL | 1120-21-4 |
| | IP from charge transfer equilibrium constant determinations (81MAU/SIE, 82LIA). | | | | | | |
| n-$C_8H_{17}CH(CH_3)_2$ | (9.68) | (157) | (656) | −66 | −278 | *EST | 6975-98-0 |
| | IP from charge transfer equilibrium constant determinations (81MAU/SIE, 82LIA). | | | | | | |
| $C_{12}Co_4O_{12}^+$ | | | | | | | |
|  | 7.45 | (−246.2) | (−1030.1) | −418.0±3.2 | −1748.9±13 | 82PIL/SKI | 17786-31-1 |
| | IP is onset of photoelectron band. See also: 81GRE/MIN. | | | | | | |
| $C_{12}F_8^+$ | | | | | | | |
|  | (≤9.1±0.1) | (≤−56) | (≤−234) | −266 | −1112 | *EST | 1554-93-4 |
| $C_{12}F_{10}^+$ | | | | | | | |
|  | (9.40±0.02) | (−115) | (−480) | −332±3 | −1387±12 | 79PRI/SAP2 | 434-90-2 |
| $C_{12}F_{12}^+$ | | | | | | | |
|  | 11.14 | (−211) | (−884) | −468 | −1959 | *EST | 32937-02-3 |
| | IP is onset of photoelectron band (84HEI/WIR). | | | | | | |
| $C_{12}F_{27}N^+$ | | | | | | | |
| $(n\text{-}C_4F_9)_3N$ | (11.3) | (−1067) | (−4466) | −1328±2 | −5556±10 | 79ERA/KOL | 311-89-7 |
| | IP is onset of photoelectron band (82ELB/DIE, 83MOL/PIK3). | | | | | | |
| $C_{12}Fe_3O_{12}^+$ | | | | | | | |
|  | (7.44) | (−247) | (−1035) | −419±6 | −1753±27 | 82PIL/SKI | 17685-52-8 |
| | IP is onset of photoelectron band (82DEK/WON). | | | | | | |

Table 1. Positive Ion Table - Continued

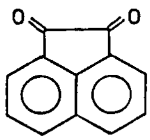
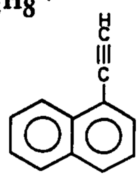
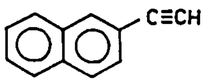
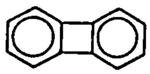
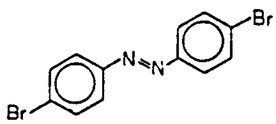
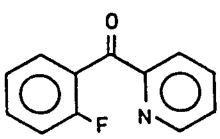
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_6O_2{}^+$ | | | | | | | |
|  | (8.6) | (305) | (1275) | 106 | 445 | *EST | 82-86-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_8{}^+$ | | | | | | | |
|  | (8.03) | (279) | (1166) | 93 | 391 | *EST | 15727-65-8 |
| | IP is onset of photoelectron band (81GLE/SCH). | | | | | | |
|  | (8.11) | (280) | (1173) | 93 | 391 | *EST | 2949-26-0 |
| | IP is onset of photoelectron band (81GLE/SCH). | | | | | | |
|  | (8.22±0.04) | (252) | (1053) | 62±0.2 | 260±1 | 81KUD/KUD | 208-96-8 |
|  | 7.56±0.02 | 279 | 1166 | 104±3 | 437±13 | 77PED/RYL | 259-79-0 |
| | IP derived from charge transfer equilibrium constant determinations is in agreement (80MAU). See also: 85DEW/TIE. | | | | | | |
| $C_{12}H_8Br_2N_2{}^+$ | | | | | | | |
|  | (9.24) | (324) | (1355) | 110.8 | 463.6 | *EST | 1601-98-5 |
| | IP from 77NUY/MES. | | | | | | |
| $C_{12}H_8FNO^+$ | | | | | | | |
|  | 9.11 | (222) | (927) | 11 | 48 | *EST | 6238-65-9 |
| | IP from 80GRU/SCH. See also: 82LEV/LIA. | | | | | | |

**Table 1. Positive Ion Table - Continued**

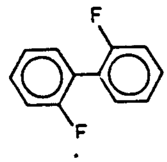
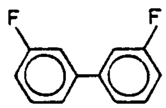
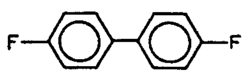
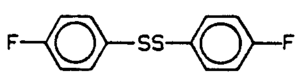
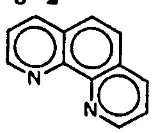
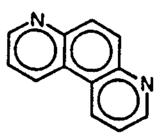
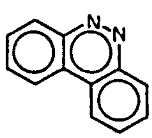
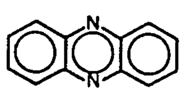
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_8F_2{}^+$ | | | | | | | |
|  | (8.35±0.02) | (147) | (616) | −45±1 | −190±5 | 64SMI/GOV | 388-82-9 |
|  | (8.35±0.02) | (146) | (611) | −47 | −195 | *EST | 396-64-5 |
|  | (8.00±0.02) | (138) | (577) | −47±1 | −195±5 | 64SMI/GOV | 398-23-2 |
| $C_{12}H_8F_2S_2{}^+$ | | | | | | | |
|  | (≤8.4) | (≤109) | (≤456) | −85 | −354 | *EST | 405-31-2 |
| | IP from 82GIO/BOC. | | | | | | |
| $C_{12}H_8N_2{}^+$ | | | | | | | |
|  | (8.3) | (270) | (1130) | 79 | 329 | *EST | 66-71-7 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.35±0.02 | (269) | (1127) | 77 | 321 | *EST | 230-07-9 |
|  | (7.9) | (277) | (1159) | 95 | 397 | 77SCH/PET | 230-17-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.33±0.02 | 274 | 1148 | 82±0.7 | 344±3 | 80ARS | 92-82-0 |

**Table 1. Positive Ion Table - Continued**

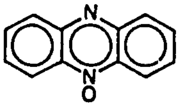
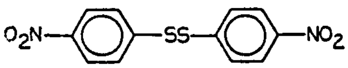
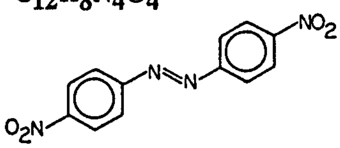
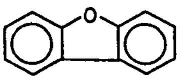
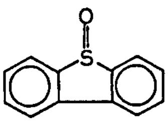
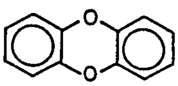
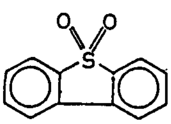
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_8N_2O^+$ | | | | | | | |
|  | 8.00±0.02 | (247) | (1036) | 63 | 264 | *EST | 304-81-4 |
| $C_{12}H_8N_2O_4S_2^+$ | | | | | | | |
|  | (≤8.98)<br>IP from 82GIO/BOC. | (≤258) | (≤1080) | 51 | 214 | *EST | 100-32-3 |
| $C_{12}H_8N_4O_4^+$ | | | | | | | |
|  | (9.97)<br>IP from 77NUY/MES. | (314) | (1312) | 83.6 | 349.8 | *EST | |
| $C_{12}H_8O^+$ | | | | | | | |
|  | 7.9±0.05 | 202 | 845 | 20±1 | 83±5 | 77PED/RYL | 132-64-9 |
| $C_{12}H_8OS^+$ | | | | | | | |
|  | (8.1)<br>IP is onset of photoelectron band. | (206) | (863) | 19 | 81 | *EST | 1013-23-6 |
| $C_{12}H_8O_2^+$ | | | | | | | |
|  | (7.5)<br>IP is onset of photoelectron band. | (158) | (661) | −15 | −63 | 82SHA | 262-12-4 |
| $C_{12}H_8O_2S^+$ | | | | | | | |
|  | (8.9)<br>IP is onset of photoelectron band. | (171) | (714) | −35 | −145 | *EST | 1016-05-3 |

Table 1. Positive Ion Table - Continued

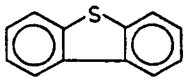
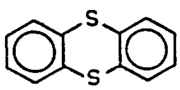
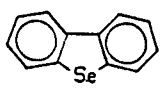
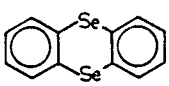
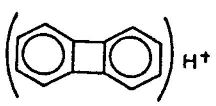
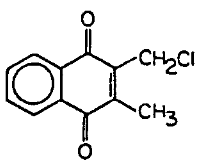
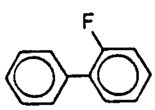
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_8S^+$ | | | | | | | |
|  | 7.90±0.03 | 231 | 967 | 49±0.7 | 205±1 | 79SAB | 132-65-0 |
| $C_{12}H_8S_2^+$ | | | | | | | |
|  | (7.7) | (201) | (840) | 23±1 | 97±6 | 77PED/RYL | 92-85-3 |
| | IP is onset of photoelectron band (81TRA/RED). | | | | | | |
| $C_{12}H_8Se^+$ | | | | | | | |
|  | (≤7.86) | (≤243) | (≤1018) | 62 | 260 | *EST | 244-95-1 |
| | IP from 82TRA/ROD. | | | | | | |
| $C_{12}H_8Se_2^+$ | | | | | | | |
|  | (≤7.89) | (≤231) | (≤968) | 49 | 207 | *EST | |
| | IP from 82TRA/ROD. | | | | | | |
| $C_{12}H_9^+$ | | | | | | | |
|  | | 267 | 1116 | | | | |
| | From proton affinity of biphenylene. (RN 259-79-0). PA = 203.4 kcal/mol, 851. kJ/mol. | | | | | | |
| $C_{12}H_9ClO_2^+$ | | | | | | | |
|  | (9.25) | (242) | (1010) | 28 | 118 | *EST | 31599-79-8 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{12}H_9F^+$ | | | | | | | |
|  | (8.20±0.02) | (185) | (774) | −4 | −17 | *EST | 321-60-8 |

**Table 1. Positive Ion Table - Continued**

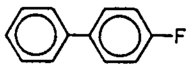
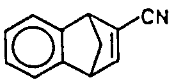
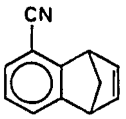
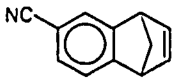
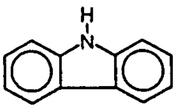
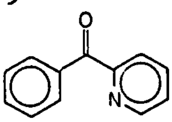
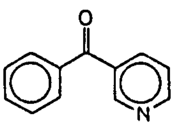
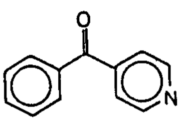
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_9F^+$ | | | | | | | |
|  | (8.00±0.02) | (180) | (755) | −4 | −17 | *EST | 324-74-3 |
| $C_{12}H_9N^+$ | | | | | | | |
|  | (8.5)<br>IP is onset of photoelectron band. | (294) | (1228) | 98 | 408 | *EST | 71906-57-5 |
|  | (8.7)<br>IP is onset of photoelectron band. | (301) | (1259) | 100 | 420 | *EST | 61346-79-0 |
|  | (8.7)<br>IP is onset of photoelectron band. | (300) | (1255) | 99 | 416 | *EST | 16513-60-3 |
|  | 7.57±0.03 | 229 | 959 | 55±0.2 | 229±1 | 81KUD/KUD2 | 86-74-8 |
| $C_{12}H_9NO^+$ | | | | | | | |
|  | 9.06<br>IP from 82LEV/LIA, 80GRU/SCH. | (247) | (1032) | 38 | 158 | *EST | 91-02-1 |
|  | (9.6±0.1) | (261) | (1090) | 39 | 164 | *EST | 5424-19-1 |
|  | (9.6±0.1) | (261) | (1090) | 39 | 164 | *EST | 14548-46-0 |

Table 1. Positive Ion Table - Continued

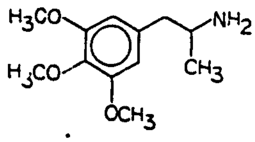
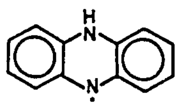
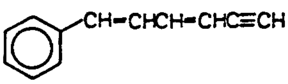
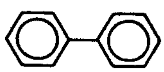
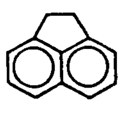
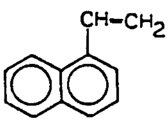
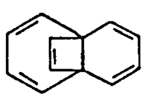
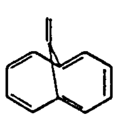
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_{12}H_9NO_3^+$** | | | | | | | |
|  | (≤8.16±0.06) | (≤90) | (≤376) | −98 | −411 | *EST | 22199-17-3 |
| **$C_{12}H_9N_2^+$** | | | | | | | |
|  | | 224 | 938 | | | | |
| | From proton affinity of phenazine (RN 92-82-0). PA = 223.7 kcal/mol, 936. kJ/mol. | | | | | | |
| **$C_{12}H_{10}^+$** | | | | | | | |
|  | (7.9) | (244) | (1019) | 61.5 | 257.3 | 62MOM/BRA | 940-50-1 |
| | IP from 74KOP/SCH. | | | | | | |
|  | 7.95±0.02 | 226.9 | 949.4 | 43.6±0.3 | 182.3±1.4 | 77PED/RYL | 92-52-4 |
| | See also: 74KOP/SCH. | | | | | | |
|  | (7.68) | (214) | (896) | 37±0.2 | 155±1 | 81KUD/KUD | 83-32-9 |
| | IP from charge transfer equilibrium constant determinations (80MAU, re-evaluated). | | | | | | |
|  | (7.7) | (229) | (958) | 51 | 215 | *EST | 826-74-4 |
| | IP is onset of photoelectron band (81GLE/SCH). | | | | | | |
|  | (≤8.1) | (≤286) | (≤1197) | 99 | 415 | *EST | 19539-78-7 |
|  | (7.5) | (269) | (1127) | 96 | 403 | *EST | 10474-24-5 |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |

Table 1. Positive Ion Table - Continued

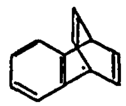
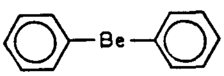
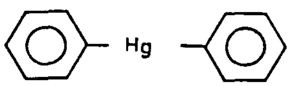
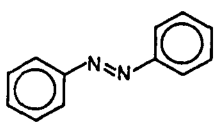
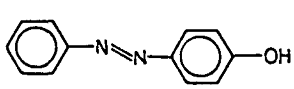
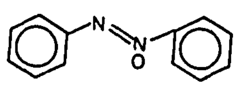
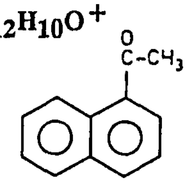
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{10}^+$ | | | | | | | |
|  | (8.0) | (259) | (1083) | 74 | 311 | *EST | 7322-47-6 |
| | IP is onset of photoelectron band (82HAS/NEU). | | | | | | |
| $C_{12}H_{10}Be^+$ | | | | | | | |
|  | (9.20±0.10) | (285) | (1193) | 73±5 | 305±21 | 80TEL/RAB | 22300-89-6 |
| $C_{12}H_{10}Hg^+$ | | | | | | | |
|  | 8.30±0.03 | 285 | 1192 | 93.5±0.8 | 391.4±3.2 | 77PED/RYL | 587-85-9 |
| | See also: 81FUR/PIA. | | | | | | |
| $C_{12}H_{10}N_2^+$ | | | | | | | |
|  | (8.2) | (286) | (1195) | 97±0.7 | 404±3 | 77SCH/PET | 17082-12-1 |
| | IP is onset of photoelectron band. See also: 81NAT/FRA. | | | | | | |
| $C_{12}H_{10}N_2O^+$ | | | | | | | |
|  | 7.6 | (229) | (958) | 54 | 225 | *EST | 20714-70-9 |
| | IP is onset of photoelectron band (81MIL/MIL, 82LEV/LIA). | | | | | | |
|  | (8.1) | (269) | (1124) | 81.7±0.6 | 342±2.4 | 86KIR/ACR | 495-48-7 |
| | IP is onset of photoelectron band (81MIL/CIL). | | | | | | |
| $C_{12}H_{10}O^+$ | | | | | | | |
|  | (8.23) | (185) | (773) | -5±2 | -21±8 | *EST | 941-98-0 |

**Table 1. Positive Ion Table - Continued**

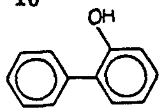
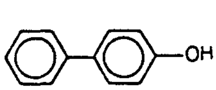
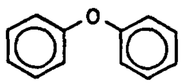
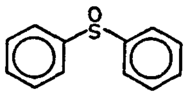
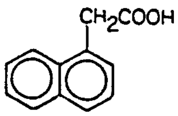
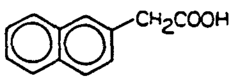
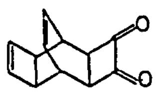
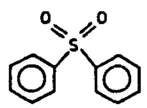
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{10}O^+$ | | | | | | | |
|  | (7.80±0.02) | (181) | (756) | 0.7 | 3 | *EST | 90-43-7 |
|  | (7.78±0.03) | (180) | (754) | 0.7 | 3 | *EST | 92-69-3 |
|  | 8.09±0.03 | 183 | 766 | -3.6±0.4 | -14.9±1.8 | 77PED/RYL | 101-84-8 |
| $C_{12}H_{10}OS^+$ | | | | | | | |
|  | (8.3) | (217) | (908) | 26±0.7 | 107±3 | 77PED/RYL | 945-51-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{10}O_2^+$ | | | | | | | |
|  | (7.71) | (111) | (464) | -67 | -280 | *EST | 86-87-3 |
| | IP is onset of photoelectron band (83KLA/KOV). | | | | | | |
|  | (8.05) | (118) | (495) | -67 | -282 | *EST | 581-96-4 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (8.5) | (227) | (948) | 31 | 128 | *EST | |
| | IP is onset of photoelectron band (85ALB/HEL). | | | | | | |
| $C_{12}H_{10}O_2S^+$ | | | | | | | |
|  | 9.16±0.03 | 183 | 765 | -28±0.7 | -119±3 | 77PED/RYL | 127-63-9 |
| | See: 81TRA/RED. | | | | | | |

**Table 1. Positive Ion Table - Continued**

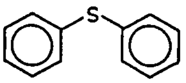
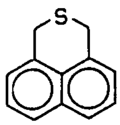
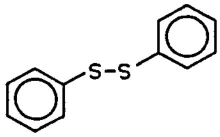
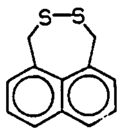
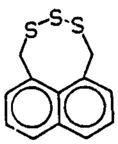
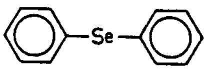
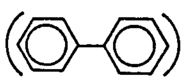
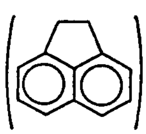
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{10}S^+$ | | | | | | | |
|  | 7.86±0.04 | 236 | 989 | 55±0.7 | 231±3 | 77PED/RYL | 139-66-2 |
| | See also: 81TRA/RED. | | | | | | |
|  | (7.91) | (232) | (972) | 50 | 209 | *EST | |
| | IP is onset of photoelectron band (81GUT/BES). | | | | | | |
| $C_{12}H_{10}S_2^+$ | | | | | | | |
|  | ≤8.3 | ≤250 | ≤1045 | 58±1 | 244±4 | 77PED/RYL | 882-33-7 |
| | IP from 82GIO/BOC. | | | | | | |
|  | (7.4) | (223) | (931) | 52 | 217 | *EST | 75574-98-0 |
| | IP is onset of photoelectron band (81GUT/BES). | | | | | | |
| $C_{12}H_{10}S_3^+$ | | | | | | | |
|  | (7.2) | (221) | (925) | 55 | 230 | *EST | 75574-99-1 |
| | IP is onset of photoelectron band (81GUT/BES). | | | | | | |
| $C_{12}H_{10}Se^+$ | | | | | | | |
|  | (≤7.79) | (≤248) | (≤1038) | 68.4±1.2 | 286.4±5.2 | 77PED/RYL | 1132-39-4 |
| | IP from 82TRA/ROD. | | | | | | |
| $C_{12}H_{11}^+$ | | | | | | | |
|  $H^+$ | | 213 | 892 | | | | |
| | From proton affinity of biphenyl (RN 92-52-4). PA = 196.1 kcal/mol, 820. kJ/mol. | | | | | | |
|  $H^+$ | | 199 | 834 | | | | |
| | From proton affinity of acenaphthene (RN 83-32-9). PA = 203.5 kcal/mol, 851. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

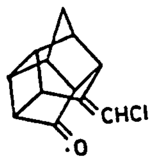
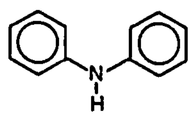
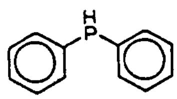
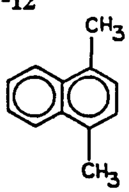
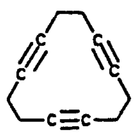
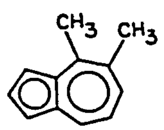
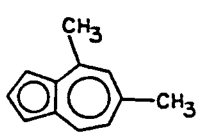
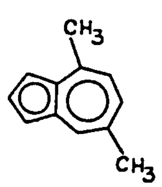
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{11}ClO^+$ | | | | | | | |
|  | 9.0<br>IP from 84MAR/KAY. | (204) | (853) | –4 | –15 | *EST | |
| $C_{12}H_{11}N^+$ | | | | | | | |
|  | 7.16±0.04 | 217 | 910 | 52±0.7 | 219±3 | 78STE | 122-39-4 |
| $C_{12}H_{11}P^+$ | | | | | | | |
|  | (7.80±0.01) | (234) | (979) | 54 | 226 | *EST | 829-85-6 |
| $C_{12}H_{12}^+$ | | | | | | | |
|  | 7.78±0.03 | 199 | 834 | 20 | 83 | 69STU/WES | 571-58-4 |
|  | (9.0)<br>IP is onset of photoelectron band. | (344) | (1441) | 137 | 573 | 80BAR/STR | 60323-50-4 |
|  | (≤7.18±0.03) | (≤219) | (≤915) | 53 | 222 | *EST | 56594-77-5 |
|  | (≤7.29±0.03) | (≤221) | (≤924) | 53 | 221 | *EST | 56594-78-6 |
|  | (≤7.20±0.03) | (≤219) | (≤916) | 53 | 221 | *EST | 46030-99-3 |

Table 1. Positive Ion Table - Continued

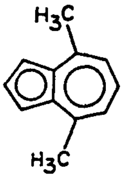
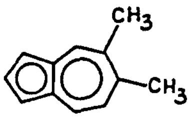
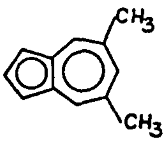
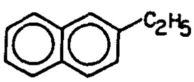
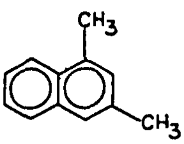
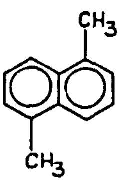
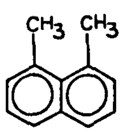
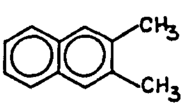
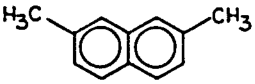
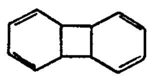
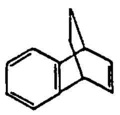
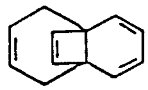
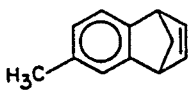
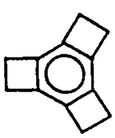
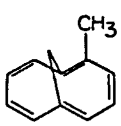
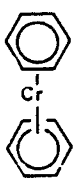
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{12}^+$ | | | | | | | |
|  | (≤7.27±0.03) | (≤221) | (≤923) | 53 | 222 | *EST | 7206-52-2 |
|  | (≤7.17±0.03) | (≤218) | (≤915) | 53 | 223 | *EST | 10556-12-4 |
|  | (≤7.08±0.03) | (≤216) | (≤906) | 53 | 223 | *EST | 56594-76-4 |
|  | 7.95<br>IP from 83KLA/KOV. | (203) | (853) | 20 | 86 | *EST | 939-27-5 |
|  | (≤7.86±0.03) | (≤201) | (≤840) | 20 | 82 | 69STU/WES | 575-41-7 |
|  | (≤7.85±0.03) | (≤201) | (≤839) | 20 | 82 | 69STU/WES | 571-61-9 |
|  | (7.5)<br>IP is onset of photoelectron band (81GUT/BES). | (199) | (832) | 26.0±0.2 | 108.7±1 | 77PED/RYL | 569-41-5 |
|  | (≤7.89±0.03) | (≤202) | (≤845) | 20 | 84 | 69STU/WES | 581-40-8 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{12}^+$ | | | | | | | |
|  | (≤7.89±0.03) | (≤202) | (≤844) | 20 | 83 | 69STU/WES | 582-16-1 |
|  | (7.7) | (269) | (1125) | 91 | 382 | *EST | 21657-71-6 |
| | IP is onset of photoelectron band (81GLE/GUB). | | | | | | |
|  | (8.2) | (235) | (984) | 46 | 193 | *EST | 7322-46-5 |
| | IP is onset of photoelectron band (82HAS/NEU). | | | | | | |
|  | (≤8.0) | (≤257) | (≤1076) | 73 | 304 | *EST | 38310-32-6 |
|  | (≤8.12±0.05) | (≤247) | (≤1033) | 60 | 250 | *EST | 4897-73-8 |
|  | (8.15±0.05) | (312) | (1306) | 124 | 520 | *EST | 60323-52-6 |
| | IP from 81HEI/KOV. | | | | | | |
|  | (7.5) | (239) | (1002) | 66 | 278 | *EST | 58790-01-5 |
| | IP from 84AND/CER. | | | | | | |
| $C_{12}H_{12}Cr^+$ | | | | | | | |
|  | 5.40 | 177 | 741 | 53±2 | 220±8 | 77PED/RYL | 1271-54-1 |
| | IP from 82CAB/COW. | | | | | | |

## Table 1. Positive Ion Table - Continued

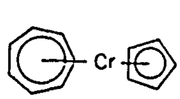
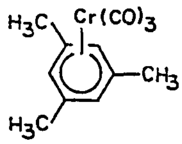
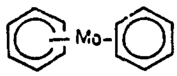
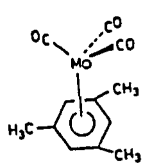
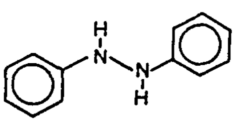
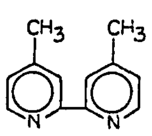
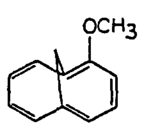
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_{12}H_{12}Cr^+$** | | | | | | | |
|  | (5.4) | (260) | (1087) | 135 | 566 | *EST | 12093-81-1 |
| | IP is onset of photoelectron band (85DAV/GAR). | | | | | | |
| **$C_{12}H_{12}CrO_3^+$** | | | | | | | |
|  | (6.8) | (45) | (190) | −111±2 | −466±10 | 77PED/RYL | 12129-67-8 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_{12}H_{12}Mo^+$** | | | | | | | |
|  | (≤5.52±0.05) | (≤223) | (≤935) | 96±5 | 402±20 | 77PED/RYL | 12129-68-9 |
| **$C_{12}H_{12}MoO_3^+$** | | | | | | | |
|  | (7.0) | (60) | (251) | −101±3 | −424±13 | 82PIL/SKI | 12089-15-5 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_{12}H_{12}N_2^+$** | | | | | | | |
|  | | | | 78 | 326 | 69BEN/CRU | 122-66-7 |
| | A value of 7.78 eV has been reported for the adiabatic IP of this compound. Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. | | | | | | |
|  | (8.2) | (241) | (1008) | 52 | 217 | *EST | 1134-35-6 |
| | IP is onset of photoelectron band (83DOB/HIL). | | | | | | |
| **$C_{12}H_{12}O^+$** | | | | | | | |
|  | (7.0) | (186) | (778) | 25 | 103 | *EST | |
| | IP is onset of photoelectron band (84AND/CER). | | | | | | |

**Table 1. Positive Ion Table - Continued**

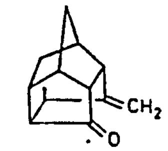
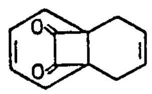
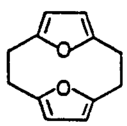
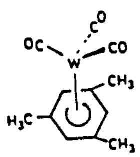
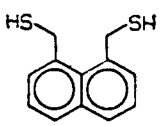
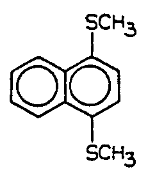
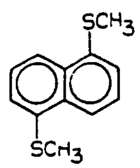
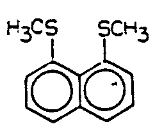
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{12}O^+$ | | | | | | | |
|  | ≤8.95<br>IP from 84MAR/KAY. | (≤206) | (≤864) | 0 | 0 | *EST | |
| $C_{12}H_{12}O_2{}^+$ | | | | | | | |
|  | (8.3)<br>IP is onset of photoelectron band. | (185) | (775) | −6 | −26 | *EST | 21377-44-6 |
|  | (7.60)<br>IP is onset of photoelectron band. | (148) | (620) | −27 | −113 | *EST | 73650-68-7 |
| $C_{12}H_{12}O_3W^+$ | | | | | | | |
|  | (7.0)<br>IP is onset of photoelectron band. | (74) | (309) | −87±4 | −366±15 | 84ALT/CON2 | 12129-69-0 |
| $C_{12}H_{12}S_2{}^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band (81GUT/BES). | (225) | (940) | 47 | 197 | *EST | 60948-99-4 |
|  | 7.4<br>IP is onset of photoelectron band. | (214) | (895) | 43 | 181 | *EST | 10075-73-7 |
|  | (7.3)<br>IP is onset of photoelectron band. | (212) | (885) | 43 | 181 | *EST | 10075-74-8 |
|  | (7.2)<br>IP is onset of photoelectron band | (215) | (901) | 49 | 206 | *EST | 7343-31-9 |

**Table 1. Positive Ion Table - Continued**

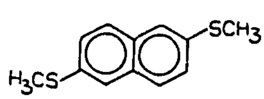
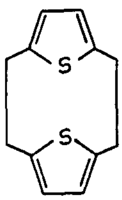
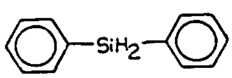
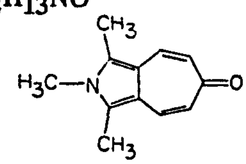
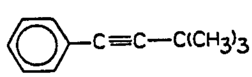
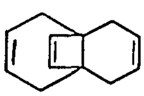
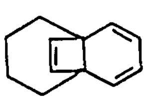
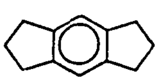
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{12}S_2^+$ | | | | | | | |
|  | 7.1 | (207) | (866) | 43 | 181 | *EST | 10075-77-1 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.95) | (258) | (1079) | 75 | 312 | *EST | 73650-69-8 |
| $C_{12}H_{12}Si^+$ | | | | | | | |
|  | (8.8) | (248) | (1037) | 45 | 188 | *EST | 775-12-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{13}NO^+$ | | | | | | | |
|  | (7.3) | (176) | (734) | 7 | 30 | *EST | |
| | IP is onset of photoelectron band (84GLE/BIS). | | | | | | |
| $C_{12}H_{14}^+$ | | | | | | | |
|  | (8.32±0.08) | (244) | (1020) | 52 | 217 | *EST | 4250-82-2 |
| | IP from 81ELB/LIE. See also: 85ORL/BOG. | | | | | | |
|  | (≤8.7) | (≤247) | (≤1032) | 46 | 193 | *EST | 20295-17-4 |
|  | (≤8.0) | (≤229) | (≤958) | 44 | 186 | *EST | 24139-33-1 |
|  | (7.94) | (193) | (809) | 10 | 43 | *EST | 495-52-3 |

Table 1. Positive Ion Table - Continued

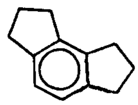
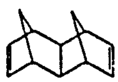
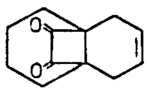
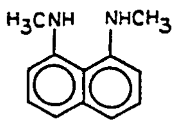
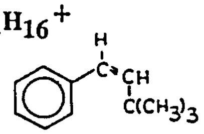
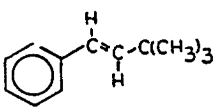
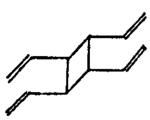
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{14}^+$ | | | | | | | |
|  | (8.09) | (200) | (836) | 13 | 55 | *EST | 1076-17-1 |
|  | (8.2) | (255) | (1068) | 66 | 277 | *EST | |
| | IP from 81PAD/PAT. | | | | | | |
| $C_{12}H_{14}O_2^+$ | | | | | | | |
|  | (8.1) | (152) | (638) | −34 | −144 | *EST | 21377-45-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{15}N_2^+$ | | | | | | | |
|  | | 181 | 757 | | | | |
| | From proton affinity of N,N'-dimethyl-1,8-naphthalenediamine (RN 20734-56-9). PA = 230.0 kcal/mol, 962. kJ/mol. | | | | | | |
| $C_{12}H_{16}^+$ | | | | | | | |
|  | 8.29±0.04 | (207) | (866) | 16±1 | 66±4 | 77PED/RYL | 3740-05-4 |
| | See also: 81KOB/ARA. | | | | | | |
|  | 7.80±0.04 | (188) | (786) | 8±2 | 33±9 | 77PED/RYL | 3846-66-0 |
| | See also: 81KOB/ARA. | | | | | | |
|  | (≤9.16) | (≤300) | (≤1255) | 88.7 | 371.1 | 83GLE/HAI2 | 82865-42-7 |
| | IP from 83GLE/HAI2 | | | | | | |
|  | (≤9.02) | (≤294) | (≤1231) | 86.2 | 360.7 | 83GLE/HAI2 | 87753-95-5 |
| | IP from 83GLE/HAI2 | | | | | | |

**Table 1. Positive Ion Table - Continued**

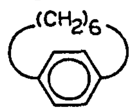
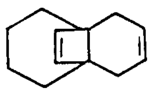
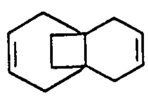
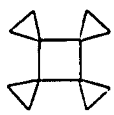
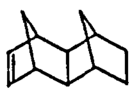
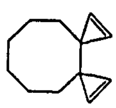
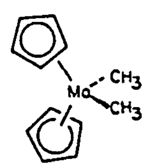
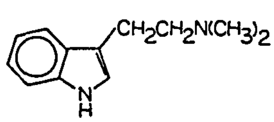
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{16}^+$ | | | | | | | |
|  | (7.5) | (196) | (821) | 23 | 97 | •EST | 53011-74-8 |
| | IP is onset of photoelectron band. | | | Name prob wrong | | | |
|  | (≤8.9) | (≤223) | (≤934) | 18 | 75 | •EST | 24139-32-0 |
|  | (8.7) | (278) | (1161) | 77 | 322 | •EST | 5103-78-6 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.22) | (≤326) | (≤1365) | 137 | 572 | •EST | 24375-17-5 |
|  | (8.6) | (231) | (968) | 33 | 138 | •EST | 262-30-6 |
| | IP from 81PAD/PAT. | | | | | | |
|  | (8.2) | (331) | (1385) | 142 | 594 | •EST | 64371-17-1 |
| | IP from 82SPA/KOR. | | | | | | |
| $C_{12}H_{16}Mo^+$ | | | | | | | |
|  | (≤6.1±0.1) | (≤226) | (≤943) | 85±1 | 354±6 | 82PIL/SKI | 39333-52-3 |
| $C_{12}H_{16}N_2^+$ | | | | | | | |
|  | (7.3) | (201) | (842) | 33 | 138 | •EST | 61-50-7 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

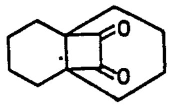
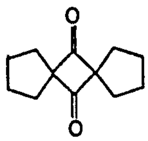
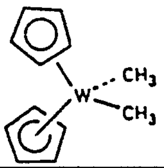
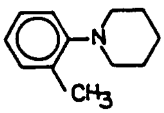
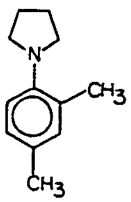
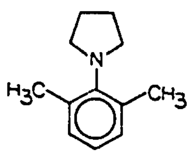
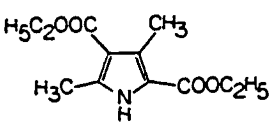
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{16}O_2^+$ | | | | | | | |
|  | 8.5 | (133) | (558) | −63 | −262 | *EST | 21377-46-8 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (8.9±0.01) | (161) | (675) | −44 | −184 | *EST | 5011-61-0 |
| | IP from 84OLI/FLE. | | | | | | |
| $C_{12}H_{16}W^+$ | | | | | | | |
|  | (5.8) | (220) | (919) | 86±1 | 359±6 | 82PIL/SKI | 39333-53-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{17}N^+$ | | | | | | | |
|  | (7.1) | (169) | (706) | 5 | 21 | *EST | 7250-70-6 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
|  | (≤7.60) | (≤219) | (≤918) | 44 | 185 | *EST | 81506-12-9 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (7.0) | (199) | (834) | 38 | 159 | *EST | 64175-53-7 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
| $C_{12}H_{17}NO_4^+$ | | | | | | | |
|  | (≤8.15) | (≤4) | (≤15) | −184 | −771 | *EST | 2436-79-5 |
| | IP from 81CAU/GIA. | | | | | | |

Table 1. Positive Ion Table - Continued

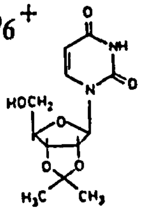
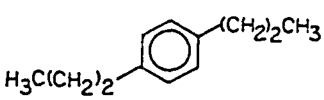
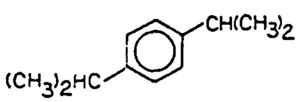
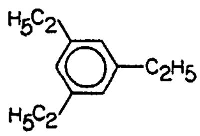
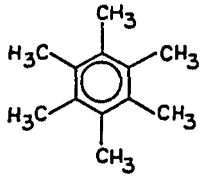
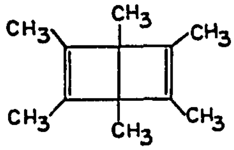
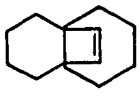
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{17}N_2O_6^+$ | | | | | | | |
|  | | (−60) | (−251) | | | | |
| | From proton affinity of 2',3'-O'-isopropylideneuridine (RN 362-43-6). PA = (208) kcal/mol, (870) kJ/mol. | | | | | | |
| $C_{12}H_{18}^+$ | | | | | | | |
| n-$C_4H_9C{\equiv}CC{\equiv}C$(n-$C_4H_9$) | (8.67) | (258) | (1077) | 58 | 241 | 77PED/RYL | 1120-29-2 |
| (tert-$C_4H_9C{\equiv}C)_2$ | (8.61±0.02) | (249) | (1040) | 50±1 | 209±5 | 77KUP/SHI | 6130-98-9 |
|  | (≤8.31) | (≤176) | (≤736) | −16 | −66 | *EST | 4815-57-0 |
| | IP from 80GLE/HOP. | | | | | | |
|  | (8.35) | (175) | (732) | −18 | −75 | *EST | 100-18-5 |
|  | (8.32) | (173) | (724) | −19 | −79 | *EST | 102-25-0 |
| | IP from 84HOW/GON. | | | | | | |
|  | 7.85 | 160 | 670 | −21±0.7 | −87±3 | 77PED/RYL | 87-85-4 |
| | See also: 84HOW/GON. | | | | | | |
|  | (≤7.83) | (≤219) | (≤917) | 39 | 162 | 78GRE/LIE | 7641-77-2 |
|  | (≤9.05) | (≤198) | (≤830) | −10 | −43 | *EST | 38992-78-8 |

**Table 1. Positive Ion Table - Continued**

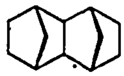
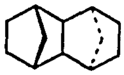
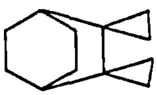
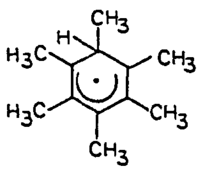
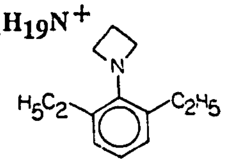
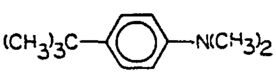
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{18}^+$ | | | | | | | |
|  | (≤9.50±0.03) | (≤219) | (≤916) | −0.2±1 | −1±5 | 73ENG/AND2 | 53862-33-2 |
|  | (≤9.57±0.03) | (≤232) | (≤968) | 11±2 | 45±8 | 73ENG/AND2 | 15914-95-1 |
|  | (8.3) | (232) | (972) | 41 | 171 | *EST | 40827-30-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{18}Hg^+$ | | | | | | | |
| $((CH_3)_3CC{\equiv}C)_2Hg$ | (9.03) | (285) | (1194) | 77 | 323 | *EST | 73838-84-3 |
| | IP is onset of photoelectron band (81FUR/PIA). | | | | | | |
| $C_{12}H_{18}O_4^+$ | | | | | | | |
| $(CH_3)_3C[C(=O)]_4C(CH_3)_3$ | (8.5) | (25) | (105) | −171 | −715 | *EST | 19909-70-7 |
| | IP from 85GLE/DOB. | | | | | | |
| $C_{12}H_{19}^+$ | | | | | | | |
|  | | 138 | 576 | | | | |
| | From proton affinity of hexamethylbenzene (RN 87-85-4). PA = 207.3 kcal/mol, 867. kJ/mol. | | | | | | |
| $C_{12}H_{19}N^+$ | | | | | | | |
|  | (≤7.82) | (≤241) | (≤1007) | 60 | 253 | *EST | 81506-11-8 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (6.90) | (158) | (661) | −1.2 | −4.9 | 85ORL/MIS | 2909-79-7 |
| | IP from 86ORL/MIS. See also: 85BAI/MIS2. | | | | | | |

Table 1. Positive Ion Table - Continued

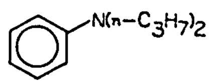
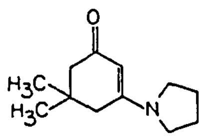
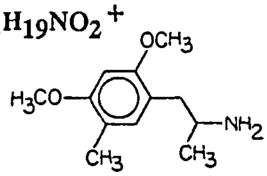
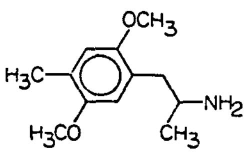
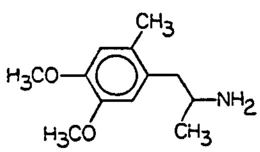
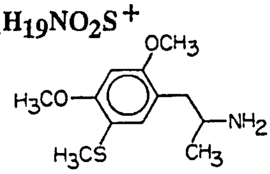
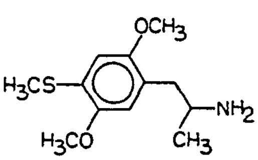
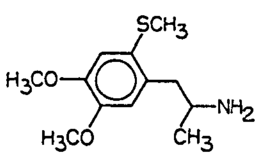
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{19}N^+$ | | | | | | | |
|  | 6.93 | (161) | (672) | 1 | 3 | *EST | 2217-07-4 |
| | IP from charge transfer equilibrium constant determinations; reference standard: IP $C_6H_5N(CH_3)_2$ = 7.12eV. (85LIA/JAC). | | | | | | |
| $C_{12}H_{19}NO^+$ | | | | | | | |
|  | (≤7.54) | (≤138) | (≤579) | −35 | −148 | *EST | 3357-16-2 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{12}H_{19}NO_2^+$ | | | | | | | |
|  | (7.2) | (87) | (366) | −79 | −329 | *EST | 79440-50-9 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
|  | (6.8) | (80) | (335) | −77 | −321 | *EST | 26011-50-7 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |
|  | (6.9) | (85) | (356) | −74 | −310 | *EST | 56966-33-7 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
| $C_{12}H_{19}NO_2S^+$ | | | | | | | |
|  | (6.9) | (92) | (385) | −67 | −281 | *EST | 79440-52-1 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
|  | (6.8) | (91) | (383) | −65 | −273 | *EST | 61638-07-1 |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |
|  | (6.9) | (94) | (393) | −65 | −273 | *EST | |
| | IP is onset of photoelectron band (81DOM/EAT). | | | | | | |

**Table 1. Positive Ion Table - Continued**

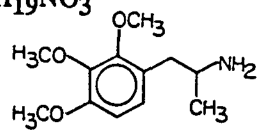
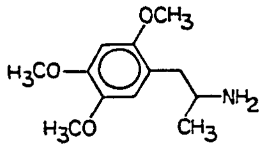
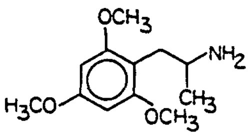
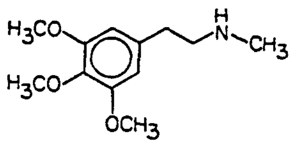
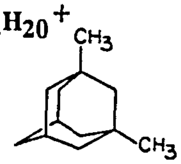
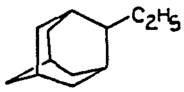
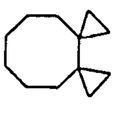
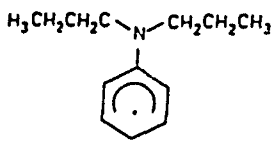
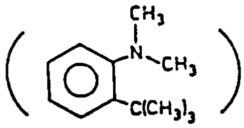
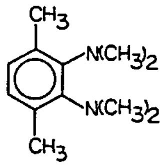
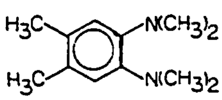
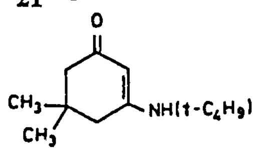
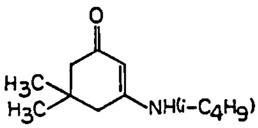
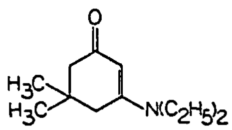
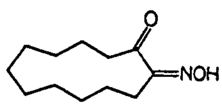
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{19}NO_3^+$ | | | | | | | |
|  | (≤8.09±0.06) | (≤88) | (≤370) | −98 | −411 | *EST | 22199-12-8 |
|  | (7.0) | (54) | (224) | −108 | −451 | *EST | 22199-15-1 |
| | IP is onset of photoelectron band (81DOM/EAT, 82LEV/LIA). | | | | | | |
|  | (≤7.76±0.06) | (≤67) | (≤279) | −112 | −470 | *EST | 22199-16-2 |
|  | (≤8.44±0.40) | (≤101) | (≤421) | −94 | −393 | *EST | 4838-96-4 |
| $C_{12}H_{20}^+$ | | | | | | | |
|  | (9.15) | (159) | (664) | −52±0.7 | −219±3 | 77STE/WAT | 702-79-4 |
|  | (9.2) | (250) | (1049) | 38±0.5 | 161±2 | 81GOD/SCH2 | 14451-87-7 |
|  | (8.6) | (233) | (976) | 35 | 146 | *EST | 64601-40-7 |
| | IP is onset of photoelectron band (82SPA/GLE). | | | | | | |
| $C_{12}H_{20}N^+$ | | | | | | | |
|  | | 138 | 578 | | | | |
| | From proton affinity of $C_6H_5N(n\text{-}C_3H_7)_2$ (RN 2217-07-4). PA = 228.6 kcal/mol, 956. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{20}N^+$ | | | | | | | |
|  H + | | 152 | 634 | | | | |
| | From proton affinity of 2-(t-$C_4H_9$)$C_6H_4N(CH_3)_2$ (RN 22025-87-2). 229.3 kcal/mol, 959. kJ/mol. | | | | | | |
| $C_{12}H_{20}N_2^+$ | | | | | | | |
|  | (7.3) | (196) | (822) | 28 | 118 | *EST | 66102-30-5 |
| | IP is onset of photoelectron band (81NEL/GRE). | | | | | | |
|  | (6.4) | (168) | (704) | 21 | 86 | *EST | 54929-05-4 |
| | IP is onset of photoelectron band (81NEL/GRE). | | | | | | |
| $C_{12}H_{21}N^+$ | | | | | | | |
| $(CH_2=C(CH_3)CH_2)_3N$ | (7.8) | (208) | (869) | 28 | 116 | *EST | |
| | IP from 79AUE/BOW. | | | | | | |
| $C_{12}H_{21}NO^+$ | | | | | | | |
|  | (≤7.69) | (≤111) | (≤464) | −66 | −278 | *EST | 27336-61-4 |
| | IP from 82PFI/GER. | | | | | | |
|  | (≤7.98) | (≤122) | (≤513) | −61 | −257 | *EST | 82663-49-8 |
| | IP from 82PFI/GER. | | | | | | |
|  | (7.3) | (116) | (486) | −52 | −218 | *EST | 65115-73-3 |
| | IP is onset of photoelectron band (82PFI/GER). | | | | | | |
| $C_{12}H_{21}NO_2^+$ | | | | | | | |
|  | (8.99±0.03) | (132) | (552) | −75 | −315 | *EST | 4422-06-4 |
| | IP from 79GOL/KUL. | | | | | | |

### Table 1. Positive Ion Table - Continued

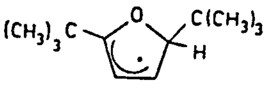
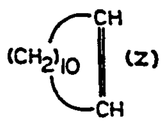
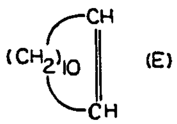
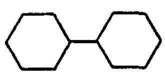
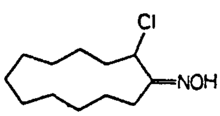
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{21}O^+$ | | | | | | | |
|  | | 87 | 366 | | | | |
| | From the proton affinity of 2,5-Di-t-butylfuran (RN 4789-40-6) (85HOU/ROL).<br>PA = 213.4 kcal/mol, 893. kJ/mol. | | | | | | |
| $C_{12}H_{22}^+$ | | | | | | | |
| 1-$C_{12}H_{22}$ | (9.90±0.02) | (228) | (956) | 0.1 | 0.4 | *EST | 765-03-7 |
| 2-$C_{12}H_{22}$ | (9.29±0.02) | (210) | (878) | −4 | −18 | *EST | 629-49-2 |
| 3-$C_{12}H_{22}$ | (9.17±0.02) | (207) | (868) | −4 | −17 | *EST | 6790-27-8 |
| 4-$C_{12}H_{22}$ | (9.14±0.03) | (207) | (865) | −4 | −17 | *EST | 22058-01-1 |
| 5-$C_{12}H_{22}$ | (9.09±0.03) | (206) | (860) | −4 | −17 | *EST | 19780-12-2 |
| $CH_2=C(t\text{-}C_4H_9)C(t\text{-}C_4H_9)=CH_2$ | (8.5) | (179) | (750) | −17 | −70 | *EST | 3378-20-9 |
| | IP is onset of photoelectron band (84HON/ZHO). | | | | | | |
| trans, trans-((tert-$C_4H_9$)CH = CH)$_2$ | (8.23±0.04) | (168) | (704) | −22 | −90 | *EST | 22430-49-5 |
|  | (8.78±0.15) | (173) | (727) | −29 | −120 | 76JEN | 1129-89-1 |
|  | (8.74±0.15) | (173) | (725) | −28 | −118 | 76JEN | 1486-75-5 |
|  | (9.41) | (164.8) | (689.5) | −52.2±.7 | −218.4±3.1 | 78MON/ROS | 92-51-3 |
| $C_{12}H_{22}ClNO^+$ | | | | | | | |
|  | (9.18±0.03) | (160) | (668) | −52 | −218 | *EST | 4806-74-0 |
| | IP from 79GOL/KUL. | | | | | | |

Table 1. Positive Ion Table - Continued

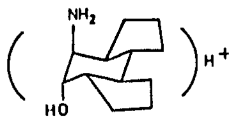
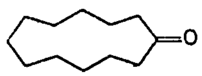
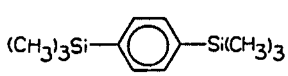
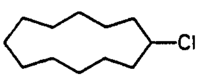
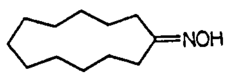
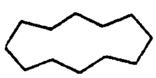
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{22}N^+$ | | | | | | | |
| $(CH_2=C(CH_3)CH_2)_3NH$ | | | | | | | |
| | | (163) | (684) | | | | |
| | From proton affinity of $(CH_2=C(CH_3)CH_2)_3N$. PA = (230.7) kcal/mol, (965.) kJ/mol. | | | | | | |
| $C_{12}H_{22}NO^+$ | | | | | | | |
|  | | 83 | 347 | | | | |
| | From proton affinity of 3-amino-tricyclo[7.3.0.0$^{4,8}$] dodecan-2-ol. PA = 220.0 kcal/mol, 920. kJ/mol. | | | | | | |
| $C_{12}H_{22}O^+$ | | | | | | | |
|  | (8.96±0.03) | (123) | (514) | −84 | −350 | *EST | 830-13-7 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_{12}H_{22}Si_2^+$ | | | | | | | |
|  | (8.45) | (132) | (554) | −62 | −261 | *EST | 13183-70-5 |
| | IP is onset of photoelectron band (82TRA/RED). | | | | | | |
| $C_{12}H_{23}Cl^+$ | | | | | | | |
|  | (9.04±0.03) | (≤143) | (≤598) | −65 | −274 | *EST | 34039-83-3 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_{12}H_{23}NO^+$ | | | | | | | |
|  | (8.84±0.03) | (154) | (643) | −50 | −210 | *EST | 946-89-4 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_{12}H_{24}^+$ | | | | | | | |
| (Z)-$(CH_3)_3CCH_2C(CH_3)=CHC(CH_3)_3$ | (8.35±0.01) | (142) | (594) | −50 | −211 | *EST | 27656-50-4 |
|  | (9.72±0.03) | (169) | (707) | −55±0.5 | −230±2 | 77PED/RYL | 294-62-2 |
| | IP from 79GOL/KUL. | | | | | | |

**Table 1. Positive Ion Table - Continued**

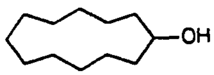
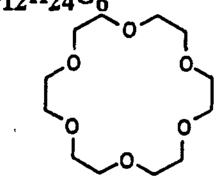
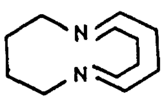
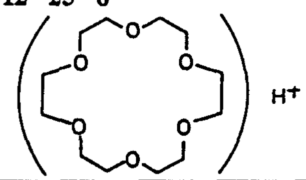
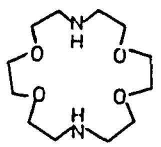
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{24}O^+$ | | | | | | | |
|  | (9.26±0.03) | (119) | (499) | −94 | −394 | *EST | 1724-39-6 |
| | IP from 79GOL/KUL. | | | | | | |
| $C_{12}H_{24}O_6^+$ | | | | | | | |
|  | 8.9 | (−22) | (−91) | −227 | −950 | *EST | 17455-13-9 |
| | IP is onset of photoelectron band (83BAK/ARM, 82LEV/LIA). | | | | | | |
| $C_{12}H_{25}N_2^+$ | | | | | | | |
|  | | 117 | 490 | | | | |
| | From proton affinity of 1,6-diazabicyclo[4.4.4]tetradecane (RN 71058-67-8). PA = 226.0 kcal/mol, 946. kJ/mol. | | | | | | |
| $C_{12}H_{25}O_6^+$ | | | | | | | |
|  | | −91 | −382 | | | | |
| | From proton affinity of 1,4,7,10,13,16-hexaoxacyclooctadecane (18-Crown-6) (RN 17455-13-9). PA = 230. kcal/mol, 962. kJ/mol. | | | | | | |
| $C_{12}H_{26}N_2O_4^+$ | | | | | | | |
|  | (≤8.4) | (≤52) | (≤218) | −141 | −592 | *EST | 23978-55-4 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{12}H_{27}BO_3^+$ | | | | | | | |
| $(n\text{-}C_4H_9O)_3B$ | (≤10.72±0.74) | (≤−27) | (≤−113) | −274±1 | −1147±4 | 77PED/RYL | 688-74-4 |
| $C_{12}H_{27}N^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_3N$ | (7.4) | (118) | (494) | −53±0.2 | −222±1 | *EST | 102-82-9 |
| | IP is onset of photoelectron band (82ELB/DIE), giving $\Delta_f H$(Ion) in good agreement with value predicted from hydrogen affinity of tertiary amines. | | | | | | |
| $C_{12}H_{27}P^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_3P$ | (7.5) | (160) | (668) | −13±8 | −56±35 | 77PED/RYL | 998-40-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{12}H_{28}N^+$ | | | | | | | |
| $(n\text{-}C_4H_9)_3NH$ | | 77 | 323 | | | | |
| | From proton affinity of $(n\text{-}C_4H_9)_3N$ (RN 102-82-9). PA = 235.4 kcal/mol, 985 kJ/mol (85BOL/HOU). | | | | | | |

**Table 1. Positive Ion Table - Continued**

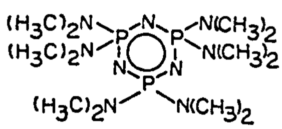
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$C_{12}H_{28}N_2^+$** | | | | | | | |
| $(n\text{-}C_3H_7)_2NN(n\text{-}C_3H_7)_2$ | (≤7.74) | (≤197) | (≤825) | 19 | 78 | *EST | 60678-69-5 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |
| $(n\text{-}C_4H_9)_2NN(C_2H_5)_2$ | (≤7.77) | (≤198) | (≤828) | 19 | 78 | *EST | 60678-68-4 |
| | Reported values of IP's of hydrazines determined by threshold measurements are usually significantly higher than the adiabatic value because of the large geometry change associated with ionization. See also: 84NEL. | | | | | | |
| **$C_{12}H_{28}Sn^+$** | | | | | | | |
| $(C_3H_7)_4Sn$ | (≤8.82) | (≤168) | (≤705) | −35±1 | −146±6 | 77PED/RYL | 2176-98-9 |
| $(iso\text{-}C_3H_7)_4Sn$ | (≤8.46) | (≤166) | (≤693) | −29±2 | −123±7 | 77PED/RYL | 2949-42-0 |
| **$C_{12}H_{30}Ge_2^+$** | | | | | | | |
| $((C_2H_5)_3Ge)_2$ | 7.48±0.01 | 90 | 375 | −83±2 | −347±8 | 80TEL/RAB | 993-62-4 |
| **$C_{12}H_{30}N_3P^+$** | | | | | | | |
| $P(N(C_2H_5)_2)_3$ | (≤7.19) | (≤112) | (≤468) | −54±2 | −226±10 | 77PED/RYL | 2283-11-6 |
| | IP from 82WOR/HAR. | | | | | | |
| **$C_{12}H_{30}Sn_2^+$** | | | | | | | |
| $[(C_2H_5)_3Sn]_2$ | (6.60±0.02) | (115) | (482) | −37±2 | −155±10 | 77PED/RYL | 993-63-5 |
| **$C_{12}H_{31}N_3OP^+$** | | | | | | | |
| $HOP(N(C_2H_5)_2)_3$ | | 9 | 37 | | | | |
| | From proton affinity of $OP(N(C_2H_5)_2)_3$ (RN 2622-07-3) (85BOL/HOU). PA = 230.0 kcal/mol, 962. kJ/mol. | | | | | | |
| **$C_{12}H_{36}Mo_2N_6^+$** | | | | | | | |
| $Mo_2((CH_3)_2N)_6$ | (6.74) | (125) | (522) | −31±3 | −128±13 | 79ADE/CAV | 51956-20-8 |
| **$C_{12}H_{36}N_6W^+$** | | | | | | | |
| $W(N(CH_3)_2)_6$ | (6.3) | (209) | (876) | 64±3 | 268±14 | 79ADE/CAV | 54935-70-5 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_{12}H_{36}N_9P_3^+$** | | | | | | | |
|  | (7.85±0.05) | (76) | (318) | −105±3 | −439±13 | 80TEL/RAB | 974-68-5 |
| **$C_{12}H_{36}Si_5^+$** | | | | | | | |
| $Si(Si(CH_3)_3)_4$ | (7.41±0.01) | (37) | (156) | −134±10 | −559±40 | 77PED/RYL | 4098-98-0 |

**Table 1. Positive Ion Table - Continued**

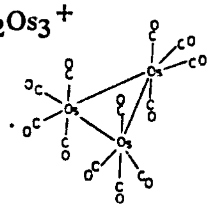
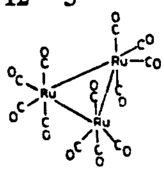
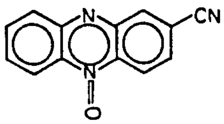
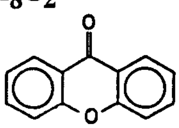
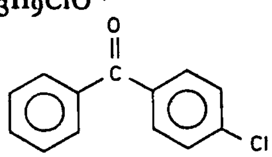
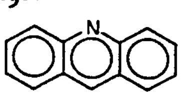
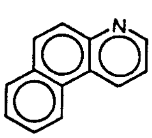
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{12}O_{12}Os_3^+$  | (7.6±0.3) | (−218) | (−911) | −393±7 | −1644±28 | 80CON | 15696-40-9 |
| | IP is onset of photoelectron band. See also: 81GRE/MIN, 82SHE/HAL. | | | | | | |
| $C_{12}O_{12}Ru_3^+$  | (7.3) | (−267) | (−1116) | −435±6 | −1820±26 | 77PED/RYL | 15243-33-1 |
| | IP is onset of photoelectron band. See also: 81GRE/MIN. | | | | | | |
| $C_{13}H_7N_3O^+$  | (8.44) | (290) | (1211) | 95 | 397 | *EST | 59019-84-0 |
| $C_{13}H_8O_2^+$  | (8.42±0.03) | (174) | (727) | −20±2 | −85±7 | 82JOH/KIM | 90-47-1 |
| $C_{13}H_9ClO^+$  | 9.64±0.04 | (229) | (959) | 7±2 | 29±8 | *EST | 134-85-0 |
| $C_{13}H_9N^+$  | 7.8 | 249 | 1044 | 69±0.2 | 291±1 | 81KUD/KUD2 | 260-94-6 |
|  | (8.14±0.02) | (244) | (1019) | 56±2 | 234±7 | 81STE/BAR | 85-02-9 |

**Table 1. Positive Ion Table - Continued**

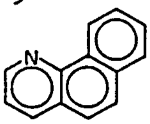
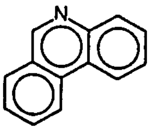
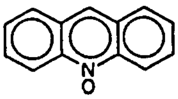
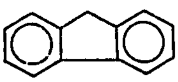
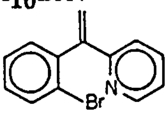
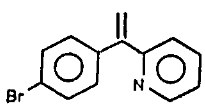
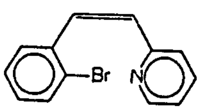
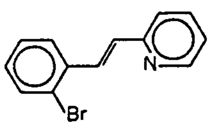
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_9N^+$ | | | | | | | |
|  | (8.04±0.02) | (240) | (1007) | 55±1 | 231±5 | 81STE/BAR | 230-27-3 |
|  | (8.31±0.02) | (250) | (1046) | 58±1 | 244±6 | 81STE/BAR | 229-87-8 |
| $C_{13}H_9NO^+$ | | | | | | | |
|  | (7.45±0.02) | (222) | (930) | 50 | 211 | *EST | 10399-73-2 |
| $C_{13}H_{10}^+$ | | | | | | | |
|  | 7.89±0.03 | 227 | 948 | 45±0.2 | 187±1 | 81KUD/KUD | 86-73-7 |
| | Value of IP from charge transfer equilibrium constant determinations (80MAU, re-evaluated) is in agreement. | | | | | | |
| $C_{13}H_{10}BrN^+$ | | | | | | | |
|  | (8.6) | (274) | (1146) | 76 | 316 | *EST | 74309-56-1 |
| | IP from 80GRU/SCH, 82LEV/LIA. | | | | | | |
|  | (8.62) | (274) | (1148) | 76 | 316 | *EST | |
|  | (8.05) | (262) | (1098) | 77 | 321 | *EST | 76293-40-8 |
| | IP from 80GRU/SCH. | | | | | | |
|  | (8.05) | (258) | (1081) | 73 | 304 | *EST | 77275-12-8 |
| | IP from 80SCH/RAM. | | | | | | |

**Table 1. Positive Ion Table – Continued**

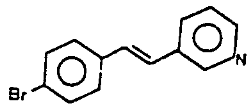
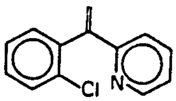
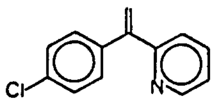
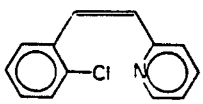
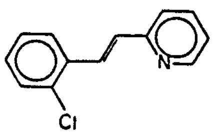
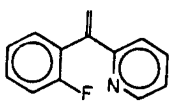
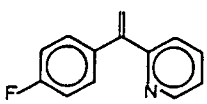
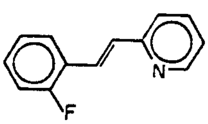
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{10}BrN^+$ | | | | | | | |
|  | (≤8.15±0.05) | (≤258) | (≤1078) | 70 | 292 | *EST | 5847-71-2 |
| $C_{13}H_{10}ClN^+$ | | | | | | | |
|  | (8.6)<br>IP from 80GRU/SCH, 82LEV/LIA. | (262) | (1096) | 64 | 266 | *EST | 74309-55-0 |
|  | (8.58) | (261) | (1094) | 64 | 266 | *EST | |
|  | (8.07)<br>IP from 80GRU/SCH. | (251) | (1051) | 65 | 272 | *EST | 5350-12-9 |
|  | 8.06±0.01<br>IP from 80SCH/RAM, 82LEV/LIA. | (247) | (1032) | 61 | 254 | *EST | 6772-77-6 |
| $C_{13}H_{10}FN^+$ | | | | | | | |
|  | (8.66)<br>IP from 82LEV/LIA, 80GRU/SCH. | (223) | (931) | 23 | 96 | *EST | 74309-53-8 |
|  | (8.68) | (223) | (933) | 23 | 96 | *EST | |
|  | (≤8.1)<br>IP from 80SCH/RAM. | (≤207) | (≤866) | 20 | 84 | *EST | 77275-10-6 |

**Table 1. Positive Ion Table - Continued**

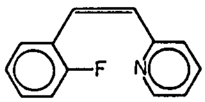
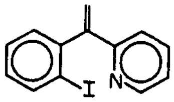
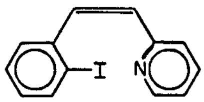
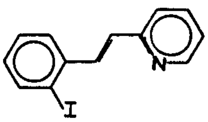
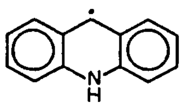
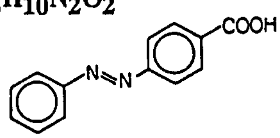
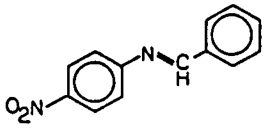
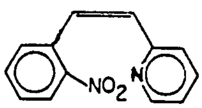
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{10}FN^+$ | | | | | | | |
|  | (8.18)<br>IP from 80GRU/SCH. | (213) | (890) | 24 | 101 | *EST | 76293-38-4 |
| $C_{13}H_{10}IN^+$ | | | | | | | |
|  | (8.3)<br>IP from 80GRU/SCH, 82LEV/LIA. | (281) | (1175) | 89 | 374 | *EST | 74309-57-2 |
|  | (7.95)<br>IP from 80GRU/SCH. | (274) | (1147) | 91 | 380 | *EST | |
|  | (7.95)<br>IP from 80SCH/RAM. | (270) | (1129) | 86 | 362 | *EST | 6772-85-6 |
| $C_{13}H_{10}N^+$ | | | | | | | |
|  | From proton affinity of acridine. (RN 260-94-6). PA = 231.9 kcal/mol, 970. kJ/mol. | 203 | 851 | | | | |
| $C_{13}H_{10}N_2O_2{}^+$ | | | | | | | |
|  | (8.3)<br>IP is onset of photoelectron band. | (198) | (828) | 6 | 27 | *EST | 37790-20-8 |
|  | (8.4)<br>IP is onset of photoelectron band. | (240) | (1005) | 47 | 195 | *EST | 69173-79-1 |
|  | (8.30)<br>IP from 80GRU/SCH. | (259) | (1086) | 68 | 285 | *EST | 50385-24-5 |

**Table 1. Positive Ion Table - Continued**

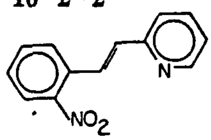
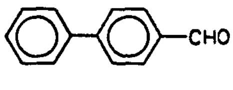
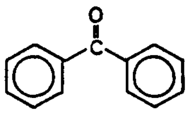
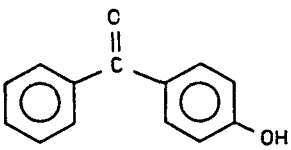
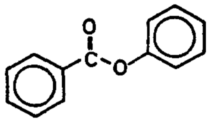
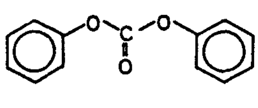
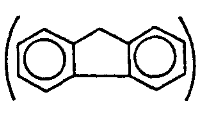
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{10}N_2O_2^+$ | | | | | | | |
|  | (8.3) | (255) | (1069) | 64 | 268 | •EST | 77340-84-2 |
| | IP from 80SCH/RAM. | | | | | | |
| $C_{13}H_{10}O^+$ | | | | | | | |
|  | (8.47±0.03) | (210) | (879) | 15±0.7 | 62±3 | •EST | 3218-36-8 |
|  | 9.05±0.05 | 221 | 923 | 12±0.7 | 50±3 | 78SAB/LAF3 | 119-61-9 |
| | IP from 78CEN/FRA, 82LEV/LIA. | | | | | | |
| $C_{13}H_{10}O_2^+$ | | | | | | | |
|  | (8.3) | (160) | (670) | −31.2±2 | −131±8 | •EST | 1137-42-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 8.99±0.02 | 173 | 724 | −34±0.7 | −143±3 | 77PED/RYL | 93-99-2 |
| $C_{13}H_{10}O_3^+$ | | | | | | | |
|  | (9.01±0.05) | (134) | (558) | −74±2 | −311±9 | 77PED/RYL | 102-09-0 |
| $C_{13}H_{11}^+$ | | | | | | | |
|  $H^+$ | | 210 | 880 | | | | |
| | From proton affinity of fluorene (RN 86-73-7). PA = 200.0 kcal/mol, 837. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

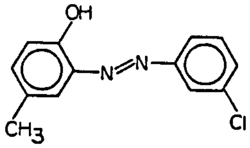
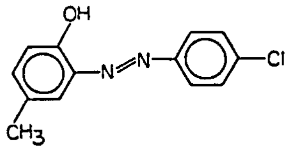
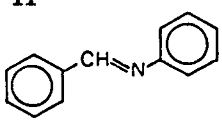
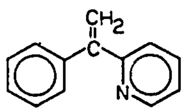
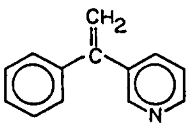
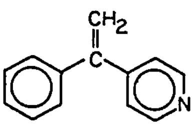
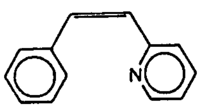
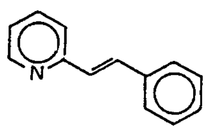
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{11}ClN_2O^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band (81MIL/MIL). | (217) | (910) | 40 | 167 | *EST | 19116-23-5 |
|  | (7.7)<br>IP is onset of photoelectron band (81MIL/MIL). | (217) | (910) | 40 | 167 | *EST | 2491-56-7 |
| $C_{13}H_{11}N^+$ | | | | | | | |
|  | 7.9<br>IP is onset of photoelectron band. | (232) | (972) | 50 | 210 | *EST | 538-51-2 |
|  | (8.65)<br>See also: 80GRU/SCH. | (270) | (1130) | 71 | 295 | *EST | 15260-65-8 |
|  | (8.73) | (269) | (1125) | 68 | 283 | *EST | 74309-58-3 |
|  | (8.90) | (277) | (1159) | 72 | 300 | *EST | 54813-56-8 |
|  | (8.15)<br>IP from 80GRU/SCH. | (264) | (1105) | 76 | 319 | *EST | 1519-59-1 |
|  | (≤7.99±0.05)<br>See also: 80SCH/RAM. | (≤252) | (≤1054) | 68 | 283 | *EST | 538-49-8 |

**Table 1. Positive Ion Table - Continued**

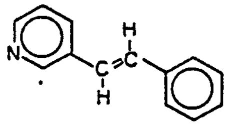
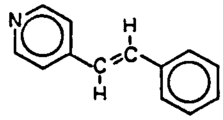
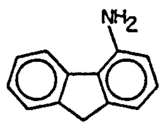
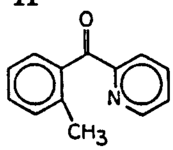
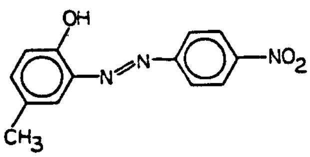
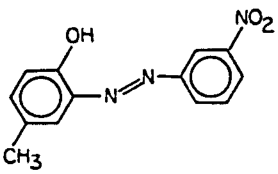
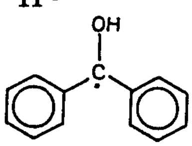
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{11}N^+$ | | | | | | | |
|  | (≤8.10±0.05)<br>See also: 80SCH/RAM. | (≤256) | (≤1072) | 69 | 290 | *EST | 5097-91-6 |
|  | (≤8.34±0.05)<br>See also: 80SCH/RAM. | (≤261) | (≤1093) | 69 | 288 | *EST | 5097-93-8 |
|  | (7.25)<br>IP is onset of photoelectron band (84GLE/SCH). | (216) | (904) | 49 | 205 | *EST | 7083-63-8 |
| $C_{13}H_{11}NO^+$ | | | | | | | |
|  | (8.72)<br>IP from 82LEV/LIA, 80GRU/SCH. | (231) | (966) | 30 | 125 | *EST | |
| $C_{13}H_{11}N_3O_3^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band (81MIL/MIL). | (221) | (924) | 43 | 181 | *EST | 1435-68-3 |
|  | (≤8.19)<br>IP from 81MIL/MIL. | (≤232) | (≤971) | 43 | 181 | *EST | 19020-84-9 |
| $C_{13}H_{11}O^+$ | | | | | | | |
|  | From proton affinity of $(C_6H_5)_2CO$ (RN 119-61-9). PA = 210.9 kcal/mol, 882. kJ/mol. | 167 | 698 | | | | |

Table 1. Positive Ion Table - Continued

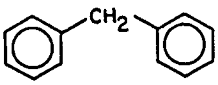
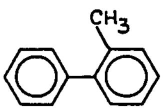
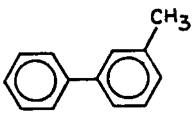
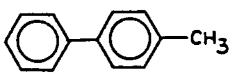
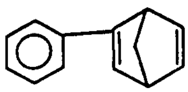
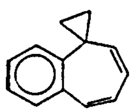
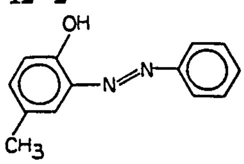
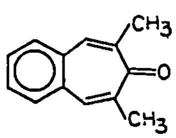
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{12}^+$ | | | | | | | |
|  | 8.55±0.03 | 230 | 965 | 33±0.7 | 140±3 | 77PED/RYL | 101-81-5 |
|  | (8.10±0.02) | (228) | (954) | 41±2 | 172±7 | 77PED/RYL | 643-58-3 |
|  | (7.95±0.02) | (219) | (917) | 36±2 | 150±8 | *EST | 643-93-6 |
|  | (7.80±0.02) | (216) | (904) | 36±2 | 151±8 | *EST | 644-08-6 |
|  | (≤9.06)<br>IP from 83HOU/RON. | (≤289) | (≤1210) | 79 | 330 | *EST | 74437-39-1 |
|  | (8.0±0.1) | (266) | (1115) | 82 | 343 | *EST | 29150-13-8 |
| $C_{13}H_{12}N_2O^+$ | | | | | | | |
|  | (7.4)<br>IP is onset of photoelectron band (81MIL/MIL). | (217) | (910) | 47 | 196 | *EST | 952-47-6 |
| $C_{13}H_{12}O^+$ | | | | | | | |
|  | (8.1)<br>IP is onset of photoelectron band. | (186) | (780) | -0.5±3 | -2±11 | 77PED/RYL | 2484-16-4 |

Table 1. Positive Ion Table - Continued

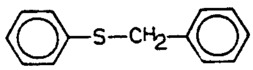
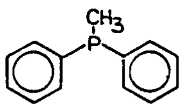
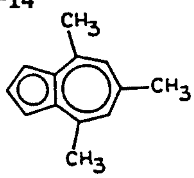
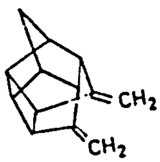
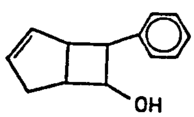
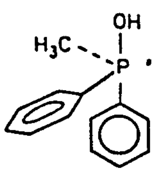
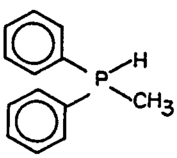
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{12}S^+$ | | | | | | | |
|  | (7.87±0.02) | (227) | (950) | 46 | 191 | *EST | 831-91-4 |
| $C_{13}H_{13}P^+$ | | | | | | | |
|  | (≤8.28±0.05)<br>IP from 82IKU/KEB. | (≤235) | (≤984) | 44 | 185 | *EST | 1486-28-8 |
| $C_{13}H_{14}^+$ | | | | | | | |
|  | (7.10) | (209) | (873) | 45 | 188 | *EST | 941-81-1 |
|  | ≤8.95<br>IP from 84MAR/KAY. | (≤222) | (≤929) | 16 | 65 | *EST | |
| $C_{13}H_{14}O^+$ | | | | | | | |
|  | (7.82)<br>IP from 81DAL/NIB. | (197) | (824) | 17 | 70 | 81DAL/NIB | 64353-61-3 |
| $C_{13}H_{14}OP^+$ | | | | | | | |
|  | From proton affinity of $(C_6H_5)_2CH_3PO$ (RN 2129-89-7) (86TRA/MUN).<br>PA = 216. kcal/mol, 904. kJ/mol. | 118 | 494 | | | | |
| $C_{13}H_{14}P^+$ | | | | | | | |
|  | From proton affinity of $(C_6H_5)_2(CH_3)P$ (RN 1486-28-8). PA = 230.3 kcal/mol, 963.5 kJ/mol. | 180 | 752 | | | | |

**Table 1. Positive Ion Table - Continued**

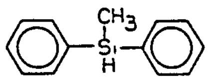
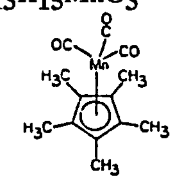
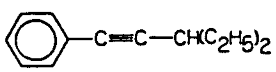
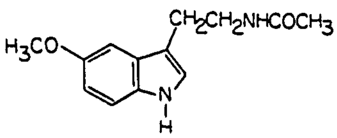
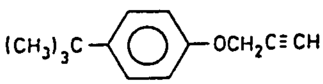
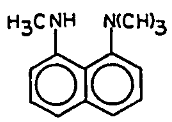
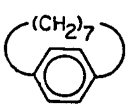
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{14}Si^+$ | | | | | | | |
|  | (8.75±0.15) | (229) | (959) | 27 | 115 | *EST | 776-76-1 |
| $C_{13}H_{15}MnO_3^+$ | | | | | | | |
|  | (7.0) | (14) | (57) | −148 | −618 | *EST | 34807-89-1 |
| | IP is onset of photoelectron band (81CAL/HUB). | | | | | | |
| $C_{13}H_{16}^+$ | | | | | | | |
|  | (8.24±0.08) | (239) | (1000) | 49 | 205 | *EST | |
| | IP from 81ELB/LIE. | | | | | | |
| $C_{13}H_{16}N_2O_2^+$ | | | | | | | |
|  | (7.03) | (109) | (454) | −54 | −224 | *EST | |
| | IP is onset of photoelectron band (83CAN/HAM). | | | | | | |
| $C_{13}H_{16}O^+$ | | | | | | | |
|  | (7.85) | (196) | (820) | 15 | 63 | 85ORL/MIS | |
| | IP from 85ORL/MIS. | | | | | | |
| $C_{13}H_{17}N_2^+$ | | | | | | | |
|  | | 78 | 327 | | | | |
| | From proton affinity of N,N,N'-trimethyl-1,8-naphthalenediamine (RN 20723-57-0).<br>PA = 235.6 kcal/mol, 986. kJ/mol. | | | | | | |
| $C_{13}H_{18}^+$ | | | | | | | |
|  | (8.0) | (195) | (817) | 11 | 45 | *EST | 3761-63-5 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

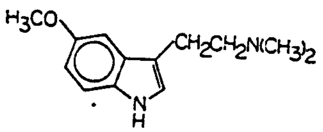
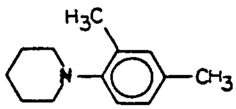
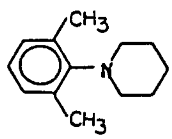
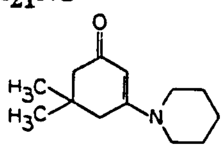
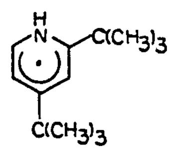
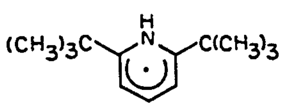
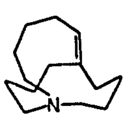
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{18}N_2O^+$ | | | | | | | |
|  | (≤7.61±0.14) | (≤172) | (≤721) | −3 | −13 | *EST | 1019-45-0 |
| $C_{13}H_{19}N^+$ | | | | | | | |
|  | (≤7.70) | (≤202) | (≤844) | 24 | 101 | *EST | 81506-14-1 |
| | IP from 82ROZ/HOU2. | | | | | | |
|  | (7.35) | (185) | (774) | 16 | 65 | *EST | 81506-15-2 |
| | IP is onset of photoelectron band (82ROZ/HOU2). | | | | | | |
| $C_{13}H_{21}NO^+$ | | | | | | | |
|  | (≤7.67) | (≤131) | (≤546) | −46 | −194 | *EST | 13358-76-4 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{13}H_{22}N^+$ | | | | | | | |
|  | | 115 | 483 | | | | |
| | From proton affinity of 2,4-di-tert-butylpyridine (RN 29939-31-9). PA = (231.4) kcal/mol, (968) kJ/mol. | | | | | | |
|  | | 113 | 473 | | | | |
| | From proton affinity of 2,6-di-tert-butylpyridine (RN 585-48-4). PA = 233.4 kcal/mol, 976. kJ/mol. | | | | | | |
| $C_{13}H_{23}N^+$ | | | | | | | |
|  | (6.8) | (184) | (770) | 27 | 114 | *EST | 84509-55-7 |
| | IP is onset of photoelectron band (82ALD/ARR). | | | | | | |

Table 1. Positive Ion Table - Continued

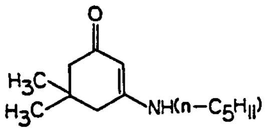
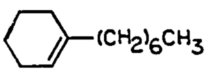
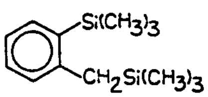
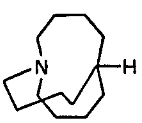
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{23}NO^+$ | | | | | | | |
|  | (≤8.07)<br>IP from 82PFI/GER. | (≤122) | (≤512) | −64 | −267 | *EST | 82663-50-1 |
| $C_{13}H_{24}^+$ | | | | | | | |
| 1-$C_{13}H_{24}$ | (9.90±0.02) | (223) | (934) | −5 | −21 | *EST | 26186-02-7 |
| 2-$C_{13}H_{24}$ | (9.28±0.02) | (205) | (856) | −9 | −39 | *EST | 28467-75-6 |
| 3-$C_{13}H_{24}$ | (9.14±0.03) | (202) | (844) | −9 | −38 | *EST | 60186-78-9 |
| 4-$C_{13}H_{24}$ | (9.07±0.03) | (200) | (837) | −9 | −38 | *EST | 60186-79-0 |
| 5-$C_{13}H_{24}$ | (9.09±0.03) | (201) | (839) | −9 | −38 | *EST | 60186-80-3 |
| 6-$C_{13}H_{24}$ | (9.05±0.03) | (200) | (835) | −9 | −38 | *EST | 42371-66-4 |
|  | (8.37±0.02) | (232) | (969) | 39±1 | 161±5 | *EST | 15232-86-7 |
| $C_{13}H_{24}Si_2^+$ | | | | | | | |
|  | (8.26)<br>IP is onset of photoelectron band (82TRA/RED). | (152) | (637) | −38 | −160 | *EST | 1899-74-7 |
| $C_{13}H_{25}N^+$ | | | | | | | |
|  | (7.3)<br>IP from 82ALD/ARR. | (157) | (657) | −11 | −47 | 81ALD/ARR | |
| $C_{13}H_{26}^+$ | | | | | | | |
| 1-$C_{13}H_{26}$ | (9.38)<br>IP from 81HOL/FIN. | (172) | (719) | −44.5 | −186.2 | *EST | 2437-56-1 |
| $((CH_3)_3C)_2C=CHCH(CH_3)_2$ | (8.31±0.01) | (136) | (569) | −56 | −233 | *EST | 50787-12-7 |

**Table 1. Positive Ion Table - Continued**

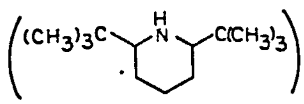
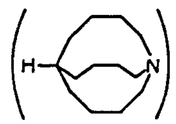
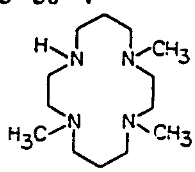
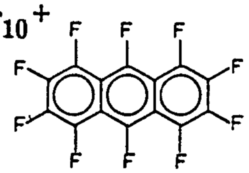
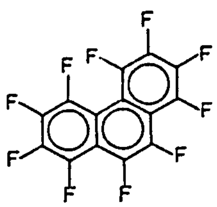
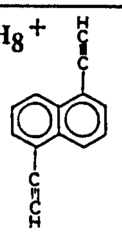
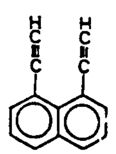
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{26}N^+$ | | | | | | | |
|  $H^+$ | | 56 | 233 | | | | |
| | From proton affinity of 2,6-di-tert-butylpiperidine (RN 29939-31-9).<br>PA = 234.3 kcal/mol, 980. kJ/mol. | | | | | | |
|  $H^+$ | | 140 | 586 | | | | |
| | From proton affinity of out-6H-1-azabicyclo[4.4.4]tetradecane.<br>PA = 214.3 kcal/mol, 896. kJ/mol. | | | | | | |
| $C_{13}H_{30}N_4{}^+$ | | | | | | | |
|  | (≤8.0)<br>IP from 83BAK/ARM. | (≤185) | (≤775) | 1 | 3 | *EST | |
| $C_{14}F_{10}{}^+$ | | | | | | | |
|  | (8.28±0.05) | (−165) | (−691) | −356 | −1490 | *EST | 1580-19-4 |
|  | (8.75±0.05) | (−160) | (−669) | −362 | −1513 | *EST | 1580-20-7 |
| $C_{14}H_8{}^+$ | | | | | | | |
|  | (7.91)<br>IP from 81GLE/SCH. | (324) | (1357) | 142 | 594 | *EST | 67665-34-3 |
|  | (7.88)<br>IP from 81GLE/SCH, 84GLE/SCH. | (330) | (1381) | 148 | 621 | *EST | 18067-44-2 |

Table 1. Positive Ion Table - Continued

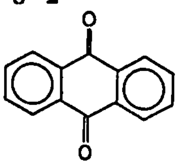
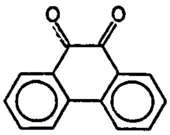
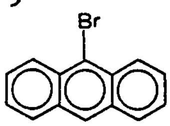
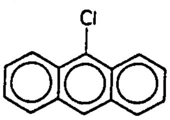
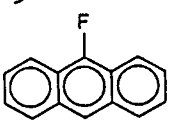
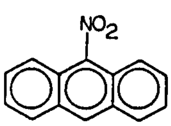
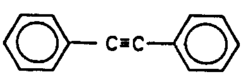
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_8O_2^+$ | | | | | | | |
|  | 9.25±0.03 | 190 | 797 | −22.8±1.6 | −95.2±6.6 | 77PED/RYL | 84-65-1 |
|  | (8.64±0.03) | (166±1) | (695±5) | −33±1 | −139±5 | 77PED/RYL | 84-11-7 |
| $C_{14}H_9Br^+$ | | | | | | | |
|  | (7.58) IP from 83KLA/KOV, 82LEV/LIA. | (236) | (986) | 61 | 255 | *EST | 1564-64-3 |
| $C_{14}H_9Cl^+$ | | | | | | | |
|  | (7.45±0.03) IP from 82LEV/LIA, 83KLA/KOV. | (221) | (924) | 49 | 205 | *EST | 716-53-0 |
| $C_{14}H_9F^+$ | | | | | | | |
|  | (7.46) IP from 83KLA/KOV, 82LEV/LIA. | (179) | (751) | 7 | 31 | *EST | 529-85-1 |
| $C_{14}H_9NO_2^+$ | | | | | | | |
|  | 7.87±0.01 IP from 82LEV/LIA, 83KLA/KOV. | (233) | (974) | 51 | 215 | *EST | 602-60-8 |
| $C_{14}H_{10}^+$ | | | | | | | |
|  | 7.90±0.02 See also: 81ELB/LIE. | 278 | 1165 | 96±1 | 403±4 | 82CHI/LIE | 501-65-5 |

Table 1. Positive Ion Table - Continued

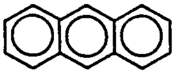
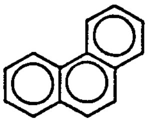
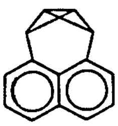
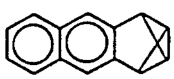
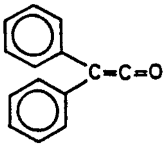
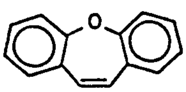
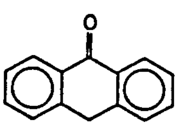
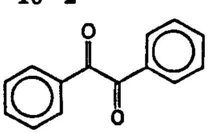
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{10}{}^+$ | | | | | | | |
|  | 7.45±0.03 | 227 | 949 | 55±0.2 | 230±1 | 79KUD/KUD4 | 120-12-7 |
| | See also: 83KLA/KOV, 84STA/MAQ. Value of IP from charge transfer equilibrium constant determination (80MAU, re-evaluated) is in agreement. | | | | | | |
|  | 7.86±0.02 | 230 | 965 | 49±0.2 | 207±1 | 79KUD/KUD4 | 85-01-8 |
| | Value of IP from charge transfer equilibrium constant determination (80MAU, re-evaluated), 7.89 eV. | | | | | | |
|  | (7.55) | (293) | (1226) | 119 | 498 | *EST | 40480-63-5 |
| | IP from 81GLE/GUB. | | | | | | |
|  | (7.71) | (247) | (1036) | 70 | 292 | *EST | 77669-79-5 |
| | IP from 81GLE/GUB. | | | | | | |
| $C_{14}H_{10}O^+$ | | | | | | | |
|  | (7.85) | (206) | (862) | 25 | 105 | 80DEM/WUL | 525-06-4 |
|  | (7.45) | (207) | (866) | 35±4 | 147±18 | *EST | 257-05-6 |
|  | (8.83±0.03) | (211) | (883) | 7 | 31 | 78KIM/WIN | 90-44-8 |
| $C_{14}H_{10}O_2{}^+$ | | | | | | | |
|  | (8.5) | (183) | (764) | −13±0.7 | −56±3 | 77PED/RYL | 134-81-6 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

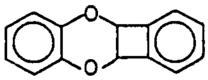
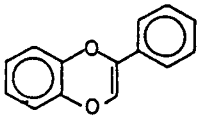
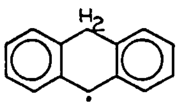
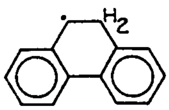
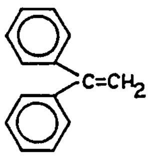
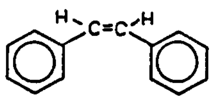
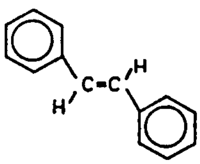
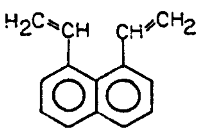
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{10}O_2^+$ | | | | | | | |
|  | (7.28±0.02)<br>IP from 81BOU/DAG. | (153) | (639) | −15 | −63 | 81BOU/DAG | |
|  | (7.60±0.02)<br>IP from 81BOU/DAG. | (171) | (716) | −4 | −17 | 81BOU/DAG | |
| $C_{14}H_{11}^+$ | | | | | | | |
|  | From proton affinity of anthracene (RN 120-12-7). PA = 207.0 kcal/mol, 866. kJ/mol. | 214 | 894 | | | | |
|  | From proton affinity of phenanthrene (RN 85-01-8). PA = 198.7 kcal/mol, 831. kJ/mol. | 216 | 906 | | | | |
| $C_{14}H_{12}^+$ | | | | | | | |
|  | (8.00±0.02) | (243) | (1018) | 59±1 | 246±4 | 77PED/RYL | 530-48-3 |
|  | (7.80±0.02) | (240) | (1005) | 60.3±0.4 | 252.4±1.6 | 77PED/RYL | 645-49-8 |
|  | 7.70±0.03 | 234 | 978 | 56±0.7 | 235±3 | 77PED/RYL | 103-30-0 |
|  | (7.72)<br>IP from GLE/SCH. | (252) | (1054) | 74 | 309 | *EST | 17935-66-9 |

**Table 1. Positive Ion Table - Continued**

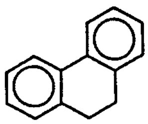
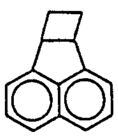
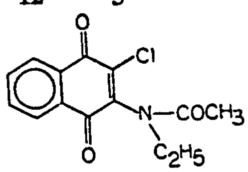
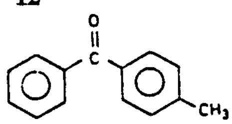
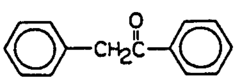
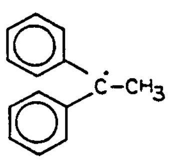
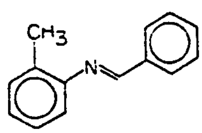
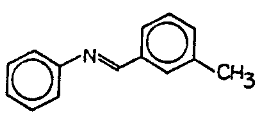
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{12}^+$ | | | | | | | |
|  | (7.55±0.02) | (216) | (903) | 42±2 | 175±8 | 77SHA/GOL | 776-35-2 |
|  | (7.60) | (265) | (1107) | 89 | 374 | *EST | |
| | IP from 82GLE/GUB. | | | | | | |
| $C_{14}H_{12}ClNO_3^+$ | | | | | | | |
|  | (8.7) | (120) | (504) | −80 | −335 | *EST | 4497-72-7 |
| | IP is onset of photoelectron band (80RED/FRE). | | | | | | |
| $C_{14}H_{12}O^+$ | | | | | | | |
|  | (9.13±0.05) | (217) | (907) | 6.1±1 | 26±4 | *EST | |
|  | (8.50) | (201) | (842) | 5±1 | 22±5 | 77PED/RYL | 451-40-1 |
| | IP is onset of photoelectron band (78CEN/FRA). | | | | | | |
| $C_{14}H_{13}^+$ | | | | | | | |
|  | | 213 | 889 | | | | |
| | From proton affinity of $(C_6H_5)_2C=CH_2$ (RN 530-48-3). PA = 211.9 kcal/mol, 887. kJ/mol. | | | | | | |
| $C_{14}H_{13}N^+$ | | | | | | | |
|  | (7.7) | (236) | (988) | 59 | 245 | *EST | 5877-55-4 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (≤8.07) | (≤245) | (≤1024) | 59 | 245 | *EST | 6906-25-8 |

**Table 1. Positive Ion Table - Continued**

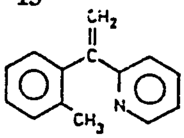
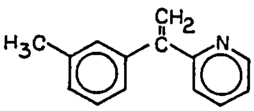
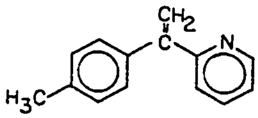
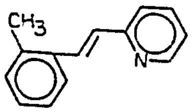
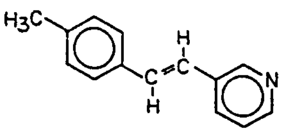
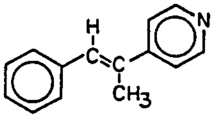
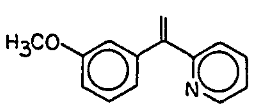
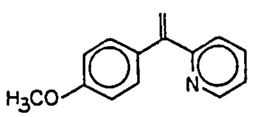
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{13}N^+$ | | | | | | | |
|  | 8.55<br>IP from 80GRU/SCH. | (261) | (1092) | 64 | 268 | *EST | 74309-54-9 |
|  | (8.48) | (258) | (1080) | 63 | 262 | *EST | |
|  | (8.45) | (257) | (1077) | 63 | 262 | *EST | |
|  | 8.01<br>IP from 80GRU/SCH, 80SCH/RAM. | (249) | (1040) | 64 | 267 | *EST | 77275-11-7 |
|  | (≤7.90±0.05) | (≤242) | (≤1012) | 60 | 250 | *EST | 6892-33-7 |
|  | (≤8.39±0.05) | (≤254) | (≤1063) | 60 | 253 | *EST | 18150-12-4 |
| $C_{14}H_{13}NO^+$ | | | | | | | |
|  | (8.27) | (225) | (942) | 34 | 144 | *EST | |
|  | (8.15) | (222) | (930) | 34 | 144 | *EST | |

**Table 1. Positive Ion Table - Continued**

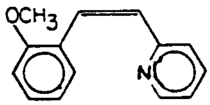
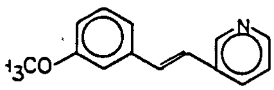
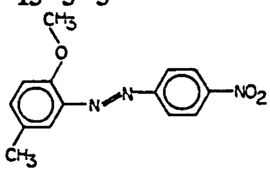
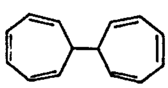
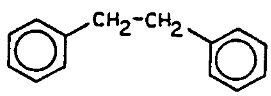
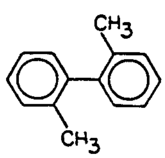
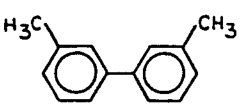
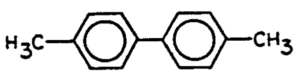
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{13}NO^+$ | | | | | | | |
|  | (7.87)<br>IP from 80GRU/SCH. | (217) | (908) | 36 | 149 | *EST | 62205-27-0 |
|  | (≤7.72±0.05) | (≤211) | (≤883) | 33 | 138 | *EST | 5847-73-4 |
| $C_{14}H_{13}N_3O_3^+$ | | | | | | | |
|  | (7.8)<br>IP is onset of photoelectron band (81MIL/MIL). | (229) | (959) | 49 | 206 | *EST | |
| $C_{14}H_{14}^+$ | | | | | | | |
|  | (8.2)<br>IP is onset of photoelectron band. | (288) | (1203) | 99 | 412 | *EST | 39473-62-6 |
|  | 8.7±0.1 | 235 | 982 | 34.2±0.4 | 143.0±1.8 | 77PED/RYL | 103-29-7 |
|  | (8.05±0.02) | (214) | (895) | 28 | 118 | *EST | 605-39-0 |
|  | (7.85±0.02) | (208) | (871) | 27 | 114 | *EST | 612-75-9 |
|  | (8.50) | (223) | (934) | 27 | 114 | *EST | 613-33-2 |

Table 1. Positive Ion Table - Continued

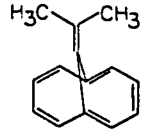
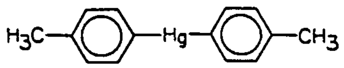
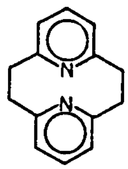
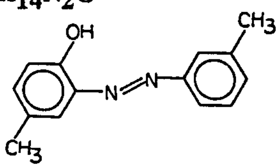
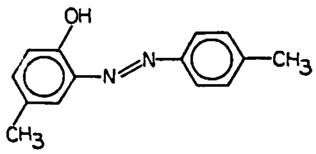
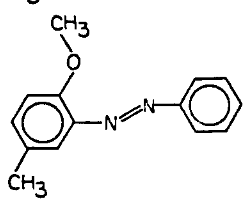
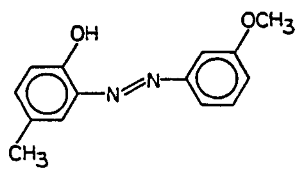
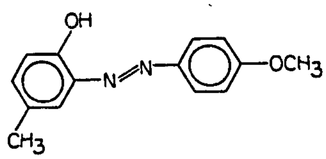
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{14}^+$ | | | | | | | |
|  | (7.7)<br>IP is onset of photoelectron band (84AND/CER). | (261) | (1094) | 84 | 351 | *EST | 88635-77-2 |
| $C_{14}H_{14}Hg^+$ | | | | | | | |
|  | (7.94)<br>IP is onset of photoelectron band (81FUR/PIA). | (261) | (1091) | 78 | 325 | *EST | 537-64-4 |
| $C_{14}H_{14}N_2^+$ | | | | | | | |
|  | (8.35) | (265) | (1109) | 72 | 303 | *EST | 6574-83-0 |
| $C_{14}H_{14}N_2O^+$ | | | | | | | |
|  | (≤7.88)<br>IP from 81MIL/MIL. | (≤221) | (≤923) | 39 | 163 | *EST | 19020-81-6 |
|  | (≤7.88)<br>IP from 81MIL/MIL. | (≤221) | (≤923) | 39 | 163 | *EST | 17739-97-8 |
|  | (7.3)<br>IP is onset of photoelectron band (81MIL/MIL). | (221) | (925) | 53 | 221 | *EST | 77046-80-1 |
| $C_{14}H_{14}N_2O_2^+$ | | | | | | | |
|  | (≤7.85)<br>IP from 81MIL/MIL. | (≤192) | (≤802) | 11 | 45 | *EST | 23375-56-6 |
|  | (≤7.76)<br>IP from 81MIL/MIL. | (≤190) | (≤794) | 11 | 45 | *EST | 15096-05-6 |

**Table 1. Positive Ion Table - Continued**

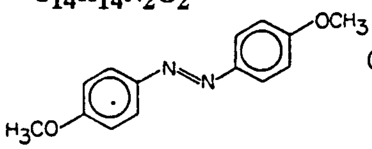
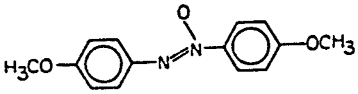
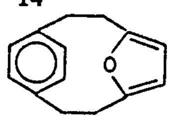
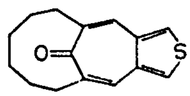
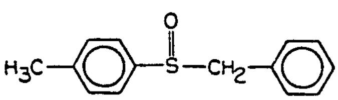
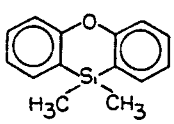
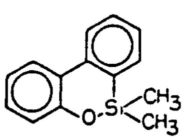
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{14}N_2O_2{}^+$ | | | | | | | |
|  | (7.72)<br>IP from 77NUY/MES. | (198) | (830) | 20 | 85 | *EST | 501-58-6 |
| $C_{14}H_{14}N_2O_3{}^+$ | | | | | | | |
|  | (≤8.06)<br>IP from 81MIL/CIL. | (≤202) | (≤844) | 16 | 66 | *EST | 1562-94-3 |
| $C_{14}H_{14}O^+$ | | | | | | | |
|  | (≤7.78) | (≤161) | (≤674) | -18 | -77 | *EST | 5040-51-7 |
| $C_{14}H_{14}OS^+$ | | | | | | | |
|  | (8.1)<br>IP is onset of photoelectron band (84GLE/BIS). | (227) | (950) | 40 | 169 | *EST | |
|  | (≤8.45)<br>IP from 81MOH/JIA. | (≤204) | (≤855) | 10 | 40 | *EST | |
| $C_{14}H_{14}OSi^+$ | | | | | | | |
|  | (8.0±0.1) | (158) | (661) | -27 | -111 | *EST | 18414-62-5 |
|  | (~7.0)<br>IP from 82TRA/RED. | (~57) | (~240) | -104 | -435 | *EST | |

Table 1. Positive Ion Table - Continued

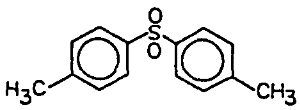
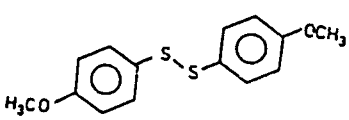
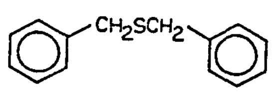
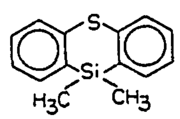
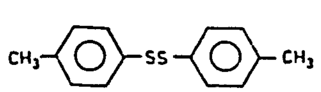
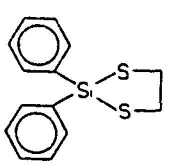
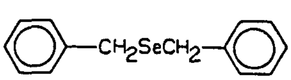
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{14}O_2S^+$ | | | | | | | |
|  | (8.66±0.04) | (151) | (634) | −48±0.7 | −202±3 | 77PED/RYL | 599-66-6 |
| $C_{14}H_{14}O_2S_2^+$ | | | | | | | |
|  | 7.6<br>IP from 82GIO/BOC. | (161) | (674) | −14 | −59 | *EST | 5335-87-5 |
| $C_{14}H_{14}S^+$ | | | | | | | |
|  | (8.05±0.02) | (232) | (969) | 46±1 | 192±4 | 77PED/RYL | 538-74-9 |
| $C_{14}H_{14}SSi^+$ | | | | | | | |
|  | (7.45)<br>IP is onset of photoelectron band (82TRA/RED). See also: 81TRA/RED. | (206) | (864) | 35 | 145 | *EST | 61431-08-1 |
| $C_{14}H_{14}S_2^+$ | | | | | | | |
|  | 7.5<br>IP is onset of photoelectron band (82GIO/BOC). | (215) | (901) | 42 | 177 | *EST | 103-19-5 |
| $C_{14}H_{14}S_2Si^+$ | | | | | | | |
|  | (8.4)<br>IP is onset of photoelectron band (83AND/CAU). | (220) | (919) | 26 | 109 | *EST | 57864-56-9 |
| $C_{14}H_{14}Se^+$ | | | | | | | |
|  | (≤7.96)<br>IP from 81BAK/ARM. | (≤243) | (≤1015) | 59 | 247 | *EST | 1842-38-2 |

**Table 1. Positive Ion Table - Continued**

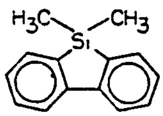
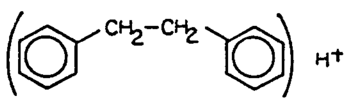
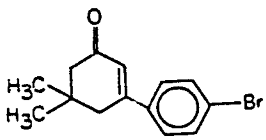
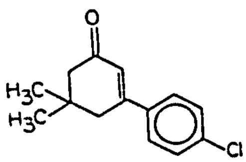
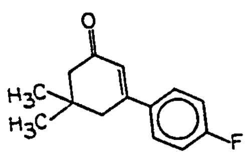
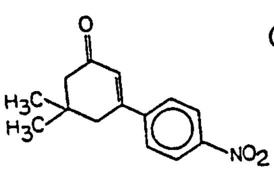
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{14}Si^+$ | | | | | | | |
|  | (7.4) | (178) | (743) | 7 | 29 | *EST | 13688-68-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{14}H_{15}^+$ | | | | | | | |
|  | | 205 | 859 | | | | |
| | From proton affinity of $C_6H_5CH_2CH_2C_6H_5$ (RN 103-29-7). PA = 194.6 kcal/mol, 814. kJ/mol. | | | | | | |
| $C_{14}H_{15}BrO^+$ | | | | | | | |
|  | (≤8.57) | (≤184) | (≤770) | −14 | −57 | *EST | 72036-54-5 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{14}H_{15}ClO^+$ | | | | | | | |
|  | (8.67) | (173) | (724) | −27 | −113 | *EST | 59344-32-0 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{14}H_{15}FO^+$ | | | | | | | |
|  | (8.90) | (124) | (518) | −82 | −341 | *EST | 72036-55-6 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{14}H_{15}NO_3^+$ | | | | | | | |
|  | (≤9.28) | (≤193) | (≤806) | −21 | −89 | *EST | 29339-45-5 |
| | IP from 82PFI/GER. | | | | | | |

**Table 1. Positive Ion Table - Continued**

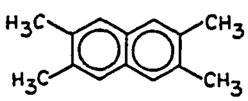
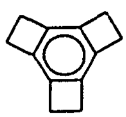
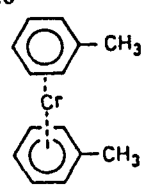
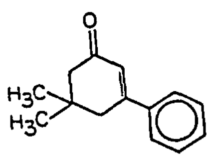
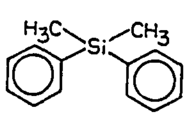
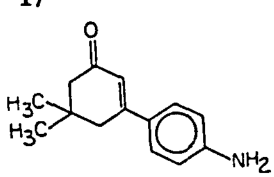
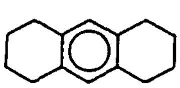
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{16}^+$ | | | | | | | |
|  | (≤7.60±0.03) | (≤180) | (≤754) | 5±0.7 | 21±3 | *EST | 1134-40-3 |
|  | (7.95±0.05) | (241) | (1007) | 57 | 240 | *EST | 54922-12-2 |
| | IP from 81HEI/KOV. | | | | | | |
| $C_{14}H_{16}Cr^+$ | | | | | | | |
|  | (≤5.24±0.1) | (≤86) | (≤360) | −35 | −146 | *EST | 12087-58-0 |
| | See also: 82CAB/COW. | | | | | | |
| $C_{14}H_{16}O^+$ | | | | | | | |
|  | (≤8.90) | (≤187) | (≤781) | −19 | −78 | *EST | 36047-17-3 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{14}H_{16}Si^+$ | | | | | | | |
|  | (8.5) | (209) | (875) | 13 | 55 | *EST | 778-24-5 |
| | IP from 81TRA/RED. | | | | | | |
| $C_{14}H_{17}NO^+$ | | | | | | | |
|  | (≤7.85) | (≤163) | (≤683) | −18 | −74 | *EST | 72036-57-8 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{14}H_{18}^+$ | | | | | | | |
|  | (7.86) | (172) | (721) | −9±0.7 | −37±3 | 77PED/RYL | 1079-71-6 |
| | IP from charge transfer equilibrium constant determinations (80MAU). | | | | | | |

Table 1. Positive Ion Table - Continued

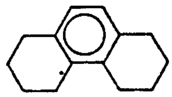
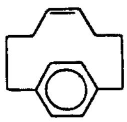
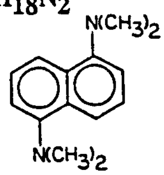
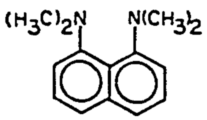
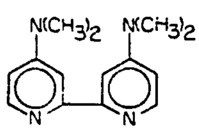
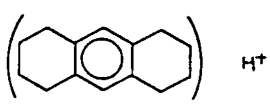
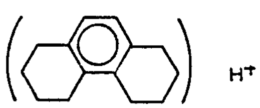
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{18}^+$ | | | | | | | |
|  | 7.89 | 174 | 727 | −8±2 | −34±8 | 77SHA/GOL | 5325-97-3 |
| | IP from charge transfer equilibrium constant determinations (80MAU). | | | | | | |
|  | (≤8.37) | (≤246) | (≤1029) | 53 | 221 | *EST | |
| | IP from 80GLE/HOP. | | | | | | |
| $C_{14}H_{18}N_2^+$ | | | | | | | |
|  | (6.70±0.02) | (200) | (839) | 46 | 193 | *EST | 10075-69-1 |
|  | (6.45±0.02) | (212) | (884) | 63 | 262 | *EST | 20734-58-1 |
| $C_{14}H_{18}N_4^+$ | | | | | | | |
|  | (7.3) | (244) | (1021) | 76 | 317 | *EST | 85698-56-2 |
| | IP is onset of photoelectron band (83DOB/HIL). | | | | | | |
| $C_{14}H_{19}^+$ | | | | | | | |
|  | | 154 | 645 | | | | |
| | From proton affinity of 1,2,3,4,5,6,7,8-octahydroanthracene (RN 1079-71-6). PA = 202.6 kcal/mol, 848. kJ/mol. | | | | | | |
|  | | 153 | 640 | | | | |
| | From proton affinity of 1,2,3,4,5,6,7,8-octahydrophenanthrene (RN 5325-97-3). PA = 204.7 kcal/mol, 856. kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

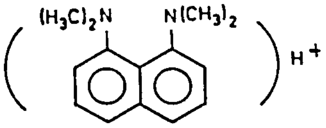
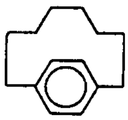
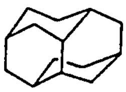
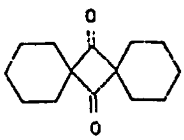
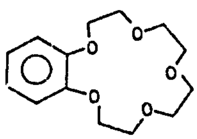
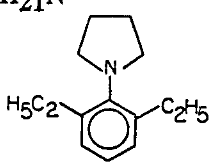
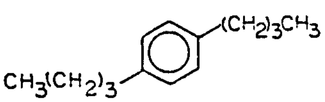
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{19}N_2^+$ | | | | | | | |
|  | | 186 | 780 | | | | |
| | From proton affinity of N,N,N',N'-tetramethyl-1,8-naphthalenediamine (RN 20734-58-1). PA = 241.8 kcal/mol, 1012. kJ/mol. | | | | | | |
| $C_{14}H_{20}^+$ | | | | | | | |
|  | (≤8.17) | (≤190) | (≤795) | 2 | 7 | *EST | 4685-74-9 |
| | IP from 80GLE/HOP. | | | | | | |
|  | (8.93) | (171.1) | (717.1) | −34.5 | −144.5 | 79CLA/KNO | 2292-79-7 |
| $C_{14}H_{20}O_2^+$ | | | | | | | |
|  | 9.0±0.05 | (141) | (589) | −67 | −279 | *EST | 950-21-0 |
| | IP from 84OLI/FLE. | | | | | | |
| $C_{14}H_{20}O_5^+$ | | | | | | | |
|  | (≤8.0) | (≤19) | (≤80) | −165 | −692 | *EST | 14098-44-3 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{14}H_{21}N^+$ | | | | | | | |
|  | (≤7.60) | (≤208) | (≤869) | 33 | 136 | *EST | 81506-13-0 |
| | IP from 82ROZ/HOU2. | | | | | | |
| $C_{14}H_{22}^+$ | | | | | | | |
|  | (≤8.40) | (≤163) | (≤681) | −31±1.4 | −129±6 | 84NES/VER | 1571-86-4 |
| | IP from 80GLE/HOP. See also: 85BAI/MIS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

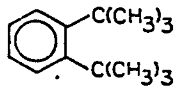
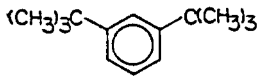
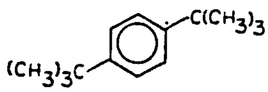
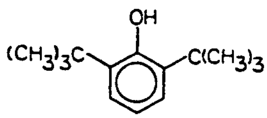
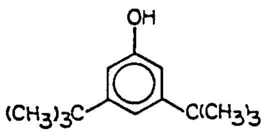
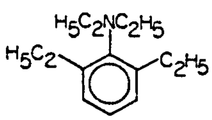
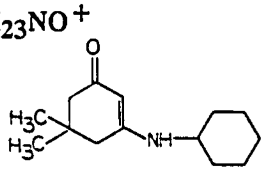
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{22}^+$ | | | | | | | |
|  | (≤8.60±0.07) | (≤185) | (≤774) | −13 | −56 | *EST | 1012-76-6 |
|  | (8.71±0.07) | (171) | (713) | −30±1.4 | −127±6 | 84NES/VER | 1014-60-4 |
|  | 8.24±0.01 | (161) | (673) | −29 | −122 | 85ORL/MIS | 1012-72-2 |
| | IP from 82LEV/LIA, 84HOW/GON, 86ORL/MIS. See also: 85BAI/MIS. | | | | | | |
| $C_{14}H_{22}O^+$ | | | | | | | |
|  | (7.70±0.02) | (112) | (468) | −66 | −275 | *EST | 128-39-2 |
| | See also: 83CET/LAP. | | | | | | |
|  | (7.90±0.02) | (109) | (455) | −73 | −307 | *EST | 1138-52-9 |
| $C_{14}H_{23}N^+$ | | | | | | | |
|  | (≤7.77) | (≤207) | (≤867) | 28 | 117 | *EST | 81506-16-3 |
| | IP from 82ROZ/HOU2. | | | | | | |
| $C_{14}H_{23}NO^+$ | | | | | | | |
|  | (≤7.75) | (≤116) | (≤486) | −63 | −262 | *EST | 1500-76-1 |
| | IP from 82PFI/GER. | | | | | | |

Table 1. Positive Ion Table - Continued

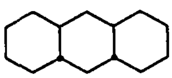
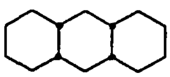
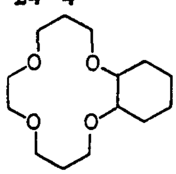
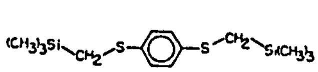
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{24}^+$ | | | | | | | |
|  | (8.8) | (145) | (606) | −58.1±0.9 | −243.2±3.8 | 77PED/RYL | |
| | IP is onset of photoelectron band (84HEI/HON). | | | | | | |
|  | (9.0) | (158) | (660) | −50 | −208 | 71ALL/WUE | |
| | IP is onset of photoelectron band (84HEI/HON). | | | | | | |
| $C_{14}H_{24}O_4^+$ | | | | | | | |
|  | (≤9.2) | (≤39) | (≤162) | −174 | −726 | *EST | |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{14}H_{26}^+$ | | | | | | | |
| 1-$C_{14}H_{26}$ | (9.89±0.02) | (218) | (913) | −10 | −41 | *EST | 765-10-6 |
| 2-$C_{14}H_{26}$ | (9.26±0.03) | (199) | (833) | −14 | −60 | *EST | 638-60-8 |
| 3-$C_{14}H_{26}$ | (9.17±0.02) | (197) | (826) | −14 | −59 | *EST | 60212-32-0 |
| 4-$C_{14}H_{26}$ | (9.11±0.03) | (196) | (820) | −14 | −59 | *EST | 60212-33-1 |
| 5-$C_{14}H_{26}$ | (9.10±0.03) | (196) | (819) | −14 | −59 | *EST | 60212-34-2 |
| 6-$C_{14}H_{26}$ | (9.09±0.02) | (196) | (818) | −14 | −59 | *EST | 3730-08-3 |
| 7-$C_{14}H_{26}$ | (9.03±0.04) | (194) | (812) | −14 | −59 | *EST | 35216-11-6 |
| $C_{14}H_{26}S_2Si_2^+$ | | | | | | | |
|  | (7.0) | (23) | (96) | −138 | −579 | *EST | 69209-20-7 |
| | IP is onset of photoelectron band (82TRA/RED). | | | | | | |
| $C_{14}H_{28}^+$ | | | | | | | |
| $((CH_3)_3C)_2C=CHC(CH_3)_3$ | (8.17±0.01) | (131) | (550) | −57 | −238 | 81HOL/FIN | 28923-90-2 |

**Table 1. Positive Ion Table - Continued**

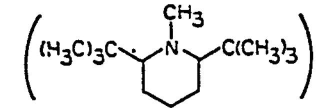
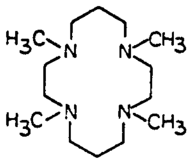
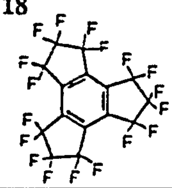
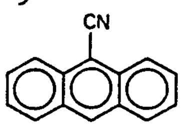
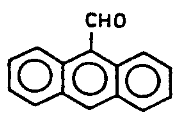
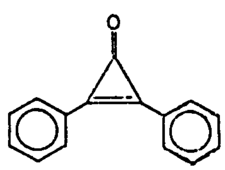
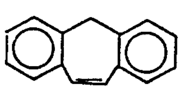
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{28}N^+$ | | | | | | | |
|  $H^+$ | | 60 | 250 | | | | |
| | From proton affinity of 1-methyl-2,6-di-tert-butylpiperidine. PA = 239.2 kcal/mol, 1001. kJ/mol. | | | | | | |
| $C_{14}H_{32}N_4^+$ | | | | | | | |
|  | (≤8.0) | (≤184) | (≤770) | −0.5 | −2 | *EST | |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{15}F_{18}^+$ | | | | | | | |
|  | 11.3 | (−530) | (−2216) | −790 | −3306 | *EST | 33021-47-5 |
| | IP is onset of photoelectron band (84HEI/WIR). | | | | | | |
| $C_{15}H_9N^+$ | | | | | | | |
|  | (7.80±0.03) | (267) | (1114) | 87±0.2 | 362±1 | *EST | 1210-12-4 |
| | See also: 83KLA/KOV. | | | | | | |
| $C_{15}H_{10}O^+$ | | | | | | | |
|  | 7.69±0.03 | (204) | (852) | 26.3±2 | 110±8 | *EST | 642-31-9 |
|  | (8.1) | (262) | (1099) | 76±2 | 318±8 | 85STE/GAM | 886-38-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{15}H_{12}^+$ | | | | | | | |
|  | (7.6) | (232) | (970) | 57±0.7 | 237±3 | *EST | 256-81-5 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

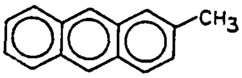
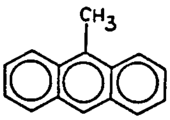
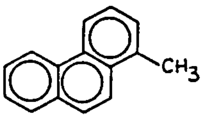
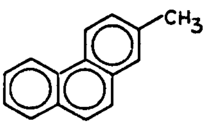
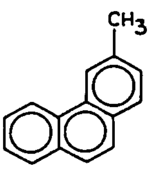
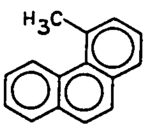
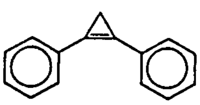
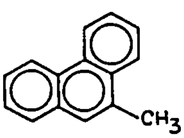
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{12}^{+}$ | | | | | | | |
|  | (7.37) | (215) | (898) | 45 | 187 | *EST | 613-12-7 |
| | IP from charge transfer equilibrium constant determinations (80MAU). | | | | | | |
|  | 7.24±0.03 | (215) | (899) | 48 | 201 | *EST | 779-02-2 |
| | See also: 80MAU, 83KLA/KOV. | | | | | | |
|  | 7.7±0.03 | (217) | (907) | 39±2 | 164±7 | *EST | 832-69-9 |
|  | (7.7) | (217) | (907) | 39±2 | 164±7 | *EST | 2531-84-2 |
|  | (7.68±0.01) | (216) | (905) | 39 | 164 | *EST | 832-71-3 |
|  | (7.70±0.02) | (222) | (929) | 44±4 | 186±15 | *EST | 832-64-4 |
|  | (7.45) | (282) | (1180) | 110 | 461 | *EST | 24168-52-3 |
|  | 7.46±0.03 | (214) | (897) | 42±0.2 | 177±1 | *EST | 883-20-5 |

**Table 1. Positive Ion Table - Continued**

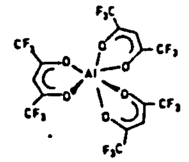
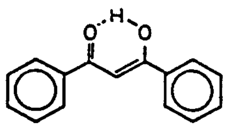
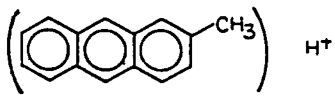
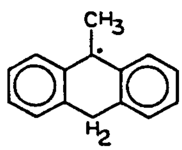
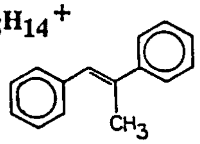
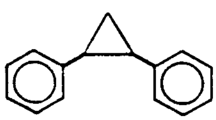
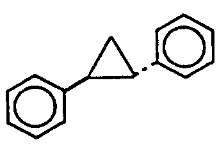
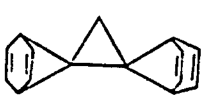
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{12}AlF_9O_6^+$ | | | | | | | |
|  | (8.7)<br>IP is onset of photoelectron band. | (−580) | (−2428) | −781±3 | −3267±13 | 80TEL/RAB | 14354-59-7 |
| $C_{15}H_{12}O_2^+$ | | | | | | | |
|  | (8.3)<br>IP is onset of photoelectron band. | (131) | (550) | −60±0.7 | −251±3 | 81FER/RIB | 120-46-7 |
| $C_{15}H_{13}^+$ | | | | | | | |
|  | From proton affinity of 2-methylanthracene (RN 613-12-7). PA = 210.3 kcal/mol, 880. kJ/mol. | 200 | 837 | | | | |
|  | From proton affinity of 9-methylanthracene (RN 779-02-2). PA = 213.9 kcal/mol, 895. kJ/mol. | 200 | 836 | | | | |
| $C_{15}H_{14}^+$ | | | | | | | |
|  | (≤8.10±0.05) | (≤236) | (≤986) | 49 | 204 | *EST | 833-81-8 |
|  | (8.20) | (249) | (1043) | 60±0.5 | 252±2 | 77PED/RYL | 1138-48-3 |
|  | (8.05) | (243) | (1016) | 57±0.7 | 239±3 | 77PED/RYL | 1138-47-2 |
|  | (8.0)<br>IP is onset of photoelectron band. | (351) | (1469) | 167 | 697 | *EST | 73045-27-9 |

**Table 1. Positive Ion Table - Continued**

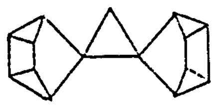
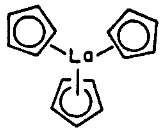
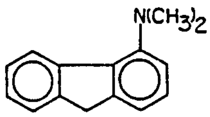
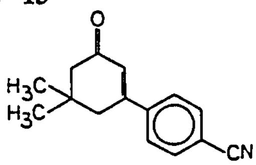
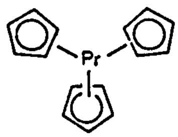
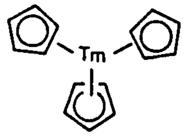
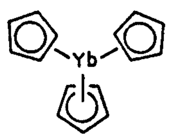
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{14}^{+}$ | | | | | | | |
|  | (7.6) | (386) | (1616) | 211 | 883 | *EST | 73050-58-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{15}H_{15}La^{+}$ | | | | | | | |
|  | (7.9±0.3) | (218) | (912) | 36±2 | 150±7 | 77PED/RYL | 1272-23-7 |
| $C_{15}H_{15}N^{+}$ | | | | | | | |
|  | (7.1) | (216) | (905) | 53 | 220 | *EST | 92013-89-3 |
| | IP is onset of photoelectron band (84GLE/SCH). | | | | | | |
| $C_{15}H_{15}NO^{+}$ | | | | | | | |
|  | (≤9.20) | (≤226) | (≤946) | 14 | 58 | *EST | 72036-56-7 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{15}H_{15}Pr^{+}$ | | | | | | | |
|  | (7.68±0.1) | (200) | (838) | 23±2 | 97±9 | 77PED/RYL | 11077-59-1 |
| $C_{15}H_{15}Tm^{+}$ | | | | | | | |
|  | (7.43±0.1) | (186) | (779) | 15±1 | 62±6 | 77PED/RYL | 1272-26-0 |
| $C_{15}H_{15}Yb^{+}$ | | | | | | | |
|  | (7.5±0.3) | (206) | (862) | 33±1 | 138±6 | 77PED/RYL | 1295-20-1 |

**Table 1. Positive Ion Table - Continued**

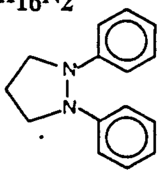
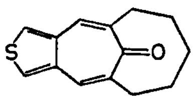
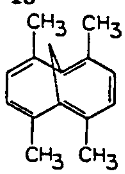
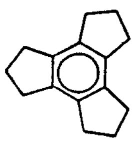
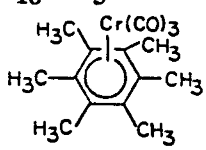
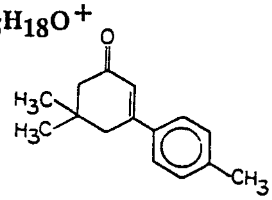
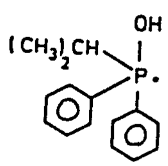
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{16}N_2^+$ | | | | | | | |
|  | (7.50±0.05) | (253) | (1059) | 80 | 335 | *EST | 63378-86-9 |
| $C_{15}H_{16}OS^+$ | | | | | | | |
|  | (8.15)<br>IP is onset of photoelectron band (84GLE/BIS). | (213) | (890) | 25 | 104 | *EST | |
| $C_{15}H_{18}^+$ | | | | | | | |
|  | (7.1)<br>IP is onset of photoelectron band (84AND/CER). | (219) | (918) | 56 | 233 | *EST | 88635-76-1 |
|  | (7.85±0.05)<br>IP from 81HEI/KOV. | (205) | (857) | 24 | 100 | *EST | 1206-79-7 |
| $C_{15}H_{18}CrO_3^+$ | | | | | | | |
|  | (6.35±0.1) | (10) | (42) | −136±3 | −571±13 | 77PED/RYL | 12088-11-8 |
| $C_{15}H_{18}O^+$ | | | | | | | |
|  | (≤8.59)<br>IP from 82PFI/GER. | (≤172) | (≤718) | −26 | −111 | *EST | 72036-52-3 |
| $C_{15}H_{18}OP^+$ | | | | | | | |
|  | From proton affinity of i-$C_3H_7(C_6H_5)_2PO$ (RN 2959-75-3)(86TRA/MUN).<br>PA = 216. kcal/mol, 904. kJ/mol. | 89 | 373 | | | | |

**Table 1. Positive Ion Table - Continued**

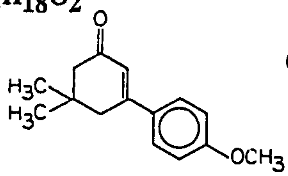
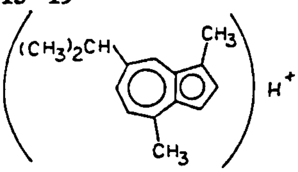
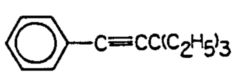
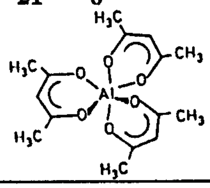
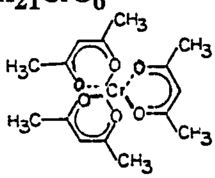
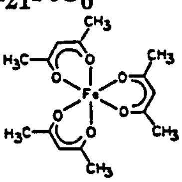
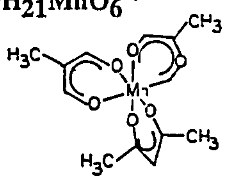
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{18}O_2{}^+$ | | | | | | | |
|  | (≤8.26) | (≤136) | (≤568) | -55 | -229 | *EST | 29339-44-4 |
| | IP from 82PFI/GER. | | | | | | |
| $C_{15}H_{19}{}^+$ | | | | | | | |
|  | | 165 | 694 | | | | |
| | From proton affinity of 1,4-dimethyl-7-isopropylazulene (RN 489-84-9). PA = 233. kcal/mol, 975. kJ/mol. | | | | | | |
| $C_{15}H_{20}{}^+$ | | | | | | | |
|  | (8.29±0.08) | (230) | (962) | 39 | 162 | *EST | 80025-09-8 |
| | IP from 81ELB/LIE. | | | | | | |
| $C_{15}H_{21}AlO_6{}^+$ | | | | | | | |
|  | (7.78±0.05) | (-220) | (-919) | -399±1 | -1669±4 | 80TEL/RAB | 13963-57-0 |
| | IP from 81WES/REI. | | | | | | |
| $C_{15}H_{21}CrO_6{}^+$ | | | | | | | |
|  | 6.95±0.2 | (-182) | (-760) | -342±2 | -1431±7 | 82PIL/SKI | 21679-31-2 |
| | IP is onset of photoelectron band(81WES/REI). | | | | | | |
| $C_{15}H_{21}FeO_6{}^+$ | | | | | | | |
|  | (7.55) | (-123) | (-515) | -297±1 | -1244±6 | 77PED/RYL | 14024-18-1 |
| | IP is onset of photoelectron band. See also: 81WES/REI. | | | | | | |
| $C_{15}H_{21}MnO_6{}^+$ | | | | | | | |
|  | (7.58±0.05) | (-135) | (-564) | -310±1 | -1295±6 | 77PED/RYL | 14284-89-0 |
| | IP from 81WES/REI. | | | | | | |

**Table 1. Positive Ion Table - Continued**

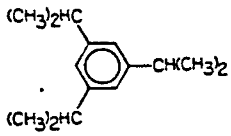
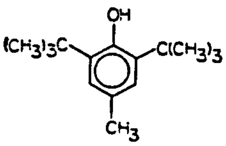
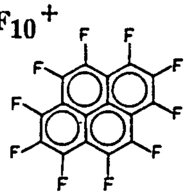
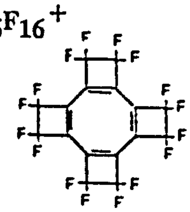
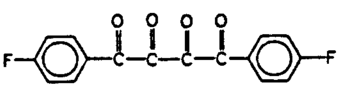
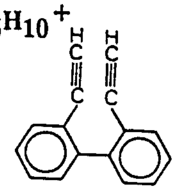
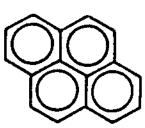
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{15}H_{24}^+$ | | | | | | | |
|  | (8.24)<br>IP from 84HOW/GON. | (158) | (661) | −32 | −134 | *EST | 717-74-8 |
| $C_{15}H_{24}O^+$ | | | | | | | |
|  | (≤7.80)<br>IP from 83CET/LAP. | (≤107) | (≤449) | −73 | −304 | *EST | 128-37-0 |
| $C_{16}F_{10}^+$ | | | | | | | |
|  | (8.36±0.05) | (−167) | (−697) | −359 | −1504 | *EST | 1493-68-1 |
| $C_{16}F_{16}^+$ | | | | | | | |
|  | 10.1<br>IP is onset of photoelectron band (84HEI/WIR). | (−347) | (−1451) | −580 | −2425 | *EST | 42858-85-5 |
| $C_{16}H_8F_2O_4^+$ | | | | | | | |
|  | (8.7)<br>IP is onset of photoelectron band (85GLE/DOB). | (39) | (165) | −161 | −674 | *EST | 97245-28-8 |
| $C_{16}H_{10}^+$ | | | | | | | |
|  | (8.2)<br>IP is onset of photoelectron band (81GLE/SCH). | (340) | (1421) | 151 | 630 | *EST | 18442-29-0 |
|  | 7.41<br>See also: 81CLA/ROB. IP value at 298 K from charge transfer equilibrium constant determinations (80MAU) = 7.50 eV. | 222 | 931 | 52±0.2 | 216±1 | 79KUD/KUD2 | 129-00-0 |

**Table 1. Positive Ion Table - Continued**

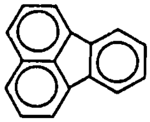
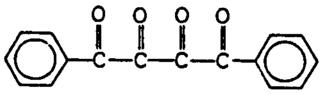
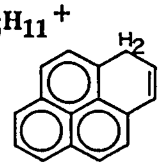
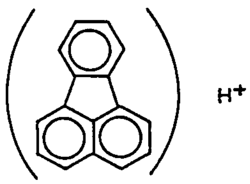
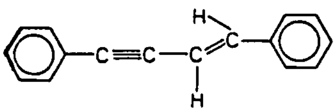
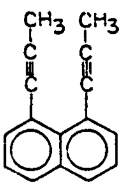
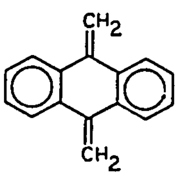
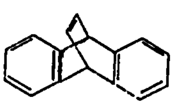
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{16}H_{10}^+$ | | | | | | | |
|  | (7.95±0.04) | (253) | (1056) | 69.2±0.3 | 289.4±1.1 | 81KUD/KUD | 206-44-0 |
| $C_{16}H_{10}O_4^+$ | | | | | | | |
|  | (8.5) | (130) | (544) | −66 | −276 | *EST | 19909-44-5 |
| | IP is onset of photoelectron band (85GLE/DOB). | | | | | | |
| $C_{16}H_{11}^+$ | | | | | | | |
|  | | 211 | 884 | | | | |
| | From proton affinity of pyrene (RN 129-00-0). PA = 206.1 kcal/mol, 862. kJ/mol. | | | | | | |
|  | | 235 | 985 | | | | |
| | From proton affinity of fluoranthene (RN 206-44-0). PA = 199.3 kcal/mol, 834. kJ/mol. | | | | | | |
| $C_{16}H_{12}^+$ | | | | | | | |
|  | (7.5) | (276) | (1154) | 103 | 430 | *EST | 13343-79-8 |
| | IP is onset of photoelectron band (80AND/BIC). | | | | | | |
|  | (7.48) | (311) | (1304) | 139 | 582 | *EST | 22360-77-6 |
| | IP from 84GLE/SCH. | | | | | | |
|  | (7.6) | (233) | (976) | 58±3 | 243±12 | *EST | 3302-51-0 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.7) | (253) | (1060) | 76 | 317 | *EST | |
| | IP is onset of photoelectron band (82HAS/NEU). | | | | | | |

Table 1. Positive Ion Table - Continued

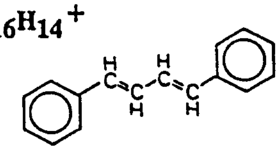
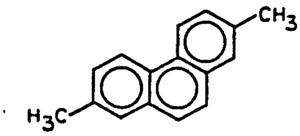
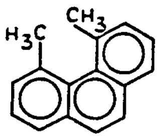
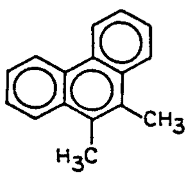
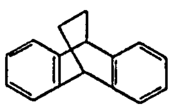
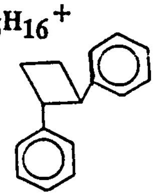
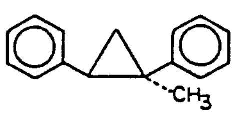
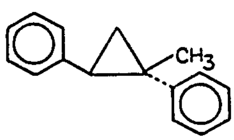
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{16}H_{14}^+$ | | | | | | | |
|  | 7.55 | 237 | 993 | 63 | 265 | 69STU/WES | 538-81-8 |
|  | 7.99±0.04 | 218 | 914 | 34±0.5 | 143±2 | 77PED/RYL | 1576-69-8 |
|  | 7.56±0.1 | 220 | 924 | 46±1 | 194±6 | 77PED/RYL | 3674-69-9 |
|  | (8.01±0.05) | (225) | (940) | 40±2 | 167±9 | 77PED/RYL | 604-83-1 |
|  | (8.1)<br>IP is onset of photoelectron band (82HAS/NEU). | (224) | (936) | 37 | 155 | *EST | |
| $C_{16}H_{16}^+$ | | | | | | | |
|  | (8.2±0.1)<br>IP from 84GRO/CHE. | (247) | (1035) | 58 | 244 | 84GRO/CHE | 20071-09-4 |
|  | (7.9)<br>IP from 81KLY/SHU. | (235) | (984) | 53 | 222 | *EST | 14161-72-9 |
|  | (7.9)<br>IP from 81KLY/SHU. | (232) | (971) | 50 | 209 | *EST | 14161-73-0 |

**Table 1. Positive Ion Table - Continued**

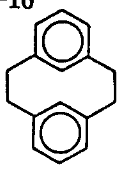
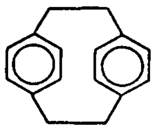
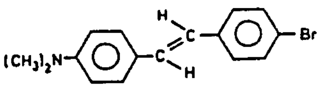
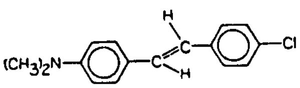
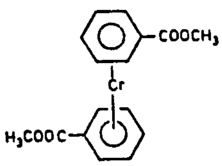
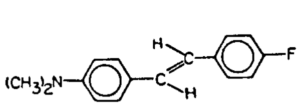
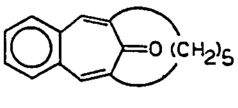
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{16}H_{16}^+$ | | | | | | | |
|  | 7.9 | (223) | (933) | 41±2 | 171±7 | 77PED/RYL | 2319-97-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | 7.8±0.1 | 239 | 998 | 59±0.7 | 246±3 | 80NIS/SAK | 1633-22-3 |
| | IP from 82LEV/LIA, 82GLE/ECK. See also: 81ZHO/KOV. | | | | | | |
| $C_{16}H_{16}BrN^+$ | | | | | | | |
|  | (≤7.04) | (≤200) | (≤835) | 37 | 156 | *EST | 2844-19-1 |
| | IP from 85CAU/FUR. | | | | | | |
| $C_{16}H_{16}ClN^+$ | | | | | | | |
|  | (≤7.05) | (≤190) | (≤796) | 28 | 116 | *EST | 69957-42-2 |
| | IP from 85CAU/FUR. | | | | | | |
| $C_{16}H_{16}CrO_4^+$ | | | | | | | |
|  | (≤5.77) | (≤35) | (≤147) | −98 | −410 | *EST | 1272-35-1 |
| | IP from 82CAB/COW. | | | | | | |
| $C_{16}H_{16}FN^+$ | | | | | | | |
|  | (6.39) | (160) | (671) | 13 | 54 | *EST | 38695-34-0 |
| | IP is onset of photoelectron band (85CAU/FUR). | | | | | | |
| $C_{16}H_{16}O^+$ | | | | | | | |
|  | (8.0) | (217) | (909) | 33±3 | 137±12 | 77PED/RYL | 25401-39-2 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

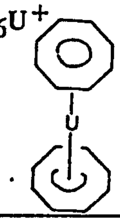
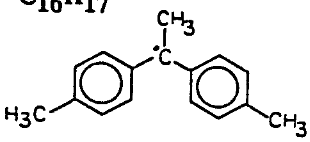
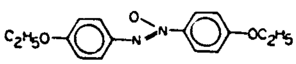
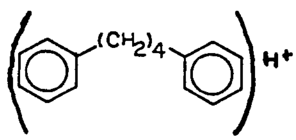
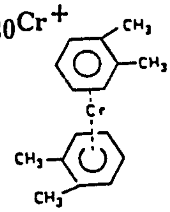
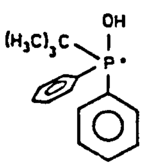
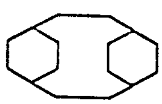
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{16}H_{16}U^+$  | ≤6.17±0.03 | (≤247) | (≤1035) | 105±3 | 439±13 | 77TEL/RAB | 11079-26-8 |
| $C_{16}H_{17}^+$  | | 193 | 809 | | | | |
| | From proton affinity of $(4\text{-}CH_3C_6H_4)_2C=CH_2$ (RN 2919-20-2). PA = 215.4 kcal/mol, 901. kJ/mol. | | | | | | |
| $C_{16}H_{18}N_2O_3^+$  | (7.2) | (166) | (695) | 0 | 0 | *EST | 4792-83-0 |
| | IP is onset of photoelectron band (81MIL/CIL). | | | | | | |
| $C_{16}H_{19}^+$  | | 194 | 810 | | | | |
| | From proton affinity of $C_6H_5(CH_2)_4C_6H_5$ (RN 1083-56-3). PA = 195.9 kcal/mol, 820. kJ/mol. | | | | | | |
| $C_{16}H_{20}Cr^+$  | (≤5.21) | (≤105) | (≤439) | −15 | −64 | *EST | 12092-21-6 |
| | IP from 82CAB/COW. | | | | | | |
| $C_{16}H_{20}OP^+$  | | 83 | 347 | | | | |
| | From proton affinity of $t\text{-}C_4H_9(C_6H_5)_2PO$ (RN 56598-35-7) (86TRA/MUN). PA = 216 kcal/mol, 904 kJ/mol. | | | | | | |
| $C_{16}H_{28}^+$  | (9.1) | (173) | (726) | −36±3 | −152±13 | 77PED/RYL | 283-68-1 |
| | IP is onset of photoelectron band (84GLE/SPA). | | | | | | |

**Table 1. Positive Ion Table - Continued**

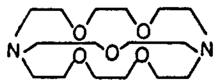
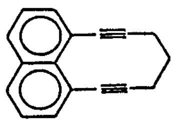
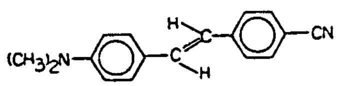
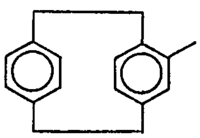
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{16}H_{32}N_2O_5^+$ | | | | | | | |
|  | (≤7.7) | (≤7) | (≤31) | −170 | −712 | *EST | 31364-42-8 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{16}H_{34}N_2^+$ | | | | | | | |
| (E)-$((CH_3)_3CCH_2C(CH_3)_2)_2N_2$ | (≤8.00) | (≤137) | (≤575) | −47±2 | −197±9 | 80ENG | 55204-43-8 |
| $C_{16}H_{36}Sn^+$ | | | | | | | |
| $(C_4H_9)_4Sn$ | (8.0) | (132) | (553) | −52±1 | −219±4 | 77PED/RYL | 1461-25-2 |
| | IP is onset of photoelectron band. | | | | | | |
| (iso-$C_4H_9)_4Sn$ | (≤8.68) | (≤165) | (≤689) | −35 | −148 | *EST | 3531-43-9 |
| $C_{16}H_{44}Si_4Ti^+$ | | | | | | | |
| $[(CH_3)_3SiCH_2]_4Ti$ | (8.0) | (−3) | (−14) | −188±8 | −786±33 | 86SIM/BEA | 33948-28-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{16}H_{44}Si_4Zr^+$ | | | | | | | |
| $((CH_3)_3SiCH_2)_4Zr$ | (8.2) | (−9) | (−36) | −198±8 | −827±33 | 86SIM/BEA | 32665-18-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{17}H_{12}^+$ | | | | | | | |
|  | (7.53) | (349) | (1458) | (175) | (732) | *EST | 32137-40-9 |
| | IP from 84GLE/SCH. | | | | | | |
| $C_{17}H_{16}N_2^+$ | | | | | | | |
|  | (≤7.31) | (≤261) | (≤1094) | 93 | 389 | *EST | |
| | IP from 85CAU/FUR. | | | | | | |
| $C_{17}H_{18}^+$ | | | | | | | |
|  | (7.6) | (226) | (947) | 51 | 214 | *EST | 24262-07-5 |
| | IP is onset of photoelectron band (81ZHO/KOV). | | | | | | |

**Table 1. Positive Ion Table - Continued**

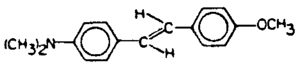
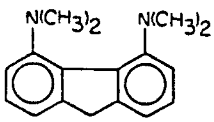
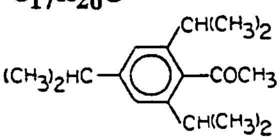
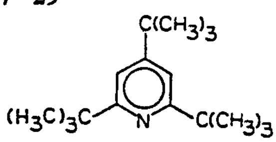
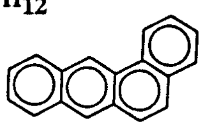
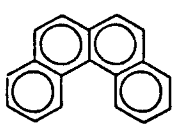
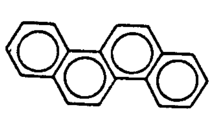
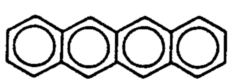
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{17}H_{19}NO^+$ | | | | | | | |
|  | (6.16) | (166) | (696) | 24 | 102 | *EST | 2844-24-8 |
| | IP is onset of photoelectron band (85CAU/FUR). | | | | | | |
| $C_{17}H_{20}N_2^+$ | | | | | | | |
|  | (6.7) | (226) | (945) | 71 | 299 | *EST | 86943-85-3 |
| | IP is onset of photoelectron band (84GLE/SCH). | | | | | | |
| $C_{17}H_{26}O^+$ | | | | | | | |
|  | (8.0) | (104) | (437) | −80 | −335 | *EST | 2234-14-2 |
| | IP is onset of photoelectron band (78CEN/FRA). | | | | | | |
| $C_{17}H_{29}N^+$ | | | | | | | |
|  | 8.20 | (133) | (558) | −56 | −233 | *EST | 20336-15-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{18}H_{12}^+$ | | | | | | | |
|  | 7.43±0.03 | 239 | 1001 | 68±0.2 | 284±1 | 79KUD/KUD2 | 56-55-3 |
| | See also: 81AKI/HAR. | | | | | | |
|  | 7.60 | 245 | 1024 | 70±0.2 | 291±1 | 79KUD/KUD2 | 195-19-7 |
|  | 7.59±0.02 | 243 | 1016 | 67.8±0.2 | 283.7±0.8 | 79KUD/KUD2 | 218-01-9 |
| | Value of IP from charge transfer equilibrium constant determinations (80MAU) is in agreement. See also: 81SHA/AKI, 80SHU/BOY. | | | | | | |
|  | 6.97±0.02 | 229 | 956 | 68±0.2 | 284±1 | 79KUD/KUD2 | 92-24-0 |
| | See also: 84STA/MAQ, 80SHU/BOY. | | | | | | |

**Table 1. Positive Ion Table - Continued**

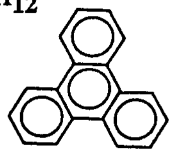
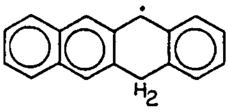
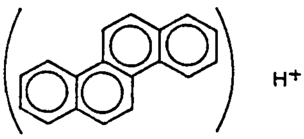
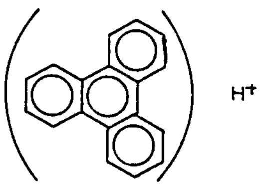
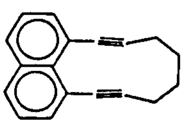
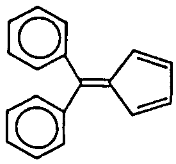
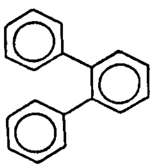
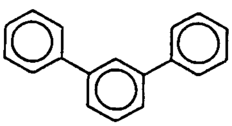
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{12}^+$ | | | | | | | |
|  | 7.84±0.01 | 245 | 1026 | 64±0.2 | 270±1 | 79KUD/KUD2 | 217-59-4 |
| | Value of IP from charge transfer equilibrium constant determinations (80MAU) is in agreement. See also: 80SHU/BOY. | | | | | | |
| $C_{18}H_{13}^+$ | | | | | | | |
|  | | 216 | 903 | | | | |
| | From proton affinity of naphthacene (RN 92-24-0). PA = 217.8 kcal/mol, 911. kJ/mol. | | | | | | |
|  | | 227 | 950 | | | | |
| | From proton affinity of chrysene (RN 218-01-9). PA = 201.6 kcal/mol, 843. kJ/mol. | | | | | | |
|  | | 232 | 970 | | | | |
| | From proton affinity of triphenylene (RN 217-59-4). PA = 198.5 kcal/mol, 830.5 kJ/mol. | | | | | | |
| $C_{18}H_{14}^+$ | | | | | | | |
|  | (7.50) | (343) | (1434) | 170 | 710 | *EST | 32137-39-6 |
| | IP from 84GLE/SCH. | | | | | | |
|  | (≤7.96) | (≤280) | (≤1170) | 96±4 | 402±15 | 77PED/RYL | 2175-90-8 |
|  | 8.0 | (252) | (1054) | 68 | 283 | *EST | 84-15-1 |
| | IP is onset of photoelectron band (83KOB, 82LEV/LIA). | | | | | | |
|  | 8.01±0.01 | (252) | (1056) | 68 | 283 | *EST | 92-06-8 |
| | IP from 82LEV/LIA. See also: 83KOB. | | | | | | |

**Table 1. Positive Ion Table - Continued**

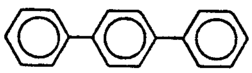
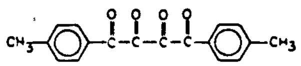
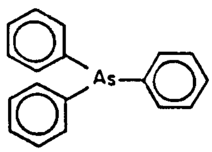
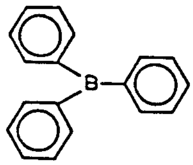
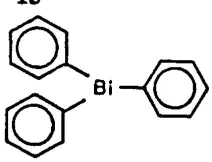
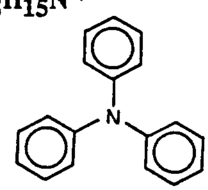
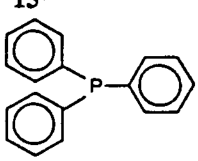
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{14}^+$ | | | | | | | |
|  | 7.78±0.01 | (247) | (1034) | 68 | 283 | *EST | 92-94-4 |
| $C_{18}H_{14}O_4^+$ | | | | | | | |
|  | (≤8.8) | (≤121) | (≤507) | −82 | −342 | *EST | 19909-64-9 |
| | IP from 85GLE/DOB. | | | | | | |
| $C_{18}H_{15}As^+$ | | | | | | | |
|  | 7.32±0.05 | 266 | 1114 | 98±3 | 408±11 | 79STE | 603-32-7 |
| $C_{18}H_{15}B^+$ | | | | | | | |
|  | (8.60±0.03) | (229) | (960) | 31±2 | 130±8 | 77PED/RYL | 960-71-4 |
| $C_{18}H_{15}Bi^+$ | | | | | | | |
|  | 7.45±0.05 | 317 | 1328 | 146±2 | 609±10 | 79STE | 603-33-8 |
| $C_{18}H_{15}N^+$ | | | | | | | |
|  | 6.80±0.04 | 176 | 734 | 19±0.2 | 78±1 | 78STE | 603-34-9 |
| $C_{18}H_{15}P^+$ | | | | | | | |
|  | 7.39±0.03 | 249 | 1041 | 78±5 | 328±21 | 79STE | 603-35-0 |
| | IP from 82IKU/KEB, 77ROS/DRA, 82LEV/LIA. | | | | | | |

**Table 1. Positive Ion Table - Continued**

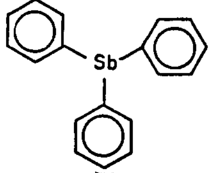
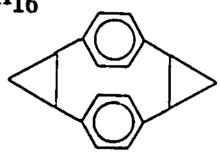
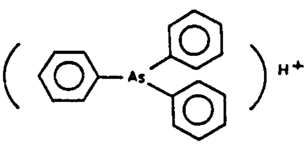
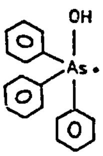
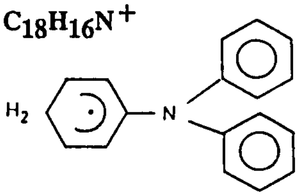
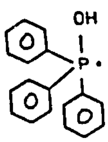
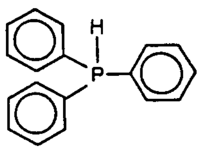
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{15}Sb^+$  | 7.26±0.05 | 271 | 1135 | 104±4 | 435±19 | 79STE | 603-36-1 |
| $C_{18}H_{16}^+$  | (7.4) | (275) | (1152) | 105 | 438 | *EST | |
| | IP is onset of photoelectron band (82GLE/ECK). | | | | | | |
| $C_{18}H_{16}As^+$  | | 247 | 1034 | | | | |
| | From proton affinity of $(C_6H_5)_3As$ (RN 603-32-7)(86TRA/MUN). PA = 216. kcal/mol, 904. kJ/mol. | | | | | | |
| $C_{18}H_{16}AsO^+$  | | 198 | 827 | | | | |
| | From proton affinity of $(C_6H_5)_3AsO$ (RN 1153-05-5) (86TRA/MUN). PA = 216. kcal/mol, 904. kJ/mol. | | | | | | |
| $C_{18}H_{16}N^+$  | | 168 | 704 | | | | |
| | From proton affinity of $(C_6H5)_3N$ (RN 603-34-9)(86TRA/MUN). PA = 216. kcal/mol, 904. kJ/mol. | | | | | | |
| $C_{18}H_{16}OP^+$  | | 154 | 644 | | | | |
| | From proton affinity of $(C_6H_5)_3PO$ (RN 791-28-6)(86TRA/MUN). PA = 216. kcal/mol, 904. kJ/mol. | | | | | | |
| $C_{18}H_{16}P^+$  | | 214 | 896 | | | | |
| | From proton affinity of $(C_6H_5)_3P$ (RN 603-35-0). PA = (230) kcal/mol, (962) kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

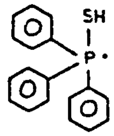
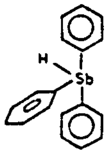
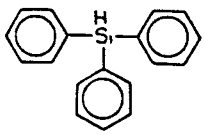
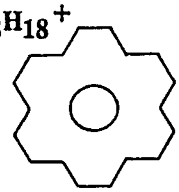
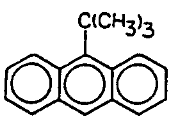
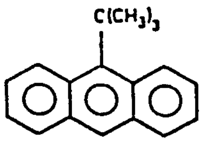
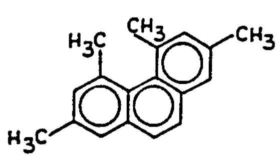
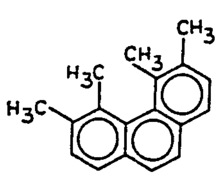
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$C_{18}H_{16}PS^+$** | | | | | | | |
|  | | 206 | 860 | | | | |
| | From proton affinity of $(C_6H_5)_3PS$ (RN 3878-45-3)(86TRA/MUN). PA = 216. kcal/mol, 904. kJ/mol. | | | | | | |
| **$C_{18}H_{16}Sb^+$** | | | | | | | |
|  | | 267 | 1119 | | | | |
| | From proton affinity of $(C_6H_5)_3Sb$ (RN 603-36-1)(86TRA/MUN). PA = 202. kcal/mol, 846. kJ/mol. | | | | | | |
| **$C_{18}H_{16}Si^+$** | | | | | | | |
|  | (8.4) | (257) | (1075) | 63 | 265 | *EST | 789-25-3 |
| | IP is onset of photoelectron band. | | | | | | |
| **$C_{18}H_{18}^+$** | | | | | | | |
|  | (6.60) | (276) | (1156) | 124±5 | 519±20 | 74OTH/BUN | 2040-73-5 |
| | IP from 82BAU/BUN. | | | | | | |
|  | (7.13) | (201) | (843) | 37 | 156 | *EST | 62337-65-9 |
| | IP from 78KLA/KOV, 83KLA/KOV. | | | | | | |
|  | 7.13 | (201) | (843) | 37 | 155 | *EST | 13719-97-6 |
| | IP from 83KLA/KOV. | | | | | | |
|  | (7.8±0.1) | (210) | (879) | 30±1 | 126±6 | 77PED/RYL | 7396-38-5 |
|  | (7.5±0.1) | (211) | (881) | 38±1 | 157±6 | 77PED/RYL | 7343-06-8 |

**Table 1. Positive Ion Table - Continued**

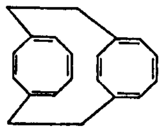
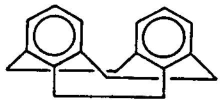
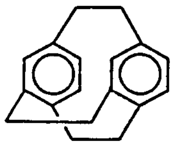
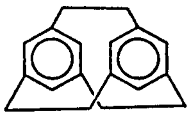
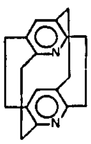
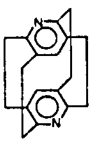
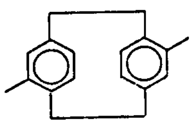
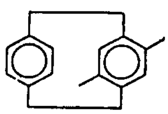
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{18}^+$ | | | | | | | |
|  | (7.3) | (221) | (926) | 53 | 222 | *EST | |
| | IP is onset of photoelectron band (84ZHO/HEI). | | | | | | |
|  | 7.8 | (222) | (931) | 43 | 178 | *EST | |
| | IP is onset of photoelectron band. | | | | | | |
|  | 7.8 | (236) | (987) | 56 | 234 | *EST | 58002-98-5 |
|  | 7.4 | (212) | (886) | 41 | 172 | *EST | 27165-88-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{18}H_{18}N_2^+$ | | | | | | | |
|  | (7.4) | (275) | (1150) | 104 | 436 | *EST | |
| | IP is onset of photoelectron band (81ZHO/HEI). | | | | | | |
|  | (7.6) | (279) | (1169) | 104 | 436 | *EST | |
| | IP is onset of photoelectron band (81ZHO/HEI). | | | | | | |
| $C_{18}H_{20}^+$ | | | | | | | |
|  | (≤7.85±0.05) | (≤225) | (≤939) | 43 | 182 | *EST | |
| | IP from 81ZHO/KOV. | | | | | | |
|  | (7.4) | (214) | (897) | 44 | 183 | *EST | |
| | IP is onset of photoelectron band (81ZHO/KOV). | | | | | | |

**Table 1. Positive Ion Table - Continued**

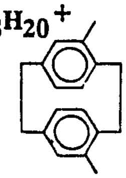
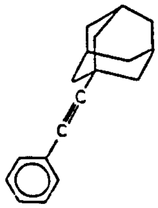
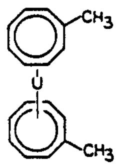
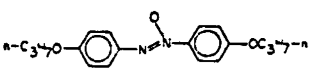
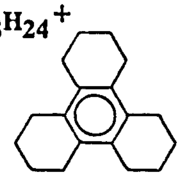
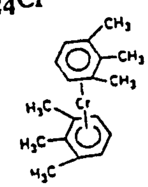
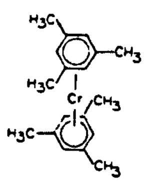
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{20}^+$ | | | | | | | |
|  | (≤7.85±0.05)<br>IP from 81ZHO/KOV. | (≤225) | (≤939) | 43 | 182 | *EST | |
|  | (8.12±0.08)<br>IP from 81ELB/LIE. | (240) | (1002) | 52 | 219 | *EST | |
| $C_{18}H_{20}U^+$ | | | | | | | |
|  | (≤6.08)<br>IP from 83GRE/PAY. | (≤229) | (≤959) | 89 | 373 | *EST | 41367-67-3 |
| $C_{18}H_{22}N_2O_3^+$ | | | | | | | |
|  | (≤7.64)<br>IP from 81MIL/CIL. | (≤167) | (≤697) | −10 | −40 | *EST | 23315-55-1 |
| $C_{18}H_{24}^+$ | | | | | | | |
|  | (7.70±0.05)<br>IP from 81HEI/KOV. | (175) | (732) | −3 | −11 | *EST | 1610-39-5 |
| $C_{18}H_{24}Cr^+$ | | | | | | | |
|  | (≤5.04)<br>IP from 82CAB/COW. | (≤134) | (≤562) | 18 | 76 | *EST | 57820-96-9 |
|  | 4.97<br>IP from 82CAB/COW. | 130 | 543 | 15±3 | 64±12 | 82PIL/SKI | 1274-07-3 |

**Table 1. Positive Ion Table - Continued**

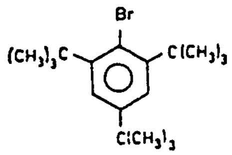
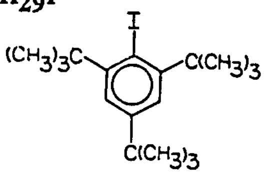
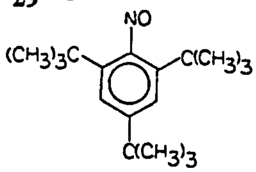
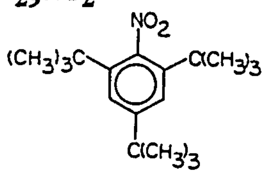
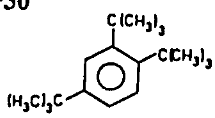
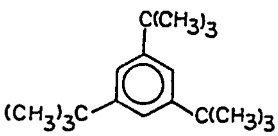
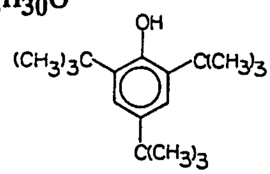
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{29}Br^+$ | | | | | | | |
|  | 8.0 | (151) | (631) | −33 | −140 | *EST | 3975-77-7 |
| | IP is onset of photoelectron band (83CET/LAP). | | | | | | |
| $C_{18}H_{29}I^+$ | | | | | | | |
|  | 7.5 | (156) | (651) | −17 | −73 | *EST | 31039-82-4 |
| | IP is onset of photoelectron band (83CET/LAP). | | | | | | |
| $C_{18}H_{29}NO^+$ | | | | | | | |
|  | (≤8.69) | (≤184) | (≤768) | −17 | −70 | *EST | 24973-59-9 |
| | IP from 83CET/LAP. | | | | | | |
| $C_{18}H_{29}NO_2^+$ | | | | | | | |
|  | (≤8.78) | (≤154) | (≤646) | −48 | −201 | *EST | 3463-37-4 |
| | IP from 83CET/LAP. | | | | | | |
| $C_{18}H_{30}^+$ | | | | | | | |
|  | (≤8.60±0.07) | (≤164) | (≤687) | −34±1.4 | −143±6 | 67ARN/SAN | 1459-11-6 |
|  | (8.19) | (131) | (548) | −58±1 | −242±4 | 77PED/RYL | 1460-02-2 |
| | IP from 84HOW/GON. See also: 83CET/LAP. | | | | | | |
| $C_{18}H_{30}O^+$ | | | | | | | |
|  | (7.5) | (80) | (335) | −93 | −389 | *EST | 732-26-3 |
| | IP is onset of photoelectron band (83CET/LAP). | | | | | | |

**Table 1. Positive Ion Table - Continued**

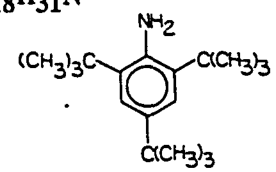
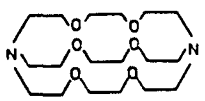
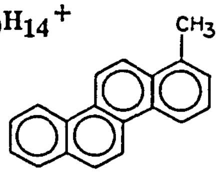
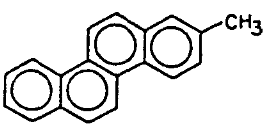
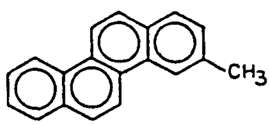
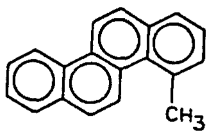
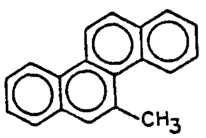
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{18}H_{31}N^+$ | | | | | | | |
|  | (6.9) | (110) | (460) | −49 | −206 | *EST | |
| | IP is onset of photoelectron band (83CET/LAP). | | | | | | |
| $C_{18}H_{36}N_2O_6^+$ | | | | | | | |
|  | (≤7.8) | (≤−28) | (≤−118) | −208 | −871 | *EST | 23978-09-8 |
| | IP from 83BAK/ARM. | | | | | | |
| $C_{18}H_{42}N_3P^+$ | | | | | | | |
| $P(N(n\text{-}C_3H_7)_2)_3$ | (≤7.05) | (≤78) | (≤325) | −85 | −355 | *EST | 5848-64-6 |
| | IP from 82WOR/HAR. | | | | | | |
| $C_{19}H_{14}^+$ | | | | | | | |
|  | (7.46±0.03) | (226) | (944) | 54 | 224 | *EST | 3351-28-8 |
| | IP from 81SHA/AKI. | | | | | | |
|  | (7.49±0.03) | (226) | (947) | 54 | 224 | *EST | 3351-32-4 |
| | IP from 81SHA/AKI. | | | | | | |
|  | (7.46±0.03) | (226) | (944) | 54 | 224 | *EST | 3351-31-3 |
| | IP from 81SHA/AKI. | | | | | | |
|  | (7.44±0.03) | (230) | (963) | 59 | 245 | *EST | 3351-30-2 |
| | IP from 81SHA/AKI. | | | | | | |
|  | (7.40±0.03) | (229) | (959) | 59 | 245 | *EST | 3697-24-3 |
| | IP from 81SHA/AKI. | | | | | | |

Table 1. Positive Ion Table - Continued

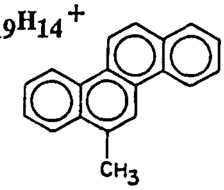
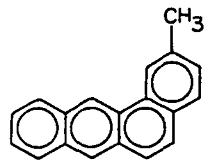
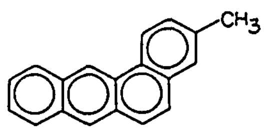
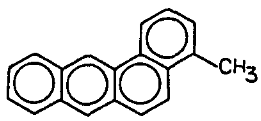
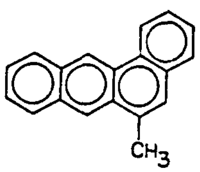
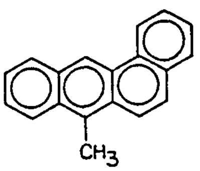
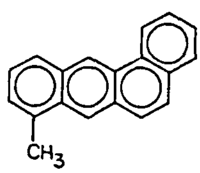
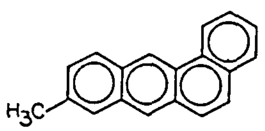
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{19}H_{14}^+$ | | | | | | | |
|  | (7.44±0.03)<br>IP from 81SHA/AKI. | (228) | (953) | 57 | 236 | *EST | 1705-85-7 |
|  | (7.30)<br>IP from 81AKI/HAR. | (224) | (938) | 56 | 234 | *EST | 2498-76-2 |
|  | (7.29)<br>IP from 81AKI/HAR. | (224) | (937) | 56 | 234 | *EST | 2498-75-1 |
|  | (7.30)<br>IP from 81AKI/HAR. | (224) | (938) | 56 | 234 | *EST | 316-49-4 |
|  | (7.33)<br>IP from 81AKI/HAR. | (225) | (941) | 56 | 234 | *EST | 316-14-3 |
|  | (7.24)<br>IP from 81AKI/HAR. | (223) | (933) | 56 | 234 | *EST | 2541-69-7 |
|  | (7.33)<br>IP from 81AKI/HAR. | (225) | (941) | 56 | 234 | *EST | 2381-31-9 |
|  | (7.31)<br>IP from 81AKI/HAR. | (224) | (939) | 56 | 234 | *EST | 2381-16-0 |

**Table 1. Positive Ion Table - Continued**

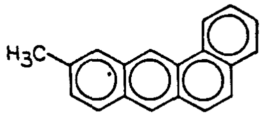
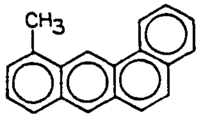
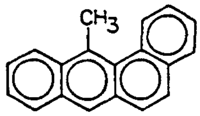
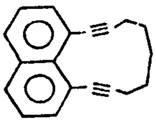
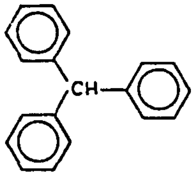
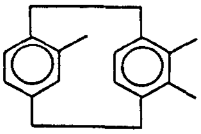
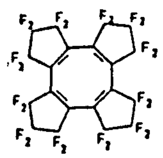
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{19}H_{14}^+$ | | | | | | | |
|  | (7.30)<br>IP from 81AKI/HAR. | (224) | (938) | 56 | 234 | *EST | 2381-15-9 |
|  | (7.30)<br>IP from 81AKI/HAR. | (224) | (938) | 56 | 234 | *EST | 6111-78-0 |
|  | (7.27)<br>IP from 81AKI/HAR. | (243) | (1015) | 75 | 314 | *EST | 2422-79-9 |
| $C_{19}H_{16}^+$ | | | | | | | |
|  | (7.48)<br>IP from 84GLE/SCH. | (337) | (1411) | 165 | 690 | *EST | 87842-94-2 |
|  | 8.34±0.03 | 257 | 1076 | 65±1 | 271±4 | 77PED/RYL | 519-73-3 |
| $C_{19}H_{22}^+$ | | | | | | | |
|  | (7.3)<br>IP is onset of photoelectron band (81ZHO/KOV). | (207) | (867) | 39 | 163 | *EST | |
| $C_{20}F_{24}^+$ | | | | | | | |
|  | 10.75<br>IP is onset of photoelectron band (84HEI/WIR). | (−761) | (−3183) | −1009 | −4220 | *EST | 32936-99-5 |

Table 1. Positive Ion Table - Continued

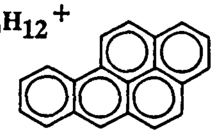
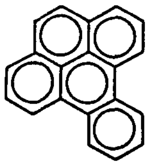
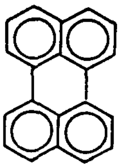
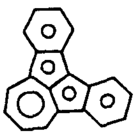
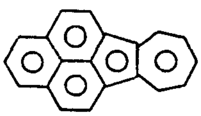
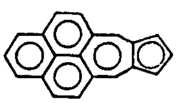
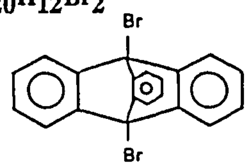
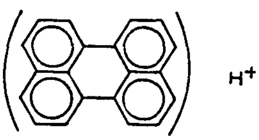
| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{12}^+$ | | | | | | | |
|  | 7.12±0.01 | 233 | 976 | 69 | 289 | 77STE/GOL | 50-32-8 |
|  | 7.41<br>IP from 79CLA/SCH. | (233) | (976) | 62 | 261 | 77STE/GOL | 192-97-2 |
|  | 6.90±0.01 | 233 | 974 | 74±1 | 308±4 | 77PED/RYL | 198-55-0 |
|  | 6.84<br>IP from 81SAT/SEK. | (270) | (1129) | 112 | 469 | *EST | 4670-86-4 |
|  | (6.58) | (269) | (1126) | 117 | 491 | *EST | 54100-60-6 |
|  | (6.76) | (273) | (1143) | 117 | 491 | *EST | 6580-41-2 |
| $C_{20}H_{12}Br_2^+$ | | | | | | | |
|  | (8.1)<br>IP from 83MAR/MAY. | (265) | (1107) | 78 | 326 | *EST | |
| $C_{20}H_{13}^+$ | | | | | | | |
|  | | 228 | 954 | | | | |
| | From proton affinity of perylene (RN 198-55-0). PA = 211.4 kcal/mol, 884. kJ/mol. | | | | | | |

Table 1. Positive Ion Table - Continued

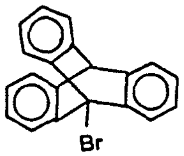
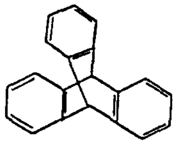
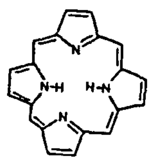
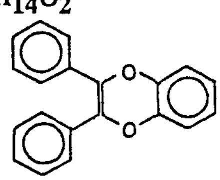
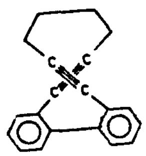
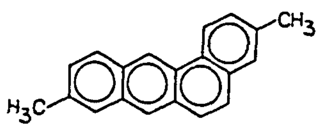
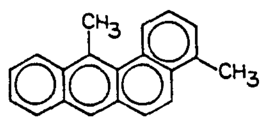
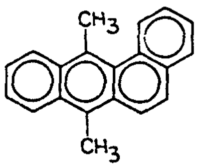
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{13}Br^+$ | | | | | | | |
|  | (7.9) | (260) | (1086) | 77 | 324 | *EST | |
| | IP is onset of photoelectron band (83MAR/MAY). | | | | | | |
| $C_{20}H_{14}^{\cdot +}$ | | | | | | | |
|  | (7.8) | (257) | (1074) | 77±3 | 322±13 | 77PED/RYL | |
| | IP is onset of photoelectron band (83MAR/MAY, 82HAS/NEU). | | | | | | |
| $C_{20}H_{14}N_4^+$ | | | | | | | |
|  | 6.6 | −86.4 | −361.5 | −238.6±0.4 | −998.3±1.7 | 70LON/FIN | 101-60-0 |
| | IP from 80DUP/ROB. | | | | | | |
| $C_{20}H_{14}O_2^+$ | | | | | | | |
|  | (7.08±0.02) | (172) | (721) | 9 | 38 | 81BOU/DAG | 75694-46-1 |
| | IP from 81BOU/DAG. | | | | | | |
| $C_{20}H_{16}^+$ | | | | | | | |
|  | (7.9) | (354) | (1481) | 172 | 719 | *EST | |
| | IP is onset of photoelectron band (81GLE/SCH). | | | | | | |
|  | (7.20) | (210) | (878) | 43.9±0.9 | 183.7±3.9 | 77PED/RYL | 316-51-8 |
| | IP from 81AKI/HAR. | | | | | | |
|  | (7.18) | (232) | (971) | 66 | 278 | *EST | 35187-19-0 |
| | IP from 81AKI/HAR. | | | | | | |
|  | (7.10) | (230) | (963) | 66.4±1.0 | 277.7±4.4 | 77PED/RYL | 57-97-6 |
| | IP from 81AKI/HAR. | | | | | | |

**Table 1. Positive Ion Table - Continued**

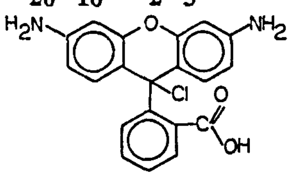
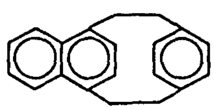
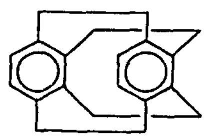
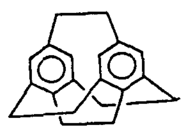
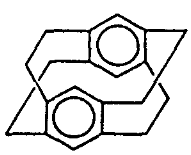
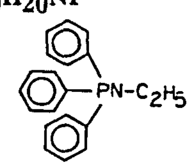
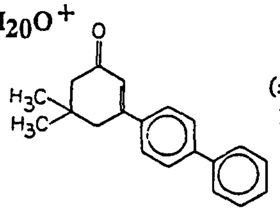
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{16}ClN_2O_3^+$ | | | | | | | |
|  | (7.80±0.05)<br>IP from 81TIM/KOR. | (157) | (656) | −23 | −97 | *EST | |
| $C_{20}H_{18}^+$ | | | | | | | |
|  | (7.4)<br>IP is onset of photoelectron band. | (244) | (1020) | 73 | 306 | *EST | 4432-72-8 |
| $C_{20}H_{20}^+$ | | | | | | | |
|  | (7.6)<br>IP is onset of photoelectron band. | (233) | (975) | 58 | 242 | *EST | |
|  | (7.4)<br>IP is onset of photoelectron band. | (226) | (944) | 55 | 230 | *EST | |
|  | (7.35)<br>IP is onset of photoelectron band (81ZHO/HEI). | (237) | (993) | 68 | 284 | *EST | |
| $C_{20}H_{20}NP^+$ | | | | | | | |
|  | (≤7.43) | (≤216) | (≤903) | 44±2 | 186±9 | 77PED/RYL | 47182-04-7 |
| $C_{20}H_{20}O^+$ | | | | | | | |
|  | (≤8.88)<br>IP from 82PFI/GER. | (≤186) | (≤778) | −19 | −79 | *EST | 72036-53-4 |

Table 1. Positive Ion Table - Continued

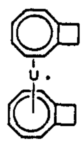
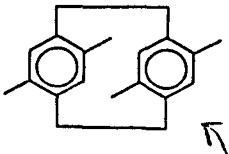
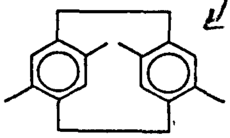
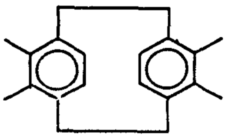
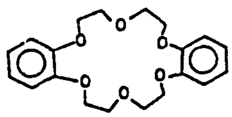
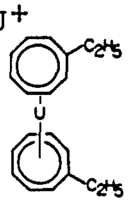
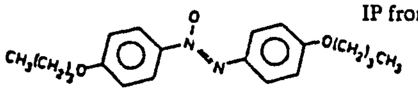
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{20}U^+$ | | | | | | | |
|  | (≤6.02) | (≤300) | (≤1256) | 161 | 675 | *EST | 70377-87-6 |
| | IP from 83GRE/PAY. | | | | | | |
| $C_{20}H_{24}^+$ | | | | | | | |
|  | (7.2) | (200) | (838) | 34 | 144 | *EST | |
| | IP is onset of photoelectron band (81ZHO/KOV). | | | | | | |
| SAME MOLECULE | | | | | | | |
|  | (≤7.55±0.05) | (≤209) | (≤872) | 34 | 144 | *EST | |
| | IP from 81ZHO/KOV. | | | | | | |
|  | ≤7.60±0.05 | (≤210) | (≤877) | 34 | 144 | *EST | |
| | IP from 81ZHO/KOV. | | | | | | |
| $C_{20}H_{24}O_6^+$ | | | | | | | |
|  | (7.5) | (1.8) | (7.6) | −171 | −716 | *EST | |
| | IP is onset of photoelectron band (83BAK/ARM). | | | | | | |
| $C_{20}H_{24}U^+$ | | | | | | | |
|  | (5.9) | (215) | (900) | 79 | 331 | *EST | 37274-10-5 |
| | IP is onset of photoelectron band (83GRE/PAY). | | | | | | |
| $C_{20}H_{26}N_2O_3^+$ | | | | | | | |
|  | (≤7.61) | (≤156) | (≤654) | −19 | −80 | *EST | 17051-01-3 |
| | IP from 81MIL/CIL. | | | | | | |

**Table 1. Positive Ion Table - Continued**

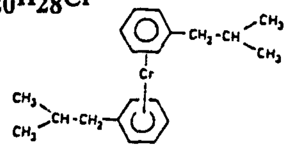
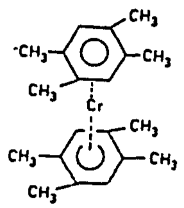
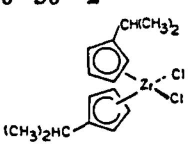
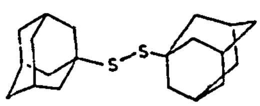
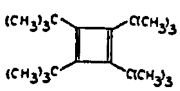
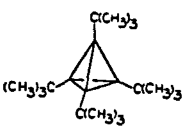
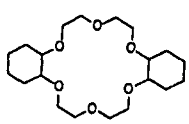
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{28}Cr^+$ | | | | | | | |
|  | (≤5.23)<br>IP from 82CAB/COW. | (≤128) | (≤538) | 8 | 33 | *EST | 51951-64-5 |
|  | (≤4.85)<br>IP from 82CAB/COW. | (≤108) | (≤454) | −3 | −14 | *EST | 57820-98-1 |
| $C_{20}H_{30}Cl_2Zr^+$ | | | | | | | |
|  | 7.1<br>IP is onset of photoelectron band (81CIL/CON). | (60) | (252) | −103±1 | −433±4 | 82PIL/SKI | 54039-38-2 |
| $C_{20}H_{30}S_2^+$ | | | | | | | |
|  | (7.5)<br>IP is onset of photoelectron band. | (125) | (524) | −48 | −200 | *EST | 34895-45-9 |
| $C_{20}H_{36}^+$ | | | | | | | |
|  | (5.9)<br>IP is onset of photoelectron band. | (226) | (946) | 90±5.5 | 377±23 | *EST | 66809-05-0 |
|  | (7.1)<br>IP is onset of photoelectron band. | (257) | (1076) | 93±5.5 | 391±23 | *EST | 66809-06-1 |
| $C_{20}H_{36}O_6^+$ | | | | | | | |
|  | (8.6)<br>IP is onset of photoelectron band. | (−59) | (−248) | −258 | −1078 | *EST | 16069-36-6 |
| $C_{20}H_{44}Hf^+$<br>$((CH_3)_3CCH_2)_4Hf$ | (8.1)<br>IP is onset of photoelectron band. | (132) | (554) | −54±9 | −228±33 | 86SIM/BEA | 50654-35-8 |

**Table 1. Positive Ion Table - Continued**

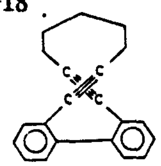
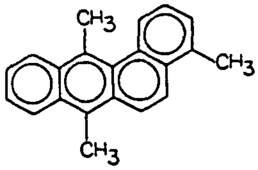
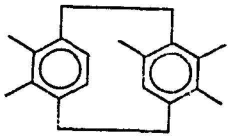
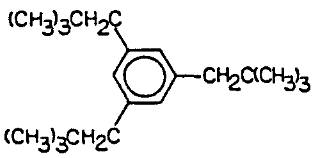
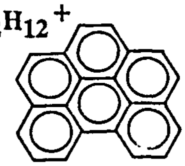
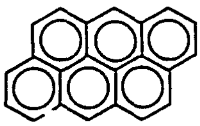
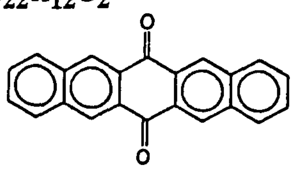
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{20}H_{44}Ti^+$ | | | | | | | |
| $((CH_3)_3CCH_2)_4Ti$ | (7.7) | (140) | (586) | −38±8 | −157±33 | 86SIM/BEA | 36945-13-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{21}H_{18}^{+\cdot}$ | | | | | | | |
|  | (7.7) | (345) | (1442) | 167 | 699 | *EST | |
| | IP is onset of photoelectron band (81GLE/SCH). | | | | | | |
|  | (7.06±0.03) | (217) | (909) | 54 | 228 | *EST | 35187-24-7 |
| | IP from 81AKI/HAR. | | | | | | |
| $C_{21}H_{26}^+$ | | | | | | | |
|  | (≤7.55±0.05) | (≤199) | (≤831) | 25 | 103 | *EST | |
| | IP from 81ZHO/KOV. | | | | | | |
| $C_{21}H_{36}^+$ | | | | | | | |
|  | (8.17) | (111) | (466) | −77 | −322 | *EST | 21411-39-2 |
| | IP from 84HOW/GON. | | | | | | |
| $C_{22}H_{12}^+$ | | | | | | | |
|  | 7.15 | 237 | 992 | 72 | 302 | 77STE/GOL | 191-24-2 |
| | See also: 80MAU. | | | | | | |
|  | (6.92±0.04) | (233) | (978) | 74 | 310 | 77STE/GOL | 191-26-4 |
| $C_{22}H_{12}O_2^+$ | | | | | | | |
|  | (8.07±0.05) | (196) | (823) | 10±2 | 44±9 | 77PED/RYL | 3029-32-1 |

Table 1. Positive Ion Table - Continued

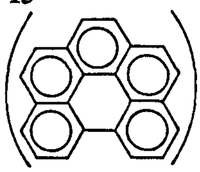
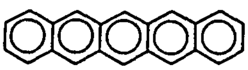
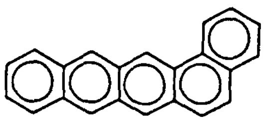
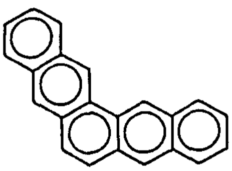
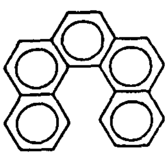
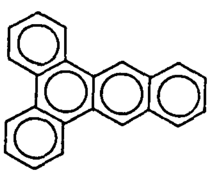
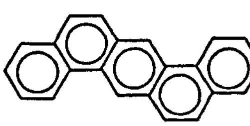
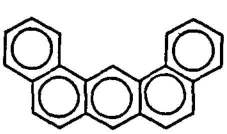
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{22}H_{13}^+$ | | | | | | | |
|  H+ | | 229 | 960 | | | | |
| | From proton affinity of 1,12-benzoperylene (RN 191-24-2). PA = 208.5 kcal/mol, 872. kJ/mol. | | | | | | |
| $C_{22}H_{14}^+$ | | | | | | | |
|  | 6.61±0.02<br>See also: 84STA/MAQ. | (237) | (992) | 85 | 354 | *EST | 135-48-8 |
|  | 7.00<br>See also: 75CLA/SCH. | (244) | (1020) | 82 | 345 | *EST | 226-88-0 |
|  | 7.27±0.02<br>See also: 79CLA/SCH. | (250) | (1046) | 82 | 345 | *EST | 222-93-5 |
|  | 7.47±0.04<br>See also: 75CLA/SCH. | (269) | (1127) | 97 | 406 | *EST | 188-52-3 |
|  | 7.39±0.02<br>See also: 75CLA/SCH, 79CLA/SCH. | 251 | 1049 | 80 | 336 | 77STE/GOL | 215-58-7 |
|  | 7.38±0.04<br>See also: 75CLA/SCH. | 250 | 1048 | 80 | 336 | 77STE/GOL | 53-70-3 |
|  | (7.40±0.02)<br>See also: 75CLA/SCH. | (251) | (1050) | 80 | 336 | 77STE/GOL | 224-41-9 |

Table 1. Positive Ion Table - Continued

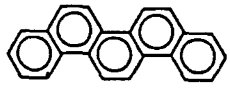
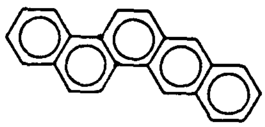
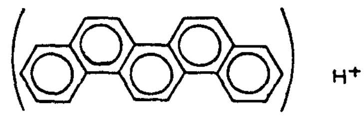
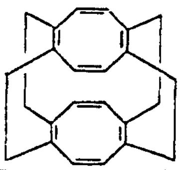
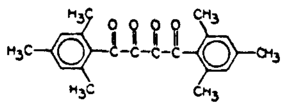
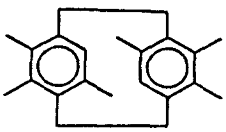
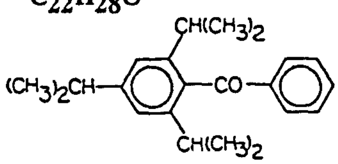
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{22}H_{14}^+$ | | | | | | | |
|  | 7.48 | (250) | (1048) | 78 | 326 | *EST | 213-46-7 |
| | IP from charge transfer equilibrium constant determinations (80MAU), in agreement with value from 79CLA/SCH. | | | | | | |
|  | (7.14±0.04) | (245) | (1024) | 80 | 336 | *EST | 214-17-5 |
| $C_{22}H_{15}^+$ | | | | | | | |
|  | | 240 | 1005 | | | | |
| | From proton affinity of picene (RN 213-46-7). PA = 203.4 kcal/mol, 851. kJ/mol. | | | | | | |
| $C_{22}H_{22}^+$ | | | | | | | |
|  | (7.35) | (256) | (1072) | 87 | 363 | *EST | |
| | IP is onset of photoelectron band (84ZHO/HEI). | | | | | | |
| $C_{22}H_{22}O_4^+$ | | | | | | | |
|  | (≤8.6) | (≤76) | (≤318) | −122 | −512 | *EST | 19909-65-0 |
| | IP from 85GLE/DOB. | | | | | | |
| $C_{22}H_{28}^+$ | | | | | | | |
|  | (7.0) | (176) | (737) | 15 | 62 | *EST | |
| | IP is onset of photoelectron band (81ZHO/KOV). | | | | | | |
| $C_{22}H_{28}O^+$ | | | | | | | |
|  | (7.9) | (137) | (574) | −45±2 | −189±7 | 82INA/MUR | 33574-11-7 |
| | IP is onset of photoelectron band (78CEN/FRA). | | | | | | |

Table 1. Positive Ion Table - Continued

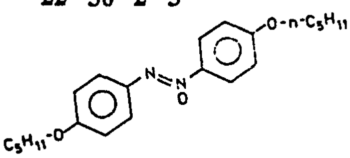
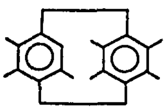
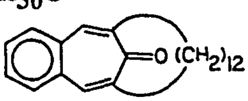
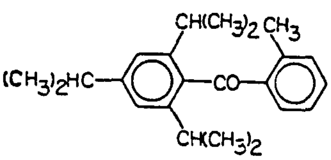
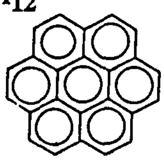
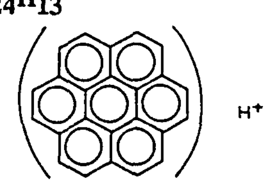
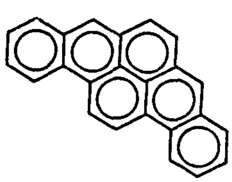
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{22}H_{30}N_2O_3$ + | | | | | | | |
|  | (≤7.63)<br>IP from 81MIL/CIL. | (≤147) | (≤616) | −29 | −120 | *EST | 19482-05-4 |
| $C_{23}H_{30}$ + | | | | | | | |
|  | (≤7.40±0.05)<br>IP from 81ZHO/KOV. | (≤182) | (≤763) | 12 | 49 | *EST | |
| $C_{23}H_{30}O$ + | | | | | | | |
|  | (≤8.15±0.03) | (≤150) | (≤626) | −38±4 | −160±15 | 77PED/RYL | 25401-43-8 |
|  | (7.6)<br>IP is onset of photoelectron band (78CEN/FRA). | (125) | (523) | −50 | −210 | *EST | 78823-28-6 |
| $C_{24}H_{12}$ + | | | | | | | |
|  | 7.29<br>IP at 298 K from charge transfer equilibria, 7.26 eV (80MAU, re-evaluated).<br>See also: 81CLA/ROB. | 245 | 1026 | 77 | 323 | 77STE/GOL | 191-07-1 |
| $C_{24}H_{13}$ + | | | | | | | |
|  | From proton affinity of coronene (RN 191-07-1). PA = 205.0 kcal/mol, 858. kJ/mol. | 238 | 995 | | | | |
| $C_{24}H_{14}$ + | | | | | | | |
|  | (6.95)<br>IP from 79CLA/SCH. | (243) | (1018) | 83 | 348 | 77STE/GOL | 189-55-9 |

**Table 1. Positive Ion Table - Continued**

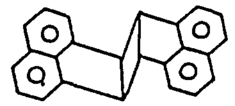
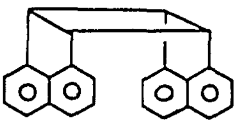
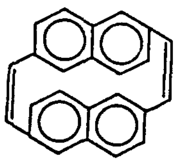
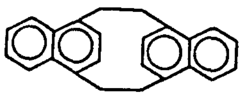
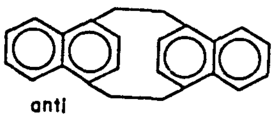
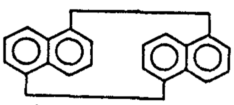
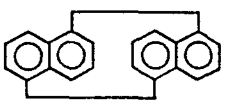
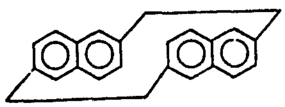
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{24}H_{16}{}^+$ | | | | | | | |
|  | (7.48) | (321) | (1342) | 148 | 620 | *EST | 14620-98-5 |
| | IP from 82GLE/GUB. | | | | | | |
|  | 7.58 | (323) | (1351) | 148 | 620 | *EST | 15065-28-8 |
| | IP from 82GLE/GUB. | | | | | | |
|  | (7.1) | (305) | (1274) | 141 | 589 | *EST | 43012-17-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{24}H_{20}{}^+$ | | | | | | | |
|  syn | (7.0) | (250) | (1046) | 89 | 371 | *EST | 14724-91-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  anti | (7.3) | (257) | (1075) | 89 | 371 | *EST | 17341-02-5 |
| | IP is onset of photoelectron band. | | | | | | |
|  achiral | (6.8) | (245) | (1027) | 89 | 371 | *EST | 54835-57-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  chiral | (7.1) | (253) | (1058) | 89 | 373 | *EST | 54835-57-3 |
| | IP is onset of photoelectron band. | | | | | | |
|  | (7.3) | (240) | (1005) | 72 | 301 | *EST | 73608-51-2 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

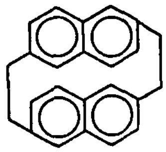
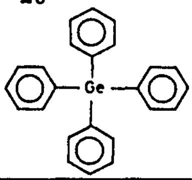
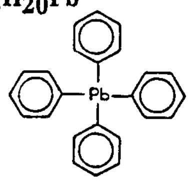
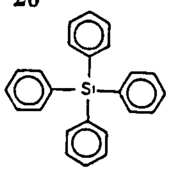
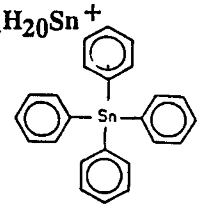
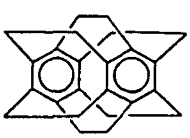
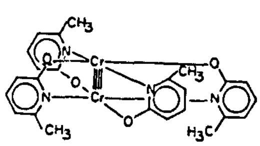
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{24}H_{20}^+$ | | | | | | | |
|  | (7.0)<br>IP is onset of photoelectron band. | (317) | (1325) | 155 | 650 | *EST | 7130-24-7 |
| $C_{24}H_{20}Ge^+$ | | | | | | | |
|  | (8.1)<br>IP is onset of photoelectron band (84NOV/POT). | (293) | (1226) | (106±6) | (445±24) | 77PED/RYL | 1048-05-1 |
| $C_{24}H_{20}Pb^+$ | | | | | | | |
|  | (8.0)<br>IP is onset of photoelectron band (84NOV/POT). | (346) | (1446) | 161±4 | 674±15 | 78STE | 595-89-1 |
| $C_{24}H_{20}Si^+$ | | | | | | | |
|  | (8.50±0.03)<br>See also: 84NOV/POT. | (278) | (1162) | 82±1 | 342±6 | 82PIL/SKI | 1048-08-4 |
| $C_{24}H_{20}Sn^+$ | | | | | | | |
|  | (8.34±0.03)<br>See also: 84NOV/POT. | (329) | (1378) | 137±2 | 573±8 | 77KAN/MOR | 595-90-4 |
| $C_{24}H_{24}^+$ | | | | | | | |
|  | (7.3)<br>IP is onset of photoelectron band. | (253) | (1057) | 84 | 353 | *EST | 60144-50-5 |
| $C_{24}H_{24}Cr_2N_4O_4^+$ | | | | | | | |
|  | (6.5)<br>IP is onset of photoelectron band. | (−41) | (−171) | −191±2 | −798±9 | 81CAV/GAR | 67634-82-6 |

**Table 1. Positive Ion Table - Continued**

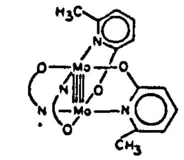
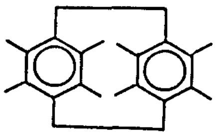
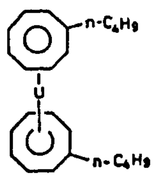
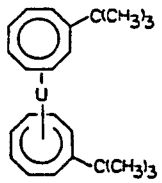
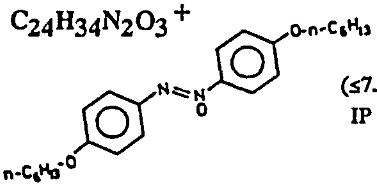
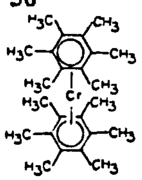
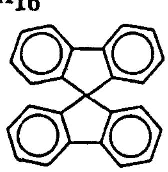
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{24}H_{24}Mo_2N_4O_4^+$ | | | | | | | |
|  | (5.5) | (−16) | (−66) | −143±2 | −597±9 | 81CAV/GAR | 67634-80-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $C_{24}H_{32}^+$ | | | | | | | |
|  | (6.9) | (168) | (702) | 9 | 36 | *EST | |
| | IP is onset of photoelectron band (81ZHO/KOV). | | | | | | |
| $C_{24}H_{32}U^+$ | | | | | | | |
|  | (≤6.05) | (≤199) | (≤831) | 59 | 247 | *EST | 37274-12-7 |
| | IP from 83GRE/PAY. | | | | | | |
|  | (≤6.03) | (≤193) | (≤809) | 54 | 227 | *EST | 63230-70-6 |
| | IP from 83GRE/PAY. | | | | | | |
| $C_{24}H_{34}N_2O_3^+$ | | | | | | | |
|  | (≤7.55) | (≤136) | (≤568) | −38 | −160 | *EST | 2587-42-0 |
| | IP from 81MIL/CIL. | | | | | | |
| $C_{24}H_{36}Cr^+$ | | | | | | | |
|  | (≤4.68) | (≤87) | (≤364) | −21±3 | −88±12 | 82PIL/SKI | 12243-39-9 |
| $C_{25}H_{16}^+$ | | | | | | | |
|  | (7.5) | (286) | (1199) | 114 | 475 | *EST | 159-66-0 |
| | IP is onset of photoelectron band. | | | | | | |

Table 1. Positive Ion Table - Continued

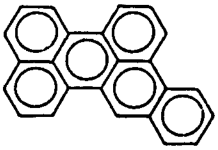
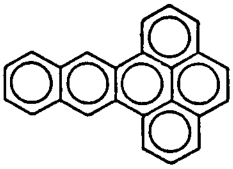
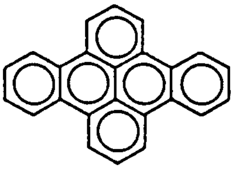
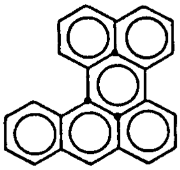
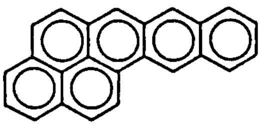
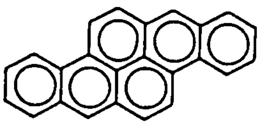
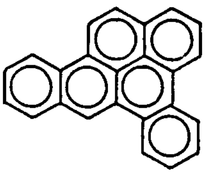
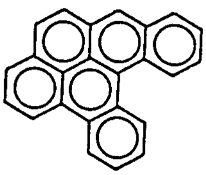
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{24}H_{14}^+$ | | | | | | | |
|  | (6.89) | (240) | (1004) | 81 | 339 | *EST | 197-70-6 |
|  | (7.35)<br>IP from 79CLA/SCH. | (253) | (1057) | 83 | 348 | *EST | 193-09-9 |
|  | 7.39<br>IP from 79CLA/SCH. | (249) | (1042) | 79 | 329 | *EST | 192-51-8 |
|  | (6.71) | (237) | (991) | 82 | 344 | *EST | 191-85-5 |
|  | (6.82)<br>IP from 79CLA/SCH. | (243) | (1015) | 85 | 357 | *EST | |
|  | (6.82)<br>IP from 79CLA/SCH. | (240) | (1006) | 83 | 348 | 77STE/GOL | 189-64-0 |
|  | (7.11)<br>IP from 79CLA/SCH. | (245) | (1025) | 81 | 339 | *EST | |
|  | (7.07)<br>IP from 79CLA/SCH. | (245) | (1026) | 82 | 344 | *EST | |

Table 1. Positive Ion Table - Continued

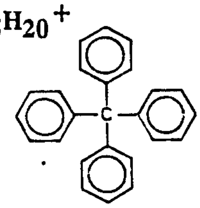
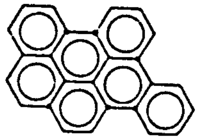
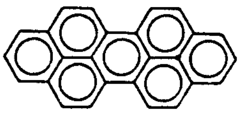
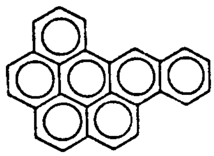
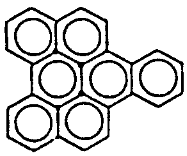
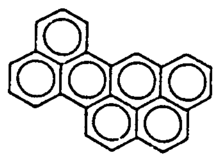
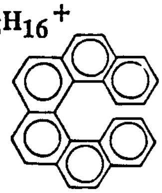
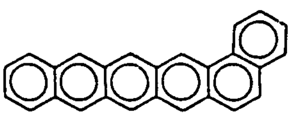
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{25}H_{20}^+$ | | | | | | | |
|  | (8.0) | (280) | (1170) | 95±1 | 398±4 | 77PED/RYL | 630-76-2 |
| | IP is onset of photoelectron band (84NOV/POT). | | | | | | |
| $C_{26}H_{14}^+$ | | | | | | | |
|  | (7.12) | (248) | (1038) | 84 | 351 | *EST | 190-95-4 |
|  | 6.72±0.02 | (241) | (1008) | 86 | 360 | *EST | 188-96-5 |
|  | (6.99) | (247) | (1034) | 86 | 360 | *EST | 5869-30-7 |
|  | (6.96) | (244) | (1022) | 84 | 351 | *EST | 190-84-1 |
|  | (6.82±0.04) | (243) | (1018) | 86 | 360 | *EST | 188-89-6 |
| $C_{26}H_{16}^+$ | | | | | | | |
|  | (7.37) | (290) | (1213) | 120 | 502 | *EST | 187-83-7 |
|  | (6.61±0.02) | (251) | (1050) | 99 | 413 | *EST | 239-98-5 |

**Table 1. Positive Ion Table - Continued**

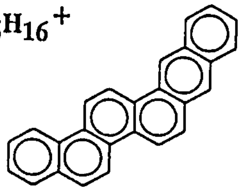
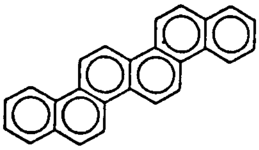
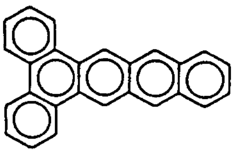
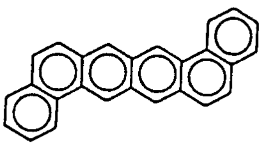
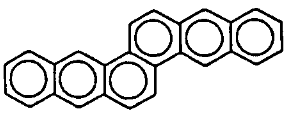
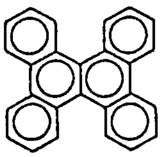
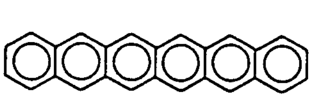
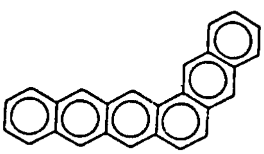
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{26}H_{16}{}^{+}$ | | | | | | | |
|  | 7.17±0.02 | (267) | (1117) | 102 | 425 | *EST | 217-42-5 |
|  | (7.36) | (262) | (1095) | 92 | 385 | *EST | 217-37-8 |
|  | 6.97±0.02<br>See also: 75CLA/SCH, 79CLA/SCH. | (255) | (1067) | 94 | 394 | *EST | 216-00-2 |
|  | (6.99±0.02)<br>See also: 75CLA/SCH. | (258) | (1078) | 96 | 403 | *EST | 227-04-3 |
|  | (6.97±0.04) | (257) | (1076) | 96 | 403 | *EST | 217-54-9 |
|  | 7.20±0.02<br>See also: 75CLA/SCH, 79CLA/SCH. | (256) | (1072) | 90 | 377 | *EST | 191-68-4 |
|  | (6.36±0.02)<br>See also: 75CLA/SCH. | (247) | (1035) | 101 | 422 | *EST | 258-31-1 |
|  | (6.92±0.02) | (258) | (1080) | 99 | 413 | *EST | 222-78-6 |

Table 1. Positive Ion Table - Continued

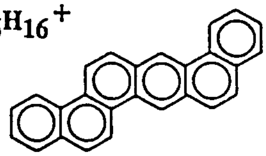
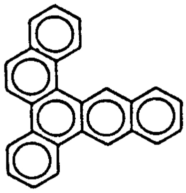
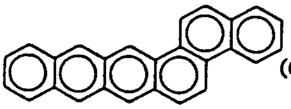
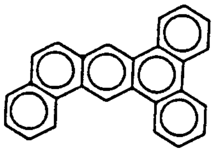
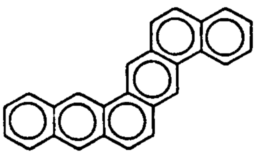
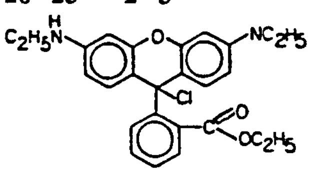
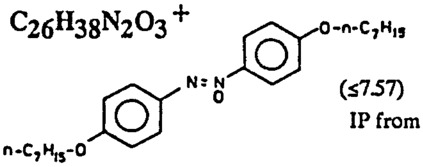
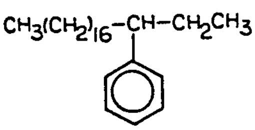
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{26}H_{16}^+$ | | | | | | | |
|  | (7.19±0.02) | (253) | (1057) | 87 | 363 | *EST | 220-77-9 |
|  | 7.15±0.02 | (258) | (1080) | 93 | 390 | *EST | 196-64-5 |
|  | (6.83±0.02) | (254) | (1062) | 96 | 403 | *EST | 220-82-6 |
|  | 7.40±0.02<br>See also: 75CLA/SCH. | (263) | (1099) | 92 | 385 | *EST | 215-26-9 |
|  | (7.20±0.02) | (262) | (1098) | 96 | 403 | *EST | 222-54-8 |
| $C_{26}H_{25}ClN_2O_3^+$ | Name in CA are Rhodamine 6G = CASN formula + struct ≠ R6G | | | | | | |
|  | (6.94±0.05)<br>IP from 81TIM/KOR. | (115) | (483) | −45 | −187 | *EST | 989-38-8 |
| $C_{26}H_{38}N_2O_3^+$ | | | | | | | |
|  | (≤7.57)<br>IP from 81MIL/CIL. | (≤127) | (≤530) | −48 | −200 | *EST | 2635-26-9 |
| $C_{26}H_{46}^+$ | | | | | | | |
|  | (8.95±0.10) | (123) | (516) | −83±1.2 | −348±5 | 77PED/RYL | 72557-70-1 |

Table 1. Positive Ion Table - Continued

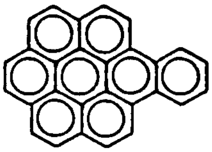
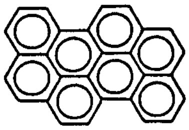
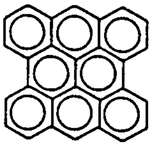
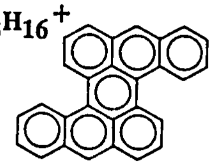
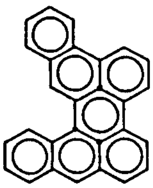
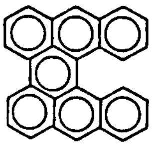
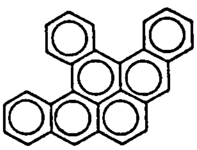
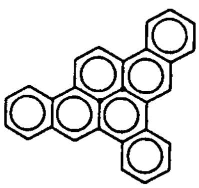
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{28}H_{14}{}^+$ | | | | | | | |
|  | (7.08) | (248) | (1037) | 84 | 353 | *EST | 190-70-5 |
|  | (6.92±0.04) | (249) | (1040) | 89 | 372 | *EST | 190-71-6 |
|  | (6.30) | (234) | (980) | 89 | 372 | *EST | 190-39-6 |
| $C_{28}H_{16}{}^+$ | | | | | | | |
|  | (6.51) | (252) | (1055) | 102 | 426 | *EST | 191-87-7 |
|  | (6.64) | (247) | (1033) | 94 | 392 | *EST | 191-81-1 |
|  | (6.51) | (247) | (1035) | 97 | 406 | *EST | 190-36-3 |
|  | (6.96)<br>IP from 79CLA/SCH. | (262) | (1098) | 102 | 426 | *EST | 191-20-8 |
|  | (6.99)<br>IP from 79CLA/SCH. | (256) | (1072) | 95 | 397 | *EST | 192-47-2 |

**Table 1. Positive Ion Table - Continued**

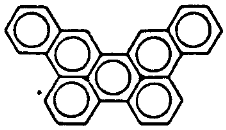
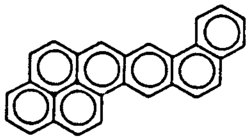
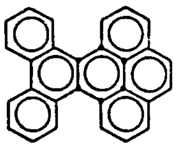
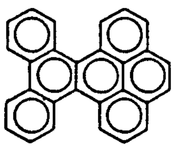
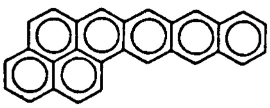
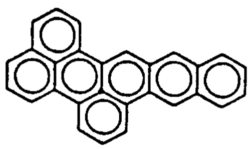
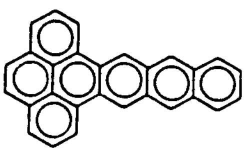
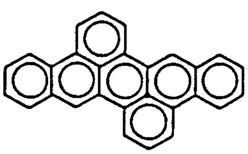
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{28}H_{16}{}^+$ | | | | | | | |
|  | (6.85) | (253) | (1058) | 95 | 397 | *EST | 197-69-3 |
|  | (6.83)<br>IP from 79CLA/SCH. | (257) | (1075) | 99 | 416 | *EST | |
|  | (7.00)<br>IP from 79CLA/SCH. | (252) | (1055) | 91 | 380 | *EST | |
|  | (7.00±0.04) | (250) | (1044) | 88 | 369 | *EST | 385-14-8 |
|  | (6.57)<br>IP from 79CLA/SCH. | (253) | (1059) | 102 | 425 | *EST | 196-45-2 |
|  | (6.82) | (254) | (1064) | 97 | 406 | *EST | 14147-38-7 |
|  | (6.95)<br>IP from 79CLA/SCH. | (260) | (1086) | 99 | 416 | *EST | 193-11-3 |
|  | (6.86) | (253) | (1059) | 95 | 397 | *EST | 197-74-0 |

**Table 1. Positive Ion Table - Continued**

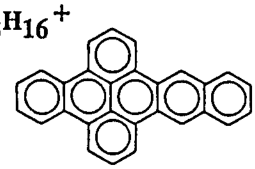
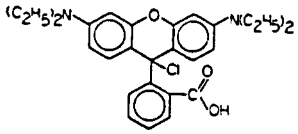
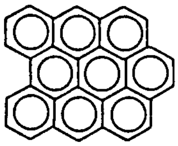
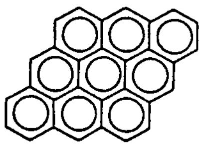
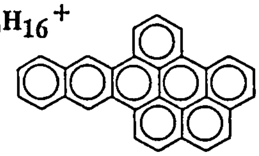
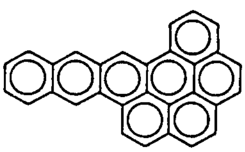
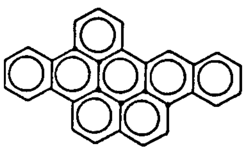
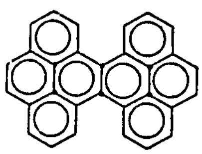
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{28}H_{16}^+$ | | | | | | | |
|  | (7.33±0.04)<br>See also: 79CLA/SCH. | (264) | (1104) | 95 | 397 | *EST | 192-59-6 |
| $C_{28}H_{32}ClN_2O_3^+$ | | | | | | | |
|  | (6.70±0.05)<br>IP from 81TIM/KOR. | (109) | (455) | −46 | −191 | *EST | |
| $C_{30}H_{14}^+$ | | | | | | | |
|  | (6.50) | (244) | (1021) | 94 | 394 | *EST | 190-31-8 |
|  | (6.42±0.02) | (244) | (1022) | 96 | 403 | *EST | 190-55-6 |
| $C_{30}H_{16}^+$ | | | | | | | |
|  | (7.04) | (269) | (1125) | 107 | 446 | *EST | 14258-76-5 |
|  | (6.78) | (265) | (1110) | 109 | 455 | *EST | 5869-31-8 |
|  | (6.97) | (254) | (1063) | 93 | 391 | *EST | 190-87-4 |
|  | (6.90±0.04) | (259) | (1086) | 100 | 420 | *EST | 385-13-7 |

**Table 1. Positive Ion Table - Continued**

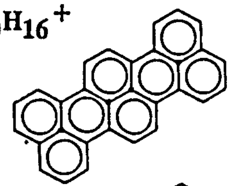
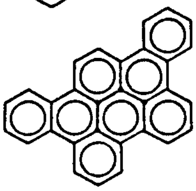
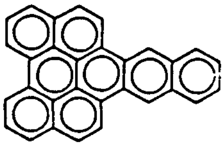
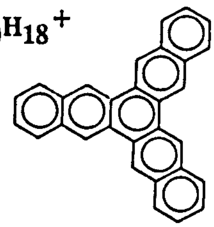
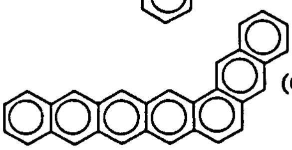
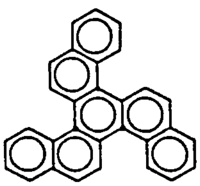
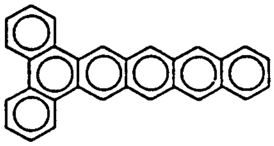
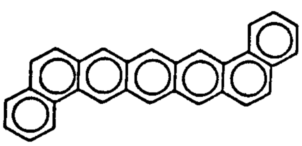
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{30}H_{16}^+$ | | | | | | | |
|  | (6.42±0.02) | (246) | (1029) | 98 | 409 | *EST | 188-72-7 |
|  | (7.13) | (260) | (1088) | 96 | 400 | *EST | 190-81-8 |
|  | (6.77) | (256) | (1072) | 100 | 419 | *EST | 190-85-2 |
| $C_{30}H_{18}^+$ | | | | | | | |
|  | (7.35±0.02) | (280) | (1171) | 110 | 462 | *EST | 196-62-3 |
|  | (6.59±0.02) | (280) | (1172) | 128 | 536 | *EST | 222-81-1 |
|  | (7.19±0.02) | (273) | (1144) | 108 | 450 | *EST | 27798-46-5 |
|  | 6.62±0.02<br>See also: 75CLA/SCH. | (263) | (1101) | 110 | 462 | *EST | 216-08-0 |
|  | (6.64±0.02) | (264) | (1103) | 110 | 462 | *EST | 227-09-8 |

**Table 1. Positive Ion Table - Continued**

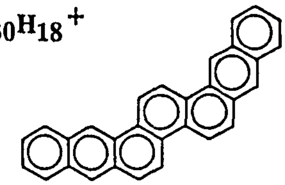
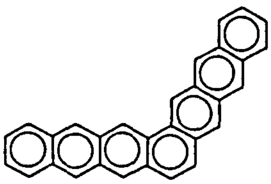
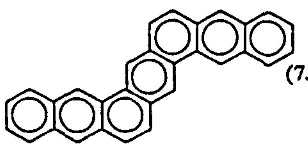
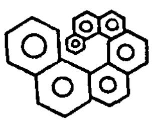
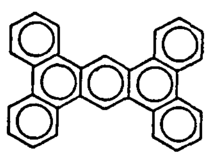
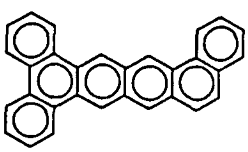
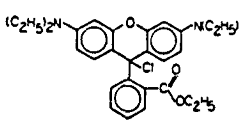
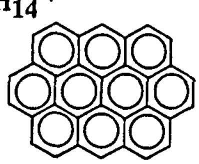
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{30}H_{18}^+$ | | | | | | | |
|  | (7.17±0.02) | (276) | (1154) | 110 | 462 | *EST | 213-44-5 |
|  | (6.89±0.02) | (274) | (1145) | 115 | 480 | *EST | 222-75-3 |
|  | (7.04±0.02) | (275) | (1150) | 113 | 472 | *EST | 222-58-2 |
|  | (7.25) | (314) | (1315) | 147 | 616 | *EST | 16914-68-4 |
|  | 7.43±0.02<br>See also: 75CLA/SCH. | (275) | (1151) | 104 | 434 | *EST | 215-11-2 |
|  | (6.99±0.02)<br>See also: 75CLA/SCH. | (269) | (1127) | 108 | 453 | *EST | 215-96-3 |
| $C_{30}H_{36}ClN_2O_3^+$ | | | | | | | |
|  | (6.58±0.05)<br>IP from 81TIM/KOR. | (99) | (416) | −52 | −219 | *EST | |
| $C_{32}H_{14}^+$ | | | | | | | |
|  | 6.71<br>See also: 81CLA/ROB. | 254 | 1062 | 99 | 415 | 77STE/GOL | 190-26-1 |

Table 1. Positive Ion Table - Continued

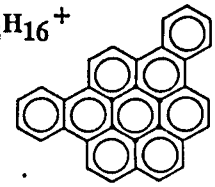
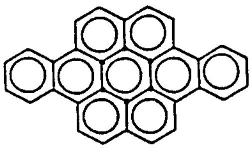
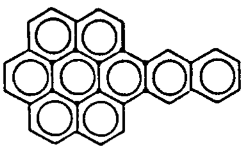
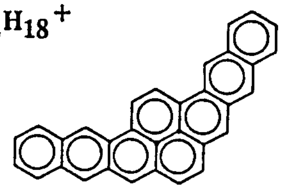
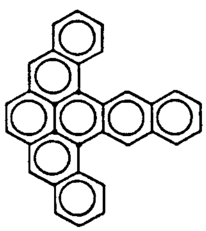
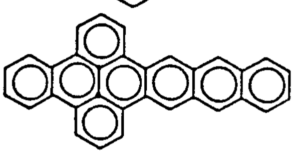
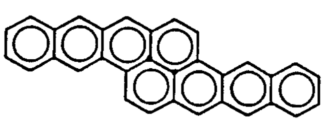
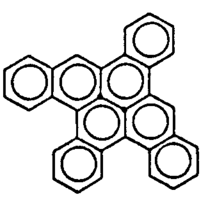
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{32}H_{16}^+$ | | | | | | | |
|  | (7.04) | (263) | (1101) | 101 | 422 | *EST | 190-66-9 |
|  | (6.92) | (260) | (1089) | 101 | 422 | *EST | 190-72-7 |
|  | (6.88) | (264) | (1104) | 105 | 440 | *EST | 190-74-9 |
| $C_{32}H_{18}^+$ | | | | | | | |
|  | (6.65)<br>IP from 79CLA/SCH. | (269) | (1125) | 115 | 483 | *EST | 189-43-5 |
|  | (6.94)<br>IP from 79CLA/SCH. | (274) | (1145) | 114 | 475 | *EST | |
|  | (6.91)<br>IP from 79CLA/SCH. | (270) | (1132) | 111 | 465 | *EST | 192-60-9 |
|  | (6.42)<br>IP from 79CLA/SCH. | (264) | (1103) | 115 | 483 | *EST | |
|  | (7.02)<br>IP from 79CLA/SCH. | (276) | (1153) | 114 | 476 | *EST | |

**Table 1. Positive Ion Table - Continued**

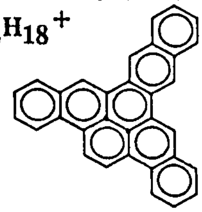
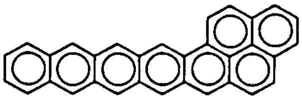
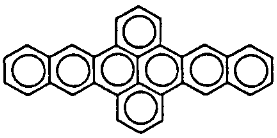
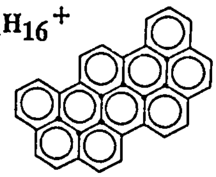
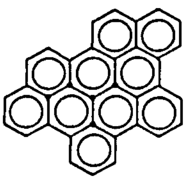
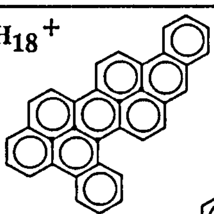
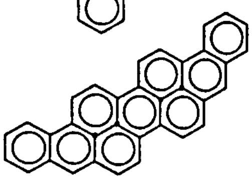
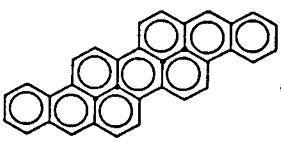
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{32}H_{18}^+$ | | | | | | | |
|  | (6.99)<br>IP from 79CLA/SCH. | (277) | (1153) | 116 | 485 | *EST | |
|  | (6.36)<br>IP from 79CLA/SCH. | (264) | (1107) | 118 | 493 | *EST | 196-46-3 |
|  | (7.30±0.04) | (279) | (1169) | 111 | 465 | *EST | 192-54-1 |
| $C_{34}H_{16}^+$ | | | | | | | |
|  | (6.74±0.02) | (261) | (1093) | 106 | 443 | *EST | 188-11-4 |
|  | 6.82±0.02 | (261) | (1092) | 104 | 434 | *EST | 187-94-0 |
| $C_{34}H_{18}^+$ | | | | | | | |
|  | (6.59±0.02) | (265) | (1109) | 113 | 473 | *EST | |
|  | (6.48±0.02) | (263) | (1102) | 114 | 477 | *EST | |
|  | (6.42±0.02) | (262) | (1097) | 114 | 477 | *EST | 190-93-2 |

Table 1. Positive Ion Table - Continued

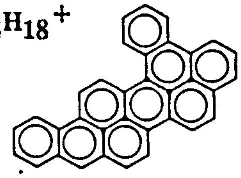
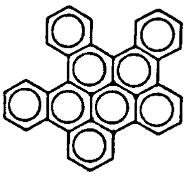
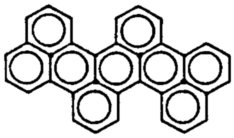
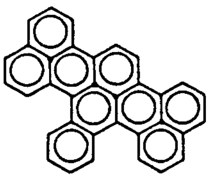
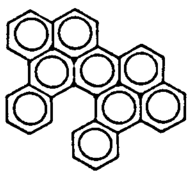
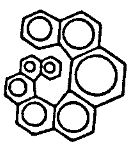
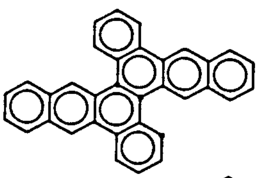
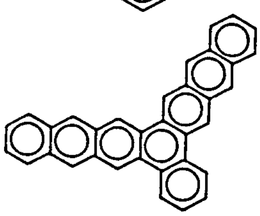
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{34}H_{18}^+$ | | | | | | | |
|  | (6.59±0.02) | (265) | (1109) | 113 | 473 | *EST | 191-46-8 |
|  | (6.84) | (267) | (1119) | 110 | 459 | *EST | 313-63-3 |
|  | (6.27±0.02) | (256) | (1073) | 112 | 468 | *EST | 191-79-7 |
|  | (6.22±0.02) | (260) | (1088) | 117 | 488 | *EST | 188-13-6 |
|  | 6.58 | (276) | (1155) | 124 | 520 | *EST | 191-53-7 |
| $C_{34}H_{20}^+$ | | | | | | | |
|  | (7.15) | (327) | (1370) | 162 | 680 | *EST | 20495-12-9 |
|  | (6.83±0.02) | (280) | (1172) | 123 | 513 | *EST | 385-15-9 |
|  | (6.90±0.02) | (286) | (1196) | 127 | 530 | *EST | 214-87-9 |

Table 1. Positive Ion Table - Continued

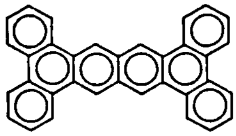
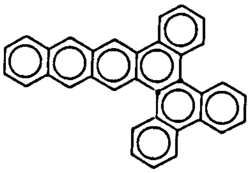
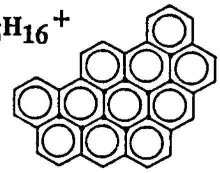
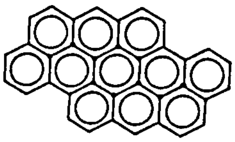
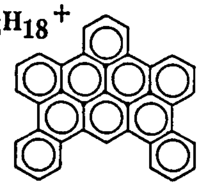
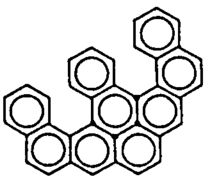
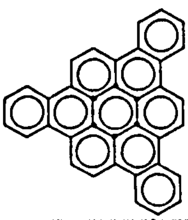
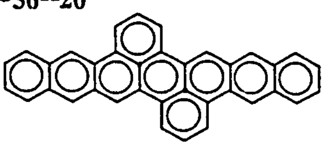
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{34}H_{20}^+$ | | | | | | | |
|  | (7.00±0.02) | (281) | (1177) | 120 | 502 | *EST | 215-95-2 |
|  | (6.73±0.02) | (278) | (1162) | 122 | 513 | *EST | 385-16-0 |
| $C_{36}H_{16}^+$ | | | | | | | |
|  | (6.76±0.02) | (267) | (1117) | 111 | 464 | *EST | 53086-28-5 |
|  | (6.70±0.04) | (265) | (1111) | 111 | 464 | *EST | 190-47-6 |
| $C_{36}H_{18}^+$ | | | | | | | |
|  | (≤7.10) | (≤284) | (≤1187) | 120 | 502 | *EST | 188-00-1 |
|  | (6.88)<br>IP from 79CLA/SCH. | (306) | (1282) | 148 | 618 | *EST | |
|  | (6.88) | (271) | (1135) | 113 | 471 | *EST | 313-62-2 |
| $C_{36}H_{20}^+$ | | | | | | | |
|  | (6.68) | (284) | (1190) | 130 | 545 | *EST | 197-73-9 |

**Table 1. Positive Ion Table - Continued**

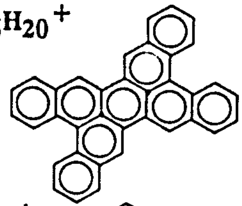
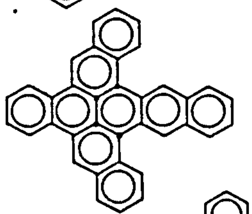
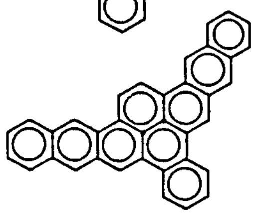
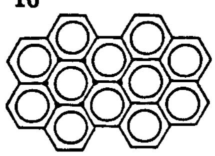
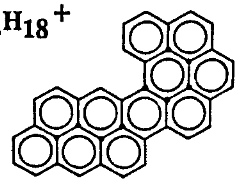
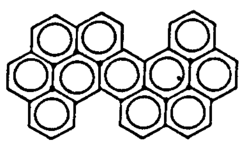
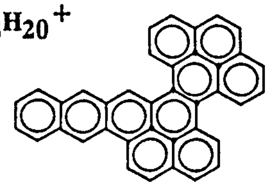
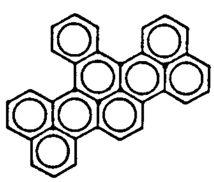
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{36}H_{20}^+$ | | | | | | | |
|  | (6.82) | (287) | (1202) | 130 | 544 | *EST | 36474-85-8 |
|  | (6.95)<br>IP from 79CLA/SCH. | (286) | (1195) | 125 | 525 | *EST | |
|  | (6.74)<br>IP from 79CLA/SCH. | (283) | (1183) | 127 | 533 | *EST | |
| $C_{38}H_{16}^+$ | | | | | | | |
|  | (6.81±0.02) | (271) | (1134) | 114 | 477 | *EST | 41163-25-1 |
| $C_{38}H_{18}^+$ | | | | | | | |
|  | (6.38±0.02) | (270) | (1132) | 123 | 516 | *EST | 190-90-9 |
|  | (6.50±0.02) | (277) | (1158) | 127 | 531 | *EST | 190-89-6 |
| $C_{38}H_{20}^+$ | | | | | | | |
|  | (6.58)<br>IP from 79CLA/SCH. | (282) | (1181) | 130 | 546 | *EST | |
|  | (6.06±0.02) | (266) | (1112) | 126 | 528 | *EST | 187-96-2 |

**Table 1. Positive Ion Table - Continued**

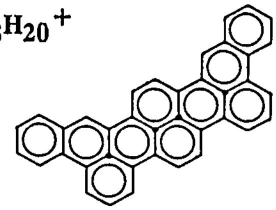
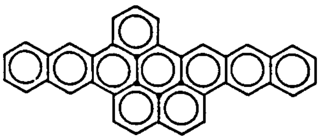
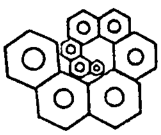
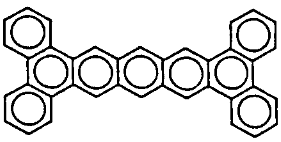
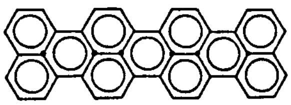
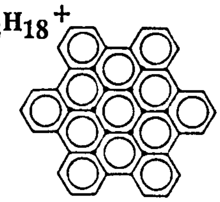
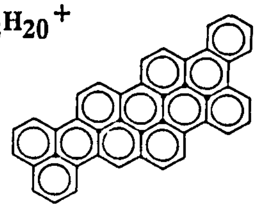
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{38}H_{20}^+$ | | | | | | | |
|  | (6.40±0.02) | (273) | (1144) | 126 | 527 | *EST | 34814-77-2 |
|  | (6.72) | (285) | (1193) | 130 | 545 | *EST | 14529-73-8 |
| $C_{38}H_{22}^+$ | | | | | | | |
|  | (7.07) | (365) | (1527) | 202 | 844 | *EST | 20495-14-1 |
|  | 6.65±0.02<br>See also: 75CLA/SCH. | (290) | (1212) | 136 | 570 | *EST | 216-07-9 |
| $C_{40}H_{20}^+$ | | | | | | | |
|  | (6.11±0.02) | (270) | (1128) | 129 | 539 | *EST | 188-73-8 |
| $C_{42}H_{18}^+$ | | | | | | | |
|  | 6.87±0.02 | (280) | (1170) | 121 | 508 | *EST | 190-24-9 |
| $C_{42}H_{20}^+$ | | | | | | | |
|  | (6.72±0.02) | (287) | (1199) | 132 | 551 | *EST | 34814-80-7 |

**Table 1. Positive Ion Table - Continued**

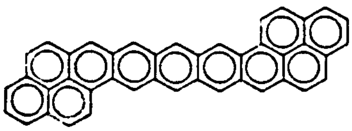
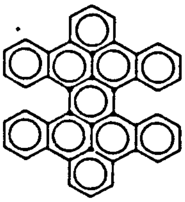
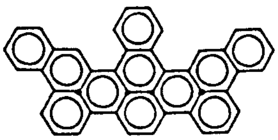
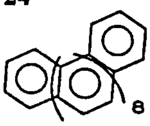
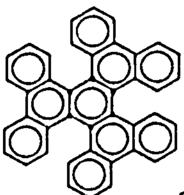
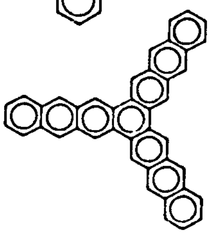
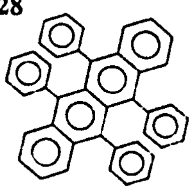
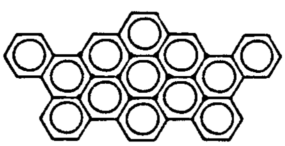
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{42}H_{22}^+$ | | | | | | | |
|  | (6.22)<br>IP from 79CLA/SCH. | (294) | (1231) | 151 | 631 | *EST | 190-09-0 |
|  | (6.71±0.02) | (283) | (1186) | 129 | 538 | *EST | 190-22-7 |
|  | (6.18±0.02) | (282) | (1181) | 140 | 585 | *EST | 34814-82-9 |
| $C_{42}H_{24}^+$ | | | | | | | |
|  | (6.99) | (390) | (1633) | 229 | 959 | *EST | 57520-29-3 |
|  | (7.52±0.02) | (356) | (1491) | 183 | 765 | *EST | 190-23-8 |
|  | (6.85±0.02) | (317) | (1326) | 159 | 665 | *EST | 214-77-7 |
| $C_{42}H_{28}^+$ | | | | | | | |
|  | 6.41<br>IP from 81SAT/SEK. | 334 | 1399 | 187±5 | 781±22 | 77PED/RYL | 517-51-1 |
| $C_{44}H_{20}^+$ | | | | | | | |
|  | (6.79±0.02) | (287) | (1199) | 130 | 544 | *EST | 70346-75-7 |

**Table 1. Positive Ion Table - Continued**

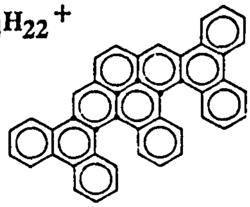
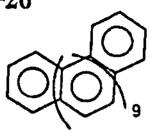
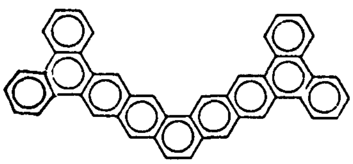
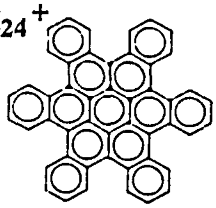
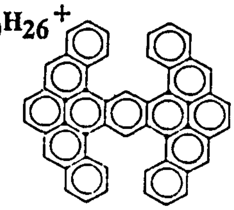
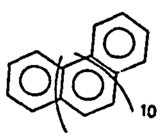
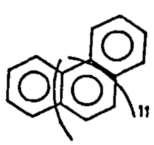
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $C_{44}H_{22}^+$ | | | | | | | |
|  | (6.80)<br>IP from 79CLA/SCH. | (333) | (1394) | 176 | 738 | *EST | |
| $C_{46}H_{26}^+$ | | | | | | | |
|  | (6.95) | (417) | (1744) | 256 | 1073 | *EST | 57468-45-8 |
|  | (6.88±0.02) | (325) | (1360) | 166 | 696 | *EST | 62662-49-1 |
| $C_{48}H_{24}^+$ | | | | | | | |
|  | (6.75) | (297) | (1242) | 141 | 590 | *EST | 1065-80-1 |
| $C_{50}H_{26}^+$ | | | | | | | |
|  | (6.70)<br>IP from 79CLA/SCH. | (329) | (1379) | 175 | 732 | *EST | 72382-92-4 |
| $C_{50}H_{28}^+$ | | | | | | | |
|  | (6.93) | (444) | (1856) | 284 | 1187 | *EST | 57468-46-9 |
| $C_{54}H_{30}^+$ | | | | | | | |
|  | (6.91) | (470) | (1968) | 311 | 1302 | *EST | 24386-06-9 |

**Table 1. Positive Ion Table - Continued**

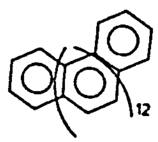
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $C_{58}H_{32}^+$ | | | | | | | |
|  | (6.88) | (497) | (2080) | 338 | 1416 | *EST | 57483-71-3 |
| $Ca^+$ | | | | | | | |
| Ca | 6.11321±0.00002 | 183.6 | 768.0 | 42.6 | 178.2 | 82TN270 | 7440-70-2 |
| | | *183.5* | *767.5* | *42.5* | *177.7* | | |
| $CaCl^+$ | | | | | | | |
| CaCl | 5.61±0.13 | 106 | 443 | −24.7±1.2 | −103.4±5.0 | 87GAR/PAR | 15606-71-0 |
| | | *106* | *444* | *−24.5±1.2* | *−102.7±5.0* | | |
| | IP and $\Delta_f H$(Ion) derived from onset of endothermic reaction (84MEY/SCH). | | | | | | |
| $CaCl_2^+$ | | | | | | | |
| $CaCl_2$ | (≤10.0) | (≤118) | (≤494) | −113 | −471 | 82TN270 | 10043-52-4 |
| | | *(≤118)* | *(≤493)* | *−113* | *−472* | | |
| | See also: 82EMO/KIE, 79LEE/POT2. | | | | | | |
| $CaH^+$ | | | | | | | |
| CaH | (5.86±0.09) | (190) | (794) | 55 | 229 | 82TN270 | 14452-75-6 |
| | | *(190)* | *(795)* | *55* | *230* | | |
| | Value for $\Delta_f H$(Ion) derived from onset energy of endothermic reaction is in good agreement (86ELK/ARI). | | | | | | |
| $CaHO^+$ | | | | | | | |
| CaOH | 5.7 | *(89)* | *(371)* | *−42.0* | *−175.7* | 87GAR/PAR | 12177-67-2 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (83MUR). See also: 81MUR. 0 K values. | | | | | | |
| $CaI^+$ | | | | | | | |
| CaI | (6.1±0.3) | (139) | (584) | −1±21 | −5±84 | 79HUB/HER | 15923-87-2 |
| | | *(137)* | *(572)* | *−4* | *−17* | | |
| $CaI_2^+$ | | | | | | | |
| $CaI_2$ | (8.7) | (139) | (581) | −62±4 | −258±17 | 85JANAF | 10102-68-8 |
| | | *(140)* | *(584)* | *−61±4* | *−255±17* | | |
| | IP is onset of photoelectron band (79LEE/POT2). See also: 82EMO/KIE. | | | | | | |
| $CaO^+$ | | | | | | | |
| CaO | (6.9) | (166) | (693) | (6±4) | (27±17) | 83PED/MAR | 1305-78-8 |
| | IP from 83MUR. | | | | | | |
| $CaO_4W^+$ | | | | | | | |
| $CaWO_4$ | (9.8) | (0) | (0) | −226 | −946 | 76DEL/HAL | |
| $Cd^+$ | | | | | | | |
| Cd | 8.993 | 234.2 | 979.7 | 26.8 | 112.0 | 82TN270 | 7440-43-9 |
| | | *234.2* | *979.8* | *26.8* | *112.1* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Ce^+$ | | | | | | | |
| Ce | 5.5387±0.0004 | 229 | 957 | 101 | 423 | 82TN270 | 7440-45-1 |
| | | *229* | *957* | *101.1* | *423.4* | | |
| $CeI_3^+$ | | | | | | | |
| $CeI_3$ | 8.7 | 101 | 422 | −100 | −417 | 82TN270 | |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| $CeO^+$ | | | | | | | |
| CeO | (4.90±0.1) | (81) | (339) | −32±3 | −134±12 | 83PED/MAR | 12014-74-3 |
| | | *(81)* | *(341)* | *−32* | *−132* | | |
| $CeS^+$ | | | | | | | |
| CeS | (6.0±0.6) | (170) | (710) | 31 | 131 | 82TN270 | 12014-82-3 |
| | | *(170)* | *(713)* | *32* | *134* | | |
| $Ce_2^+$ | | | | | | | |
| $Ce_2$ | (5.6±0.4) | (273) | (1142) | 144 | 602 | 82TN270 | 12595-88-9 |
| | | *(274)* | *(1147)* | *145* | *607* | | |
| $Cf^+$ | | | | | | | |
| Cf | 6.3 | 192 | 804 | 47 | 196 | 85KLE/WAR | 7440-71-3 |
| | See: 81CHE/GAB. | | | | | | |
| $Cl^+$ | | | | | | | |
| Cl | 12.967 | 328 | 1372 | 29.0 | 121.3 | 85JANAF | 22537-15-1 |
| | | *328* | *1371* | *28.6* | *119.6* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $ClCs^+$ | | | | | | | |
| CsCl | (7.84±0.05) | (122) | (510) | −59 | −247 | 84PAR/WEX | 7647-17-8 |
| | | *(122)* | *(512)* | *−58.4±1.8* | *−244.4±7.5* | | |
| | A value of 8.32±0.1 eV has also been reported for the ionization potential. | | | | | | |
| $ClCsNa^+$ | | | | | | | |
| NaCsCl | 3.9±0.1 | *(21)* | *(88)* | *−69* | *−288* | *EST | 95860-64-3 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| $ClCs_2^+$ | | | | | | | |
| $Cs_2Cl$ | 3.4±0.2 | *−1* | *−4* | *−79±6* | *−332±25* | 85KAP/RAD | 87331-16-6 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| $ClCu^+$ | | | | | | | |
| CuCl | (10.7±0.3) | *(265)* | *(1110)* | *19* | *78* | 79HUB/HER | 7758-89-6 |
| | 0 K values. | | | | | | |
| $ClF^+$ | | | | | | | |
| ClF | 12.65±0.01 | 280 | 1170 | −12.0±0.1 | −50.3±0.4 | 85JANAF | 7790-89-8 |
| | | *280* | *1170* | *−12.0±0.1* | *−50.2±0.4* | | |
| | See also: 84DYK/JOS. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $ClFO_2^+$ | | | | | | | |
| $ClO_2F$ | (12.41±0.10) | (278) | (1164) | −8 | −33 | 73BAR | 13637-83-7 |
| | IP from 80BAL/NIK. | | | | | | |
| $ClFO_2S^+$ | | | | | | | |
| $SO_2FCl$ | (12.4) | (151) | (632) | −135 | −564 | 81WOO | 13637-84-8 |
| • | IP is onset of photoelectron band. | | | | | | |
| $ClFO_3^+$ | | | | | | | |
| $ClO_3F$ | (12.945±0.005) | (293) | (1225) | −6 | −24 | 82TN270 | 7616-94-6 |
| | | *(295)* | *(1234)* | *−4* | *−15* | | |
| $ClF_2^+$ | | | | | | | |
| $ClF_2$ | (12.77±0.05) | (269) | (1127) | −25 | −105 | 62ARM/KRI | 24801-48-7 |
| | $\Delta_f H$(Ion) derived from appearance potential (13.78±0.07 eV) in $ClF_3$ is 261 kcal/mol, 1091 kJ/mol. | | | | | | |
| $ClF_3^+$ | | | | | | | |
| $ClF_3$ | (12.65±0.05) | (253) | (1057) | −39 | −163 | 82BAU/COX | 7790-91-2 |
| | | *(254)* | *(1061)* | *−38* | *−159* | | |
| $ClF_5S^+$ | | | | | | | |
| $SF_5Cl$ | (12.335±0.005) | (34) | (142) | −250 | −1048 | 82TN270 | 13780-57-9 |
| | | *(37)* | *(155)* | *−247* | *−1035* | | |
| $ClH^+$ | | | | | | | |
| HCl | 12.747 | 271.9 | 1137.6 | −22.1±0.04 | −92.3±0.2 | 85JANAF | 7647-01-0 |
| | | *271.4* | *1137.7* | *−22.0±0.04* | *−92.1±0.2* | | |
| | IP for formation of $HCl^+$ ($^2\Pi_{3/2}$) from 79HUB/HER, 82NAT/PEN, 77ROS/DRA, 82LEV/LIA. IP for formation of $HCl^+$ ($^2\Pi_{1/2}$) = 12.828 eV. See also: 82VON/ASB, 84WAN/DIL, 81KIM/KAT. | | | | | | |
| $ClD^+$ | | | | | | | |
| DCl | 12.754 | 271.8 | 1137.3 | −22.3±0.05 | −93.3±0.2 | 85JANAF | 7698-05-7 |
| | | *271.9* | *1137.6* | *−22.3±0.05* | *−93.1±0.2* | | |
| | IP for formation of DCl($^2\Pi_{3/2}$) from 79HUB/HER, 83PEN/NAT. | | | | | | |
| $ClHO^+$ | | | | | | | |
| HOCl | (11.12±0.01) | (238) | (995) | −19 | −78 | 82BAU/COX | 7790-92-3 |
| | | *(239)* | *(998)* | *−18* | *−75* | | |
| $ClH_2^+$ | | | | | | | |
| $H_2Cl$ | | 207 | 867 | | | | |
| | From proton affinity of HCl (RN 7647-01-0) (85MCM/KEB) re-evaluated relative to CO standard (84LIA/LIE). PA = 128.6 kcal/mol, 538 kJ/mol. | | | | | | |
| $ClH_2N^+$ | | | | | | | |
| $NH_2Cl$ | (9.85±0.02) | (240) | (1003) | 13 | 53 | *EST | 10599-90-3 |
| $ClH_3Si^+$ | | | | | | | |
| $SiH_3Cl$ | 11.4 | (215) | (899) | −48 | −201 | 81BEL/PER | 13465-78-6 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$ClI^+$** | | | | | | | |
| ICl | 10.088±0.01 | 236.8 | 990.8 | 4.2±0.02 | 17.5±0.1 | 85JANAF | 7790-99-0 |
| | | *237.2* | *992.4* | *4.6±0.2* | *19.1±0.1* | | |
| | See also: 84DYK/JOS, 71POT/PRI. | | | | | | |
| **$ClIn^+$** | | | | | | | |
| ClIn | (9.51) | (201) | (843) | −18 | −75 | 82TN270 | 13465-10-6 |
| | | *(204)* | *(852)* | *−15* | *−65* | | |
| **$ClK^+$** | | | | | | | |
| KCl | (8.0±0.4) | (133) | (557) | −51.3±0.1 | −214.7±0.4 | 85JANAF | 7447-40-7 |
| | | *(134)* | *(559)* | *−50.9±0.1* | *−212.9±0.4* | | |
| **$ClKNa^+$** | | | | | | | |
| NaKCl | 4.0±0.1 | *(26)* | *(107)* | *−67* | *−279* | *EST | 95860-66-5 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| **$ClK_2^+$** | | | | | | | |
| $K_2Cl$ | 3.5±0.2 | *10* | *44* | *−70±4* | *−294±17* | 85KAP/RAD | 95386-61-1 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| **$ClLi^+$** | | | | | | | |
| LiCl | 9.57 | 174 | 728 | −47±3 | −196±13 | 85JANAF | 7447-41-8 |
| | | *174* | *728* | *−47±3* | *−196±13* | | |
| **$ClNO^+$** | | | | | | | |
| NOCl | 10.87±0.01 | 263 | 1101 | 12 | 52 | 82BAU/COX | 2696-92-6 |
| | | *264* | *1103* | *13* | *54* | | |
| | See also: 83BIN. | | | | | | |
| **$ClNO_2^+$** | | | | | | | |
| $ClNO_2$ | (11.84) | (276) | (1155) | 3 | 13 | 82BAU/COX | 13444-90-1 |
| | | *(277)* | *(1160)* | *4* | *18* | | |
| **$ClN_3^+$** | | | | | | | |
| $ClN_3$ | (10.20±0.01) | (313.9) | (1313.4) | 78.7 | 329.3 | 83DEW/RZE | 13973-88-1 |
| **$ClNa^+$** | | | | | | | |
| NaCl | 8.92±0.06 | 162 | 679 | −43±0.5 | −181±2 | 85JANAF | 7647-14-5 |
| | | *163* | *681* | *−43±0.5* | *−180±2* | | |
| **$ClNa_2^+$** | | | | | | | |
| $Na_2Cl$ | 4.1±0.1 | *36* | *152* | *−58±4* | *−244±17* | 85KAP/RAD | 84008-89-9 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| **$ClNi^+$** | | | | | | | |
| NiCl | (11.4±0.5) | (306) | (1282) | 43±1 | 182±4 | 85JANAF | 13931-83-4 |
| | | *(306)* | *(1282)* | *43±1* | *182±4* | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $ClO^+$ | | | | | | | |
| ClO | 10.95 | 277 | 1158 | 24.4 | 101.9 | 82BAU/COX | 14989-30-1 |
| | | *277* | *1158* | *24.3* | *101.8* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $ClOP^+$ | | | | | | | |
| POCl | (11.5) | (205) | (859) | −60 | −251 | 83BIN/LAK | 21295-50-1 |
| | IP from 83BIN. | | | | | | |
| $ClOSb^+$ | | | | | | | |
| SbOCl | (10.7) | (247) | (1032) | 0 | 0 | 83BIN | 7791-08-4 |
| | IP from 83BIN. | | | | | | |
| $ClO_2^+$ | | | | | | | |
| OClO | 10.36±0.02 | 262 | 1097 | 23±2 | 97±8 | 82BAU/COX | 10049-04-4 |
| | | *263* | *1099* | *24* | *99* | | |
| | See also: 80BAL/NIK. | | | | | | |
| $ClRb^+$ | | | | | | | |
| RbCl | (8.50±0.03) | (141) | (591) | −55 | −229 | 82TN270 | 7791-11-9 |
| | | *(142)* | *(593)* | *−54* | *−227* | | |
| $ClSr^+$ | | | | | | | |
| SrCl | 5.10±0.06 | (88) | (368) | −30±2 | −124±8 | 85JANAF | 14989-33-4 |
| | | *(88)* | *(370)* | *−29±2* | *−122±8* | | |
| | See also: 84MEY/SCH. | | | | | | |
| $ClTl^+$ | | | | | | | |
| TlCl | 9.70±0.03 | 207 | 868 | −16 | −68 | 82TN270 | 7791-12-0 |
| | | *207* | *868* | *−16* | *−68* | | |
| | See also: 83BAN/BRI. | | | | | | |
| $Cl_2^+$ | | | | | | | |
| $Cl_2$ | 11.480±0.005 | 265 | 1108 | 0 | 0 | *DEF | 7782-50-5 |
| | | *265* | *1108* | *0* | *0* | | |
| | Cited ionization potential is for formation of $Cl_2^+(^2\Pi_{3/2})$ (77ROS/DRA, 82LEV/LIA, 84VAN/DEL2, 84DYK/JOS)). Formation of $Cl_2^+(^2\Pi_{1/2})$ requires 11.56 eV. See also: 81KIM/KAT. | | | | | | |
| $Cl_2Co^+$ | | | | | | | |
| $CoCl_2$ | (10.4) | (217) | (909) | −22±2 | −94±8 | 85JANAF | 7646-79-9 |
| | | *(217)* | *(908)* | *−23±2* | *−95±8* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_2Cr^+$ | | | | | | | |
| $CrCl_2$ | (9.4) | (186) | (779) | −31 | −128 | 82TN270 | 10049-05-5 |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

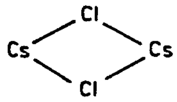
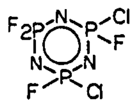
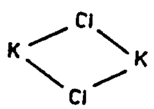
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$Cl_2CrO_2^+$** | | | | | | | |
| $Cl_2CrO_2$ | 11.6 | (139) | (581) | −129 | −538 | 82TN270 | 14977-61-8 |
| | | *(140)* | *(585)* | *−128* | *−534* | | |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cl_2Cs_2^+$** | | | | | | | |
|  | (≤9.15) | (≤53) | (≤223) | −158 | −660 | 81LIN/BES | 12258-95-6 |
| | | *(≤54)* | *(≤227)* | *−157* | *−656* | | |
| **$Cl_2F_4N_3P_3^+$** | | | | | | | |
|  | (10.97±0.3) | (−150) | (−629) | −403 | −1687 | *EST | 29871-62-3 |
| | IP from 81CLA/SOW. | | | | | | |
| **$Cl_2Fe^+$** | | | | | | | |
| $FeCl_2$ | (10.0) | (197) | (824) | −34 | −141 | 85JANAF | 7758-94-3 |
| | | *(197)* | *(823)* | *−34* | *−142* | | |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cl_2Ge^+$** | | | | | | | |
| $GeCl_2$ | (10.20±0.05) | (194) | (813) | −41±1 | −171±5 | 79TPIS | 10060-11-4 |
| | | *(195)* | *(814)* | *−41* | *−170* | | |
| | IP from 82JON/VAN. | | | | | | |
| **$Cl_2HN^+$** | | | | | | | |
| $NHCl_2$ | (9.98±0.05) | (269) | (1124) | 38 | 161 | *EST | 3400-09-7 |
| **$Cl_2H_2Si^+$** | | | | | | | |
| $SiH_2Cl_2$ | 11.4 | (183) | (765) | −80 | −335 | 81BEL/PER | 4109-96-0 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cl_2Hg^+$** | | | | | | | |
| $HgCl_2$ | 11.380±0.003 | 227 | 952 | −35±1 | −146±6 | 71JANAF | 7487-94-7 |
| | Cited ionization potential (from 83LIN/BRO) refers to formation of $HgCl_2^+(^2\Pi_{3/2g})$. Ionization potential for formation of $HgCl_2^+(^2\Pi_{1/2g})$ is 11.505±0.003 eV. See also: 81LEE/POT. | | | | | | |
| **$Cl_2K_2^+$** | | | | | | | |
|  | (≤9.60) | (≤72) | (≤303) | −149 | −623 | 82TN270 | 12258-97-8 |

**Table 1. Positive Ion Table - Continued**

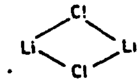
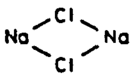
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Cl_2Li_2^+$ | | | | | | | |
|  | 10.20 | 93 | 390 | −142 | −594 | 82TN270 | 12345-57-2 |
| | | *94* | *393* | *−141* | *−591* | | |
| $Cl_2Mg^+$ | | | | | | | |
| $MgCl_2$ | (8.5) | (102) | (428) | −94 | −392 | 85JANAF | 7786-30-3 |
| | | *(102)* | *(427)* | *−94* | *−393* | | |
| | IP is onset of photoelectron band. See also: 77LEE/POT2. | | | | | | |
| $Cl_2Mn^+$ | | | | | | | |
| $MnCl_2$ | (10.8) | (186) | (778) | −63 | −264 | 82TN270 | 7773-01-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_2MoO_2^+$ | | | | | | | |
| $MoO_2Cl_2$ | (11.93±0.02) | (124) | (517) | −152 | −634 | 82TN270 | 13637-68-8 |
| $Cl_2Na_2^+$ | | | | | | | |
|  | (≤10.30) | (≤102) | (≤428) | −135±2 | −566±8 | 85JANAF | 12258-98-9 |
| | | *(≤103)* | *(≤432)* | *−134±2* | *−562±8* | | |
| $Cl_2Ni^+$ | | | | | | | |
| $NiCl_2$ | (10.8) | (231) | (968) | −18±0.1 | −74±0.3 | 82JANAF | 7718-54-9 |
| | | *(231)* | *(968)* | *−18±0.1* | *−74±0.3* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_2O^+$ | | | | | | | |
| $Cl_2O$ | 10.94 | 271 | 1136 | 19 | 80 | 82BAU/COX | 7791-21-1 |
| | | *272* | *1138* | *20* | *82* | | |
| $Cl_2OS^+$ | | | | | | | |
| $SOCl_2$ | 10.96 | (202) | (844) | −51 | −213 | 82TN270 | 7719-09-7 |
| | | *(203)* | *(847)* | *−50* | *−210* | | |
| $Cl_2O_2S^+$ | | | | | | | |
| $SO_2Cl_2$ | 12.05 | 193 | 808 | −85 | −355 | 85JANAF | 7791-25-5 |
| | | *195* | *814* | *−83* | *−349* | | |
| $Cl_2Pb^+$ | | | | | | | |
| $PbCl_2$ | (10.0) | (189) | (791) | −42±0.3 | −174±1 | 85JANAF | 7758-95-4 |
| | | *(189)* | *(793)* | *−41±0.3* | *−172±1* | | |
| | IP is onset of photoelectron band. (See: 84NOV/POT2). | | | | | | |

**Table 1. Positive Ion Table - Continued**

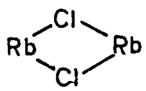
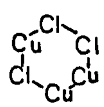
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Cl_2Rb_2^+$ | | | | | | | |
|  | (≤9.30) | (≤64) | (≤269) | −150 | −628 | 82TN270 | 12265-61-1 |
| | | *(≤65)* | *(≤271)* | *−150* | *−626* | | |
| $Cl_2S^+$ | | | | | | | |
| $SCl_2$ | 9.45±0.03 | 214 | 894 | −4 | −18 | 85JANAF | 10545-99-0 |
| | | *214* | *895* | *−4* | *−16* | | |
| | IP from 81KAU/VAH. | | | | | | |
| $Cl_2S_2^+$ | | | | | | | |
| $S_2Cl_2$ | (9.66±0.03) | (218) | (914) | −4 | −18 | 82TN270 | 10025-67-9 |
| | | *(219)* | *(915)* | *−4* | *−17* | | |
| | IP from 81KAU/VAH. | | | | | | |
| $Cl_2Se^+$ | | | | | | | |
| $SeCl_2$ | 9.25 | (206) | (860) | −8 | −32 | 82TN270 | 14457-70-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_2Se_2^+$ | | | | | | | |
| $Se_2Cl_2$ | (9.4) | (221) | (924) | 4 | 17 | 82TN270 | 10025-68-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_2Si^+$ | | | | | | | |
| $SiCl_2$ | (10.93±0.10) | (212) | (889) | −40 | −166 | 82TN270 | 13569-32-9 |
| | | *(212)* | *(889)* | *−40* | *−166* | | |
| $Cl_2Sn^+$ | | | | | | | |
| $SnCl_2$ | (10.0) | (182) | (762) | −49 | −203 | 82TPIS | 7772-99-8 |
| | | *(183)* | *(764)* | *−49±2* | *−201±10* | | |
| | IP is onset of photoelectron band (84NOV/POT2, 82LEV/LIA). | | | | | | |
| $Cl_2Sr^+$ | | | | | | | |
| $SrCl_2$ | 9.70±0.1 | *(115)* | *(481)* | *−109* | *−455* | 82EMO/KIE | 10476-85-4 |
| | See also: 82EMO/KIE, 79LEE/POT2. 0 K values. | | | | | | |
| $Cl_2Zn^+$ | | | | | | | |
| $ZnCl_2$ | 11.85 | 210 | 877 | −64 | −266 | 82TN270 | 7646-85-7 |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_3Cu_3^+$ | | | | | | | |
|  | (≤9.52) | (≤158) | (≤660) | −62±0.5 | −259±2 | 85JANAF | 11093-65-5 |
| | | *(≤158)* | *(≤660)* | *−62±0.5* | *−259±2* | | |

**Table 1. Positive Ion Table - Continued**

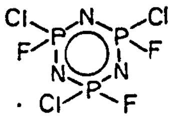
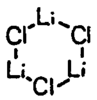
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Cl_3F_3N_3P_3^+$ | | | | | | | |
|  | (10.76±0.03) | (−5) | (−22) | −253 | −1060 | *EST | 25251-05-2 |
| | IP from 81CLA/SOW. | | | | | | |
| $Cl_3Ga^+$ | | | | | | | |
| $GaCl_3$ | 11.52 | 159 | 664 | −107 | −448 | 82TN270 | 13450-90-3 |
| $Cl_3HSi^+$ | | | | | | | |
| $SiHCl_3$ | (11.7) | (155) | (647) | −115 | −482 | 81BEL/PER | 10025-78-2 |
| | | *(156)* | *(652)* | *−114* | *−477* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_3In^+$ | | | | | | | |
| $InCl_3$ | (11.4) | (173) | (722) | −90 | −378 | 82TPIS | 10025-82-8 |
| | | *(173)* | *(724)* | *−90±2* | *−376±7* | | |
| $Cl_3La^+$ | | | | | | | |
| $LaCl_3$ | (10.6) | (67) | (282) | −177 | −741 | 82TN270 | 10099-58-8 |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| $Cl_3Li_3^+$ | | | | | | | |
|  | (10.17) | (5) | (19) | −230 | −962 | 82TN270 | 59217-69-5 |
| | | *(6)* | *(26)* | *−228* | *−955* | | |
| $Cl_3Lu^+$ | | | | | | | |
| $LuCl_3$ | (11.5±0.5) | (110) | (461) | −155 | −649 | 82TN270 | 10099-66-8 |
| $Cl_3N^+$ | | | | | | | |
| $NCl_3$ | (10.12±0.1) | (297) | (1244) | 64 | 268 | *EST | 10025-85-1 |
| $Cl_3NbO^+$ | | | | | | | |
| $NbOCl_3$ | ≤12.14 | ≤100.1 | ≤419.0 | −179.8 | −752.3 | 82TN270 | 13597-20-1 |
| | | *≤100.8* | *≤421.7* | *−179.1* | *−749.6* | | |
| $Cl_3OP^+$ | | | | | | | |
| $POCl_3$ | 11.36±0.02 | 129 | 538 | −133 | −558 | 82TN270 | 10025-87-3 |
| | | *130* | *543* | *−132* | *−553* | | |
| $Cl_3OV^+$ | | | | | | | |
| $VOCl_3$ | (11.6) | (101) | (423) | −166 | −696 | 82TN270 | 7727-18-6 |
| | | *(102)* | *(426)* | *−166* | *−693* | | |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

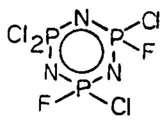
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$Cl_3P^+$** | | | | | | | |
| $PCl_3$ | 9.91 | 160 | 667 | −69 | −289 | 85JANAF | 7719-12-2 |
| | | *160* | *671* | *−68* | *−286* | | |
| | See also: 83OZG, 81CHA/FIN. | | | | | | |
| **$Cl_3PS^+$** | | | | | | | |
| $PSCl_3$ | 9.71±0.03 | 137 | 574 | −87 | −363 | 71JANAF | 3982-91-0 |
| **$Cl_3Sb^+$** | | | | | | | |
| $SbCl_3$ | (10.1±0.1) | (158) | (660) | −75 | −314 | 82TN270 | 10025-91-9 |
| | IP is onset of photoelectron band. See also: 83OZG. | | | | | | |
| **$Cl_3Si^+$** | | | | | | | |
| $SiCl_3$ | | (108) | (454) | | | | 19165-34-5 |
| | From appearance potentials, 11.91 eV in $SiHCl_3$ and 11.90 eV in $CH_3SiCl_3$. | | | | | | |
| **$Cl_4F_2N_3P_3^+$** | | | | | | | |
|  | (10.48±0.03) | (−53) | (−222) | −295 | −1233 | *EST | 25251-04-1 |
| | IP from 81CLA/SOW. | | | | | | |
| **$Cl_4Ge^+$** | | | | | | | |
| $GeCl_4$ | 11.68±0.05 | (151) | (631) | −119 | −496 | 82TN270 | 10038-98-9 |
| | | *(151)* | *(633)* | *−118* | *−494* | | |
| **$Cl_4Hf^+$** | | | | | | | |
| $HfCl_4$ | (11.7) | (59) | (246) | −211 | −883 | 81SPE | 13499-05-3 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cl_4Mo^+$** | | | | | | | |
| $MoCl_4$ | (10.5±0.1) | (152) | (636) | −90 | −377 | 82TN270 | 13320-71-3 |
| | IP from 83MAK/VER. | | | | | | |
| **$Cl_4Si^+$** | | | | | | | |
| $SiCl_4$ | 11.79±0.01 | 126 | 528 | −146 | −610 | 81BEL/PER | 10026-04-7 |
| | | *124* | *520* | *−148* | *−618* | | |
| **$Cl_4Sn^+$** | | | | | | | |
| $SnCl_4$ | (11.88±0.05) | (161) | (674) | −113 | −472 | 82TN270 | 7646-78-8 |
| | | *(162)* | *(677)* | *−112* | *−469* | | |
| **$Cl_4Th^+$** | | | | | | | |
| $ThCl_4$ | (12.7±0.3) | (62) | (259) | −231 | −966 | 82TN270 | 10026-08-1 |
| | | *(62)* | *(260)* | *−230.8* | *−965.6* | | |
| **$Cl_4Ti^+$** | | | | | | | |
| $TiCl_4$ | 11.65±0.15 | (86) | (361) | −182 | −763 | 85JANAF | 7550-45-0 |
| | | *(86)* | *(362)* | *−182* | *−762* | | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $Cl_4U^+$ | | | | | | | |
| $UCl_4$ | 9.18 | 18 | 76 | −193 | −810 | 82TN270 | 10026-10-5 |
| $Cl_4V^+$ | | | | | | | |
| $VCl_4$ | (9.2) | (86) | (362) | −126 | −526 | 82TN270 | 7632-51-1 |
| | | *(87)* | *(364)* | *−125* | *−524* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_4W^+$ | | | | | | | |
| $WCl_4$ | (8.0) | (104) | (436) | −80±8 | −336±33 | 85JANAF | 13470-13-8 |
| | | *(104)* | *(436)* | *−80±8* | *−336±33* | | |
| $Cl_4Zr^+$ | | | | | | | |
| $ZrCl_4$ | (11.2) | (50) | (211) | −208 | −870 | 82TN270 | 10026-11-6 |
| | | *(51)* | *(212)* | *−208* | *−869* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_5Mo^+$ | | | | | | | |
| $MoCl_5$ | (8.7) | (94) | (392) | −107 | −448 | 85JANAF | 10241-05-1 |
| | | *(94)* | *(393)* | *−106* | *−446* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_5Nb^+$ | | | | | | | |
| $NbCl_5$ | (10.97) | (85) | (355) | −168 | −703 | 85JANAF | 10026-12-7 |
| | | *(85)* | *(357)* | *−168* | *−701* | | |
| $Cl_5P^+$ | | | | | | | |
| $PCl_5$ | 10.7 | (157) | (657) | −90 | −375 | 82TN270 | 10026-13-8 |
| | | *(158)* | *(662)* | *−88* | *−370* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_5Re^+$ | | | | | | | |
| $ReCl_5$ | (9.2) | (136) | (570) | −76 | −318 | 82TN270 | 13596-35-5 |
| | IP is onset of photoelectron band. | | | | | | |
| $Cl_5Sb^+$ | | | | | | | |
| $SbCl_5$ | (10.8) | (155) | (648) | −94 | −394 | 82TN270 | 7647-18-9 |
| | | *(155)* | *(650)* | *−94* | *−392* | | |
| | IP is onset of photoelectron band (81ELB/DIE). | | | | | | |
| $Cl_5Ta^+$ | | | | | | | |
| $TaCl_5$ | 11.08 | 73 | 304 | −183 | −765 | 85JANAF | 7721-01-9 |
| | | *73* | *306* | *−182* | *−763* | | |
| $Cl_5W^+$ | | | | | | | |
| $WCl_5$ | (8.5) | (97) | (407) | −99±8 | −413±33 | 85JANAF | 13470-14-9 |
| | | *(98)* | *(409)* | *−98±8* | *−411±33* | | |
| | IP is onset of photoelectron band. | | | | | | |

**Table 1. Positive Ion Table - Continued**

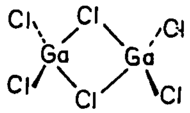
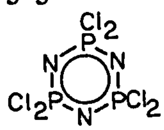
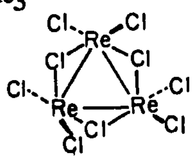
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$Cl_6Ga_2^+$** | | | | | | | |
|  | (11.4) | (30) | (125) | −233 | −975 | 82TN270 | 15654-66-7 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cl_6N_3P_3^+$** | | | | | | | |
|  | 9.8 | (51) | (213) | −175 | −732 | 69BEN/CRU | 940-71-6 |
| | IP is onset of photoelectron band. See also: 81CLA/SOW. | | | | | | |
| **$Cl_6Si_2^+$** | | | | | | | |
| $Si_2Cl_6$ | (10.4) | (−4) | (−16) | −244 | −1019 | 81BEL/PER | 13465-77-5 |
| | See also: 81KHV/ZYK. | | | | | | |
| **$Cl_6W^+$** | | | | | | | |
| $WCl_6$ | (9.5) | (83) | (347) | −136 | −570 | 81WOO | 13283-01-7 |
| | | | | *−136* | *−570* | | |
| **$Cl_9Re_3^+$** | | | | | | | |
|  | (8.7) | (64) | (266) | −137 | −573 | 82TN270 | 14973-59-2 |
| | IP is onset of photoelectron band. | | | | | | |
| **$Cm^+$** | | | | | | | |
| Cm | 6.09±0.02 | 233 | 974 | 92 | 386 | 85KLE/WAR | 7440-51-9 |
| | See also: 81CHE/GAB. | | | | | | |
| **$Co^+$** | | | | | | | |
| Co | 7.864±0.001 | 283 | 1184 | 102 | 425 | 82TN270 | 7440-48-4 |
| | | *282* | *1182* | *101* | *423* | | |
| | See also: 82DYK/GRA. | | | | | | |
| **$CoH^+$** | | | | | | | |
| CoH | (7.3±0.1) | *(287)* | *(1203)* | *(119)* | *(496)* | 81ARM/BEA | 14994-20-8 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM4). See also: 81ARM/HAL. IP from 81ARM/BEA. 0 K values. | | | | | | |
| **$CoHO^+$** | | | | | | | |
| CoOH | | *220* | *920* | | | | 12314-24-8 |
| | $\Delta_f H$(Ion) from photodissociation onset, proton affinity of CoO(84CAS/FRE). 0 K values. | | | | | | |
| **$CoO^+$** | | | | | | | |
| CoO | 8.9±0.2 | *(277)* | *(1159)* | *72±3* | *301±13* | 79HUB/HER | 1307-96-6 |
| | $\Delta_f H$(Ion) from 81ARM/HAL, 82ARM/HAL. See also: 81KAP/STA. 0 K values. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Cr^+$ | | | | | | | |
| Cr | 6.766 | 250.8 | 1049.4 | 94.8 | 396.6 | 82TN270 | 7440-47-3 |
| | | *250.3* | *1047.3* | *94.3* | *394.5* | | |
| $CrF^+$ | | | | | | | |
| CrF | (8.4±0.3) | (199) | (831) | 5 | 21 | 81WOO | 13943-42-5 |
| $CrF_2^+$ | | | | | | | |
| $CrF_2$ | (10.1±0.3) | (181) | (758) | −52 | −216 | 81WOO | 10049-10-2 |
| $CrF_3^+$ | | | | | | | |
| $CrF_3$ | (12.2±0.3) | (124) | (517) | −158 | −660 | 81WOO | 7788-97-8 |
| $CrH^+$ | | | | | | | |
| CrH | | *(274)* | *(1145)* | | | | 13966-79-5 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). See also: 81ARM/HAL. 0 K values. | | | | | | |
| $CrO^+$ | | | | | | | |
| CrO | 7.85±0.02 | (233) | (975) | 52±7 | 218±29 | 83PED/MAR | 12018-00-7 |
| | | *(230)* | *(961)* | *49±3* | *203±12* | | |
| | IP from 83DYK/GRA. $\Delta_f H$(Ion) at 0 K from 81ARM/HAL, 82ARM/HAL. See also: 81BAL/GIG, 81KAP/STA. | | | | | | |
| $CrO_2^+$ | | | | | | | |
| $CrO_2$ | (10.3±0.5) | *(223)* | *(935)* | *−14* | *−59* | 82TN270 | 12018-01-8 |
| | 0 K values. | | | | | | |
| $CrO_2P^+$ | | | | | | | |
| $CrPO_2$ | (8.0±0.5) | *(236)* | *(989)* | *52±3* | *218±13* | 81BAL/GIG | |
| | IP from 81BAL/GIG. 0 K values. | | | | | | |
| $CrO_3^+$ | | | | | | | |
| $CrO_3$ | (11.6±0.5) | (175) | (733) | −92 | −386 | 82TN270 | 1333-82-0 |
| $Cs^+$ | | | | | | | |
| Cs | 3.894 | 108.0 | 451.8 | 18.2 | 76.1 | 82TN270 | 7440-46-2 |
| | | *108.3* | *453.3* | *18.5* | *77.6* | | |
| | See also: 84ASA/YAS, 85SCH/WEI. | | | | | | |
| $CsF^+$ | | | | | | | |
| CsF | (8.80±0.10) | (117) | (488) | −86 | −361 | 84PAR/WEX | 13400-13-0 |
| | | *(117)* | *(490)* | *−85.8±1.8* | *−359.0±7.5* | | |
| $CsHO^+$ | | | | | | | |
| CsOH | (7.3±0.15) | (106) | (445) | −62 | −259 | 81LIN/BES | 21351-79-1 |
| $CsH_2O^+$ | | | | | | | |
| $CsOH_2$ | | 36 | 149 | | | | |
| | $\Delta_f H$(Ion) from equilibrium constant determination (69SEA/DZI). | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $CsI^+$ | | | | | | | |
| CsI | 7.10±0.05 | 127 | 531 | −37 | −154 | 84PAR/WEX | 7789-17-5 |
| | | *128* | *535* | *−35.9±3.4* | *−150±14* | | |
| | See also: 82EMO/HOR, 82LEL/BAL, 84VIS/HIL. | | | | | | |
| $CsK^+$ | | | | | | | |
| KCs | (3.9±0.1) | *(119)* | *(498)* | *(29)* | *(122)* | 79HUB/HER | |
| | IP from 85KAP/SCH. 0 K values. | | | | | | |
| $CsLi^+$ | | | | | | | |
| LiCs | (4.1±0.1) | *(134)* | *(562)* | *(40)* | *(166)* | 79HUB/HER | 12018-59-6 |
| | IP from 85KAP/SCH. 0 K values. | | | | | | |
| $CsNa^+$ | | | | | | | |
| NaCs | (4.05±0.04) | *(128)* | *(535)* | *(35)* | *(144)* | 79HUB/HER | 12018-60-9 |
| | IP from 85KAP/SCH. 0 K values. | | | | | | |
| $CsO^+$ | | | | | | | |
| CsO | 6.22 | 153.6 | 642.8 | 10.2 | 42.7 | 82TPIS | 24774-39-8 |
| | | *154.1* | *644.9* | *10.7±5* | *44.8±21* | | |
| | IP from 84BUT/KUD. | | | | | | |
| $CsRb^+$ | | | | | | | |
| RbCs | 3.7±0.1 | 96 | 401 | 11 | 44 | 86IGE/WED | 12331-83-8 |
| | IP from 85KAP/SCH. | | | | | | |
| $Cs_2^+$ | | | | | | | |
| $Cs_2$ | 3.7±0.1 | (111) | (464) | 26±0.1 | 107±0.3 | 85JANAF | 12184-83-7 |
| | | *(112)* | *(469)* | *27±0.1* | *112±0.3* | | |
| | IP from 85KAP/RAD, 85KAP/SCH. See also: 83HEL/MOL. | | | | | | |
| $Cs_2MoO_4^+$ | | | | | | | |
| $Cs_2MoO_4$ | (7.0) | (−114) | (−479) | −276 | −1154 | 81LIN/BES | |
| $Cs_2O^+$ | | | | | | | |
| $Cs_2O$ | 4.41±0.03 | (80) | (333) | −22 | −92 | 81LIN/BES | 20281-00-9 |
| | IP from 77ROS/DRA, 84BUT/KUD. | | | | | | |
| $Cu^+$ | | | | | | | |
| Cu | 7.72634±0.00002 | 259.0 | 1083.8 | 80.9 | 338.3 | 82TN270 | 7440-50-8 |
| | | *258.8* | *1082.7* | *80.6* | *337.2* | | |
| $CuF^+$ | | | | | | | |
| CuF | 10.15±0.02 | (235) | (984) | 1 | 5 | 81WOO | 13478-41-6 |
| | | *(231)* | *(967)* | *−3* | *−12* | | |
| | IP from 80DYK/FAY. See also: 77EHL/WAN. | | | | | | |
| $CuF_2^+$ | | | | | | | |
| $CuF_2$ | (12.7) | (229) | (958) | −64 | −267 | 81WOO | 7789-19-7 |
| | | *(230)* | *(960)* | *−63* | *−265* | | |
| | IP is onset of photoelectron band (80DYK/FAY). See also: 77EHL/WAN. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$CuH^+$** | | | | | | | |
| CuH | (9.5) | *(289)* | *(1208)* | *70* | *291* | 79HUB/HER | |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (86ELK/ARM4). IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). 0 K values. | | | | | | |
| **$CuO^+$** | | | | | | | |
| CuO | | (286±8) | (1197±33) | 73±10 | 306±41 | 85JANAF | 1317-38-0 |
| | $\Delta_fH$(Ion) from (81KAP/STA). Ion/molecule bracketing results. | | | | | | |
| **$CuSn^+$** | | | | | | | |
| CuSn | (7.2±1.0) | *(277)* | *(1161)* | *111* | *466* | 79HUB/HER | 12054-11-4 |
| | 0 K values. | | | | | | |
| **$Cu_2^+$** | | | | | | | |
| $Cu_2$ | 7.894±0.015 | 298 | 1247 | 116 | 485 | 85JANAF | 12190-70-4 |
| | | *298* | *1247* | *116* | *485* | | |
| | IP from 83POW/HAN. | | | | | | |
| **$D^+$** | | | | | | | |
| D | 13.602 | 366.6 | 1534.0 | 52.98 | 221.67 | 82TN270 | 16873-17-9 |
| | | *366.2* | *1532.1* | *52.52* | *219.76* | | |
| **$DH^+$** | | | | | | | |
| HD | 15.44477±0.00007 | 356.2 | 1490.5 | .077 | .32 | 85JANAF | 13983-20-5 |
| | | *356.2* | *1490.5* | *.079* | *.33* | | |
| **$DLi^+$** | | | | | | | |
| LiD | 7.7±0.1 | (211) | (884) | 33.7 | 141.1 | 82TN270 | 13587-16-1 |
| | | *(211)* | *(884)* | *33.7* | *141.1* | | |
| **$D_2^+$** | | | | | | | |
| $D_2$ | 15.46660±0.0001 | 356.7 | 1492.2 | 0 | 0 | *DEF | 7782-39-0 |
| | | *356.7* | *1492.2* | *0* | *0* | | |
| | IP from 79HUB/HER. | | | | | | |
| **$D_2O^+$** | | | | | | | |
| $D_2O$ | 12.635±0.007 | 231.8 | 970.0 | −59.56 | −249.20 | 85JANAF | 7789-20-0 |
| | | *232.5* | *972.8* | *−58.85* | *−246.25* | | |
| **$D_3O^+$** | | | | | | | |
| $D_3O$ | 4.3±0.1 | | | | | | 24847-51-6 |
| | IP from 84GEL/POR. | | | | | | |
| **$Dy^+$** | | | | | | | |
| Dy | 5.9390±0.0006 | 206 | 863 | 69 | 290 | 82TN270 | 7429-91-6 |
| | | *207.0* | *866.1* | *70.0* | *293.1* | | |
| **$DyF^+$** | | | | | | | |
| DyF | (6.0±0.3) | *(101)* | *(422)* | *−38* | *−157* | 79HUB/HER | |
| | 0 K values. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$DyO^+$** | | | | | | | |
| DyO | (6.08±0.1) | (122) | (512) | −18±10 | −75±42 | 83PED/MAR | 12175-28-9 |
| | | *(121)* | *(508)* | *−19* | *−79* | | |
| **$Er^+$** | | | | | | | |
| Er | 6.1077±0.0006 | 217 | 906 | 76 | 317 | 82TN270 | 7440-52-0 |
| | | *216.9* | *907.6* | *76.1* | *318.3* | | |
| **$ErF^+$** | | | | | | | |
| ErF | (6.3±0.3) | *(105)* | *(441)* | *−40* | *−167* | 79HUB/HER | |
| | 0 K values. | | | | | | |
| **$ErF_2{}^+$** | | | | | | | |
| $ErF_2$ | (7.0±0.3) | (−3) | (−11) | −164 | −686 | 82TN270 | |
| **$ErI_3{}^+$** | | | | | | | |
| $ErI_3$ | 9.0 | 125 | 524 | −82 | −344 | 82TN270 | 13813-42-8 |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| **$ErO^+$** | | | | | | | |
| ErO | (6.30±0.1) | (135) | (566) | −10±5 | −42±21 | 83PED/MAR | 12280-61-4 |
| | | *(132)* | *(554)* | *−13* | *−54* | | |
| | See also: 80MUR/HIL. | | | | | | |
| **$Es^+$** | | | | | | | |
| Es | 6.52±0.10 | 182 | 762 | 31.8±3 | 133±13 | 85KLE/WAR | 7429-92-7 |
| **$Eu^+$** | | | | | | | |
| Eu | 5.67045±0.0003 | 172 | 722 | 42 | 175 | 82TN270 | 7440-53-1 |
| | | *173.1* | *724.2* | *42.3* | *177.1* | | |
| **$EuO^+$** | | | | | | | |
| EuO | (6.48±0.1) | (139) | (582) | −10 | −43 | 83PED/MAR | 12020-60-9 |
| | See also: 81BAL/GIG, 85BAL/GIG. | | | | | | |
| **$EuO_2V^+$** | | | | | | | |
| $EuVO_2$ | (8) | *(108)* | *(450)* | *−77* | *−322* | 83BAL/GIG | 88762-30-5 |
| | IP from 83BAL/GIG. 0 K values. | | | | | | |
| **$EuO_3Ti^+$** | | | | | | | |
| $EuTiO_3$ | (6.5±0.5) | (−62) | (−260) | −212±7 | −887±28 | 85BAL/GIG | 12020-61-0 |
| | IP from 85BAL/GIG. | | | | | | |
| **$EuO_3V^+$** | | | | | | | |
| $EuVO_3$ | 8.1±0.5 | *(4)* | *(17)* | *(−183)* | *(−764)* | 83BAL/GIG | 39432-21-8 |
| | IP from 83BAL/GIG. 0 K values. | | | | | | |
| **$EuS^+$** | | | | | | | |
| EuS | (6.8±0.3) | (184) | (769) | 27 | 113 | 82TN270 | 12020-65-4 |
| | | *(180)* | *(751)* | *23* | *95* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $F^+$ | | | | | | | |
| F | 17.422 | 420.7 | 1760.2 | 19.0±0.1 | 79.4±0.3 | 85JANAF | 14762-94-8 |
| | | *420.2* | *1758.2* | *18.5±0.1* | *77.4±0.3* | | |
| $FGa^+$ | | | | | | | |
| GaF | (9.6±0.5) | (167) | (699) | −54 | −227 | 79HUB/HER | 13966-78-4 |
| . | | *(167)* | *(700)* | *−54* | *−226* | | |
| | A value of 10.7±0.6 eV has also been reported for this ionization potential. | | | | | | |
| $FGe^+$ | | | | | | | |
| GeF | 7.46 | 166 | 694 | −6 | −26 | 81WOO | 14929-46-5 |
| | | *166* | *694* | *−6* | *−26* | | |
| | IP from 79HUB/HER. | | | | | | |
| $FH^+$ | | | | | | | |
| HF | 16.044±0.003 | 304.9 | 1275.5 | −65.1±0.2 | −272.5±0.8 | 85JANAF | 7664-39-3 |
| | | *304.9* | *1275.5* | *−65.1±0.2* | *−272.5±0.8* | | |
| | See also: 81KIM/KAT, 81BIE/ASB. | | | | | | |
| $FHO^+$ | | | | | | | |
| HOF | 12.71±0.01 | 270 | 1128 | −23±1 | −98±4 | 82BAU/COX | 14034-79-8 |
| $FH_2^+$ | | | | | | | |
| $H_2F$ | | 184 | 767 | | | | |
| | From proton affinity of HF (RN 7664-39-3). A value of 205 kcal/mol, 859 kJ/mol is derived from the appearance potential of this ion from $(HF)_2$. PA = 117 kcal/mol, 489.5 kJ/mol. | | | | | | |
| $FH_3Si^+$ | | | | | | | |
| $SiH_3F$ | 11.7 | (180) | (752) | −90±5 | −377±21 | 78JANAF | 13537-33-2 |
| | IP is onset of photoelectron band. | | | | | | |
| $FHo^+$ | | | | | | | |
| HoF | (6.1±0.3) | *(103)* | *(431)* | *−38* | *−158* | 79HUB/HER | 16087-66-4 |
| | 0 K values. | | | | | | |
| $FI^+$ | | | | | | | |
| IF | 10.62 | 222.2 | 929.9 | −22.7±0.9 | −94.8±3.8 | 85JANAF | 13873-84-2 |
| | | *222.7* | *931.8* | *−22.2±0.9* | *−92.9±3.8* | | |
| | IP from 84DYK/JOS. | | | | | | |
| $FIn^+$ | | | | | | | |
| InF | (9.6±0.5) | *(177)* | *(740)* | *−44* | *−186* | 79HUB/HER | 13966-95-5 |
| | 0 K values. | | | | | | |
| $FMg^+$ | | | | | | | |
| MgF | (7.68) | (120.5) | (504) | −56.6±2.0 | −236.8±8.4 | 85JANAF | 14953-28-7 |
| | | *(121)* | *(505)* | *−56.5±2.0* | *−236.4±8.4* | | |
| $FMn^+$ | | | | | | | |
| MnF | (8.3±0.2) | (173) | (723) | −19 | −78 | 81WOO | 13569-25-0 |

**Table 1. Positive Ion Table - Continued**

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $FMo^+$ | | | | | | | |
| MoF | (8.0±0.3) | (249) | (1044) | 65 | 272 | 81WOO | 60388-18-3 |
| $FN^+$ | | | | | | | |
| NF | 12.26±0.01 | *338* | *1415* | *55.5±0.5* | *232.2±2.1* | 84BER/GRE | 13967-06-1 |
| | IP from 82DYK/JON. $\Delta_f H$(Ion) from 84BER/GRE. See also: 79DUD/BAL. 0 K values. | | | | | | |
| $FNO^+$ | | | | | | | |
| NOF | 12.63±0.03 | 275 | 1152 | −16 | −67 | 82TN270 | 7789-25-5 |
| | | *276* | *1154* | *−16* | *−65* | | |
| $FNO_2^+$ | | | | | | | |
| $NO_2F$ | (13.09) | (276) | (1154) | −26±5 | −109±21 | 85JANAF | 10022-50-1 |
| | | *(277)* | *(1160)* | *−25±5* | *−103±21* | | |
| $FNS^+$ | | | | | | | |
| NSF | 11.51±0.04 | 260 | 1090 | −5±0.9 | −21±4 | 73LAR/JOH | 18820-63-8 |
| $FNa_2^+$ | | | | | | | |
| $Na_2F$ | 4.0±0.1 | *5* | *20* | *−87±3* | *−366±13* | 85KAP/RAD | 87331-13-3 |
| | IP from 85KAP/RAD. 0 K values. | | | | | | |
| $FNd^+$ | | | | | | | |
| FNd | (5.0±0.3) | (81) | (338) | −34 | −144 | 81WOO | |
| | A 298 K heat of formation of -161 kJ/mol, -38.5 kcal/mol (79HUB/HER) or -159 kJ/mol, -38.0 kcal/mol (82TN270) has also been recommended for NdF. | | | | | | |
| $FO^+$ | | | | | | | |
| OF | 12.77 | 320 | 1341 | 26±2 | 109±8 | 82BAU/COX | 12061-70-0 |
| | | *320* | *1341* | *26* | *109* | | |
| $FO_2^+$ | | | | | | | |
| $O_2F$ | (12.6±0.2) | (294) | (1229) | 3±0.5 | 13±2 | 85JANAF | 15499-23-7 |
| | | *(294)* | *(1230)* | *3±0.5* | *14±2* | | |
| $FP^+$ | | | | | | | |
| PF | (≤9.74±0.01) | (≤212) | (≤887) | −12.5±5 | −52±21 | 85JANAF | 16027-92-2 |
| | | *(≤212)* | *(≤888)* | *−12±5* | *−51±21* | | |
| | $\Delta_f H$(Ion) from appearance potential determinations (84BER/GRE). IP from 82DYK/JON2. See also: 75TOR/WES, 82LEV/LIA. | | | | | | |
| $FPb^+$ | | | | | | | |
| PbF | (7.5±0.3) | (154) | (644) | −19 | −80 | 81WOO | 14986-72-2 |
| | | *(154)* | *(646)* | *−19* | *−78* | | |
| $FS^+$ | | | | | | | |
| SF | 10.09 | (236) | (987) | 3±1 | 13±6 | 85JANAF | 16068-96-5 |
| | | *(233)* | *(973)* | *2.9±1.5* | *12±6* | | |
| | $\Delta_f H$(Ion) from appearance potential determination (80GOM/HAA); corresponding IP = 9.9 eV. IP from 85LOS/WIL. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | kJ/mol | $\Delta_fH$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $FS_2^+$ | | | | | | | |
| SSF | | 194 | 811 | | | | |
| | From appearance potential determinations (85LOS/WIL). | | | | | | |
| $FSi^+$ | | | | | | | |
| SiF | 7.28 | 163 | 682 | −5±6 | −20±25 | 83WAL | 11128-24-8 |
| · | | *166* | *680* | *−5±6* | *−22±25* | | |
| | IP from 79HUB/HER. | | | | | | |
| $FSm^+$ | | | | | | | |
| SmF | (5.7±0.3) | (68) | (286) | −63 | −264 | 79HUB/HER | 17209-59-5 |
| | | *(73)* | *(307)* | *−58* | *−243* | | |
| $FSn^+$ | | | | | | | |
| SnF | (7.04) | (142) | (593) | −21 | −86 | 81WOO | 13966-74-0 |
| $FSr^+$ | | | | | | | |
| SrF | (5.0±0.3) | (45) | (188) | −70.4±2.0 | −294.6±8.4 | 85JANAF | 13569-27-2 |
| | | *(45)* | *(189.5)* | *−70.0±2.0* | *−292.9±8.4* | | |
| $FTl^+$ | | | | | | | |
| TlF | 10.52 | 199 | 833 | −43 | −182 | 82TN270 | 7789-27-7 |
| | | *199* | *833* | *−43* | *−182* | | |
| $FW^+$ | | | | | | | |
| WF | (8.5±1) | (282) | (1180) | 86 | 360 | 81WOO | 51621-16-0 |
| $FXe^+$ | | | | | | | |
| XeF | (10.3) | *(252)* | *(1057)* | *15.3* | *64.0* | 79HUB/HER | 16757-14-5 |
| | $\Delta_fH$(Ion) from appearance potential determinations. IP is $\Delta_fH$(Ion)-$\Delta_fH$(Neutral). 0 K values. | | | | | | |
| $FY^+$ | | | | | | | |
| YF | (6.3±0.3) | *(121)* | *(507)* | *−24* | *−101* | 79HUB/HER | 13981-88-9 |
| | 0 K values. | | | | | | |
| $F_2^+$ | | | | | | | |
| $F_2$ | 15.697±0.003 | 362.0 | 1514.5 | 0 | 0 | *DEF | 7782-41-4 |
| | | *362.0* | *1514.5* | | | | |
| | IP from 84VAN/DEL2. See also: 84DYK/JOS, 81KIM/KAT, 81BIE/ASB. | | | | | | |
| $F_2Fe^+$ | | | | | | | |
| $FeF_2$ | (11.3±0.3) | (177) | (740) | −84 | −350 | 81WOO | 7789-28-8 |
| | | *(177)* | *(741)* | *−83* | *−349* | | |
| $F_2Ge^+$ | | | | | | | |
| $GeF_2$ | (11.65) | (132) | (551) | −137 | −573 | 81WOO | 13940-63-1 |
| | IP from 82JON/VAN3. | | | | | | |
| $F_2HN^+$ | | | | | | | |
| $HNF_2$ | (11.53±0.08) | (250) | (1047) | −16±1 | −65±6 | 69PAN/ZER | 10405-27-3 |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $F_2HO_2S^+$ | | | | | | | |
| $F_2SOOH$ | | 38 | 159 | | | | |
| | From proton affinity of $F_2SO_2$ (RN 2699-79-8) (85MCM/KEB, 85MCM/KEB2) re-evaluated relative to CO standard (84LIA/LIE). PA = 146.2 kcal/mol, 612. kJ/mol. | | | | | | |
| $F_2H_2Si^+$ | | | | | | | |
| $SiH_2F_2$ | 12.2 | (92) | (386) | −189±5 | −791±21 | 85JANAF | 13824-36-7 |
| | | *(94)* | *(395)* | *−187±5* | *−782±21* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $F_2IP^+$ | | | | | | | |
| $PF_2I^+$ | (9.8) | *(84)* | *(350)* | *−142.3±1* | *−595.4±4.2* | 84BER/GRE | 13819-11-9 |
| | IP is onset of photoelectron band. 0 K values. | | | | | | |
| $F_2Kr^+$ | | | | | | | |
| $KrF_2$ | 13.1±0.05 | 317 | 1325 | 14±0.7 | 60±3 | 67GUN | 13773-81-4 |
| $F_2Mg^+$ | | | | | | | |
| $MgF_2$ | (13.4±0.4) | (136) | (569) | −173 | −724 | 82TN270 | 7783-40-6 |
| | | *(137)* | *(571)* | *−172* | *−722* | | |
| $F_2Mn^+$ | | | | | | | |
| $MnF_2$ | (11.4) | (137) | (575) | −125 | −525 | 81WOO | 7782-64-1 |
| $F_2Mo^+$ | | | | | | | |
| $MoF_2$ | (9.00±0.15) | (167) | (700) | −40 | −168 | 81WOO | 20205-60-1 |
| $F_2MoO_2^+$ | | | | | | | |
| $MoO_2F_2$ | (13.0±0.3) | (56) | (236) | −243 | −1018 | 81WOO | 13824-57-2 |
| $F_2N^+$ | | | | | | | |
| $NF_2$ | 11.628±0.01 | 275 | 1153 | 8 | 31 | 84BER/GRE | 3744-07-8 |
| | | *276.5* | *1156.8* | *8.3* | *34.9* | | |
| | IP from 84BER/GRE. See also: 79DUD/BAL. | | | | | | |
| $F_2NS^+$ | | | | | | | |
| $NSF_2$ | | 253 | 1060 | | | | |
| | From appearance potential (15.47 eV) in $NSF_3$. | | | | | | |
| $F_2N_2^+$ | | | | | | | |
| (E)-$N_2F_2$ | (12.8) | (315) | (1316) | 19±1 | 81±5 | 85JANAF | 13776-62-0 |
| | | *(316)* | *(1321)* | *21±1* | *86±5* | | |
| $F_2Nd^+$ | | | | | | | |
| $F_2Nd$ | (5.6±0.3) | (−29) | (−120) | −158 | −660 | 81WOO | |
| $F_2O^+$ | | | | | | | |
| $OF_2$ | 13.11±0.01 | 308 | 1290 | 5.9±0.4 | 24.5±1.6 | 85JANAF | 7783-41-7 |
| | | *309* | *1292* | *6.4±0.4* | *26.8±1.6* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | kJ/mol | $\Delta_fH$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $F_2OS^+$ | | | | | | | |
| $SOF_2$ | 12.25 | (164) | (688) | −118±8 | −494±32 | 87HER | 7783-42-8 |
| | | *(166)* | *(693)* | *−117±8* | *−489±32* | | |
| | See also: 81COS/LLO. | | | | | | |
| $F_2O_2S^+$ | | | | | | | |
| $SO_2F_2$ | 13.04±0.01 | 119 | 499 | −181±2 | −759±8 | 87HER | 2699-79-8 |
| | | *121* | *508* | *−179±2* | *−750±8* | | |
| $F_2O_2W^+$ | | | | | | | |
| $WO_2F_2$ | (12.5±0.3) | (70) | (291) | −219 | −915 | 81WOO | 14118-73-1 |
| | IP from 81MAL/MEL. | | | | | | |
| $F_2P^+$ | | | | | | | |
| $PF_2$ | 8.847±0.010 | 90 | 378.5 | −115±0.5 | −482±2.1 | 84BER/GRE | 13873-52-4 |
| | | *90* | *375* | *−114.4±0.5* | *−478.6±2.1* | | |
| | IP from 84BER/GRE. See also: 75TOR/WES, 82LEV/LIA. | | | | | | |
| $F_2Pb^+$ | | | | | | | |
| $PbF_2$ | (11.5) | (162) | (677) | −103 | −432 | 81WOO | 7783-46-2 |
| | | *(163)* | *(681)* | *−102* | *−429* | | |
| | IP is onset of photoelectron band(83NOV/POT2). | | | | | | |
| $F_2Pt^+$ | | | | | | | |
| $PtF_2$ | (11.85±0.25) | (247) | (1032) | −26±6 | −111±25 | 83KOR/BON | 18820-56-9 |
| | IP from 83KOR/BON. | | | | | | |
| $F_2S^+$ | | | | | | | |
| $SF_2$ | (10.08) | (161) | (676) | −71±4 | −297±17 | 87HER | 13814-25-0 |
| | | *(162)* | *(678)* | *−70±4* | *−295±17* | | |
| | See also: 80GOM/HAA, 85LOS/WIL. | | | | | | |
| $F_2S_2^+$ | | | | | | | |
| FSSF | 10.62±0.02 | 176 | 739 | −68±2 | −286±10 | 87HER | 13709-35-8 |
| | | *177* | *742* | *−67±2* | *−283±10* | | |
| | IP from 85LOS/WIL. | | | | | | |
| $SSF_2$ | 10.41±0.02 | 169 | 707 | −71±2 | −297±10 | 87HER | 101947-30-2 |
| | IP from 85LOS/WIL. See also: 84COO/KRO, 82LEV/LIA. | | | | | | |
| $F_2Si^+$ | | | | | | | |
| $SiF_2$ | 10.78±0.05 | (108) | (450) | −141±2 | −590±8 | 83WAL | 13966-66-0 |
| | | *(108)* | *(451)* | *−141±2* | *−589±8* | | |
| $F_2Sn^+$ | | | | | | | |
| $SnF_2$ | (11.1) | (140) | (586) | −116 | −485 | 81WOO | 7783-47-3 |
| | IP is onset of photoelectron band (83NOV/POT2). | | | | | | |
| $F_2Ti^+$ | | | | | | | |
| $TiF_2$ | (12.2±0.5) | (125) | (524) | −156 | −653 | 81WOO | 13814-20-5 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $F_2W^+$ | | | | | | | |
| $WF_2$ | (9.0±0.3) | (182) | (763) | −25 | −105 | 81WOO | 33963-15-4 |
| $F_2Xe^+$ | | | | | | | |
| $XeF_2$ | 12.35±0.01 | 259 | 1085 | −26±0.2 | −107±1 | 72JOH/MAL | 13709-36-9 |
| $F_2Zr^+$ | | | | | | | |
| $F_2Zr$ | (12.0±0.5) | (143) | (600) | −133±5 | −558±21 | 85JANAF | 13842-94-9 |
| | | *(144)* | *(602)* | *−133±5* | *−556±21* | | |
| $F_3Fe^+$ | | | | | | | |
| $FeF_3$ | (12.5±0.3) | (101) | (421) | −188 | −785 | 81WOO | 7783-50-8 |
| | | *(101)* | *(424)* | *−187* | *−782* | | |
| $F_3HN^+$ | | | | | | | |
| $F_2NFH$ | | 199 | 832 | | | | |
| | From proton affinity of $NF_3$ (RN 7783-54-2) (85MCM/KEB) re-evaluated relative to CO standard (84LIA/LIE). PA = 136.9 kcal/mol, 573. kJ/mol. | | | | | | |
| $F_3HOP^+$ | | | | | | | |
| $P(OH)F_3$ | | −91 | −383 | | | | |
| | From proton affinity of $POF_3$ (RN 13478-20-1). PA = 167.8 kcal/mol, 702. kJ/mol. | | | | | | |
| $F_3HP^+$ | | | | | | | |
| $HPF_3$ | | −20 | −86 | | | | |
| | From proton affinity of $PF_3$ (RN 7783-55-3). PA = 166.5 kcal/mol, 697. kJ/mol. | | | | | | |
| $F_3HSi^+$ | | | | | | | |
| $SiHF_3$ | (14.0) | (36) | (150) | −287±5 | −1201±21 | 85JANAF | 13465-71-9 |
| | | *(37)* | *(157)* | *−285±5* | *−1194±21* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $F_3H_2OSi^+$ | | | | | | | |
| $SiF_3OH_2$ | | (−264) | (−1103) | | | | |
| | From proton affinity of $SiF_3OH$ (84REE/MUJ). PA = (162) kcal/mol, (676) kJ/mol. | | | | | | |
| $F_3Mn^+$ | | | | | | | |
| $MnF_3$ | (12.57±0.2) | (104) | (434) | −186 | −779 | 81WOO | 7783-53-1 |
| $F_3Mo^+$ | | | | | | | |
| $MoF_3$ | (9.88±0.10) | (87) | (361) | −141 | −592 | 81WOO | 20193-58-2 |
| | | *(87)* | *(364)* | *−141* | *−589* | | |
| $F_3MoS^+$ | | | | | | | |
| $MoSF_3$ | (13.0±0.3) | (134) | (559) | −166±6 | −695±27 | 80MAL/ALI | 67374-76-9 |
| | IP from 80MAL/ALI, 80MAL/ALI2. | | | | | | |
| $F_3N^+$ | | | | | | | |
| $NF_3$ | 13.00±0.02 | 268 | 1122 | −31±0.3 | −132±1 | 85JANAF | 7783-54-2 |
| | | *270* | *1128* | *−30±0.3* | *−126±1* | | |
| | See also: 84BER/GRE, 84BER/GRE2, 79DUD/BAL. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $F_3NO^+$ | | | | | | | |
| $NOF_3$ | 13.26±0.01 | (267) | (1116) | −39±5 | −163±21 | 85JANAF | 13847-65-9 |
| | | *(269)* | *(1124)* | *−37±5* | *−155±21* | | |
| $F_3NS^+$ | | | | | | | |
| $NSF_3$ | (12.0) | (192) | (802) | −85±0.5 | −356±2 | 70O'H/HUB | 15930-75-3 |
| | IP is onset of photoelectron band. | | | | | | |
| $F_3OP^+$ | | | | | | | |
| $POF_3$ | 12.76±0.01 | (−5) | (−23) | −300±2 | −1254±8 | 85JANAF | 13478-20-1 |
| | | *(−3)* | *(−14)* | *−298±2* | *−1245±8* | | |
| | See also: 83NES/MIL. | | | | | | |
| $F_3OV^+$ | | | | | | | |
| $VOF_3$ | (13.88±0.05) | (25) | (105) | −295.0±7.0 | −1234±29 | 75FLE/SVE | 13709-31-4 |
| $F_3P^+$ | | | | | | | |
| $PF_3$ | 11.44 | (35) | (146) | −229±1 | −958±4 | 85JANAF | 7783-55-3 |
| | | *(36)* | *(151)* | *−228±1* | *−953±4* | | |
| | IP from 84BER/GRE. See also: 83NES/MIL, 75TOR/WES, 82LEV/LIA. | | | | | | |
| $F_3PS^+$ | | | | | | | |
| $F_3PS$ | ≤11.05±0.035 | (≤14) | (≤57) | −241±15 | −1009±63 | 85JANAF | 2404-52-6 |
| | | *(≤16)* | *(≤65)* | *−239±15* | *−1001±63* | | |
| $F_3Sb^+$ | | | | | | | |
| $SbF_3$ | (12.1) | (80) | (334) | −199 | −833 | 81WOO | 7783-56-4 |
| | IP is onset of photoelectron band(83NOV/POT). | | | | | | |
| $F_3Si^+$ | | | | | | | |
| $SiF_3$ | (9.3) | (−24) | (−99) | −239±5 | −1000±21 | 83WAL | |
| | | *(−23)* | *(−96)* | *−238±5* | *−996±21* | | |
| | From appearance potential (13.33 eV) in $CH_3SiF_3$. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $F_3Ti^+$ | | | | | | | |
| $TiF_3$ | (10.5±0.5) | (−36) | (−151) | −278 | −1164 | 81WOO | 7783-57-5 |
| | | *(−35)* | *(−147)* | *−277* | *−1160* | | |
| $F_3W^+$ | | | | | | | |
| $WF_3$ | (9.0±0.2) | (81) | (337) | −127 | −531 | 81WOO | 51621-17-1 |
| $F_3Xe^+$ | | | | | | | |
| $XeF_3$ | | 234 | 981 | | | | |
| | From appearance potential (13.10 eV) in $XeF_4$. | | | | | | |
| $F_4Ge^+$ | | | | | | | |
| $GeF_4$ | (15.5) | (73) | (306) | −284 | −1190 | 81WOO | 7783-58-6 |
| | IP is onset of photoelectron band (75LLO/ROB). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | kJ/mol | $\Delta_f H$(Neutral) kcal/mol | kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $F_4HSi^+$ | | | | | | | |
| $SiF_3FH$ | | −140 | −588 | | | | |
| | From proton affinity of $SiF_4$( RN 7783-61-1)(84REE/MUJ). PA = 120.2 kcal/mol, 503. kJ/mol. | | | | | | |
| $F_4Mo^+$ | | | | | | | |
| $MoF_4$ | (9.9) | (0) | (1) | −228 | −954 | 81WOO | 23412-45-5 |
| | | *(1)* | *(4)* | *−227* | *−951* | | |
| $F_4MoO^+$ | | | | | | | |
| $MoOF_4$ | 13.8 | 2 | 6 | −317 | −1325 | 86BUR/FAW | 14459-59-7 |
| | | *3* | *13* | *−315* | *−1318* | | |
| | IP is onset of photoelectron band (81VOV/DUD). | | | | | | |
| $F_4MoS^+$ | | | | | | | |
| $MoSF_4$ | (12.6±0.3) | (58) | (245) | −232±7 | −971±29 | 80MAL/ALI | 70487-60-4 |
| | IP from 80MAL/ALI, 80MAL/ALI2. | | | | | | |
| $F_4N_2^+$ | | | | | | | |
| $N_2F_4$ | 11.94±0.03 | 267 | 1119 | −8 | −33 | 84BER/GRE | 10036-47-2 |
| | | *270* | *1131* | *−5* | *−21* | | |
| | IP from 84BER/GRE. | | | | | | |
| $F_4ORe^+$ | | | | | | | |
| $ReOF_4$ | 10.5 | −22 | −91 | −264 | −1104 | 86BUR/FAW | 17026-29-8 |
| | IP is onset of photoelectron band (81VOV/DUD). | | | | | | |
| $F_4OS^+$ | | | | | | | |
| $SOF_4$ | (12.3) | (61) | (254) | −223±11 | −933±44 | 87HER | 13709-54-1 |
| | IP is onset of photoelectron band (81COS/LLO). | | | | | | |
| $F_4OW^+$ | | | | | | | |
| $WOF_4$ | 13.6 | −28 | −119 | −342 | −1431 | 86BUR/FAW | 13520-79-1 |
| | | *−27* | *−111* | *−340* | *−1423* | | |
| | IP is onset of photoelectron band (81VOV/DUD). | | | | | | |
| $F_4P_2^+$ | | | | | | | |
| $P_2F_4$ | ≤9.28 | *≤−56* | *≤−235* | *−270* | *−1130* | 84BER/GRE | 13824-74-3 |
| | IP from 84BER/GRE, 82LEV/LIA. 0 K values. | | | | | | |
| $F_4Pb^+$ | | | | | | | |
| $PbF_4$ | (10.4±0.3) | (42) | (175) | −198 | −828 | 81WOO | 7783-59-7 |
| | | *(41)* | *(170)* | *−197* | *−823* | | |
| $F_4Pt^+$ | | | | | | | |
| $PtF_4$ | (12.83±0.28) | (171) | (714) | −125±6 | −524±25 | 83KOR/BON | 13455-15-7 |
| | IP from 83KOR/BON. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $F_4S^+$ | | | | | | | |
| $SF_4$ | 12.03±0.05 | 95 | 397 | −182±5 | −763±21 | 85JANAF | 7783-60-0 |
| | | *98* | *408* | *−181±5* | *−757±21* | | |
| | See also: 81COS/LLO. | | | | | | |
| $F_4SW^+$ | | | | | | | |
| $WSF_4$ | (≤12.0±0.2) | (≤5) | (≤21) | ≤−272±9 | ≤−1137±38 | 81MAL/ALI | 41831-80-5 |
| | IP from 81MAL/ALI. | | | | | | |
| $F_4S_2^+$ | | | | | | | |
| $F_3SSF$ | (10.15±0.10) | (76) | (319) | −158±6 | −660±24 | 87HER | 27245-05-2 |
| | IP from 80GOM/HAA. | | | | | | |
| $F_4Si^+$ | | | | | | | |
| $SiF_4$ | (15.7) | (−24) | (−100) | −386.0±0.3 | −1615±1 | 85JANAF | 7783-61-1 |
| | | *(−23)* | *(−94)* | *−384.6±0.3* | *−1609±1* | | |
| | IP is onset of photoelectron band. (75LLO/ROB, 82BIE/ASB, 82LEV/LIA) | | | | | | |
| $F_4U^+$ | | | | | | | |
| $UF_4$ | (9.51) | (−163) | (−681) | −382 | −1599 | 82TN270 | 10049-14-6 |
| | | *(−162)* | *(−676)* | *−381* | *−1594* | | |
| $F_4W^+$ | | | | | | | |
| $WF_4$ | (9.89±0.10) | (−18) | (−75) | −246 | −1029 | 81WOO | 13766-47-7 |
| $F_4Xe^+$ | | | | | | | |
| $XeF_4$ | 12.65±0.1 | 242 | 1015 | −49±0.2 | −206±1 | 72JOH/MAL | 13709-61-0 |
| $F_5I^+$ | | | | | | | |
| $IF_5$ | 12.943±0.005 | 106 | 445 | −201±0.5 | −840±2 | 85JANAF | 7783-66-6 |
| | | *108* | *453* | *−199±0.5* | *−832±2* | | |
| $F_5Mo^+$ | | | | | | | |
| $MoF_5$ | 10.5±0.3 | −54 | −228 | −297±1 | −1241±4 | 85JANAF | 13819-84-6 |
| | | *−53* | *−223* | *−295±1* | *−1236±4* | | |
| | IP from 80MAL/ALI2. | | | | | | |
| $F_5ORe^+$ | | | | | | | |
| $ReOF_5$ | (13.2±0.1) | (21) | (88) | −283 | −1186 | 81WOO | 23377-53-9 |
| $F_5P^+$ | | | | | | | |
| $PF_5$ | (15.1) | (−33) | (−139) | −381 | −1596 | 82TN270 | 7647-19-0 |
| | | *(−30)* | *(−127)* | *−379* | *−1584* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $F_5S^+$ | | | | | | | |
| $SF_5$ | 10.5±0.1 | 23 | 97 | −219 | −915.9 | 81BAB/STR | 10546-01-7 |
| | | *25* | *106* | *−216* | *−906* | | |
| | IP from charge exchange bracketing experiments (81BAB/STR);<br>$\Delta_fH$(Ion) from equilibrium: $CF_3^+ + SF_6 = SF_5^+ + CF_4$ (81BAB/STR). | | | | | | |

**Table 1. Positive Ion Table - Continued**

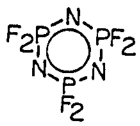
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$F_5U^+$** | | | | | | | |
| $UF_5$ | (11.4) | (−200) | (−837) | −463 | −1937 | 82TN270 | 13775-07-0 |
| | | *(−199)* | *(−832)* | *−462* | *−1932* | | |
| **$F_5W^+$** | | | | | | | |
| $WF_5$ | (10.03±0.10) | (−103) | (−429) | −334 | −1397 | 81WOO | 19357-83-6 |
| **$F_6Mo^+$** | | | | | | | |
| $MoF_6$ | (14.5±0.1) | (−38) | (−159) | −372.4±0.2 | −1558±1 | 85JANAF | 7783-77-9 |
| | | *(−36)* | *(−152)* | *−370.7±0.2* | *−1551± 1* | | |
| **$F_6N_3P_3^+$** | | | | | | | |
|  | 11.58 | (−245) | (−1024) | −512 | −2141 | *EST | 15599-91-4 |
| | IP form 82LEV/LIA and 81CLA/SOW. | | | | | | |
| **$F_6Re^+$** | | | | | | | |
| $ReF_6$ | (11.0) | (−69) | (−288) | −322 | −1349 | 84BAR/YEH | 10049-17-9 |
| | IP from 80VOV/DUD. | | | | | | |
| **$F_6S^+$** | | | | | | | |
| $SF_6$ | 15.33±0.03 | 62 | 259 | −291.7±0.2 | −1220.5±.8 | 85JANAF | 2551-62-4 |
| | | *65* | *273* | *−288.3±0.2* | *−1206.5±.8* | | |
| | See also: 82BIE/ASB. | | | | | | |
| **$F_6U^+$** | | | | | | | |
| $UF_6$ | 14.00±0.10 | −190 | −796 | −513 | −2147 | 82TN270 | 7783-81-5 |
| | | *−189* | *−791* | *−512* | *−2141* | | |
| **$F_6Xe^+$** | | | | | | | |
| $XeF_6$ | 12.19±0.02 | 214 | 897 | −67±0.5 | −279±2 | 72JOH/MAL | 13693-09-9 |
| **$F_7Re^+$** | | | | | | | |
| $ReF_7$ | (14.1±0.1) | (−16) | (−69) | −342±3 | −1429±13 | 84BAR/YEH | 17029-21-9 |
| **$Fe^+$** | | | | | | | |
| Fe | 7.870 | 281 | 1175 | 99 | 416 | 82TN270 | 7439-89-6 |
| | | *280* | *1173* | *99* | *414* | | |
| | See also: 82DYK/GRA. | | | | | | |
| **$FeH^+$** | | | | | | | |
| FeH | | (283) | (1184) | | | | 15600-68-7 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM3). See also: 81ARM/HAL, 84HAL/KLE. | | | | | | |
| **$FeHO^+$** | | | | | | | |
| FeOH | 7.9±0.2 | 211 | 884 | | | 80MUR | 12315-09-2 |
| | | *(214)* | *(895)* | *32* | *133* | | |
| | IP from 80MUR. $\Delta_f H$(Ion) at 298 K from proton affinity of FeO (84CAS/FRE). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $FeI^+$ | | | | | | | |
| FeI | (7.8±0.5) | *(247)* | *(1033)* | *(67)* | *(280)* | 84GRA/ROS2 | |
| | $\Delta_fH$(Ion) from 84GRA/ROS2. Cited IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). See also: 85GRA/ROS. 0 K values. | | | | | | |
| $FeI_2^{+\cdot}$ | | | | | | | |
| $FeI_2$ | 9.3 | *(233)* | *(976)* | *(19)* | *(79)* | 84GRA/ROS2 | 7783-86-0 |
| | IP from 84GRA/ROS. See also: 84GRA/ROS2, 85GRA/ROS. 0 K values. | | | | | | |
| $FeO^+$ | | | | | | | |
| FeO | 8.9±0.1 | 265.2 | 1109.7 | 60.0±5 | 251.0±21 | 85JANAF | 1345-25-1 |
| | | *265.3* | *1109.8* | *60.0±5* | *251.1±21* | | |
| | IP from 82ARM/HAL. See also: 84JAC/JAC, 81ARM/HAL, 81KAP/STA, 80MUR. | | | | | | |
| $FeV^+$ | | | | | | | |
| VFe | (5.4) | *(302)* | *(1264)* | *177* | *743* | 85HET/FRE | |
| | $\Delta_fH$(Ion) and IP from 85HET/FRE. 0 K values. | | | | | | |
| $Fe_2^+$ | | | | | | | |
| $Fe_2$ | 6.30±0.01 | *325* | *1361* | *180* | *753* | 82SHI/GIN | 12596-01-9 |
| | IP from 84ROH/COX. 0 K values. | | | | | | |
| $Fm^+$ | | | | | | | |
| Fm | 6.64±0.11 | | | | | | 7440-72-4 |
| $Ga^+$ | | | | | | | |
| Ga | 5.999 | 203 | 851 | 65.0 | 272.0 | 85JANAF | 7440-55-3 |
| | | *203* | *850* | *64.8* | *271.0* | | |
| | See also: 85HIR/STR. | | | | | | |
| $GaI^+$ | | | | | | | |
| GaI | (9.0±0.3) | (219) | (915) | 11.1 | 46.4 | 79HUB/HER | 15605-68-2 |
| | | *(219)* | *(917)* | *11.6* | *48.5* | | |
| $GaI_3^+$ | | | | | | | |
| $GaI_3$ | 9.40 | 183 | 765 | −34 | −142 | 82TN270 | 13450-91-4 |
| $GaO^+$ | | | | | | | |
| GaO | (9.4±0.5) | (257) | (1074) | 40±10 | 167±42 | 83PED/MAR | 12024-08-7 |
| | | *(257)* | *(1074)* | *40* | *167* | | |
| $Gd^+$ | | | | | | | |
| Gd | 6.1502±0.0006 | 237 | 991 | 95 | 398 | 82TN270 | 7440-54-2 |
| | | *237.2* | *992.3* | *95.3* | *398.9* | | |
| $GdO^+$ | | | | | | | |
| GdO | (5.75±0.1) | (116) | (486) | −16±3 | −69±13 | 83PED/MAR | 12024-77-0 |
| | | *(116)* | *(484)* | *−17* | *−71* | | |
| | See also: 80MUR/HIL. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$GdS^+$** | | | | | | | |
| GdS | (6.9±0.6) | *(197)* | *(825)* | *38* | *159* | 82TN270 | 12134-74-6 |
| | 0 K values. | | | | | | |
| **$Ge^+$** | | | | | | | |
| Ge | 7.899 | 272.2 | 1138.7 | 90.0 | 376.6 | 82TN270 | 7440-56-4 |
| | | *271.5* | *1135.9* | *89.3* | *373.8* | | |
| **$GeH_4^+$** | | | | | | | |
| $GeH_4$ | 11.33 | 283 | 1184 | 22 | 91 | 64GUN/GRE | 7782-65-2 |
| | | *285* | *1195* | *24* | *102* | | |
| **$GeH_5^+$** | | | | | | | |
| $GeH_5$ | | 221 | 926 | | | | |
| | From proton affinity of $GeH_4$ (RN 7782-65-2) (80SEN/ABE). PA = 166.2 kcal/mol, 695. kJ/mol. | | | | | | |
| **$GeI_2^+$** | | | | | | | |
| $GeI_2$ | (8.9) | (216) | (906) | 11.2 | 46.9 | 82TN270 | 13573-08-5 |
| | IP is onset of photoelectron band (83JON/VAN). | | | | | | |
| **$GeI_4^+$** | | | | | | | |
| $GeI_4$ | (9.42) | (204) | (852) | −14 | −57 | 82TN270 | 13450-95-8 |
| | | *(205)* | *(857)* | *−12.3* | *−51.5* | | |
| **$GeO^+$** | | | | | | | |
| GeO | 11.25±0.01 | 250 | 1044 | −9.9±0.7 | −41±3 | 84RAU/SCH | 20619-16-3 |
| | | *250* | *1044* | *−9.9* | *−41* | | |
| **$GeS^+$** | | | | | | | |
| GeS | 9.98±0.02 | 252 | 1055 | 22 | 92 | 82TN270 | 12025-32-0 |
| **$GeSe^+$** | | | | | | | |
| GeSe | (9.3) | (230) | (964) | 23 | 96 | 77PED/RYL | 12065-10-0 |
| | | *(237)* | *(993)* | *23* | *96* | | |
| | IP is onset of photoelectron band. | | | | | | |
| **$GeSi^+$** | | | | | | | |
| GeSi | 8.2±0.3 | *315* | *1319* | *126* | *528* | 79HUB/HER | 12025-36-4 |
| | 0 K values. | | | | | | |
| **$Ge_2^+$** | | | | | | | |
| $Ge_2$ | (7.8) | (293) | (1226) | 113 | 473 | 86KIN/NAG | 12596-05-3 |
| | | *(293)* | *(1224)* | *113* | *473* | | |
| **$Ge_2H_6^+$** | | | | | | | |
| $Ge_2H_6$ | (12.5±0.3) | (327) | (1368) | 38.8 | 162 | 64GUN/GRE | 13818-89-8 |
| **$Ge_3H_8^+$** | | | | | | | |
| $Ge_3H_8$ | (9.6±0.3) | (276) | (1153) | 54.2 | 227 | 64GUN/GRE | 14691-44-2 |

## Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $H^+$ | | | | | | | |
| H | 13.598 | 365.7 | 1530.0 | 52.10 | 217.999 | 85JANAF | 12385-13-6 |
| | | *365.2* | *1528.0* | *51.63* | *216.035* | | |
| $HHe^+$ | | | | | | | |
| HHe | | 323 | 1352 | | | | 13766-24-0 |
| | $\Delta_fH$(Ion) from 79HUB/HER. Corresponding proton affinity of He = 42.5 kcal/mol, 178. kJ/mol. | | | | | | |
| $HI^+$ | | | | | | | |
| HI | 10.386±0.001 | 245.8 | 1028.5 | 6.3±0.05 | 26.4±0.2 | 85JANAF | 10034-85-2 |
| | | *246.3* | *1030.6* | *6.8±0.05* | *28.5±0.2* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $HK^+$ | | | | | | | |
| KH | (8.0±1.0) | (214) | (895) | 29±3 | 123±15 | 85JANAF | 7693-26-7 |
| | | *(215)* | *(896)* | *30±3* | *126±15* | | |
| | IP from 82FAR/SRI. | | | | | | |
| $HKO^+$ | | | | | | | |
| KOH | (7.50±0.15) | (117) | (491) | −56 | −233 | 81LIN/BES | 1310-58-3 |
| | | *(119)* | *(497)* | *−54* | *−227* | | |
| | See also: 82FAR/SRI. | | | | | | |
| $HKr^+$ | | | | | | | |
| KrH | | 264 | 1105 | | | | |
| | From proton affinity of Kr (RN 7439-90-9). PA = 101.6 kcal/mol, 425. kJ/mol. | | | | | | |
| $HLi^+$ | | | | | | | |
| LiH | 7.7 | (211) | (882) | 33.3±0.01 | 139.2±0.04 | 79HUB/HER | 7580-67-8 |
| | | *(211)* | *(882)* | *33.3±0.01* | *139.4±0.04* | | |
| | IP from 79HUB/HER. | | | | | | |
| $HLi_2O^+$ | | | | | | | |
| $Li_2OH$ | | 37 | 155 | | | | |
| | From reaction enthalpies of $Li_2OH^+$ ions (84BUT/KUD). Corresponding proton affinity of $Li_2O$ (RN 12057-24-8) is 289 kcal/mol, 1208 kJ/mol. | | | | | | |
| $HMgO^+$ | | | | | | | |
| MgOH | 7.5±0.3 | *(143)* | *(599)* | *−30* | *−125* | 81MUR | 12141-11-6 |
| | $\Delta_fH$(Ion) from 81MUR. 0 K values. | | | | | | |
| $HMn^+$ | | | | | | | |
| MnH | (7.8) | *(242)* | *(1011)* | *(61)* | *(256)* | 79HUB/HER | 14452-76-7 |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (86ELK/ARM2). See also: 81ARM/HAL. IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). 0 K values. | | | | | | |
| $HMn_2^+$ | | | | | | | |
| $Mn_2H$ | | *(284)* | *(1186)* | | | | |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (86ARM). 0 K value. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $HMo^+$ | | | | | | | |
| MoH | | *(331)* | *(1385)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction. 0 K value. | | | | | | |
| $HN^+$ | | | | | | | |
| NH | 13.49±0.01 | 401.1 | 1678.2 | 90.0±4.0 | 376.6±16.7 | 85JANAF | 13774-92-0 |
| | | *401.1* | *1678.1* | *90.0±4.0* | *376.5±16.7* | | |
| | $\Delta_f H$(Ion) from appearance potential determination (85GIB/GRE). | | | | | | |
| $HNO^+$ | | | | | | | |
| NOH | | 274.3 | 1147.7 | | | | |
| | | *274.8* | *1149.8* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (82KUT/GOO). | | | | | | |
| HNO | (10.1) | (256.3) | (1072.3) | 24 | 100 | 82BAU/COX | 14332-28-6 |
| | | *(256.8)* | *(1074.4)* | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (82KUT/GOO).<br>IP is $\Delta_f H$(Ion)-$\Delta_f H$(Neutral). | | | | | | |
| $HNOS^+$ | | | | | | | |
| HN=S=O | (11.3) | (302) | (1265) | 41.7 | 175 | 82OLE/TUR | 13817-04-4 |
| | IP is onset of photoelectron band. | | | | | | |
| $HNO_2^+$ | | | | | | | |
| $HNO_2$ | ≤11.3 | 234 | 977 | −19 | −80 | 82BAU/COX | 7782-77-6 |
| | | *≤243* | *≤1018* | *−17* | *−72* | | |
| | $\Delta_f H$(Ion) at 298 K from proton affinity of $NO_2$ (RN 10102-44-0) (84POL/MUN).<br>PA = 140 kcal/mol, 586 kJ/mol. | | | | | | |
| $HNO_3^+$ | | | | | | | |
| $HNO_3$ | 11.95±0.01 | 244 | 1018 | −32 | −135 | 82BAU/COX | 7697-37-2 |
| | | *246* | *1028* | *−30* | *−125* | | |
| $HN_2^+$ | | | | | | | |
| $HN_2$ | | *247.5* | *1035.5* | | | | |
| | From proton affinity of $N_2$; threshold determination (82LEV/LIA) gives the same value.<br>PA = 118.2 kcal/mol, 494.5 kJ/mol. | | | | | | |
| $HN_2O^+$ | | | | | | | |
| HNNO | | 246 | 1031 | | | | |
| | From proton affinity of $N_2O$ (RN 10024-97-2). See also: 85MCM/KEB, 85MCM/KEB2.<br>PA = 138.8 kcal/mol, 581 kJ/mol. | | | | | | |
| $HN_3^+$ | | | | | | | |
| $HN_3$ | 10.72±0.025 | 317.5 | 1328.3 | 70.3 | 294.1 | 82TN270 | 7782-79-8 |
| | | *318.9* | *1334.8* | *71.8* | *300.5* | | |
| $HNb^+$ | | | | | | | |
| NbH | | *(330)* | *(1380)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction. 0 K value. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$HNe^+$** | | | | | | | |
| NeH | | 318 | 1329 | | | | |
| | $\Delta_fH$(Ion) from 68CHU/RUS. Corresponding proton affinity of Ne = 48.1 kcal/mol, 201. kJ/mol. | | | | | | |
| **$HNi^+$** | | | | | | | |
| NiH | (≤9.0) | *(291)* | *(1216)* | *>(83)* | *>(347)* | 79HUB/HER | 14332-32-2 |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (86ELK/ARM4). See also: 80ARM/BEA, 81ARM/HAL. IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). 0 K values. | | | | | | |
| **$HO^+$** | | | | | | | |
| OH | 13.00 | 309.1 | 1293.3 | 9.3±0.3 | 39.0±1.2 | 85JANAF | 3352-57-6 |
| | | *309.0* | *1292.7* | *9.2±0.3* | *38.4±1.2* | | |
| | $\Delta_fH$(Ion) from appearance potential measurements; IP derived from $\Delta_fH$(Ion)-$\Delta_fH$(Neutral) is in good agreement with the experimentally determined value of 13.01 eV. See also: 84VAN/DEL. | | | | | | |
| **$HOSr^+$** | | | | | | | |
| SrOH | 5.1±0.2 | *74* | *309* | *−44* | *−183* | 83MUR | |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (83MUR); IP is $\Delta_fH$(Ion) - $\Delta_fH$(Neutral). 0 K values. | | | | | | |
| **$HO_2^+$** | | | | | | | |
| $HO_2$ | 11.35±0.01 | 264.2 | 1105.5 | 2.5 | 10.5 | 82TN270 | 3170-83-0 |
| | | *264.9* | *1108.5* | *3.2* | *13.4* | | |
| | IP from 81DYK/JON. Value of $\Delta_fH$(Ion) from appearance potential measurements corrected to 298 K: 264.8 kcal/mol, 1107.9 kJ/mol. | | | | | | |
| **$HO_2S^+$** | | | | | | | |
| OSOH | | 143 | 597 | | | | |
| | From proton affinity of $SO_2$ (RN 7446-09-5) (85MCM/KEB, 85MCM/KEB2) re-evaluated relative to CO standard (84LIA/LIE). PA = 152.1 kcal/mol, 636. kJ/mol. | | | | | | |
| **$HO_3S^+$** | | | | | | | |
| $O_2SOH$ | | (133) | (557) | | | | |
| | From proton affinity of $SO_3$ (RN 7446-11-9). PA = (138) kcal/mol, (577) kJ/mol. | | | | | | |
| **$HP^+$** | | | | | | | |
| PH | 10.18±0.1 | 291 | 1218 | 56±2 | 236±8 | 86BER/CUR | 13967-14-1 |
| | | *291* | *1219* | *57±2* | *237±8* | | |
| | $\Delta_fH$(Ion) from 79HUB/HER, 86BER/CUR. IP from 86BER/CUR. | | | | | | |
| **$HPd^+$** | | | | | | | |
| PdH | | *(281)* | *(1176)* | | | | |
| | $\Delta_fH$(Ion) from onset of endothermic reaction (86ELK/ARM). 0 K value. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $HS^+$ | | | | | | | |
| SH | 10.37±0.01 | 272.4 | 1139.8 | 33.3±1.2 | 139.3±5.0 | 85JANAF | 13940-21-1 |
| | | *271.8* | *1137.0* | *32.6±1.2* | *136.5±5.0* | | |
| | IP from 79DUN/DYK, $\Delta_f H$(Ion) from 83PRE/TZE, in good agreement with earlier results. See also: 81SMI/ADA. | | | | | | |
| $HSc^+$ | | | | | | | |
| ScH | | *239* | *999* | | | | 33486-02-1 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 87SUN/ARI. 0 K values. | | | | | | |
| $HSe^+$ | | | | | | | |
| SeH | (9.79) | *(258)* | *(1080)* | *(32)* | *(135)* | 79HUB/HER | 13940-22-2 |
| | 0 K values. | | | | | | |
| $HSi^+$ | | | | | | | |
| SiH | 7.89±0.07 | 272.0 | 1138.0 | 90.0±2.0 | 376.7±8.4 | 85JANAF | 13774-94-2 |
| | | *271.5* | *1136.2* | *89.6±2.0* | *374.9±8.4* | | |
| | $\Delta_f H$(Ion) from 84ELK/ARM. IP from 87BOO/ARM. | | | | | | |
| $HTe^+$ | | | | | | | |
| TeH | (9.09) | (244) | (1020) | 34 | 143 | 79HUB/HER | 13940-36-8 |
| $HTi^+$ | | | | | | | |
| TiH | (6.0) | *(265)* | *(1109)* | *(127)* | *(532)* | 79HUB/HER | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (86ELK/ARM). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). 0 K values. | | | | | | |
| $HU^+$ | | | | | | | |
| UH | | 256 | 1070 | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (77ARM/HOD). | | | | | | |
| $HV^+$ | | | | | | | |
| VH | | *(282)* | *(1179)* | | | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). 0 K value. | | | | | | |
| $HXe^+$ | | | | | | | |
| XeH | | 247 | 1034 | | | | |
| | From proton affinity of Xe (RN 7440-63-3). PA = 118.6 kcal/mol, 496. kJ/mol. | | | | | | |
| $HY^+$ | | | | | | | |
| YH | | *(238)* | *(995)* | | | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction. 0 K value. | | | | | | |
| $HZn^+$ | | | | | | | |
| ZnH | (9.4) | (241) | (1008) | (25) | (106) | 79HUB/HER | |
| | From proton affinity of Zn (RN 7440-66-6). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $HZr^+$ | | | | | | | |
| ZrH | | | | 123.4 | 516.3 | 85JANAF | |
| | | *(301)* | *(1260)* | *123.6* | *517.3* | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction. 0 K value. | | | | | | |
| $H_2{}^+$ | | | | | | | |
| $H_2$ | 15.42589±0.00005 | 355.7 | 1488.3 | 0 | 0 | *DEF | 1333-74-0 |
| | | *355.7* | *1488.3* | *0* | *0* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $H_2I^+$ | | | | | | | |
| $H_2I$ | | 225 | 941 | | | | |
| | From proton affinity of HI (RN 10034-85-2) results of 85MCM/KEB re-evaluated relative to CO standard (84LIA/LIE). PA = 147.1 kcal/mol, 615. kJ/mol. | | | | | | |
| $H_2I_2Si^+$ | | | | | | | |
| $SiH_2I_2$ | (9.4) | (208) | (896) | −9±5 | −38±20 | 85JANAF | 13760-02-6 |
| | | *(206)* | *(861)* | *−7±5* | *−28±20* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $H_2KO^+$ | | | | | | | |
| $KOH_2$ | | (47) | (198) | | | | |
| | $\Delta_f H$(Ion) from equilibrium constant determination (69SEA/DZI). | | | | | | |
| $H_2N^+$ | | | | | | | |
| $NH_2$ | 11.14±0.01 | 302.0 | 1263.8 | 45.1±0.3 | 188.7±1.3 | 85GIB/GRE | 15194-15-7 |
| | | *302.7* | *1266.4* | *45.8±0.3* | *191.6±1.3* | | |
| | $\Delta_f H$(Ion) from appearance potential determination is in agreement. IP from 85GIB/GRE. | | | | | | |
| $H_2NO^+$ | | | | | | | |
| $H_2NO$ | | 224.6 | 939.7 | | | | |
| | $\Delta_f H$(Ion) from appearance potential determination (82KUT/GOO). | | | | | | |
| $H_2N_2{}^+$ | | | | | | | |
| (Z)-HN=NH | (9.52±0.05) | (275) | (1150) | 55 | 232 | 82CAS/GOD | 28647-38-3 |
| (E)-HN=NH | (9.59±0.01) | (272) | (1137) | 51 | 212 | 82CAS/GOD | 3618-05-1 |
| $H_2N_3{}^+$ | | | | | | | |
| $H_2NNN$ | | (257) | (1075) | | | | |
| | From proton affinity of $HN_3$ (RN 7782-79-8) (84BEA/EYE). PA = 179 kcal/mol, 749 kJ/mol. | | | | | | |
| $H_2NaO^+$ | | | | | | | |
| $NaOH_2$ | | 71 | 296 | | | | |
| | From proton affinity of NaOH (RN 1310-73-2) (69SEA/DZI). PA = 248 kcal/mol, 1036 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $H_2O^+$ | | | | | | | |
| $H_2O$ | 12.612±0.010 | 233.0 | 975.0 | −57.80 | −241.83 | 85JANAF | 7732-18-5 |
| | | *233.7* | *977.9* | *−57.10* | *−238.92* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $H_2O_2^+$ | | | | | | | |
| $H_2O_2$ | 10.54 | 210 | 881 | −32.6 | −136.3 | 82BAU/COX | 7722-84-1 |
| | | *212* | *887* | *−31.1* | *−130.0* | | |
| | See also: 77ASH/BUR, 81KIM/KAT. | | | | | | |
| $H_2P^+$ | | | | | | | |
| $PH_2$ | 9.824±0.002 | 261 | 1093 | 33.3 | 139.5 | 86BER/CUR | |
| | | *261* | *1090* | *34.0±0.6* | *142.2±2.5* | | |
| | IP from 86BER/CUR. See also: 82DYK/JON2. 0 K values. | | | | | | |
| $H_2S^+$ | | | | | | | |
| $H_2S$ | 10.453±0.008 | 236 | 988 | −4.9 | −20.5±0.8 | 85JANAF | 7783-06-4 |
| | | *237* | *991* | *−4.2* | *−17.6±0.8* | | |
| | IP is average of several spectroscopic and photoionization-onset determinations (77ROS/DRA, 82LEV/LIA, 84BLA/WAL, 83PRE/TZE). See also: 81SMI/ADA, 81WAL/BLA, 81KIM/KAT. | | | | | | |
| $H_2S_2^+$ | | | | | | | |
| $H_2S_2$ | (9.3) | (218) | (913) | 4 | 16 | 82TN270 | 13465-07-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $H_2Sc^+$ | | | | | | | |
| HScH | | *(238)* | *(996)* | | | | 13598-30-6 |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (84TOL/BEA). See also: 87SUN/ARI. 0 K value. | | | | | | |
| $H_2Se^+$ | | | | | | | |
| $H_2Se$ | 9.882±0.001 | 235 | 983 | 7 | 30 | 82TN270 | 7783-07-5 |
| | | *236* | *987* | *8* | *34* | | |
| $H_2Si^+$ | | | | | | | |
| $SiH_2$ | 8.92±0.07 | 276.1 | 1155.2 | 69±2 | 289±8 | 87BOO/ARM | 13825-90-6 |
| | IP and $\Delta_f H$(Ion) from 87BOO/ARM, in agreement with unpublished data of R.R. Corderman and J.L. Beauchamp. See also: 83DYK/JON2, 84CHA/HIL. | | | | | | |
| $H_2Te^+$ | | | | | | | |
| $H_2Te$ | 9.138±0.005 | 235 | 982 | 24 | 100 | 82TN270 | 7783-09-7 |
| $H_3^+$ | | | | | | | |
| $H_3$ | | 264.5 | 1106.6 | | | | 12184-91-7 |
| | | *265* | *1107* | | | | |
| | From proton affinity of $H_2$ (RN 1333-74-0) (84ADA/SMI). PA = 101.2 kcal/mol, 423.4 kJ/mol. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $H_3ISi^+$ | | | | | | | |
| $SiH_3I$ | (9.5) | (219) | (915) | −0.5±4 | −2±17 | 85JANAF | 13598-42-0 |
| | | *(221)* | *(925)* | *2±4* | *8±17* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $H_3N^{+\cdot}$ | | | | | | | |
| $NH_3$ | 10.16±0.01 | 223.2 | 934.0 | −11.0 | −45.9±0.4 | 85JANAF | 7664-41-7 |
| | | *224.9* | *941.0* | *−9.3* | *−38.9±0.4* | | |
| | See also: 81KIM/KAT, 73RAB/KAR. | | | | | | |
| $H_3NO^+$ | | | | | | | |
| $NH_2OH$ | 10.00 | (221) | (923) | −10 | −42 | 69BEN/CRU | 7803-49-8 |
| | IP from 83KOP/MOL. See also: 81KIM/KAT, 82KUT/GOO. | | | | | | |
| $H_3O^+$ | | | | | | | |
| $H_3O$ | | 141 | 591 | | | | |
| | | *143* | *597* | | | | |
| | $\Delta_fH$(Ion) at 298 K from proton affinity of $H_2O$; $\Delta_fH$(Ion) at 0 K from appearance potential from $(H_2O)_2$ (77NG/TRE). PA = 166.5 kcal/mol, 697. kJ/mol. | | | | | | |
| $H_3O_2^+$ | | | | | | | |
| $H_2OOH$ | | 171 | 716 | | | | |
| | From proton affinity of $H_2O_2$ (RN 7722-84-1). PA = 162. kcal/mol, 678. kJ/mol. | | | | | | |
| $H_3O_4S^+$ | | | | | | | |
| $(HO)_3SO$ | | (21) | (88) | | | | |
| | From proton affinity of $H_2SO_4$ (RN 7664-93-9). PA = (169) kcal/mol, (707) kJ/mol. | | | | | | |
| $H_3P^+$ | | | | | | | |
| $PH_3$ | 9.869±0.002 | 229 | 957 | 1.3±0.4 | 5.4±1.7 | 61GUN/GRE | 7803-51-2 |
| | | *231* | *966* | *3.1* | *13.3* | | |
| | IP from 83MAR/REI, 86BER/CUR. See also: 82COW/KEM. | | | | | | |
| $H_3S^+$ | | | | | | | |
| $H_3S$ | | 190 | 797 | | | | |
| | From proton affinity of $H_2S$ (RN 7783-06-4). See also: 83PRE/TZE2, 84BLA/WAL, 83ERM/AKO. PA = 170.2 kcal/mol, 712. kJ/mol. | | | | | | |
| $H_3Sb^+$ | | | | | | | |
| $SbH_3$ | 9.54±0.03 | 255 | 1066 | 35 | 145 | 82TN270 | 7803-52-3 |
| | | *257* | *1074* | *37* | *153* | | |
| $H_3Se^+$ | | | | | | | |
| $H_3Se$ | | 202 | 843 | | | | |
| | From proton affinity of $H_2Se$ (RN 7783-07-5). PA = 171.3 kcal/mol, 717. kJ/mol. | | | | | | |
| $H_3Si^+$ | | | | | | | |
| $SiH_3$ | 8.14±0.01 | 237.1 | 992 | 48.5±1.5 | 202.9±6.3 | 87BOO/ARM | 13765-44-1 |
| | IP from 83DYK/JON2. See also: 84CHA/HIL, 85DIN/CAS, 87BOO/ARM. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $H_3Te^+$ | | | | | | | |
| $TeH_3$ | | 214 | 894 | | | | |
| | $\Delta_f H$(Ion) from proton affinity of $H_2Te$ (RN7783-09-7)(86KAR/JAS). PA = 176 kcal/mol, 736 kJ/mol. | | | | | | |
| $H_4N^+$ | | | | | | | |
| $NH_4$ | (4.73±0.06) | (151) | (630) | | | | |
| | $\Delta_f H$(Ion) from proton affinity of $NH_3$(RN 7664-41-7). IP from neutralized ion-beam spectroscopy data (82GEL/CLE). PA = (204.0) kcal/mol, (854.) kJ/mol. | | | | | | |
| $H_4N_2^+$ | | | | | | | |
| $N_2H_4$ | 8.1±0.15 | (210) | (876) | 22.8±0.2 | 95.3±0.8 | 85JANAF | 302-01-2 |
| | | *(213)* | *(891)* | *26.1±0.2* | *109.4±0.8* | | |
| | From charge transfer equilibrium constant determinations(84MAU/NEL). See also: 81KIM/KAT. | | | | | | |
| $H_4N_4^+$ | | | | | | | |
| (E)-$H_2NN=NNH_2$ | (≤8.99) | (≤260) | (≤1089) | 53 | 222 | 82TN270 | 54410-57-0 |
| $H_4P^+$ | | | | | | | |
| $PH_4$ | | 178 | 746 | | | | |
| | From proton affinity of $PH_3$ (RN 7803-51-2). PA = 188.6 kcal/mol, 789. kJ/mol. | | | | | | |
| $H_4P_2^+$ | | | | | | | |
| $P_2H_4$ | 8.8±0.1 | (219) | (918) | 16 | 69 | *EST | 13445-50-6 |
| | IP is onset of photoelectron band. | | | | | | |
| $H_4Si^+$ | | | | | | | |
| $SiH_4$ | 11.65 | 277 | 1159 | 8 | 35 | 81BEL/PER | 7803-62-5 |
| | | *280* | *1170* | *11* | *46* | | |
| $H_4Sn^+$ | | | | | | | |
| $SnH_4$ | (10.75) | (287) | (1200) | 39 | 163 | 82TN270 | 2406-52-2 |
| | | *(290)* | *(1212)* | *42* | *175* | | |
| | The $SnH_4^+$ ion has not been observed. | | | | | | |
| $H_5N_2^+$ | | | | | | | |
| $NH_3NH_2$ | | 184 | 770 | | | | |
| | From proton affinity of hydrazine (RN 302-01-2). PA = 204.7 kcal/mol, 856. kJ/mol. | | | | | | |
| $H_5Si^+$ | | | | | | | |
| $SiH_5$ | | (219) | (917) | | | | |
| | From proton affinity of $SiH_4$ (RN 7803-62-5). PA = (155) kcal/mol, (648) kJ/mol. | | | | | | |
| $H_6Si_2^+$ | | | | | | | |
| $Si_2H_6$ | (9.7) | (243) | (1016) | 19 | 80 | 81BEL/PER | 1590-87-0 |
| | | *(247)* | *(1032)* | *23* | *96* | | |
| | IP is onset of photoelectron band. See also: 84CHA/HIL. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $H_8Si_3^+$ | | | | | | | |
| $Si_3H_8$ | (9.2) | (241) | (1009) | 29 | 121 | 81BEL/PER | 7783-26-8 |
| | IP is onset of photoelectron band. | | | | | | |
| $H_{10}Si_4^+$ | | | | | | | |
| $Si_4H_{10}$ | (8.9) | (244) | (1021) | 39 | 162 | 81WAL | 7783-29-1 |
| | IP is onset of photoelectron band. | | | | | | |
| $He^+$ | | | | | | | |
| He | 24.587 | 567.0 | 2372 | 0 | 0 | *DEF | 7440-59-7 |
| | | *567.0* | *2372* | *0* | *0* | | |
| $HeNe^+$ | | | | | | | |
| HeNe | 20.87 | *481.3* | *2013.9* | *−0.028* | *−0.12* | 79HUB/HER | 12162-16-2 |
| | $\Delta_f H$(Ion) from 78DAB/HER. 0 K values. | | | | | | |
| $He_2^+$ | | | | | | | |
| $He_2$ | 22.223 | *512.4* | *2144.1* | *−0.02* | *−0.09* | 79HUB/HER | 12184-98-4 |
| | IP from 79HUB/HER. 0 K values. | | | | | | |
| $Hf^+$ | | | | | | | |
| Hf | 6.78 | 304 | 1273 | 148 | 619 | 82TN270 | 7440-58-6 |
| | | *304* | *1273* | *148* | *619* | | |
| | IP from 76MEG/MOO. | | | | | | |
| $HfO^+$ | | | | | | | |
| HfO | (7.55±0.1) | (190) | (795) | 16±3 | 67±13 | 83PED/MAR | 12029-22-0 |
| | | *(192)* | *(804)* | *18* | *76* | | |
| $Hg^+$ | | | | | | | |
| Hg | 10.437 | 255.3 | 1068.3 | 14.7 | 61.3 | 82TN270 | 7439-97-6 |
| | | *256.1* | *1071.5* | *15.4* | *64.5* | | |
| | See also: 84LIN/LIA. | | | | | | |
| $HgI_2^+$ | | | | | | | |
| $HgI_2$ | 9.5088±0.0022 | 215.2 | 900.3 | −4.1 | −17.2 | 82TN270 | 7774-29-0 |
| | | *216.7* | *906.6* | *−2.6* | *−10.9* | | |
| | Cited ionization potential (83LIN/TZE) refers to formation of $HgI_2^+(^2\Pi_{3/2})$. Ionization potential for formation of $HgI_2^+(^2\Pi_{1/2})$ is 10.1953±0.0025 eV. See also: 81LEE/POT. | | | | | | |
| $Hg_2^+$ | | | | | | | |
| $Hg_2$ | 9.103±0.010 | 237 | 992 | 27 | 114 | 82HIL | 12596-25-7 |
| | | *239* | *1000* | *29* | *122* | | |
| | IP from 84LIN/LIA. | | | | | | |
| $Ho^+$ | | | | | | | |
| Ho | 6.0216±0.0006 | 211 | 882 | 72 | 301 | 82TN270 | 7440-60-0 |
| | | *211.2* | *883.6* | *72.3* | *302.6* | | |

**Table 1. Positive Ion Table - Continued**

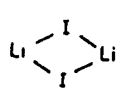
| ION Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| **$HoO^+$** | | | | | | | |
| HoO | (6.17±0.1) | (128) | (534) | −15±6 | −61±25 | 83PED/MAR | 12281-10-6 |
| | | *(126)* | *(528)* | *−16* | *−67* | | |
| | See also: 80MUR/HIL. | | | | | | |
| **$I^+$** | | | | | | | |
| I | 10.451 | 266.5 | 1115.2 | 25.5 | 106.8 | 82BAU/COX | 14362-44-8 |
| | | *266.6* | *1115.6* | *25.6* | *107.2* | | |
| | See also: 81HOA/CAB, 85GRA/ROS. | | | | | | |
| **$IK^+$** | | | | | | | |
| KI | (7.21±0.3) | (136) | (570) | −30.0±0.5 | −125.5±2.1 | 85JANAF | 7681-11-0 |
| | | *(137)* | *(573)* | *−29.2±0.5* | *−122.1±2.1* | | |
| | See also: 82EMO/HOR. | | | | | | |
| **$ILi^+$** | | | | | | | |
| LiI | (7.5) | (151) | (633) | −21.7±2.0 | −91.0±8.4 | 85JANAF | 10377-51-2 |
| | | *(152)* | *(635)* | *−21.3±2.0* | *−89.1±8.4* | | |
| | IP is onset of photoelectron band. | | | | | | |
| **$INa^+$** | | | | | | | |
| NaI | 7.64±0.02 | 157 | 659 | −18.6 | −77.8 | 82TN270 | 7681-82-5 |
| | | *158* | *662* | *−17.9* | *−74.9* | | |
| | See also: 82EMO/HOR, 83HIL/GIN, 84HIL, 82LEL/BAL. | | | | | | |
| **$IRb^+$** | | | | | | | |
| RbI | (7.12±0.1) | (132) | (554) | −32 | −133 | 79HUB/HER | 7790-29-6 |
| | | *(133)* | *(558)* | *−30.9* | *−129.3* | | |
| | See also: 82EMO/HOR. | | | | | | |
| **$ITl^+$** | | | | | | | |
| TlI | 8.47±0.02 | 197 | 824 | 2 | 7 | 82TN270 | 7790-30-9 |
| | | *197* | *823* | *1* | *6* | | |
| | See: 83BAN/BRI. | | | | | | |
| **$I_2^+$** | | | | | | | |
| $I_2$ | 9.3995±0.0012 | 231.7 | 969.3 | 14.9 | 62.4 | 82BAU/COX | 7553-56-2 |
| | | *232.4* | *972.4* | *15.7* | *65.5* | | |
| | See also: 81HOA/CAB, 85GRA/ROS, 81KIM/KAT. | | | | | | |
| **$I_2Li_2^+$** | | | | | | | |
|  | (≤9.23±0.06) | (≤126) | (≤529) | −87±4 | −362±17 | 85JANAF | 37279-36-0 |
| | | *(≤127)* | *(≤532)* | *−85±4* | *−356±17* | | |
| **$I_2Mg^+$** | | | | | | | |
| $MgI_2$ | (9.57±0.03) | (180) | (751) | −41 | −172 | 82TN270 | 10377-58-9 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $I_2O_2W^+$ | | | | | | | |
| $WO_2I_2$ | (10.4±0.4) | (137.5) | (575.4) | −102.3 | −428.0 | 76DEL/HAL | 14447-89-3 |
| $I_2Pb^+$ | | | | | | | |
| $PbI_2$ | 8.86±0.03 | *(205)* | *(856)* | *0.2±1* | *1±4* | 85JANAF | 10101-63-0 |
| | Onset of photoelectron band: 8.6 eV. See: 84NOV/POT2. 0 K values. | | | | | | |
| $I_2Sn^+$ | | | | | | | |
| $SnI_2$ | 8.83±0.1 | 204 | 854 | 0.5 | 2 | 82TPIS | 10294-70-9 |
| | IP from 83HIL/GIN, 84NOV/POT2. | | | | | | |
| $I_2Sr^+$ | | | | | | | |
| $SrI_2$ | (8.3) | (126) | (526) | −65.7±1.5 | −275±6 | 85JANAF | 10476-86-5 |
| | | *(126)* | *(529)* | *−65.0±1.5* | *−272±6* | | |
| | IP is onset of photoelectron band (79LEE/POT2). See also: 82EMO/KIE. | | | | | | |
| $I_3La^+$ | | | | | | | |
| $LaI_3$ | 8.8 | 119 | 498 | −84 | −351 | 82TN270 | |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| $I_3Nd^+$ | | | | | | | |
| $NdI_3$ | 8.7 | 124 | 519 | −76 | −320 | 82TN270 | 13813-24-6 |
| | IP is onset of photoelectron band (83RUS/GOO). | | | | | | |
| $I_4Ti^+$ | | | | | | | |
| $TiI_4$ | (9.1) | (143) | (600) | −66±2 | −278±8 | 85JANAF | 7720-83-4 |
| | | *(145)* | *(606)* | *−65±2* | *−272±8* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $I_4Zr^+$ | | | | | | | |
| $ZrI_4$ | (9.3) | (128) | (534) | −95±2 | −363±8 | 85JANAF | 13986-26-0 |
| | | *(130)* | *(544)* | *−85±2* | *−357±8* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $In^+$ | | | | | | | |
| In | 5.786 | 191.7 | 801.9 | 58.2 | 243.7 | 82TN270 | 7440-74-6 |
| | | *191.6* | *802.6* | *58.2* | *243.3* | | |
| | See also: 82GOM/CHA, 85KAP/LEL. | | | | | | |
| $InS^+$ | | | | | | | |
| InS | (7.0±0.5) | *(218)* | *(911)* | *57* | *236* | 79HUB/HER | 12030-14-7 |
| | 0 K values. | | | | | | |
| $InSe^+$ | | | | | | | |
| InSe | (7.1±0.5) | *(218)* | *(913)* | *55* | *228* | 79HUB/HER | 1312-42-1 |
| | 0 K values. | | | | | | |
| $InTe^+$ | | | | | | | |
| InTe | (7.6±0.5) | *(230)* | *(962)* | *55* | *229* | 79HUB/HER | 12030-19-2 |
| | 0 K values. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $In_2^+$ | | | | | | | |
| $In_2$ | (5.8±0.3) | *(227)* | *(949)* | *93* | *389* | 79HUB/HER | 61178-97-0 |
| | 0 K values. | | | | | | |
| $In_2O^+$ | | | | | | | |
| $In_2O$ | 8.0±0.2 | (174) | (728) | −10 | −43 | 82TPIS | 12030-22-7 |
| | | *(175)* | *(734)* | *−9±5* | *−38±20* | | |
| | IP from 85KAP/LEL, 77ROS/DRA. See also: 82GOM/CHA. | | | | | | |
| $Ir^+$ | | | | | | | |
| Ir | 9.02 | 367 | 1535 | 159 | 665 | 82TN270 | 7439-88-5 |
| | | *366.8* | *1534.6* | *158.8* | *664.3* | | |
| | IP from 79RAU/ACK. | | | | | | |
| $IrO^+$ | | | | | | | |
| IrO | (10.1) | *(367)* | *(1535)* | *(134)* | *(561)* | 79HUB/HER | 12030-48-7 |
| | 0 K values. | | | | | | |
| $IrO_3^+$ | | | | | | | |
| $IrO_3$ | (11.9) | (276) | (1156) | 2 | 8 | 82TN270 | 12030-50-1 |
| $K^+$ | | | | | | | |
| K | 4.341 | 121.4 | 507.8 | 21.3±0.1 | 89.0±0.4 | 85JANAF | 7440-09-7 |
| | | *121.6* | *508.7* | *21.5±0.1* | *89.9±0.4* | | |
| $KLi^+$ | | | | | | | |
| LiK | 4.57±0.04 | 123 | 514 | 17 | 73 | 86IGE/WED | 12030-83-0 |
| | IP from 85KAP/SCH. | | | | | | |
| $KNa^+$ | | | | | | | |
| NaK | 4.41636±0.00017 | *134.2* | *561.5* | *32.4* | *135.4* | 86ZGE/WED | 12056-29-0 |
| | IP from 81LEU/HOF, 85KAP/RAD. 0 K values. | | | | | | |
| $KO^+$ | | | | | | | |
| KO | 7.09±0.1 | 178 | 745 | 15±5 | 61±21 | 83PED/MAR | 12401-70-6 |
| | | *179* | *747* | *15±5* | - *63±21* | | |
| | IP from 82LEV/LIA, 84BUT/KUD. | | | | | | |
| $KRb^+$ | | | | | | | |
| KRb | (3.9±0.1) | *(120)* | *(500)* | *(30)* | *(124)* | 79HUB/HER | 12333-39-0 |
| | IP from 85KAP/SCH. 0 K values. | | | | | | |
| $K_2^+$ | | | | | | | |
| $K_2$ | 4.0637±0.0002 | 124.0 | 518.9 | 30.3 | 126.9 | 79HUB/HER | 25681-80-5 |
| | | *124.8* | *522.3* | *31.1* | *130.3* | | |
| | IP from 85KAP/RAD, 85BRO/CHE, in good agreement with values from 81LEU/HOF, 78HER/SCH, and 84DAO/PET. | | | | | | |
| $K_2O^+$ | | | | | | | |
| $K_2O$ | 4.96±0.2 | (80) | (336) | −34±4 | −142±15 | 79BYK/ELI | 12136-45-7 |
| | IP from 84BUT/KUD. See also: 82FAR/SRI, 84DAO/PET. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $K_2O_2^+$ | | | | | | | |
| $K_2O_2$ | (5) | (44) | (184) | −71±4 | −298±15 | 79BYK/ELI | 17014-71-0 |
| $Kr^+$ | | | | | | | |
| Kr | 13.9997±0.00001 | 322.8 | 1350.8 | 0 | 0 | *DEF | 7439-90-9 |
| | | *322.8* | *1350.8* | *0* | *0* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $KrXe^+$ | | | | | | | |
| KrXe | 11.760±0.014 | *270.8* | *1132.9* | *−0.42* | *−1.77* | 79HUB/HER | 12521-42-5 |
| | See: 82DEH/PRA, 85PRA/DEH2. 0 K values. | | | | | | |
| $Kr_2^+$ | | | | | | | |
| $Kr_2$ | 12.866±0.003 | *296.3* | *1240.9* | *−0.36* | *−1.51* | 79HUB/HER | 12596-40-6 |
| | IP from 82PRA/DEH. 0 K values. | | | | | | |
| $La^+$ | | | | | | | |
| La | 5.577 | 232 | 969 | 103 | 431 | 82TN270 | 7439-91-0 |
| | | *231.7* | *969.4* | *103.1* | *431.3* | | |
| $LaO^+$ | | | | | | | |
| LaO | 4.90±0.1 | 84 | 352 | −29±2 | −121±10 | 83PED/MAR | 12031-20-8 |
| | | *85* | *354* | *−28* | *−119* | | |
| $LaPt^+$ | | | | | | | |
| LaPt | (5.4±0.8) | (243) | (1018) | 119±5 | 497±21 | 81NAP/GIN | 12142-67-5 |
| | IP from 81NAP/GIN. | | | | | | |
| $Li^+$ | | | | | | | |
| Li | 5.392 | 162.4 | 679.6 | 38.1 | 159.4 | 82TN270 | 7439-93-2 |
| | | *162.0* | *678.0* | *37.7* | *157.8* | | |
| | See also: 81NAK/ASA. | | | | | | |
| $LiNa^+$ | | | | | | | |
| LiNa | 5.05±0.04 | 137 | 572 | 20 | 85 | 86IGE/WED | 12333-49-2 |
| | IP from 85KAP/SCH. | | | | | | |
| $LiO^+$ | | | | | | | |
| LiO | (8.45±0.20) | (214) | (894) | 19±0.5 | 79±2 | 83PED/MAR | 12142-77-7 |
| | | *(214)* | *(894)* | *19±0.5* | *79±2* | | |
| | See also: 81NAK/ASA, 79WU/KUD, 84BUT/KUD. | | | | | | |
| $LiOH_2^+$ | | | | | | | |
| $LiOH_2$ | | 69 | 289 | | | | |
| | From proton affinity of LiOH (RN 1310-58-3). PA = 241 kcal/mol, 1007 kJ/mol. | | | | | | |
| $LiRb^+$ | | | | | | | |
| LiRb | 4.3±0.1 | 116 | 485 | 17 | 70 | 86IGE/WED | 12031-70-8 |
| | IP from 85KAP/SCH. | | | | | | |

Table 1. Positive Ion Table - Continued

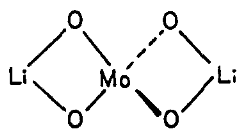
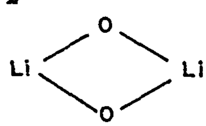
| ION / Neutral | Ionization potential eV | $\Delta_f H$(Ion) kcal/mol | $\Delta_f H$(Ion) kJ/mol | $\Delta_f H$(Neutral) kcal/mol | $\Delta_f H$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $Li_2^+$ | | | | | | | |
| $Li_2$ | 5.1127±0.0003 | 169.5 | 709.2 | 51.6±0.7 | 215.9±3.0 | 85JANAF | 14452-59-6 |
| | | *169.4* | *708.8* | *51.5±0.7* | *215.5±3.0* | | |
| | IP from 83MCG/SCH. See also: 82BIS/DEM. | | | | | | |
| $Li_2MoO_4^+$ | | | | | | | |
|  | (9.7±0.5) | (−22) | (−94) | −246 | −1030 | 81LIN/BES | |
| $Li_2O^+$ | | | | | | | |
| $Li_2O$ | 6.19±0.20 | (103) | (430) | −40 | −167 | 81LIN/BES | 12057-24-8 |
| | | *(103)* | *(431)* | *−40* | *−166* | | |
| | See also: 82IKE/TAM, 81NAK/ASA, 79WU/KUD. | | | | | | |
| $Li_2O_2^+$ | | | | | | | |
|  | (7.88±0.2) | *(84)* | *(350)* | *−98±12* | *−410±50* | 79WU/KUD | 12031-80-0 |
| | IP from 79WU/KUD. 0 K values. | | | | | | |
| $Li_2O_3Si^+$ | | | | | | | |
| $Li_2SiO_3$ | 8.3±0.2 | −99 | −415 | −291 | −1216 | 81NAK/ASA | |
| | IP from 81NAK/ASA. | | | | | | |
| $Li_2O_4W^+$ | | | | | | | |
| $Li_2WO_4$ | (9.2±0.5) | (−29) | (−122) | −241 | −1010 | 81LIN/BES | |
| $Li_3O^+$ | | | | | | | |
| $Li_3O$ | (4.54±0.2) | *(50)* | *(210)* | *−54±10* | *−228±42* | 79WU/KUD | 69235-02-5 |
| | IP from 79WU/KUD. 0 K values. | | | | | | |
| $Lu^+$ | | | | | | | |
| Lu | 5.4259±0.00001 | 227 | 951 | 102 | 428 | 82TN270 | 7439-94-3 |
| | | *227.4* | *951.3* | *102.2* | *427.8* | | |
| $LuO^+$ | | | | | | | |
| LuO | (6.79±0.1) | (153) | (640) | −3.5 | −14.6 | 82TN270 | 12032-02-9 |
| | | *(153)* | *(642)* | *−3* | *−13* | | |
| | A value of 2±17 kJ/mol, 0.5±4 kcal/mol has also been recommended for the 298 K heat of formation of LuO (83PED/MAR). See also: 80MUR/HIL. | | | | | | |
| $Md^+$ | | | | | | | |
| Md | 6.74±0.12 | | | | | | 7440-11-1 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Mg^+$ | | | | | | | |
| Mg | 7.646 | 211.6 | 885.4 | 35.3 | 147.7 | 82TN270 | 7439-95-4 |
| | | *211.3* | *884.2* | *35.0* | *146.5* | | |
| | See also: 81SAS/HAR. | | | | | | |
| $MgO^+$ | | | | | | | |
| MgO | 9.7 | (236±8) | (997±33) | 13.4 | 56.1 | 79HUB/HER | 1309-48-4 |
| | | *(238±8)* | *(997±33)* | *13.5* | *56.5* | | |
| | $\Delta_f H$(Ion) from 81KAP/STA. See also: 81MUR. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $Mg_2H^+$ | | | | | | | |
| MgHMg | | 78 | 327 | | | | |
| | From proton affinity of $Mg_2$ (RN 29904-79-8). PA = (219) kcal/mol, (916) kJ/mol. | | | | | | |
| $Mn^+$ | | | | | | | |
| Mn | 7.435 | 239 | 998 | 67 | 281 | 82TN270 | 7439-96-5 |
| | | *238* | *996* | *67* | *279* | | |
| $MnO^+$ | | | | | | | |
| MnO | 8.65±0.2 | *(240)* | *(1005)* | *41* | *170* | 67CHE/BAR | 1344-43-0 |
| | IP from 82ARM/HAL. See also: 81ARM/HAL, 81KAP/STA. 0 K values. | | | | | | |
| $Mn_2^+$ | | | | | | | |
| $Mn_2$ | 6.9±0.4 | *(280)* | *(1172)* | *(121±7)* | *(506±29)* | 83ERV/LOH | 12596-53-1 |
| | IP from 83ERV/LOH. 0 K values. | | | | | | |
| $Mo^+$ | | | | | | | |
| Mo | 7.099 | 321.0 | 1343.1 | 157.3 | 658.1 | 82TN270 | 7439-98-7 |
| | | *320.6* | *1341.5* | *156.9* | *656.6* | | |
| $MoNa_2O_4^+$ | | | | | | | |
| $Na_2MoO_4$ | (7.2) | (−87) | (−364) | −253 | −1059 | 82TN270 | |
| $MoO^+$ | | | | | | | |
| MoO | (8.0±0.6) | (267) | (1119) | 83±5 | 347±21 | 83PED/MAR | 12058-07-0 |
| | | *(267)* | *(1119)* | *83±5* | *347±21* | | |
| $MoO_2^+$ | | | | | | | |
| $MoO_2$ | (9.2) | (213) | (890) | −2±3 | −8±13 | 85JANAF | |
| | | *(213)* | *(892)* | *−2±3* | *−6±13* | | |
| $MoO_3^+$ | | | | | | | |
| $MoO_3$ | (11.8±0.5) | (186) | (777) | −87 | −362 | 81WOO | 1313-27-5 |
| | | *(187)* | *(781)* | *−86* | *−358* | | |

Table 1. Positive Ion Table - Continued

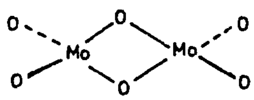
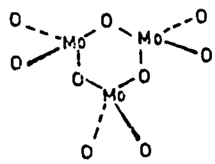
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Mo_2O_6^+$ | | | | | | | |
|  | 12.1±0.6 | (201) | (841) | −78 | −326 | 82TN270 | 12412-19-0 |
| | IP from 77ROS/DRA, 85KAP/LEL. | | | | | | |
| $Mo_3O_9^+$ | | | | | | | |
|  | (12.0±1.0) | (−174) | (−729) | −451 | −1887 | 82TN270 | 12163-83-6 |
| | See also: 85KAP/LEL. | | | | | | |
| $N^+$ | | | | | | | |
| N | 14.534 | 448.2 | 1875.0 | 113.0 | 472.7 | 82TN270 | 17778-88-0 |
| | | *447.7* | *1873.1* | *112.5* | *470.8* | | |
| $NO^+$ | | | | | | | |
| NO | 9.26436±0.00006 | 235.33 | 984.61 | 21.82 | 91.28 | 82BAU/COX | 10102-43-9 |
| | | *235.33* | *984.65* | *21.69* | *90.78* | | |
| | See: 83SEA/CHU, 84MUL/SAN, 83EBA/ANE for confirming high precision measurements. See also: 81KIM/STE, 82FAN/GIA, 81KIM/KAT. | | | | | | |
| $NO_2^+$ | | | | | | | |
| $NO_2$ | 9.75±0.01 | 233 | 974 | 7.9 | 33.2 | 82BAU/COX | 10102-44-0 |
| | | *233* | *977* | *8.6* | *36.0* | | |
| | Ionization involves a bent-linear transition with a broad Franck-Condon envelope and weak onset. Selected IP consistent with occurrence of reaction: ($NO_2^+$ + $C_6H_5CF_3$ → $C_6H_5CF_3^+$ + $NO_2$)(78AUS/LIA). See also: 81KIM/KAT, 82KAT/SHI. | | | | | | |
| $NP^+$ | | | | | | | |
| NP | 11.85 | 298 | 1248 | 25±1 | 105±5 | 85JANAF | 17739-47-8 |
| | | *299* | *1249* | *25±1* | *106±5* | | |
| $NS^+$ | | | | | | | |
| NS | 8.87±0.01 | 268 | 1119 | 63±25 | 264±105 | 85JANAF | 51801-08-2 |
| | | *268* | *1119* | *63±25* | *263±105* | | |
| | IP from 79HUB/HER. | | | | | | |
| $NTi^+$ | | | | | | | |
| TiN | (6) | *(250)* | *(1045)* | *112* | *466* | 79HUB/HER | 25583-20-4 |
| | 0 K values. | | | | | | |
| $NZr^+$ | | | | | | | |
| ZrN | (7.9±0.4) | (352.7) | (1475.6) | 170.5 | 713.4 | 85JANAF | 25658-42-8 |
| | | *(352.9)* | *(1476.5)* | *170.7* | *714.3* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $N_2^+$ | | | | | | | |
| $N_2$ | 15.5808 | 359.3 | 1503.3 | 0 | 0 | *DEF | 7727-37-9 |
| | | *359.3* | *1503.3* | *0* | *0* | | |
| | IP from 79HUB/HER. See also: 84STE/MAR, 81ARM/TAR, 81KIM/KAT. | | | | | | |
| $N_2O^{+\cdot}$ | | | | | | | |
| $N_2O$ | 12.886 | 316.8 | 1325.4 | 19.6 | 82.1 | 82BAU/COX | 10024-97-2 |
| | | *317.6* | *1328.8* | *20.4* | *85.5* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $N_2O_4^+$ | | | | | | | |
| $N_2O_4$ | 10.8±0.2 | (251) | (1051) | 2 | 9 | 82BAU/COX | 10544-72-6 |
| | | *(254)* | *(1061)* | *5* | *19* | | |
| | See also: 82CHO/FRO. | | | | | | |
| $N_2O_5^+$ | | | | | | | |
| $N_2O_5$ | (11.9) | (277) | (1159) | 3 | 11 | 82BAU/COX | 10102-03-1 |
| | | *(280)* | *(1173)* | *6* | *25* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $Na^+$ | | | | | | | |
| Na | 5.139 | <u>144.1</u> | <u>603.1</u> | 25.6±0.2 | 107.3±0.7 | 85JANAF | 7440-23-5 |
| | | *<u>144.2</u>* | *<u>603.4</u>* | *25.7±0.2* | *107.6±0.7* | | |
| | See also: 84PET/DAO. | | | | | | |
| $NaO^+$ | | | | | | | |
| NaO | (7.41) | (190.9) | (798.7) | 20.0±10.0 | 83.7±41.8 | 85JANAF | 12401-86-4 |
| | | *(191.2)* | *(800.0)* | *20.3±10.0* | *85.0±41.8* | | |
| | IP from 84BUT/KUD. | | | | | | |
| $NaRb^+$ | | | | | | | |
| NaRb | 4.32±0.04 | 115 | 481 | 15 | 64 | 86IGE/WED | 12333-61-8 |
| | IP from 85KAP/SCH. | | | | | | |
| $Na_2^+$ | | | | | | | |
| $Na_2$ | 4.88898±0.00016 | <u>146.7</u> | <u>613.8</u> | 34.0±0.3 | 142.1±1.2 | 85JANAF | 25681-79-2 |
| | | *<u>147.3</u>* | *<u>616.3</u>* | *34.6±0.3* | *144.6±1.2* | | |
| | IP from 81LEU/HOF, in agreement with values from 82MAR/CHE, 85KAP/RAD, 84PET/DAO, 78HER/SCH. $\Delta_f H$(Ion) in agreement with that derived from data of 83WAG/ISE. | | | | | | |
| $Na_2Cl^+$ | | | | | | | |
| $Na_2Cl$ | 4.15±0.22 | *(59)* | *(245)* | *−37* | *−155* | 83PET/DAO | |
| | IP from 83PET/DAO. 0 K values. | | | | | | |
| $Na_2O^+$ | | | | | | | |
| $Na_2O$ | (5.06±0.4) | (110) | (461) | −6 | −27 | 83PET/DAO | 1313-59-3 |
| | | *(111)* | *(465)* | *−5* | *−23* | | |
| | IP from 83PET/DAO. See also: 84BUT/KUD. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Nb^+$ | | | | | | | |
| Nb | 6.88 | 334 | 1397 | 175±2 | 733±8 | 85JANAF | 7440-03-1 |
| | | *333* | *1394* | *174.5±2* | *730±8* | | |
| $NbO^+$ | | | | | | | |
| NbO | (6.1) | (186±53) | (778.5±222) | 48±5 | 200±21 | 85JANAF | 12034-57-0 |
| | | *(187±53)* | *(780±222)* | *48±5* | *199±21* | | |
| | $\Delta_f H$(Ion) from 81KAP/STA. IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $Nd^+$ | | | | | | | |
| Nd | 5.5250±0.0006 | 205.80 | 861.08 | 78 | 328 | 82TN270 | 7440-00-8 |
| | | *206.04* | *862.08* | *78.5* | *328.6* | | |
| $NdO^+$ | | | | | | | |
| NdO | (4.97±0.1) | (84) | (354) | −30±3 | −126±12 | 83PED/MAR | 12035-20-0 |
| | | *(84)* | *(354)* | *−30±3* | *−126±12* | | |
| $Ne^+$ | | | | | | | |
| Ne | 21.56471±0.00001 | 497.29 | 2080.66 | 0 | 0 | *DEF | 7440-01-9 |
| | | *497.29* | *2080.66* | *0* | *0* | | |
| $NeKr^+$ | | | | | | | |
| NeKr | (13.950±0.003) | *(321.5)* | *(1345.3)* | *−0.15* | *−0.62* | 79HUB/HER | |
| | IP from 82PRA/DEH2. 0 K values. | | | | | | |
| $NeXe^+$ | | | | | | | |
| NeXe | (12.094±0.004) | *(278.7)* | *(1166.3)* | *−0.15* | *−0.63* | 79HUB/HER | 58984-40-0 |
| | IP from 82PRA/DEH2. See also: 85PRA/DEH2. 0 K values. | | | | | | |
| $Ne_2^+$ | | | | | | | |
| $Ne_2$ | 20.33±0.08 | *469* | *1961* | *−0.047* | *−0.195* | 79HUB/HER | 12185-05-6 |
| | IP from 84TRE/POL. See also: 79HUB/HER. 0 K values. | | | | | | |
| $Ni^+$ | | | | | | | |
| Ni | 7.635 | 278.9 | 1166.8 | 102.8 | 430.1 | 82TN270 | 7440-02-0 |
| | | *278.4* | *1164.8* | *102.3* | *428.1* | | |
| | See also: 82DYK/GRA. | | | | | | |
| $NiO^+$ | | | | | | | |
| NiO | 9.5±0.2 | (290) | (1214) | 71±4 | 297±17 | 83PED/MAR | 1313-99-1 |
| | IP from 81ARM/HAL, 82ARM/HAL, 77ROS/DRA. See also: 81KAP/STA. | | | | | | |
| $No^+$ | | | | | | | |
| No | 6.84±0.12 | | | | | | 10028-14-5 |
| $Np^+$ | | | | | | | |
| Np | 6.2657±0.0005 | 256 | 1070 | 111 | 465 | 85KLE/WAR | 7439-99-8 |
| $NpO^+$ | | | | | | | |
| NpO | (5.7±0.1) | (130) | (546) | −1±10 | −4±42 | 83PED/MAR | 12202-03-8 |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$O^+$** | | | | | | | |
| O | 13.618 | 373.6 | 1563.1 | 59.6 | 249.2±0.1 | 85JANAF | 17778-80-2 |
| | | *373.0* | *1560.7* | *59.0* | *246.8±0.1* | | |
| **$OP^+$** | | | | | | | |
| PO | 8.39±0.01 | 186 | 777 | −8±3 | −33±13 | 83PED/MAR | 14452-66-5 |
| | | *186* | *778* | *−8* | *−32* | | |
| | IP from 82DYK/MOR. See also: 81BAL/GIG. | | | | | | |
| **$OPb^+$** | | | | | | | |
| PbO | 9.08±0.10 | 224 | 939 | 15±3 | 63±13 | 79HUB/HER | 1317-36-8 |
| | | *227* | *949* | *17* | *73* | | |
| | See also: 83SEM/RYK, 84NIK/OVC. | | | | | | |
| **$OPd^+$** | | | | | | | |
| PdO | (9.1) | *(293)* | *(1224)* | *83* | *346* | 79HUB/HER | 1314-08-5 |
| | 0 K values. | | | | | | |
| **$OPr^+$** | | | | | | | |
| PrO | (4.90±0.1) | (79) | (331) | −34±4 | −142±17 | 82TN270 | 12035-81-3 |
| | | *(75)* | *(314)* | *−38* | *−159* | | |
| **$OPt^+$** | | | | | | | |
| PtO | (10.1±0.3) | (334) | (1397) | 101 | 423 | 79HUB/HER | 12035-82-4 |
| | | *(339)* | *(1417)* | *106* | *443* | | |
| **$ORb^+$** | | | | | | | |
| RbO | 6.69 | 168.6 | 705.3 | 14.3 | 59.8 | 82TPIS | 12509-27-2 |
| | | *168.9* | *706.6* | *14.6±5* | *61.1±20* | | |
| | IP from 84BUT/KUD. | | | | | | |
| **$ORb_2^+$** | | | | | | | |
| $Rb_2O$ | 4.63 | 25.8 | 107.8 | −81.0±2.0 | −338.9±8.4 | 82TPIS | 18088-11-4 |
| | | *26.7* | *111.6* | *−80.1* | *−335.1* | | |
| | IP from 84BUT/KUD. | | | | | | |
| **$ORh^+$** | | | | | | | |
| RhO | (9.3) | (309) | (1294) | 95±10 | 397±42 | 83PED/MAR | 12137-18-7 |
| **$ORu^+$** | | | | | | | |
| RuO | (8.7) | (290) | (1211) | 89±10 | 372±42 | 83PED/MAR | 12143-05-4 |
| **$OS^+$** | | | | | | | |
| SO | 10.32±0.02 | 239.2 | 1000.7 | 1.2±0.3 | 5.0±1.3 | 85JANAF | 13827-32-2 |
| | | *239.2* | *1000.7* | *1.2±0.3* | *5.0±1.3* | | |
| **$OS_2^+$** | | | | | | | |
| $S_2O$ | 10.54±0.04 | 231 | 965 | −12±0.2 | −52±1 | 86NIM/ELL | 20901-21-7 |
| | | *230* | *962* | *−13±0.2* | *−55±1* | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $OSi^+$ | | | | | | | |
| SiO | 11.43 | 239.6 | 1002.4 | −24.0±2 | −100.4±8.4 | 85JANAF | 10097-28-6 |
| | | *239.3* | *1001.2* | *−24.3±2* | *−101.6±8.4* | | |
| | IP from 82LEV/LIA, 79HUB/HER. See also: 81NAK/ASA. | | | | | | |
| $OSm^+$ | | | | | | | |
| SmO | 5.55±0.1 | 100 | 418 | −28±3 | −117±12 | 83PED/MAR | 12035-88-0 |
| | | *97* | *405* | *−31* | *−130* | | |
| $OSn^+$ | | | | | | | |
| SnO | 9.60±0.02 | 226 | 944 | 4.2 | 17.5 | 81LAU/BRI | 21651-19-4 |
| | | *226* | *945* | *4.6* | *19.2* | | |
| | IP from 82DYK/MOR2. | | | | | | |
| $OSr^+$ | | | | | | | |
| SrO | 7.0±0.15 | (158.2) | (662.8) | −3.2±4 | −13.4±16.7 | 85JANAF | 1314-11-0 |
| | | *(158.7)* | *(663.9)* | *−2.7±4* | *−11.5±16.7* | | |
| | $\Delta_f H$(Ion) from onset of endothermic reaction (83MUR);IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). | | | | | | |
| $OTa^+$ | | | | | | | |
| TaO | (7.92±0.1) | (228.6) | (956.7) | 46.0±15 | 192.5±62.8 | 85JANAF | 12035-90-4 |
| | | *(228.9)* | *(957.9)* | *46.3±15* | *193.7±62.8* | | |
| $OTb^+$ | | | | | | | |
| TbO | (5.62±0.1) | (113) | (471) | −17±3 | −71±12 | 83PED/MAR | 12035-91-5 |
| | | *(111)* | *(463)* | *−19* | *−79* | | |
| $OTe^+$ | | | | | | | |
| TeO | 8.72 | 218 | 910 | 16±5 | 69±21 | 83PED/MAR | 13451-17-7 |
| | | *218* | *912* | *17* | *71* | | |
| $OTh^+$ | | | | | | | |
| ThO | 6.1±0.1 | (133) | (557) | −7±2 | −31±10 | 83PED/MAR | 12035-93-7 |
| | | *(134)* | *(559)* | *−7* | *−29* | | |
| $OTi^+$ | | | | | | | |
| TiO | 6.56±0.03 | 164.3 | 687.3 | 13.0±2.0 | 54.4±8.4 | 85JANAF | 12137-20-1 |
| | | *164.2* | *686.8* | *12.9±2.0* | *53.9±8.4* | | |
| | IP from 84DYK/GRA. See also: 80MUR/HIL, 82BAN/CHA, 85BAL/GIG, 81KAP/STA. | | | | | | |
| $OTm^+$ | | | | | | | |
| TmO | (6.44±0.1) | *(130)* | *(542)* | *−19* | *−79* | 82TN270 | 12281-29-7 |
| | See also: 80MUR/HIL. 0 K values. | | | | | | |
| $OU^+$ | | | | | | | |
| UO | (5.65±0.2) | (136) | (570) | 6±2 | 25±10 | 83PED/MAR | 12035-97-1 |
| | | *(136)* | *(568)* | *6* | *23* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $OV^+$ | | | | | | | |
| VO | (7.5) | (203.4) | (851.2) | 30.5±5.0 | 127.6±20.9 | 85JANAF | 12035-98-2 |
| | | *(203.5)* | *(851.4)* | *30.5±5.0* | *127.8±20.9* | | |
| | $\Delta_f H$(Ion) from onset energy of endothermic reaction (84ARI/ARM, 85ELK/ARM). IP is $\Delta_f H$(Ion) - $\Delta_f H$(Neutral). See also: 81KAP/STA. | | | | | | |
| $OW^{+\cdot}$ | | | | | | | |
| WO | (9.1±1) | (311.5) | (1303.1) | 101.6±10.0 | 425.1±41.8 | 85JANAF | 12035-99-3 |
| | | *(311.6)* | *(1303.7)* | *101.7±10.0* | *425.7±41.8* | | |
| $OY^+$ | | | | | | | |
| YO | 5.85±0.15 | 124 | 518 | −11±2 | −46±10 | 83PED/MAR | 12036-00-9 |
| | | *124* | *519* | *−11* | *−45* | | |
| | See also: 80MUR/HIL. | | | | | | |
| $OYb^+$ | | | | | | | |
| YbO | (6.55±0.1) | (147) | (615) | −4±2 | −17±8 | 83PED/MAR | 25578-79-4 |
| $OZn^+$ | | | | | | | |
| ZnO | | *(275±8)* | *(1151±33)* | | | | |
| | $\Delta_f H$(Ion) from 81KAP/STA. 0 K values. | | | | | | |
| $OZr^+$ | | | | | | | |
| ZrO | (6.1±0.3) | (154.7) | (647.1) | 14.0±12.0 | 58.6±50.2 | 85JANAF | 12036-01-0 |
| | | *(154.9)* | *(648.2)* | *14.2±12.0* | *59.6±50.2* | | |
| | See also: 81KAP/STA. | | | | | | |
| $O_2^+$ | | | | | | | |
| $O_2$ | 12.071±0.001 | 278.5 | 1165.3 | 0 | 0 | *DEF | 7782-44-7 |
| | | *278.4* | *1164.7* | *0* | *0* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $O_2P^+$ | | | | | | | |
| $PO_2$ | (10.5±0.1) | (175) | (733) | −67 | −280 | 85JANAF | 12164-97-5 |
| | | *(176)* | *(736)* | *−66* | *−277* | | |
| $O_2Pt^+$ | | | | | | | |
| $PtO_2$ | (11.2±0.3) | (299) | (1253) | 41 | 172 | 82TN270 | 1314-15-4 |
| $O_2Rh^+$ | | | | | | | |
| $RhO_2$ | (10.0) | (275) | (1149) | 44 | 184 | 82TN270 | 12137-27-8 |
| $O_2S^+$ | | | | | | | |
| $SO_2$ | 12.32±0.02 | 213 | 892 | −70.9±0.1 | −296.8±0.2 | 85JANAF | 7446-09-5 |
| | | *214* | *894* | *−70.3±0.1* | *−294.3±0.2* | | |
| | See also: 81SMI/STE, 84ORI/SRI, 81KIM/KAT. | | | | | | |
| $O_2Sn_2^+$ | | | | | | | |
| $Sn_2O_2$ | (9.8±0.5) | (166) | (695) | −60 | −251 | 82TN270 | 12534-17-7 |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $O_2Th^+$ | | | | | | | |
| $ThO_2$ | (8.7±0.15) | (82) | (341) | −119 | −498 | 82TN270 | 1314-20-1 |
| | | *(82)* | *(344)* | *−118* | *−495* | | |
| $O_2Ti^+$ | | | | | | | |
| $TiO_2$ | (9.54±0.1) | (149) | (625) | (−71) | (−299) | 85BAL/GIG | 13463-67-7 |
| | | *(149)* | *(623)* | *(−71)* | *(−297)* | | |
| | See also: 82BAN/CHA, 85BAL/GIG. | | | | | | |
| $O_2U^+$ | | | | | | | |
| $UO_2$ | (5.4±0.1) | (13) | (55) | −111±1 | −466±5 | 80GRE | 1344-57-6 |
| | | *(14)* | *(57)* | *−111* | *−464* | | |
| $O_2W^+$ | | | | | | | |
| $WO_2$ | (9.6±0.3) | (240) | (1003) | 18±6 | 77±29 | 85JANAF | 12036-22-5 |
| | | *(240)* | *(1005)* | *19±6* | *79±29* | | |
| | See also: 81BAL/GIG. | | | | | | |
| $O_2Zr^+$ | | | | | | | |
| $ZrO_2$ | (9.5±0.3) | (151) | (631) | −68±11 | −286±46 | 85JANAF | 1314-23-4 |
| | | *(150)* | *(629)* | *−68±11* | *−284±46* | | |
| $O_3^+$ | | | | | | | |
| $O_3$ | 12.43 | 321 | 1342 | 34 | 143 | 82TN270 | 10028-15-6 |
| | | *321* | *1344* | *35* | *145* | | |
| | IP from 84KAT/SHI. | | | | | | |
| $O_3Ru^+$ | | | | | | | |
| $RuO_3$ | (11.2) | (240) | (1003) | −19 | −78 | 82TN270 | 12036-36-1 |
| $O_3S^+$ | | | | | | | |
| $SO_3$ | 12.80±0.04 | 200 | 839 | −94.6±0.2 | −395.8±0.7 | 85JANAF | 7446-11-9 |
| | | *202* | *845* | *−93.2±0.2* | *−390.0±0.7* | | |
| | See also: 81SMI/STE. | | | | | | |
| $O_3Sn_3^+$ | | | | | | | |
| $Sn_3O_3$ | (9.8±0.5) | (100) | (419) | −126 | −527 | 82TN270 | 12534-28-0 |
| $O_3Ti_2^+$ | | | | | | | |
| $Ti_2O_3$ | (8.3±0.5) | *(39)* | *(164)* | *(−152)* | *(−636)* | 85BAL/GIG2 | 1344-54-3 |
| | IP from 85BAL/GIG2. 0 K values. | | | | | | |
| $O_3U^+$ | | | | | | | |
| $UO_3$ | (10.5±0.5) | (51) | (213) | −191±5 | −800±20 | 80GRE | 1344-58-7 |
| $O_3W^+$ | | | | | | | |
| $WO_3$ | (11.8±0.6) | (202) | (846) | −70 | −293 | 81WOO | 1314-35-8 |
| | | *(203)* | *(851)* | *−69* | *−288* | | |
| | See also: 81BAL/GIG. | | | | | | |

Table 1. Positive Ion Table - Continued

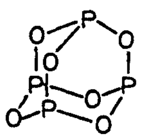
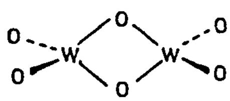
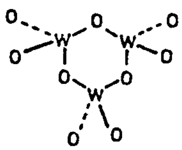
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $O_4Os^+$ | | | | | | | |
| $OsO_4$ | 12.320 | 204 | 852 | -81 | -337 | 82TN270 | 20816-12-0 |
| $O_4Ru^+$ | | | | | | | |
| $RuO_4$ | 12.15±0.03 | 236 | 988 | -44 | -184 | 82TN270 | 20427-56-9 |
| | | *238* | *994* | *-43* | *-178* | | |
| $O_4SnW^+$ | | | | | | | |
| $SnWO_4$ | (10.8)<br>0 K values. | *(41)* | *(172)* | *-208* | *-870* | 82TN270 | 14553-36-7 |
| $O_4Sn_4^+$ | | | | | | | |
| $Sn_4O_4$ | (9.2±0.5) | (19) | (80) | -193 | -808 | 82TN270 | |
| $O_4SrW^+$ | | | | | | | |
| $SrWO_4$ | (9.4) | (-33) | (-139) | -250 | -1046 | 76DEL/HAL | |
| $O_4Ti_2^+$ | | | | | | | |
| $Ti_2O_4$ | (10.5±0.5)<br>0 K values. | *(-19)* | *(-79)* | *(-261)* | *(-1092)* | 85BAL/GIG3 | |
| $O_5Sn_2W^+$ | | | | | | | |
| $Sn_2WO_5$ | (8.4)<br>0 K values. | *(-75)* | *(-315)* | *-269* | *-1125* | 82TN270 | |
| $O_6P_4^+$ | | | | | | | |
|  | (9.5) | (-293) | (-1227) | -512±8 | -2144±33 | 85JANAF | 10248-58-5 |
| | | *(-288)* | *(-1203)* | *-507±6* | *-2120±33* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $O_6W_2^+$ | | | | | | | |
|  | (12.2±0.2) | (3) | (11) | -278 | -1164 | 85JANAF | 12165-16-1 |
| | | *(4)* | *(17)* | *-277* | *-1158* | | |
| $O_7Re_2^+$ | | | | | | | |
| $Re_2O_7$ | (12.7±0.2) | (30) | (124) | -263 | -1101 | 81WOO | 1314-68-7 |
| $O_9W_3^+$ | | | | | | | |
|  | (12.0±0.2) | (-191) | (-800) | -468 | -1958 | 82TN270 | 12165-37-6 |

Table 1. Positive Ion Table - Continued

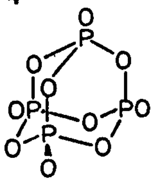
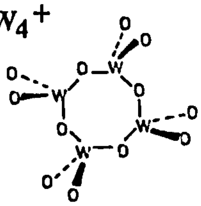
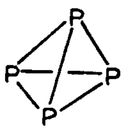
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $O_{10}P_4{}^+$ | | | | | | | |
|  | (13.3±0.2) | (−371)<br>*(−363)* | (−1551)<br>*(−1517)* | −677±2<br>*−669±2* | −2834±9<br>*−2800±9* | 85JANAF | 16752-60-6 |
| $O_{12}W_4{}^+$  | (12.0±0.2) | (−372) | (−1557) | −649 | −2715 | 82TN270 | 12165-45-6 |
| $Os^+$ | | | | | | | |
| Os | 8.28<br>IP from 79RAU/ACK. | 380 | 1590 | 189 | 791 | 82TN270 | 7440-04-2 |
| $P^+$ | | | | | | | |
| P | 10.486 | 317<br>*317* | 1328<br>*1328* | 75.6±0.2<br>*75.4±0.2* | 316.4±1.0<br>*315.6±1.0* | 85JANAF | 7723-14-0 |
| $PS^+$ | | | | | | | |
| PS | (9.0) | (245)<br>*(245)* | (1024)<br>*(1024)* | 36±1<br>*36±1* | 151±4<br>*151±4* | 79HUB/HER | 12281-36-6 |
| $PSe^+$ | | | | | | | |
| PSe | (8.2)<br>0 K values. | *(232)* | *(971)* | *43* | *180* | 79HUB/HER | 12509-41-0 |
| $P_2{}^+$ | | | | | | | |
| $P_2$ | 10.53<br>IP from 79HUB/HER. | (277.2)<br>*(277.6)* | (1159.7)<br>*(1161.5)* | 34.3±0.5<br>*34.8±0.5* | 143.7±2.1<br>*145.5±2.1* | 85JANAF | 12185-09-0 |
| $P_3{}^+$ | | | | | | | |
| $P_3$ | (7.85±0.2) | (241) | (1006) | 59.4±4 | 249±16 | 74BEN/MAR | 55030-78-9 |
| $P_4{}^+$ | | | | | | | |
|  | 9.08±0.05 | 223<br>*225* | 935<br>*942* | 14±0.5<br>*16±0.5* | 59±2<br>*66±2* | 85JANAF | 12185-10-3 |
| $Pa^+$ | | | | | | | |
| Pa | 5.89±0.12 | 270 | 1131 | 135 | 563 | 85KLE/WAR | 7440-13-3 |

**Table 1. Positive Ion Table - Continued**

| ION / Neutral | Ionization potential eV | $\Delta_fH$(Ion) kcal/mol | $\Delta_fH$(Ion) kJ/mol | $\Delta_fH$(Neutral) kcal/mol | $\Delta_fH$(Neutral) kJ/mol | Neutral reference | CAS registry number |
|---|---|---|---|---|---|---|---|
| $Pb^+$ | | | | | | | |
| Pb | 7.416 | 217.6 | 910.5 | 46.6 | 195.0 | 82TN270 | 7439-92-1 |
| | | *217.8* | *911.1* | *46.8* | *195.6* | | |
| | See also: 83SEM/RYK, 84NIK/OVC. | | | | | | |
| $PbS^+$ | | | | | | | |
| PbS | (8.5±0.5) | (228) | (954) | 32 | 134 | 79HUB/HER | 1314-87-0 |
| | | *(229)* | *(956)* | *32* | *136* | | |
| $PbSe^+$ | | | | | | | |
| PbSe | (8.4±0.5) | *(224)* | *(935)* | *30* | *125* | 79HUB/HER | 12069-00-0 |
| | 0 K values. | | | | | | |
| $PbTe^+$ | | | | | | | |
| PbTe | (≤8.04) | *(≤220)* | *(≤922)* | *35* | *146* | 79HUB/HER | 1314-91-6 |
| | 0 K values. | | | | | | |
| $Pb_2^+$ | | | | | | | |
| $Pb_2$ | (6.1±0.3) | (214) | (897) | (74) | (308) | 79HUB/HER | 12596-92-8 |
| | | *(215)* | *(901)* | *(75)* | *(312)* | | |
| | IP from 82SAI/YAM. | | | | | | |
| $Pd^+$ | | | | | | | |
| Pd | 8.34 | 283 | 1183 | 90 | 378 | 82TN270 | 7440-05-3 |
| | | *282* | *1182* | *90* | *377* | | |
| $PdSi^+$ | | | | | | | |
| PdSi | (8.4±0.5) | *(318)* | *(1329)* | *124* | *519* | 79HUB/HER | 12137-77-8 |
| | 0 K values. | | | | | | |
| $Pd_2^+$ | | | | | | | |
| $Pd_2$ | (7.7±0.3) | *(341)* | *(1426)* | *163* | *683* | 79HUB/HER | 12596-93-9 |
| | 0 K values. | | | | | | |
| $Pm^+$ | | | | | | | |
| Pm | 5.582 | | | | | | |
| $Pr^+$ | | | | | | | |
| Pr | 5.464±0.006 | 211 | 883 | 85 | 356 | 82TN270 | 7440-10-0 |
| | | *211.2* | *883.9* | *85.2* | *356.7* | | |
| $Pt^+$ | | | | | | | |
| Pt | 8.61 | 334 | 1396 | 135 | 565 | 82TN270 | 7440-06-4 |
| | | *333* | *1395* | *134.9* | *564.4* | | |
| | IP from 79RAU/ACK. See also: 81GUP/NAP. | | | | | | |
| $Pu^+$ | | | | | | | |
| Pu | 6.03±0.10 | 222 | 927 | 82.5 | 345 | 85KLE/WAR | 7440-07-5 |
| | IP from 81CHE/GAB. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_fH$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_fH$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Ra^+$ | | | | | | | |
| Ra | 5.279 | 160 | 668 | 38 | 159 | 82TN270 | 7440-14-4 |
| | IP from 70MOO. | | | | | | |
| $Rb^+$ | | | | | | | |
| Rb | 4.177 | 116 | 484 | 19.3±0.1 | 80.9±0.4 | 85JANAF | 7440-17-7 |
| | | *116* | *485* | *19.6±0.1* | *82.2±0.4* | | |
| $Rb_2^+$ | | | | | | | |
| $Rb_2$ | (3.9±0.1) | (117.0) | (489.6) | 27.1±0.6 | 113.3±2.5 | 85JANAF | |
| | | *(118.0)* | *(493.6)* | *28.0±0.6* | *117.3±2.5* | | |
| | IP from 85KAP/SCH. | | | | | | |
| $Re^+$ | | | | | | | |
| Re | 7.76 | 363 | 1519 | 184 | 770 | 82TN270 | 7440-15-5 |
| | | *363* | *1518* | *184* | *769* | | |
| | IP from 79RAU/ACK. | | | | | | |
| $Rh^+$ | | | | | | | |
| Rh | 7.46 | 305 | 1275 | 133 | 557 | 82TN270 | 7440-16-6 |
| | | *305* | *1275* | *133* | *556* | | |
| | See also: 81HAQ/GIN. | | | | | | |
| $RhTi^+$ | | | | | | | |
| TiRh | (8.2±1.0) | *(342)* | *(1431)* | *153* | *640* | 79HUB/HER | 12600-90-7 |
| | 0 K values. | | | | | | |
| $Rh_2^+$ | | | | | | | |
| $Rh_2$ | (7.1±1.0) | *(363)* | *(1518)* | *199* | *833* | 79HUB/HER | 12596-98-4 |
| | 0 K values. | | | | | | |
| $Rn^+$ | | | | | | | |
| Rn | 10.748 | 247.9 | 1037.0 | 0 | 0 | *DEF | 10043-92-2 |
| | | *247.9* | *1037.0* | *0* | *0* | | |
| | IP from 70MOO. | | | | | | |
| $Ru^+$ | | | | | | | |
| Ru | (7.37) | (324) | (1354) | 154 | 643 | 82TN270 | 7440-18-8 |
| | | *(323)* | *(1352)* | *153* | *641* | | |
| $S^+$ | | | | | | | |
| S | 10.360 | 305 | 1275 | 66.2±0.1 | 277.0±0.3 | 85JANAF | 7704-34-9 |
| | | *304* | *1272* | *65.6±0.1* | *274.7±0.3* | | |
| | See also: 86LIA/NG, 79DUN/DYK. | | | | | | |
| $SSe^+$ | | | | | | | |
| SeS | (9.2±0.2) | *(243)* | *(1015)* | *30* | *127* | 83GRA/WIE | 7446-34-6 |
| | IP from 83GRA/WIE, 77LEV/LIA. 0 K values. | | | | | | |

**Table 1. Positive Ion Table - Continued**

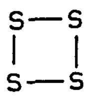
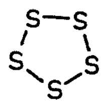
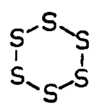
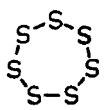
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $SSn^+$ | | | | | | | |
| SnS | (8.8) | (231) | (968) | 28 | 119 | 82TN270 | 1314-95-0 |
| | IP is onset of photoelectron band. | | | | | | |
| $STi^+$ | | | | | | | |
| TiS | (7.1±0.3) | (237) | (990) | 73 | 305 | 82TN270 | 12039-07-5 |
| $SY^+$ | | | | | | | |
| YS | (6.0) | (180) | (754) | 42 | 175 | 82TN270 | 12210-79-6 |
| | | *(180)* | *(755)* | *42* | *176* | | |
| $S_2^+$ | | | | | | | |
| $S_2$ | 9.356±0.002 | 246.5 | 1031.3 | 30.7±0.1 | 128.6±0.3 | 85JANAF | 23550-45-0 |
| | | *246.4* | *1031.0* | *30.7±0.1* | *128.3±0.3* | | |
| | IP from 86LIA/NG. See also: 83ROS/GRA, 83GRA/WIE. | | | | | | |
| $S_3^+$ | | | | | | | |
| $S_3$ | (9.68±0.03) | (257) | (1076) | 34±2 | 142±8 | 85JANAF | 12597-03-4 |
| | See also: 83ROS/GRA. | | | | | | |
| $S_4^+$ | | | | | | | |
|  | (10.1) | (270) | (1131) | 35±2 | 146±8 | 85JANAF | 19269-85-3 |
| | $\Delta_f H$(Ion) from appearance potential of 11.94±0.05 in $S_6$. IP from 83ROS/GRA. | | | | | | |
| $S_5^+$ | | | | | | | |
|  | (8.60±0.05) | (224) | (939) | 26±2 | 109±8 | 85JANAF | 12597-10-3 |
| | See also: 83ROS/GRA. | | | | | | |
| $S_6^+$ | | | | | | | |
|  | (9.00±0.03) | (232) | (971) | 24±2 | 102±8 | 85JANAF | 13798-23-7 |
| | See also: 83ROS/GRA. | | | | | | |
| $S_7^+$ | | | | | | | |
|  | (8.67±0.03) | (227) | (951) | 27±2 | 114±8 | 85JANAF | 21459-04-1 |
| | See also: 83ROS/GRA. | | | | | | |

Table 1. Positive Ion Table - Continued

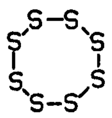
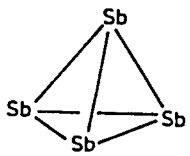
| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $S_8^+$ | | | | | | | |
|  | (9.04±0.03) | (232) | (972) | 24.0±0.2 | 100.4±0.6 | 85JANAF | 10544-50-0 |
| | | *(233)* | *(976)* | *25.0±0.2* | *104.4±0.6* | | |
| | See also: 83ROS/GRA. | | | | | | |
| $Sb^+$ | | | | | | | |
| Sb | 8.641 | 261.9 | 1096.0 | 62.7 | 262.3 | 82TN270 | 7440-36-0 |
| | | *261.9* | *1095.7* | *62.6* | *262.0* | | |
| | It has been suggested (83MAZ) that this value of the IP is too high. | | | | | | |
| $Sb_2^+$ | | | | | | | |
| $Sb_2$ | (9.3±0.2) | (271) | (1133) | 56 | 236 | 82TN270 | 32679-33-7 |
| | | *(271)* | *(1134)* | *57* | *237* | | |
| | The cited ionization potential is from a spectroscopic determination. Threshold determinations have led to values of 8.4±0.3, 8.64±0.06, 8.7±0.3, 8.9±0.3, and 9.5±0.5 eV. | | | | | | |
| $Sb_4^+$ | | | | | | | |
|  | (7.40±0.10) | (220) | (919) | 49 | 205 | 82TN270 | 12597-17-0 |
| | | *(221)* | *(924)* | *50* | *210* | | |
| | IP from 84ELB/KUD. | | | | | | |
| $Sc^+$ | | | | | | | |
| Sc | 6.54 | 241 | 1009 | 90 | 378 | 82TN270 | 7440-20-2 |
| | | *241* | *1007* | *90* | *376* | | |
| | See: 85DYK/GRA. | | | | | | |
| $Se^+$ | | | | | | | |
| Se | 9.752 | 279.2 | 1168.0 | 54.27 | 227.07 | 82TN270 | 7782-49-2 |
| | | *279.0* | *1167.3* | *54.11* | *226.40* | | |
| $SeSn^+$ | | | | | | | |
| SeSn | (8.6) | (229) | (959) | 31 | 129 | 79HUB/HER | 1315-06-6 |
| | | *(228)* | *(953)* | *29* | *123* | | |
| | IP is onset of photoelectron band. | | | | | | |
| $SeTe^+$ | | | | | | | |
| SeTe | (8.5±0.2) | (227) | (948) | 31 | 128 | 83GRA/WIE | 12067-42-4 |
| | IP from 83GRA/WIE. | | | | | | |
| $SeY^+$ | | | | | | | |
| SeY | (6.1±1) | *(90)* | *(376)* | *-51* | *-213* | 79HUB/HER | 12067-44-6 |
| | 0 K values. | | | | | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Se_2^+$ | | | | | | | |
| $Se_2$ | 8.70±0.05 | 236 | 985 | 35 | 146 | 82TN270 | 12185-17-0 |
| | | *236* | *987* | *35* | *148* | | |
| | See also: 83POT/NOV, 83GRA/WIE. | | | | | | |
| $Si^+$ | | | | | | | |
| Si · | 8.15172±0.00003 | 295 | 1236 | 108±2 | 450±8 | 82TN270 | 7440-21-3 |
| | | *295* | *1233* | *106±2* | *446±8* | | |
| $Si_2^+$ | | | | | | | |
| $Si_2$ | (7.4) | (311.6) | (1303.9) | 141.0±3 | 589.9±13 | 85JANAF | 12597-35-2 |
| | | *(311.0)* | *(1301.1)* | *140.3±3* | *587.1±13* | | |
| $Sm^+$ | | | | | | | |
| Sm | 5.6437±0.0006 | 180 | 751 | 49.4 | 206.7 | 82TN270 | 7440-19-9 |
| | | *179* | *751* | *49.3* | *206.1* | | |
| $Sn^+$ | | | | | | | |
| Sn | 7.344 | 241.5 | 1010.7 | 72.2 | 302.1 | 82TN270 | 7440-31-5 |
| | | *241.5* | *1010.6* | *72.2* | *302.0* | | |
| $Sr^+$ | | | | | | | |
| Sr | 5.695 | 170 | 713 | 39±0.5 | 164±2 | 85JANAF | 7440-24-6 |
| | | *170* | *713* | *39±0.5* | *164±2* | | |
| $Ta^+$ | | | | | | | |
| Ta | 7.40 | 358 | 1496 | 187 | 782 | 85JANAF | 7440-25-7 |
| | | *357* | *1495* | *186.7* | *781.4* | | |
| | IP from 79RAU/ACK. | | | | | | |
| $Tb^+$ | | | | | | | |
| Tb | 5.8639±0.0006 | 228 | 955 | 93 | 389 | 82TN270 | 7440-27-9 |
| | | *228.6* | *956.4* | *93.4* | *390.6* | | |
| $Tc^+$ | | | | | | | |
| Tc | (7.28) | (330) | (1380) | 162 | 678 | 82TN270 | 7440-26-8 |
| $Te^+$ | | | | | | | |
| Te | 9.009 | 255 | 1066 | 47 | 197 | 82TN270 | 22541-49-7 |
| | | *255* | *1066* | *47* | *197* | | |
| $TeY^+$ | | | | | | | |
| YTe | (6.0±1.0) | *(206)* | *(860)* | *67* | *281* | 79HUB/HER | 12187-04-1 |
| | 0 K values. | | | | | | |
| $Te_2^+$ | | | | | | | |
| $Te_2$ | 8.29±0.03 | 223 | 933 | 32 | 133 | 79HUB/HER | 10028-16-7 |
| | | *224* | *936* | *32* | *136* | | |
| | See also: 83GRA/WIE. | | | | | | |

Table 1. Positive Ion Table - Continued

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| $Th^+$ | | | | | | | |
| Th | 6.08 | 283 | 1184 | 143 | 597 | 85KLE/WAR | 7440-29-1 |
| | | *283* | *1184* | *143* | *597* | | |
| $Ti^+$ | | | | | | | |
| Ti | 6.82 | 270 | 1128 | 112 | 470 | 82TN270 | 7440-32-6 |
| | | *269* | *1125* | *112* | *467* | | |
| $Tl^+$ | | | | | | | |
| Tl | 6.108 | 184.4 | 771.6 | 43.5 | 182.2 | 82TN270 | 7440-28-0 |
| | | *184.5* | *772.1* | *43.7* | *182.8* | | |
| $Tl_2^+$ | | | | | | | |
| $Tl_2$ | (6.5±0.5) | *(223)* | *(932)* | *73* | *305* | 80BAL/PIA | 76939-73-6 |
| | IP from 80BAL/PIA. 0 K values. | | | | | | |
| $Tm^+$ | | | | | | | |
| Tm | 6.18 | 198 | 828 | 55 | 232 | 82TN270 | 7440-30-4 |
| | | *198* | *830* | *55.8* | *233.4* | | |
| $U^+$ | | | | | | | |
| U | 6.1912 | 270 | 1128 | 127 | 531 | 85KLE/WAR | 7440-61-1 |
| | | *270* | *1128* | *127* | *531* | | |
| | IP from 70EME/KHO, 76SOL/MAY. See also: 81CHE/GAB. | | | | | | |
| $V^+$ | | | | | | | |
| V | 6.74 | 278 | 1165 | 123±2 | 515±8 | 85JANAF | 7440-62-2 |
| | | *278* | *1162* | *122±2* | *512±8* | | |
| | See also: 85DYK/GRA. | | | | | | |
| $W^+$ | | | | | | | |
| W | 7.60 | 379 | 1584 | 203.4±1.5 | 851.0±6.3 | 85JANAF | 7440-33-7 |
| | | *378* | *1582* | *203.7±1.5* | *849.8±6.3* | | |
| $Xe^+$ | | | | | | | |
| Xe | 12.130 | 279.7 | 1170.4 | 0 | 0 | *DEF | 7440-63-3 |
| | | *279.7* | *1170.4* | *0* | *0* | | |
| | See also: 81KIM/KAT. | | | | | | |
| $Xe_2^+$ | | | | | | | |
| $Xe_2$ | 11.13±0.02 | *256* | *1072* | *−0.53* | *−2.22* | 79HUB/HER | 12185-19-2 |
| | See also: 82POL/DEH. 0 K values. | | | | | | |
| $Y^+$ | | | | | | | |
| Y | (6.22) | (244) | (1021) | 101 | 421 | 82TN270 | 7440-65-5 |
| | | *(244)* | *(1021)* | *100.5* | *420.4* | | |
| | IP from 73GAR/REE. | | | | | | |
| $Yb^+$ | | | | | | | |
| Yb | 6.254 | 180 | 755 | 36 | 152 | 82TN270 | 7440-64-4 |
| | | *180.7* | *756.2* | *36.5* | *152.8* | | |

**Table 1. Positive Ion Table - Continued**

| ION<br>Neutral | Ionization potential<br>eV | $\Delta_f H$(Ion)<br>kcal/mol | <br>kJ/mol | $\Delta_f H$(Neutral)<br>kcal/mol | <br>kJ/mol | Neutral<br>reference | CAS registry<br>number |
|---|---|---|---|---|---|---|---|
| **$Zn^+$** | | | | | | | |
| Zn | 9.394 | 247.8 | 1036.8 | 31.2 | 130.4±0.2 | 85JANAF | 7440-66-6 |
| | | *247.7* | *1036.3* | *31.0* | *129.9±0.2* | | |
| **$Zr^+$** | | | | | | | |
| Zr | 6.84 | 303 | 1270 | 146±2 | 610±8 | 85JANAF | 7440-67-7 |
| | | *302* | *1262* | *144±2* | *602±8* | | |

**Table 2. Negative Ion Table**

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$e^-$** | | | | | | $\Delta_f H(AH)=$ 218 | 82TN270 |
| $e^-$ | | | | | | $BDE(A-H)=$ 1312 | 82TN270 |
| * | 0 | | 1312 [f] | 1308 [h] | Def | | 82TN270 |
| **$Ag^-$** | | | | | | | |
| $Ag^-$ | | | | | | $\Delta_f H(A)=$ 285 | 82TN270 |
| * | 159±1 [b] | 1.302±0.007 | | | LPES | | 85HOT/LIN |
| **$Al^-$** | | | | | | $\Delta_f H(AH)=$ 259±1 | 82TN270 |
| $Al^-$ | | | | | | $BDE(A-H)=$ 285±3 | 81KAN/MOO |
| * | 284±5 [a] | 0.441±0.010 | 1554±4 [e] | | LPES | | 85HOT/LIN |
| **$AlBeF_6^-$** | | | | | | | |
| $BeF_2\cdot\cdot AlF_4^-$ | | | | | | | |
| | −2921±21 [c] | | *182±10* | | TDAs | | 80NIK/SOR |
| **$AlBeF_7K^-$** | | | | | | | |
| $KBeF_3\cdot\cdot AlF_4^-$ | | | | | | | |
| | −3522±21 [c] | | *192±8* | | TDAs | | 80NIK/SOR |
| **$AlBeF_7Na^-$** | | | | | | | |
| $NaBeF_3\cdot\cdot AlF_4^-$ | | | | | | | |
| | −3497±21 [c] | | *192±8* | | TDAs | | 80NIK/SOR |
| **$AlF_2^-$** | | | | | | | |
| $AlF_2^-$ | | | | | | $\Delta_f H(A)=$ −749±13 | 81WOO |
| | −971±13 | 2.25±0.13 | | | TDEq | EA: 111 kJ < EA(F), new EA(F) data used | 74SRI/UY |
| **$AlF_4^-$** | | | | | | | |
| $AlF_3\cdot\cdot F^-$ | | | | | | | |
| * | −1945±10 [c] | | *488±8* | | TDAs | Summary of literature data plus new work. Recommended average value | 86NIK/IGO |
| | −1972±21 [c] | | *498±7* | | TDAs | $F^-A$: 1100K; $\Delta_f H(AlF_4^-)$: 298K | 80SID/NIK |
| | −1964±14 [c] | | *495±11* | | TDEq | $F^-A$: 93±1 kJ > $UF_4$ | 79NIK/SKO |
| | −1954±12 [c] | | *500±8* | | TDEq | $F^-A$:17 kJ > $ScF_3$ | 81NIK/SID |
| | −2092±13 | | *628±42* [k] | | TDEq | $2AlF_2 + AlF_2^- = 2AlF + AlF_4^-$ | 74SRI/UY |
| | −1949±16 [c] | | *496±13* | | TDEq | $KF_2^- + KAlF_4 = AlF_4^- + 2KF$ | 80GUS/PYA |
| **$AlF_5K^-$** | | | | | | | |
| $KF\cdot\cdot AlF_4^-$ | | | | | | | |
| | −2397±33 [c] | | *120±8* | | TDAs | | 79GUS/GOR |
| **$AlF_7Mn^-$** | | | | | | | |
| $MnF_3\cdot\cdot AlF_4^-$ | | | | | | | |
| | −2950±60 | | | | TDAs | | 84KOR/CHI |
| **$AlO^-$** | | | | | | | |
| $AlO^-$ | | | | | | $\Delta_f H(A)=$ 67±8 | 85JANAF |
| | −282±21 [b] | 3.62±0.13 | | | TDEq | EA: near EA(Cl) | 72SRI/UY |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$AlO_2^-$** | | | | | | |
| $AlO_2^-$ | | | | | *$\Delta_f H(A)$= −130* | *82KAS/CHE* |
| −583±13 [b] | 4.05±0.13 | | | TDEq | | 72SRI/UY |
| | | | | | EA: 42 kJ > EA(Cl), new data for $\Delta_f H(AlO_2)$ and EA(Cl) used | |
| **$Al_2F_7^-$** | | | | | | |
| $AlF_3\cdot\cdot AlF_4^-$ | | | | | | |
| −3394±15 [c] | | *204±4* | *175±8* | TDAs | | 80SID/NIK |
| −3393±33 | | | | TDAs | | 79GUS/GOR |
| **$Al_2F_8K^-$** | | | | | | |
| $KAlF_4\cdot\cdot AlF_4^-$ | | | | | | |
| −4011±42 [c] | | *147±6* | *123±10* | TDAs | | 80SID/NIK |
| **$Al_2F_8Na^-$** | | | | | | |
| $NaAlF_4\cdot\cdot AlF_4^-$ | | | | | | |
| −4006±42 [c] | | *166±9* | *141±13* | TDAs | | 80SID/NIK |
| **$ArBr^-$** | | | | | | |
| $Ar\cdot\cdot Br^-$ | | | | | | |
| −219 [c] | | *6* | | Mobl | | 84GAT |
| **$As^-$** | | | | | | |
| $As^-$ | | | | | *$\Delta_f H(A)$= 303±2* | *82TN270* |
| * 224±5 [b] | 0.81±0.03 | | | PD | | 85HOT/LIN |
| **$AsBr^-$** | | | | | | |
| $AsBr^{-\cdot}$ | | | | | | |
| 7 | 1.3 | | | EIAP | From $AsBr_3$ | 76PAB/BEN |
| **$AsBr_2^-$** | | | | | | |
| $AsBr_2^-$ | | | | | | |
| | 3.5±0.1 | | | EIAP | From $AsBr_3$ | 78PAB/MAR |
| −303 | 3.5 | | | EIAP | From $AsBr_3$ | 76PAB/BEN |
| **$AsCl^-$** | | | | | | |
| $AsCl^{-\cdot}$ | | | | | | |
| −9 | 1.3 | | | EIAP | From $AsCl_3$ | 76PAB/BEN |
| **$AsClF_3^-$** | | | | | | |
| $AsF_3\cdot\cdot Cl^-$ | | | | | | |
| * −1121±12 [c] | | *108±8* [g] | *78±8* | IMRE | | 85LAR/MCM |
| **$AsCl_2^-$** | | | | | | |
| $AsCl_2^-$ | | | | | *$\Delta_f H(A)$= 67±21* | *82TN270* |
| −273 | 2.2 | | | EIAP | From $AsCl_3$ | 76PAB/BEN |
| | 2.2±0.1 | | | EIAP | From $AsCl_3$ | 78PAB/MAR |
| **$AsF^-$** | | | | | | |
| $AsF^{-\cdot}$ | | | | | | |
| | 1.3 | | | EIAP | From $AsF_3$ | 76PAB/BEN |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$AsF_2^-$** | | | | | | | |
| $AsF_2^-$ | | | | | | | |
| | −543 | 0.8 | | | EIAP | From $AsF_3$ | 76PAB/BEN |
| | | 0.8±0.1 | | | EIAP | From $AsF_3$ | 78PAB/MAR |
| **$AsF_4^-$** | | | | | | | |
| $AsF_3\cdot\cdot F^-$ | | | | | | | |
| * | −1236±13 [c] | | *202±8* [g] | *172±8* | IMRE | | 85LAR/MCM |
| **$AsH^-$** | | | | | | | |
| $AsH^{-\cdot}$ | | | | | | | |
| | | 1.0±0.1 | | | PD | | 77RAC/FEL |
| | <167 | | | | IMRB | $As^- + AsH_3 \rightarrow$ | 74WYA/HOL |
| | | <1.1 | | | IMRB | From $AsH_3$ | 64EBI/KRA |
| **$AsH_2^-$** | | | | | | *$\Delta_f H(AH)=$ 67±1* | *82TN270* |
| $AsH_2^-$ | | | | | *D-EA* | *BDE(A−H)= 326±33* | |
| * | 52±26 [a] | | 1515±26 [g] | 1483±25 | IMRB | Between $PH_3$, $H_2S$ | 74WYA/HOL |
| * | | 1.27±0.03 | | | PD | | 72SMY/BRA2 |
| | <41±20 [a] | <1.1±0.5 [d] | <1505±19 | | EIAP | From $AsH_3$ | 64EBI/KRA |
| **$As_2^-$** | | | | | | | |
| $As_2^-$ | | | | | | *$\Delta_f H(A)=$ 190±3* | *73BEN/MAR* |
| | | <0.8 | | | PD | | 77FEL/RAC |
| | 180±19 | 0.1±0.2 [i] | | | EIAP | From $As_4$ | 73BEN/MAR |
| **$As_2H^-$** | | | | | | | |
| $As_2H^-$ | | | | | | | |
| | <288 | | | | IMRB | $As^- + AsH_3 \rightarrow As_2H^- + H_2$ | 74WYA/HOL |
| **$As_3^-$** | | | | | | | |
| $As_3^-$ | | | | | | *$\Delta_f H(A)=$ 241±16* | *73BEN/MAR* |
| | 160±18 | 0.8±0.4 [i] | | | EIAP | From $As_4$ | 73BEN/MAR |
| **$Au^-$** | | | | | | *$\Delta_f H(AH)=$ 295±2* | *82TN270* |
| $Au^-$ | | | | | | *BDE(A−H)= 289±4* | *82TN270* |
| * | 144±6 [a] | 2.309 | 1379±4 [e] | | LPD | | 85HOT/LIN |
| **$AuF_6^-$** | | | | | | | |
| $AuF_6^{-\cdot}$ | | | | | | | |
| | | >1.0 | | | NBIP | | 80COM/REI |
| **$B^-$** | | | | | | *$\Delta_f H(AH)=$ 450±2* | *82TN270* |
| $B^-$ | | | | | | *BDE(A−H)= 211±10* | *85JANAF* |
| * | 416±13 [a] | 0.277±0.010 | 1497±11 [e] | 1468±13 [h] | LPES | | 85HOT/LIN |
| **$BBrCl_2^-$** | | | | | | | |
| $BCl_2Br^{-\cdot}$ | | | | | | *$\Delta_f H(A)=$ −337±42* | *85JANAF* |
| | −403±61 [b] | 0.7±0.2 | | | NBIP | | 80ROT/MAT |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$BBr_2Cl^-$** | | | | | | |
| $BBr_2Cl^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -272±42* | *85JANAF* |
| -363±61 [b] | 0.9±0.2 | | | NBIP | | 80ROT/MAT |
| **$BBr_3^-$** | | | | | | |
| $BBr_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -206* | *82TN270* |
| -285±20 [b] | 0.8±0.2 | | | NBIP | | 80ROT/MAT |
| **$BClF_3^-$** | | | | | | |
| $BF_3\cdot\cdot Cl^-$ | | | | | | |
| • -1473±12 [c] | | *109±8* [g] | *81±8* | IMRE | | 85LAR/MCM |
| **$BCl_2^-$** | | | | | *$\Delta_f H(AH)$= -248±4* | *71JANAF* |
| $BCl_2^-$ | | | | | | |
| -144±109 [b] | 0.6 | | | Est2 | Est: from IP, EA of isoelectronic $NO_2$, $BF_2$, $AlF_2$ | 82JANAF |
| **$BCl_3^-$** | | | | | | |
| $BCl_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -404±1* | *82TN270* |
| -436±20 [b] | 0.3±0.2 | | | NBIP | | 80ROT/MAT |
| **$BCl_3F^-$** | | | | | | |
| $BCl_3\cdot\cdot F^-$ | | | | | | |
| <-890 | | *>238* [k] | | IMRB | $F^-$A: > $SF_5$ | 72STO/NEL |
| **$BCl_4^-$** | | | | | | |
| $BCl_3\cdot\cdot Cl^-$ | | | | | | |
| -920±6 | | *289±8* [k] | | Latt | | 77KRI/TIT |
| **$BF_2^-$** | | | | | *$\Delta_f H(AH)$= -734±3* | *85JANAF* |
| $BF_2^-$ | | | | | *BDE(A-H)= 362±17* | *85JANAF* |
| -796±26 [b] | 2.13±0.13 | 1468±29 [e] | 1436±31 [h] | IMRE | EA: 122 kJ < EA(F), new EA(F) used | 74SRI/UY |
| **$BF_2O^-$** | | | | | *$\Delta_f H(AH)$= -1092±8* | *82TN270* |
| $BF_2O^-$ | | | | | *BDE(A-H)= 473±23* | *85JANAF* |
| <-1002±25 | | <1619±33 [f] | | IMRB | $DO^-$ + $BF_3$→ | 72STO/NEL |
| **$BF_3^-$** | | | | | | |
| $BF_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -1137±2* | *85JANAF* |
| | 0.0±0.2 | | | NBIP | See also: 72STO/NEL | 80ROT/MAT |
| | 2.6 | | | SI | | 69PAG/GOO |
| **$BF_4^-$** | | | | | | |
| $BF_3\cdot\cdot F^-$ | | | | | | |
| • -1687±25 [c] | | *301±21* [g] | *266±8* | IMRE | | 85LAR/MCM |
| -1716±44 [c] | | *330±40* | | TDEq | | 84PYA/GUS |
| -1773±26 | | *385±25* [k] | | Latt | | 84MAL/ROS |
| -1779±21 | | *393±21* [k] | | Latt | | 77KRI/TIT |
| <-1812 | | | | TDEq | $BF_3$ + $BF_2^-$ = $BF_4^-$ + BF | 74SRI/UY |
| <-1368 | | | | IMRB | $F^-$A: > $SF_5$ | 72STO/NEL |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $BH_4^-$ | | | | | | |
| $BH_3\cdot\cdot H^-$ | | | | | | |
| < 197±28 | | | | IMRB | $HO^- + B_2H_6 \rightarrow$ | 68DUN |
| −96±21 | | *341* [k] | | Latt | | 55ALT |
| −85±8 | | *322±8* [k] | | Latt | | 77KRI/TIT |
| $BKO_2^-$ | | | | | | |
| $KBO_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −672±10* | *85FAR/SRI* |
| −785±31 [b] | 1.2±0.2 | | | EIAP | From $K_2BO_2F$ | 76SHE/ILJ |
| $BNaO_2^-$ | | | | | | |
| $NaBO_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −644±42* | *82TN270* |
| −782±63 [b] | 1.4±0.2 | | | EIAP | From $Na_2BO_2F$ | 76SHE/ILJ |
| $BO^-$ | | | | | | |
| $BO^-$ | | | | | | |
| −196±17 [b] | 2.84±0.09 | | | TDEq | | 71SRI/UY |
| | | | | | EA(BO) < EA(Cl) by 75 kJ, new $\Delta_f H$(BO.) and EA(Cl) used | |
| | > 2.48 | | | TDEq | | 70JEN |
| $BO_2^-$ | | | | | *$\Delta_f H(AH)$= −562±4* | *82TN270* |
| $BO_2^-$ | | | | | *BDE(A−H)= 479±6* | *82TN270* |
| −736±18 | 4.51±0.21 [i] | 1356±26 [e] | | TDEq | | 83SID/RUD |
| −617±15 [b] | 3.28±0.13 | | | TDEq | | 71SRI/UY |
| | | | | | EA($BO_2$) < EA(Cl) by 32 kJ, new $\Delta_f H(BO_2)$ and EA(Cl) used | |
| | 3.4±0.5 | | | EIAP | From $K_2BO_2F$ | 76SHE/ILJ |
| | 4.19±0.31 | | | TDEq | | 70JEN |
| $BeF_3^-$ | | | | | | |
| $BeF_2\cdot\cdot F^-$ | | | | | | |
| −1477±15 [c] | | *407±10* | | TDEq | $F^-$A: 83±7 kJ < $AlF_3$ | 80NIK/SOR |
| $BeH^-$ | | | | | | |
| $BeH^-$ | | | | | *$\Delta_f H(A)$= 344* | *79HUB/HER* |
| 276 [b] | 0.7±0.1 | | | PD | | 77RAC/FEL |
| $Be_2F_5^-$ | | | | | | |
| $Be_2F_4\cdot\cdot F^-$ | | | | | | |
| | | *464±8* | | TDEq | $F^-$A: 26±8 kJ < $AlF_3$ | 80NIK/SOR |
| $Be_2F_6K^-$ | | | | | | |
| $KF\cdot\cdot Be_2F_5^-$ | | | | | | |
| −617 [c] | | *290±10* | | TDAs | | 80NIK/SOR |
| $Be_2F_6Na^-$ | | | | | | |
| $NaF\cdot\cdot Be_2F_5^-$ | | | | | | |
| −564 [c] | | *273±10* | | TDAs | | 80NIK/SOR |
| $Be_3F_7^-$ | | | | | | |
| $BeF_2\cdot\cdot Be_2F_5^-$ | | | | | | |
| −969 [c] | | *175±10* | | TDAs | | 80NIK/SOR |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$Be_3F_8K^-$** | | | | | | | |
| $KBeF_3\cdot\cdot Be_2F_5^-$ | | | | | | | |
| | −1482±21 [c] | | *188±8* | | TDAs | | 80NIK/SOR |
| **$Bi^-$** | | | | | | | |
| $Bi^-$ | | | | | | *$\Delta_f H(A)$= 207±4* | *82TN270* |
| • | 116±5 [b] | 0.946±0.010 | | | LPES | | 85HOT/LIN |
| **$Br^-$** | | | | | | *$\Delta_f H(AH)$= −36* | *85JANAF* |
| $Br^-$ | | | | | | *BDE(A−H)= 366* | *82BAU/COX* |
| • | −213±1 [a] | 3.365±0.003 | 1354 [e] | 1331±1 [h] | PLA | | 85HOT/LIN |
| | | | 1349±9 [g] | 1326±8 | IMRE | | 86TAF |
| **$BrClH^-$** | | | | | | | |
| $HCl\cdot\cdot Br^-$ | | | | | | | |
| • | −387±9 [c] | | *82±8* | *54±11* | TDAs | | 85CAL/KEB |
| **$BrCl_2^-$** | | | | | | | |
| $BrCl_2^-$ | | | | | | | |
| | < −464 | | *> 251* [k] | | PDis | | 79LEE/SMI |
| **$BrCl_2P^-$** | | | | | | | |
| $PBrCl_2^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −188±42* | |
| | −335±61 [b] | 1.5±0.2 | | | NBIP | | 76MAT/ROT |
| **$BrFH^-$** | | | | | | | |
| $HF\cdot\cdot Br^-$ | | | | | | | |
| • | −557±10 [c] | | *71±8* | | Est | Extrapolated from other bihalide data | 84LAR/MCM3 |
| **$BrHI^-$** | | | | | | | |
| $HBr\cdot\cdot I^-$ | | | | | | | |
| • | −292±9 [c] | | *67±8* | *43±11* | TDAs | | 85CAL/KEB |
| **$BrHNO_3^-$** | | | | | | | |
| $HBr\cdot\cdot NO_3^-$ | | | | | | | |
| | −438±10 [c] | | *94±8* | *78±7* | TDEq | | 77DAV/FEH |
| **$BrH_2O^-$** | | | | | | | |
| $HOH\cdot\cdot Br^-$ | | | | | | | |
| | −517 [c] | | *62* | *37* | TDAs | | 82BUR/HAY |
| | | | *53±8* | *29±8* | TDAs | | 70ARS/YAM |
| **$BrI^-$** | | | | | | | |
| $IBr^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 41±1* | *82TN270* |
| | −205±11 [b] | 2.5±0.1 | | | NBIP | | 72BAE |
| | | 2.5±0.1 | | | NBIP | | 73AUE/HUB |
| | | 2.7±0.2 | | | EnCT | | 71CHU/BER |
| | | 1.62±0.05 | | | NBIP | Vertical EA | 76HUB/KLE |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$BrK^-$** | | | | | | |
| $KBr^{-\cdot}$ | | | | | $\Delta_f H(A)=$ -180±2 | *85JANAF* |
| -239 [b] | 0.6 | | | Scat | | 79DEV/WIJ |
| **$BrKr^-$** | | | | | | |
| $Kr\cdot\cdot Br^-$ | | | | | | |
| -221 [c] | | *8* | | Mobl | | 84GAT |
| **$BrNa^-$** | | | | | | |
| $NaBr^{-\cdot}$ | | | | | $\Delta_f H(A)=$ -143±8 | *82TN270* |
| -234 [b] | 0.9 | | | Scat | | 79DEV/WIJ |
| **$BrO^-$** | | | | | $\Delta_f H(AH)=$ -79±8 | *76BEN* |
| $BrO^-$ | | | | | $BDE(A-H)=$ 423±13 | *82TN270* |
| <-20±21 | >1.5±0.2 [i] | <1590±29 [f] | | Endo | $Br^- + O_2 \rightarrow$ | 77VOG/DRE |
| **$BrO_2S^-$** | | | | | | |
| $SO_2\cdot\cdot Br^-$ | | | | | | |
| -590±10 [c] | | *81±8* | *53±11* | TDAs | | 85CAL/KEB |
| **$BrPb^-$** | | | | | | |
| $PbBr^-$ | | | | | | |
| | 0.9±0.2 | | | EIAP | From $PbBr_2$ | 67HAS/BLO |
| **$BrXe^-$** | | | | | | |
| $Xe\cdot\cdot Br^-$ | | | | | | |
| -227 [c] | | *14* | | Mobl | | 84GAT |
| **$Br_2^-$** | | | | | | |
| $Br_2^{-\cdot}$ | | | | | $\Delta_f H(A)=$ 31 | *82BAU/COX* |
| * | 2.5±0.1 | | | NBIP | | 72BAE |
| | 2.4 | | | ECD | Vertical EA: 1.6 eV | 81AYA/WEN |
| | 2.5±0.1 | | | EnCT | | 71CHU/BER |
| | 2.6±0.2 | | | NBIP | | 77DIS/LAC2 |
| | 2.6±0.2 | | | EnCT | | 73HUG/LIF |
| | 2.9±0.1 | | | EIAP | From $CBr_4$ | 71DEC/FRA |
| | 1.47±0.05 | | | NBIP | Vertical EA | 76HUB/KLE |
| **$Br_2ClP^-$** | | | | | | |
| $PBr_2Cl^{-\cdot}$ | | | | *Est2* | $\Delta_f H(A)=$ -152±42 | |
| -309±61 [b] | 1.6±0.2 | | | NBIP | | 76MAT/ROT |
| **$Br_2Ge^-$** | | | | | | |
| $GeBr_2^{-\cdot}$ | | | | | $\Delta_f H(A)=$ -63±8 | *82TN270* |
| <-217 [b] | >1.6 | | | EIAP | From $GeBr_4$ | 77PAB/MAR |
| **$Br_2H^-$** | | | | | | |
| $HBr\cdot\cdot Br^-$ | | | | | | |
| * -336±9 [c] | | *86±8* | *58±11* | TDAs | | 85CAL/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$Br_2I^-$** | | | | | | |
| $IBr_2^-$ | | | | | | |
| −251 | | *95* [k] | | Latt | | 77FIN/GAT |
| **$Br_2Si^-$** | | | | | | |
| $SiBr_2^{-:}$ | | | | | | |
| | >1.7 | | | EIAP | From $SiBr_4$ | 77PAB/MAR |
| **$Br_2Sn^-$** | | | | | | |
| $SnBr_2^{-\cdot}$ | | | | | | |
| −54 | 1.3 | | | EIAP | From $SnBr_4$ | 77PAB/PER |
| **$Br_3Ge^-$** | | | | | | |
| $GeBr_3^-$ | | | | | | |
| | >0.9 | | | EIAP | From $GeBr_4$ | 77PAB/MAR |
| **$Br_3P^-$** | | | | | | |
| $PBr_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −139±8* | *82TN270* |
| −293±23 [b] | 1.6±0.2 | | | NBIP | | 76MAT/ROT |
| **$Br_3Si^-$** | | | | | *$\Delta_f H(AH)$= −318±2* | *82TN270* |
| $SiBr_3^-$ | | | | | | |
| | >1.5±0.2 | | | EIAP | From $SiBr_4$ | 77PAB/MAR |
| **$Br_3Sn^-$** | | | | | *$\Delta_f H(AH)$= −318±8* | *82TN270* |
| $SnBr_3^-$ | | | | | *BDE(A−H)= 349±28* | *77PAB/PER* |
| | 3.08±0.01 | | | EIAP | From $SnBr_4$ | 78PAB/MAR |
| <−484 | >3.1 | | | EIAP | From $SnBr_4$ | 77PAB/PER |
| **$Br_3Ti^-$** | | | | | | |
| $TiBr_3^-$ | | | | | *$\Delta_f H(A)$= −377±42* | *74BEN/PAB* |
| | 0.76±0.01 | | | EIAP | From $TiBr_4$ | 78PAB/MAR |
| −452±15 | 0.8±0.3 | | | EIAP | From $TiBr_4$ | 74BEN/PAB |
| **$C^-$** | | | | | *$\Delta_f H(AH)$= 596* | *82TN270* |
| $C^-$ | | | | | *BDE(A−H)= 339±1* | *82TN270* |
| * 595±1 [a] | 1.263 | 1529±1 [e] | 1506±2 [h] | LPD | | 85HOT/LIN |
| | >1.2±1.0 | | | EIAP | From graphite | 54HON |
| **$CBrF_3^-$** | | | | | | |
| $CF_3Br^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −652* | *78KUD/KUD* |
| −740 [b] | 0.9±0.2 | | | NBIP | | 78COM/REI2 |
| **$CBr_3^-$** | | | | | *$\Delta_f H(AH)$= 24±5* | *84BIC/MIN* |
| $Br_3C^-$ | | | | | *BDE(A−H)= 402±7* | *82MCM/GOL* |
| 40±29 [b] | 1.7±0.2 | 1546±34 [f] | 1514±38 [h] | SI | | 69PAG/GOO |
| **$CBr_4^-$** | | | | | | |
| $Br_4C^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 84±3* | *84BIC/MIN* |
| −115 [b] | 2.1 | | | SI | | 69PAG/GOO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CClF_2^-$ | | | | | $\Delta_f H(AH)$= −484±2 | 77PED/RYL |
| $CF_2Cl^-$ | | | | | BDE(A−H)= 425±4 | 82MCM/GOL |
| −431±35 [a] | 1.6±0.3 | 1583±33 [c] | 1550±37 [h] | NBAP | From $CF_2Cl_2$ | 78DIS/LAC |
| | > 1.9 | | | EIAP | From $CF_3Cl$ | 79ILL/SCH |
| $CClF_2O^-$ | | | | | | |
| $CF_2{=}O\cdot\cdot Cl^-$ | | | | | | |
| • −920±11 [c] | | 52±8 [g] | 28±8 | IMRE | | 85LAR/MCM |
| < −728±25 | | | | IMRB | $ClCO^-$ or $ClF^-$ + $CF_2O$ → | 76KAR/KLE |
| $CClO^-$ | | | | | | |
| $ClCO^-$ | | | | | | |
| < −356 | | > 21 [k] | | EIAP | From $Cl_2CO$ | 76KAR/KLE |
| $CClO_2^-$ | | | | | | |
| $CO_2\cdot\cdot Cl^-$ | | | | | | |
| • −654±2 [c] | | 33 | 9 | TDAs | | 80KEE/LEE |
| | | 32±8 | 9±8 | TDEq | | 86HIR/SHO |
| $CClS_2^-$ | | | | | | |
| $CS_2\cdot\cdot Cl^-$ | | | | | | |
| • −159±10 [c] | | 49±8 [g] | 24±8 | IMRE | | 85LAR/MCM |
| $CCl_2^-$ | | | | | $\Delta_f H(AH)$= 109±4 | 83WEI/BEN |
| $CCl_2^{-\cdot}$ | | | | | BDE(A−H)= 272±17 | 85LIA/KAR |
| −10±42 [b] | 1.8±0.3 | 1411±46 [c] | | NBAP | From $CCl_4$,$CFCl_3$,$CHCl_3$ | 78DIS/LAC |
| | 2.5±0.6 | | | EIAP | From $CCl_4$, $CHCl_3$, $CH_2Cl_2$ | 80SCH/ILL |
| $CCl_2F^-$ | | | | | $\Delta_f H(AH)$= −281 | 78KUD/KUD |
| $CCl_2F^-$ | | | | | BDE(A−H)= 425±4 | 82MCM/GOL |
| | > 2.4±0.2 | < 1506±23 [c] | | EIAP | From $CF_2Cl_2$ | 79ILL/SCH |
| | 1.1±0.3 | | | NBAP | From $CFCl_3$ | 78DIS/LAC |
| $CCl_2FO^-$ | | | | | | |
| $CCl_2{=}O\cdot\cdot F^-$ | | | | | | |
| < −590±50 | | | | IMRB | $FCO^-$ + $CCl_2O$ → | 76KAR/KLE |
| $CCl_2F_2^-$ | | | | | | |
| $CCl_2F_2^{-\cdot}$ | | | | | $\Delta_f H(A)$= −477±5 | 77PED/RYL |
| −516±25 [b] | 0.4±0.2 | | | NBIP | | 78DIS/LAC |
| $CCl_3^-$ | | | | | $\Delta_f H(AH)$= −105±2 | 77PED/RYL |
| $CCl_3^-$ | | | | | BDE(A−H)= 401±4 | 82MCM/GOL |
| • −141±28 [a] | 2.3±0.3 [d] | 1494±26 [g] | 1461±25 | IMRB | > acetone, ≤ $C_5H_6$ | 72BOH/LEE |
| | 2.6±0.2 | | | EIAP | From $CCl_4$ | 80SCH/ILL |
| | > 1.9 | | | EIAP | From $CFCl_3$ | 79ILL/SCH |
| | 1.3±0.3 | | | NBAP | From $CHCl_3$, $CCl_4$ | 78DIS/LAC |
| | > 2.1±0.3 | | | EIAP | From $CFCl_3$ | 61CUR |
| | 1.44±0.05 | | | SI | | 66GAI/KAY |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$CCl_3F^-$** | | | | | | |
| $CCl_3F^{-\cdot}$ | | | | | *$\Delta_fH(A)$= −268±8* | *77PED/RYL* |
| −374±37 [b] | 1.1±0.3 | | | NBIP | | 78DIS/LAC |
| **$CCl_3O^-$** | | | | | | |
| $CCl_2{=}O\cdot\cdot Cl^-$ | | | | | | |
| • −498±9 [c] | | *52±8* [g] | *27±8* | IMRE | | 85LAR/MCM |
| −460±8 | | | | IMRB | | 76KAR/KLE |
| **$CCl_4^-$** | | | | | | |
| $CCl_4^{-\cdot}$ | | | | | *$\Delta_fH(A)$= −97±3* | *77PED/RYL* |
| −290±22 [b] | 2.0±0.2 | | | NBIP | | 83LAC/MAN |
| | 2.0±0.2 | | | NBIP | | 78DIS/LAC |
| | 2.1±0.1 | | | SI | | 66GAI/KAY |
| **$CCl_5^-$** | | | | | | |
| $CCl_4\cdot\cdot Cl^-$ | | | | | | |
| −384±7 [c] | | *59±3* | *25±4* | TDAs | | 74DOU/DAL |
| **$CF^-$** | | | | | | |
| $CF^{-\cdot}$ | | | | | *$\Delta_fH(A)$= 255* | *85JANAF* |
| | >3.3±0.3 | | | EIAP | From $C_2F_4$ | 70THY/MAC2 |
| **$CFN^-$** | | | | | | |
| $FCN^{-\cdot}$ | | | | | *$\Delta_fH(A)$= 36±17* | *85JANAF* |
| −318 | 2.9 [i] | | | EIAP | From $CF_3NC$ | 86HEN/ILL |
| | >4.0 | | | EIAP | From $PF_2CN$ | 74HAR/RAN |
| **$CFO^-$** | | | | *Est* | *$\Delta_fH(AH)$= −380* | |
| $FCO^-$ | | | | | *BDE(A−H)= 415±29* | *81DYK/JON2* |
| −444±10 | 2.7 [i] | *104* [k] | | EIAP | From $CF_2O$ | 70THY/MAC |
| −435 [a] | 2.3±0.5 [d] | 1475±19 | | EIAP | From HCOF | 77KAR/KLE |
| | 3.3 | | | EIAP | From $(CF_3)_2CO$ | 70HAR/THY |
| **$CFOS^-$** | | | | | | |
| $COS\cdot\cdot F^-$ | | | | | | |
| • −524±11 [c] | | *133±8* [g] | *103±8* | IMRE | | 85LAR/MCM |
| **$CFO_2^-$** | | | | | | |
| $CO_2\cdot\cdot F^-$ | | | | | | |
| • −775±11 [c] | | *133±8* [g] | *103±8* | IMRE | | 85LAR/MCM |
| −780±15 [c] | | *138±13* | | IMRE | | 78MCM/NOR |
| **$CFS_2^-$** | | | | | | |
| $CS_2\cdot\cdot F^-$ | | | | | | |
| • −262±11 [c] | | *131±8* [g] | *101±8* | IMRE | | 85LAR/MCM |
| **$CF_2^-$** | | | | | | |
| $CF_2^{-\cdot}$ | | | | | *$\Delta_fH(A)$= −205±13* | *85LIA/KAR* |
| <−102 | | | | IMRB | $O^- + CH_2F_2 \rightarrow$ | 76DAW/JEN |
| | <1.3±0.8 | | | EIAP | From c−$C_4F_8$ | 72HAR/THY2 |
| | >0.2 | | | EIAP | From $C_2F_4$ | 70THY/MAC2 |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$CF_2^-$** | | | | | | | |
| $CF_2^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -205±13* | *85LIA/KAR* |
| | | 2.6 | | | SI | | 69PAG/GOO |
| **$CF_2N^-$** | | | | | | | |
| $CF_2N^-$ | | | | | | | |
| | <-222 | | | | EIAP | From $CF_3NC$ | 86HEN/ILL |
| **$CF_3^-$** | | | | | | *$\Delta_f H(AH)$= -695±1* | *78KUD/KUD* |
| $CF_3^-$ | | | | | | *BDE(A-H)= 443±7* | *86TSA* |
| * | -648±10 [a] | 1.84±0.16 [d] | 1577±9 [g] | 1545±8 | IMRE | | 79BAR/SCO |
| * | | 2.82±0.01 | | | PD | Vertical detachment energy | 75RIC/STE4 |
| | | 1.9±0.3 | | | NBAP | From $CF_4$ | 78DIS/LAC |
| | | >2.0±0.2 | | | EIAP | From $C_3F_8$ | 74HAR/FRA |
| | | >2.4±0.5 | | | EIAP | From $C_2F_6$ | 74HAR/FRA |
| | | 2.2±0.3 | | | EIAP | From $CF_4$ | 74HAR/FRA |
| | -683 | 2.2 | | | EIAP | From $CF_4$ | 74FRA/WAN |
| | -651 | 1.9 | | | EIAP | From $CF_4$ | 73WAN/MAR |
| | | 3.1±0.2 | | | EIAP | From $CF_4$ | 72LIF/GRA |
| | | 2.1±0.3 | | | EIAP | From $C_2F_4$ | 70THY/MAC2 |
| | | 1.8±0.2 | | | EIAP | From $CF_3OF$ | 70THY/MAC |
| | | 2.7±0.2 | | | EIAP | From $CF_4$ | 70MAC/THY |
| | | 2.5 | | | EIAP | From $(CF_3)_2CO$ | 70HAR/THY |
| | | <2.6 | | | EIAP | From $C_2F_6$ | 69MAC/THY |
| | | 2.0 | | | EIAP | From $C_3F_8$ | 69LIF/GRA |
| | | 3.3 | | | EIAP | From $C_2F_6$ | 63BIB/CAR |
| | | 2.0±0.2 | | | SI | | 69PAG/GOO |
| | | | | 1539±8 | IMRE [o] | | 79BAR/SCO |
| **$CF_3I^-$** | | | | | | | |
| $CF_3I^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -590±21* | *78KUD/KUD* |
| | | 1.6±0.2 | | | NBIP | | 78COM/REI2 |
| | | 1.4±0.2 | | | NBIP | | 76TAN/MAT |
| | | 2.2±0.2 | | | NBIP | | 73MCN/LAC |
| **$CF_3N^-$** | | | | | | | |
| $CF_3N^{-\cdot}$ | | | | | | | |
| | <145±39 | | | | EIAP | From $CF_3NC$ | 86HEN/ILL |
| **$CF_3NO^-$** | | | | | | | |
| $CF_3NO^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -527* | |
| | <-720 [b] | >2.0±0.2 | | | EIAP | From$(CF_3)_2NO$ | 77HAR |
| **$CF_3O^-$** | | | | | | *$\Delta_f H(AH)$= -876±21* | *79KLO/SEP* |
| $CF_2{=}O\cdot\cdot F^-$ | | | | | | *BDE(A-H)= 452±13* | *68CZA/CAS* |
| * | -1062±13 [c] | 4.35±0.48 [d] | *178±8 [g]* | *142±8* | IMRE | | 83LAR/MCM |
| | -1030±17 [c] | | *146±13* | | IMRE | | 78MCM/NOR |
| | -937±25 | | | | IMRB | | 76KAR/KLE |
| | | >1.9±0.2 | | | EIAP | From $CF_3OOCF_3$ | 72MAC/THY |
| | | 1.9±0.1 | | | EIAP | From $CF_3OF$ | 70THY/MAC |
| | | 1.3 | | | SI | | 69PAG/GOO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CF_3O_3S^-$ | | | | | | |
| $CF_3SO_3^-$ | | | | | | |
| | 4.9±0.3 | | | IMRB | | 86VIG |
| | | | | | $\Delta_{acid}G$: $CF_3SO_3H < FSO_3H < H_2SO_4 < HPO_3 < HI$, $\Delta_{acid}G(CF_3SO_3H) <$ 1312 kJ | |
| • | | <1312±8 | | EIAP | From $CF_3SO_3H$,anhydride | 86ADA/SMI |
| $CF_3S^-$ | | | | | | |
| $CF_3S^-$ | | | | | | |
| | 1.8 | | | SI | | 69PAG/GOO |
| $CFeO^-$ | | | | | | |
| $Fe(CO)^-$ | | | | | | |
| • | 1.260±0.022 | | | LPES | | 79ENG/LIN2 |
| 68±25 | | | | EIAP | From $Fe(CO)_5$ | 76COM/STO |
| $CI^-$ | | | | | | |
| $CI^{-}\cdot$ | | | | | *$\Delta_f H(A)=$ 552* | *76REF/FRA2* |
| <363 [b] | >2.0 | | | Endo | $I^- + CO \rightarrow$ | 77VOG/MIS |
| 222±21 | 3.4±0.2 [i] | | | Endo | $I^- + CO \rightarrow$ | 76REF/FRA2 |
| $CIO^-$ | | | | | | |
| $ICO^-$ | | | | | | |
| −412 | 3.1 | | | Endo | $I^- + COS \rightarrow$ | 76REF |
| $CIO_2^-$ | | | | | | |
| $CO_2\cdot\cdot I^-$ | | | | | | |
| • −605±1 [c] | | *23* | *2* | TDAs | | 80KEE/LEE |
| $CN^-$ | | | | | *$\Delta_f H(AH)=$ 135* | *82TN270* |
| $CN^-$ | | | | | *BDE(A−H)= 518±8* | *82MCM/GOL* |
| • 74±9 [a] | 3.74±0.17 [d] | 1469±8 [g] | 1438±8 | IMRE | | 79BAR/SCO |
| • | 3.82±0.02 | 1461±10 [c] | | PI | | 69BER/CHU |
| 74 | | | | Endo | $I^- + (CN)_2 \rightarrow$ | 77REF/FRA |
| −105±19 | 3.2±0.1 [i] | | | EIAP | From $CH_3CN$ | 71DEC/BAF |
| | 3.2 | | | SI | | 74CHA/PAG |
| | 2.8 | | | SI | | 72PAG |
| | 2.80±0.02 | | | SI | New DH(H−CN) used | 63NAP/PAG |
| | | | 1447±8 | IMRE[o] | | 79BAR/SCO |
| $CNO^-$ | | | | | | |
| $CNO^-$ | | | | | | |
| 142 | | | | EIAP | From $MeNO_2$ | 72DID/FRA |
| 190±13 | | | | EIAP | From $MeNO_2$ | 69TSU/YOK2 |
| $CNO^-$ | | | | | *$\Delta_f H(AH)=$ −105±12* | *86SPI/PER* |
| $NCO^-$ | | | | | *BDE(A−H)= 477±26* | *70OKA* |
| • −192±21 [a] | 3.59±0.36 [d] | 1443±9 [g] | 1415±8 | IMRE | | 80WIG/BEA |
| | >2.6±0.4 | | | EIAP | From $PF_2NCO$ | 72THY |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CNO_4^-$ | | | | | | |
| $CO_2\cdot\cdot NO_3^-$ | | | | | | |
| • −740±2 [c] | | *39* | *8±1* | TDAs | | 80KEE/LEE |
| $CNS^-$ | | | | | *$\Delta_f H(AH)$= 128±2* | *82TN270* |
| $SCN^-$ | | | | | *BDE(A−H)= 464±6* | *63NAP/PAG* |
| | | 1375±25 [g] | 1343±21 | IMRB | Acid: HNCS | 84BIE/GRA |
| | 2.0 | | | SI | | 72PAG |
| | 2.15±0.02 | | | SI | From $(SCN)_2$ | 63NAP/PAG |
| $CNSe^-$ | | | | | | |
| $SeCN^-$ | | | | | | |
| | 2.6 | | | SI | | 69PAG/GOO |
| $CN_2^-$ | | | | | | |
| $CN_2^{-\cdot}$ | | | | | | |
| <649 | | | | IMRB | $O^- + CH_2N_2$ or $(CN)_2 \rightarrow$ | 79DAW/NOE |
| $CN_3O_6^-$ | | | | | *$\Delta_f H(AH)$= −2±2* | *77PED/RYL* |
| $(NO_2)_3C^-$ | | | | | | |
| | 3.1 | | | EIAP | From $C(NO_2)_4$ | 67JAE/HEN |
| $CO^-$ | | | | | | |
| $CO^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −110* | *82TN270* |
| −243 | 1.4 | | | EnCT | | 76REF/FRA2 |
| $COS^-$ | | | | | | |
| $COS^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −142±1* | *77PED/RYL* |
| −187±20 [b] | 0.5±0.2 | | | NBIP | | 75COM/REI |
| | >0.4 | | | ECD | | 83CHE/WEN |
| $CO_2^-$ | | | | | | |
| $CO_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −394* | *82TN270* |
| | | | | | | 75COM/REI |
| $CO_3^-$ | | | | | | |
| $CO\cdot\cdot O_2^-$ | | | | | | |
| >−210 [c] | | *<57* | | IMRB | $CO\cdot\cdot O_2^- + O_2 \rightarrow O_4^- + CO$ | 70ADA/BOH |
| $CO_3^-$ | | | | | | |
| $CO_2\cdot\cdot O^{-\cdot}$ | | | | | | |
| −503±6 [c] | 3.3±0.2 [i] | *218±4* | | PDis | | 80HIL/VES |
| −502 | | | | NBAP | From ethylene carbonate | 83COM/REI |
| | >3.079 | | | LPES | | 79NOV/ENG |
| | 3.3±0.1 | | | PD | | 77VES/MAU |
| −469±12 [c] | | *183±10* | | PDis | | 77VES/MAU |
| | 2.7±0.1 | | | PD | | 77HON/WOO |
| | >2.80 | *>190* [k] | | IMRE | $O_3^- + CO_2 = CO_3^- + O_2$ | 77DOT/DAV |
| | | *174±10* | | PDis | | 76MOS/COS |
| | 1.8±0.2 | | | PD | | 72BUR |
| −469 [c] | | *183* | | PDis | | 79SMI/LEE |
| | 3.1±0.2 | | | CIDT | | 78TIE/WU |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $CO_3^-$ | | | | | | | |
| $CO_2\cdot\cdot O^{-\cdot}$ | | | | | | | |
| | −455 [c] | | *169* | | PDis | | 78SMI/LEE |
| | −520±23 [c] | | *234±21* [g] | *201±21* | IMRE | $O_3^- + CO_2 = CO_3^- + O_2$ | 70ADA/BOH |
| $CO_4^-$ | | | | | | | |
| $CO_2\cdot\cdot O_2^-$ | | | | | | | |
| | −542±20 [c] | | *106±19* | | PDis | | 77VES/MAU |
| | −515±10 | | | | IMRE | $O_4^- + CO_2 = CO_4^- + O_2$ | 70ADA/BOH |
| | −510±9 [c] | | | *51±5* | kine | | 66PAC/PHE2 |
| $CO_5S^-$ | | | | | | | |
| $CO_2\cdot\cdot SO_3^-$ | | | | | | | |
| | −981±17 [c] | | *27±1* | *1±1* | TDAs | | 80KEE/LEE |
| $CS^-$ | | | | | | | |
| $CS^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 268* | *79HUB/HER* |
| • | 248 [b] | 0.205±0.021 | | | LPES | | 82BUR/FEI |
| | | > 1.6±0.3 | | | EIAP | From COS | 72THY |
| $CS_2^-$ | | | | | | | |
| $CS_2^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 117±1* | *77PED/RYL* |
| • | 68±11 [b] | 0.51±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.53±0.11 | | | IMRE | | 85GRI/CAL |
| | | 0.895±0.200 | | | LPES | | 86OAK/ELL |
| | | 0.6±0.1 | | | ECD | | 83CHE/WEN |
| | | 1.0±0.2 | | | NBIP | | 75COM/REI |
| | | 0.5±0.2 | | | EnCT | | 73HUG/LIF |
| | | 0.9±0.3 | | | IMRB | Between $NH_2^-$, $C^-$ | 61KRA/MUL |
| $CH^-$ | | | | | | *$\Delta_f H(AH)$= 390±8* | *82TN270* |
| $CH^{-\cdot}$ | | | | | | *BDE(A−H)= 423±18* | *79HUB/HER* |
| • | 477±27 [a] | 1.238±0.008 | 1616±18 [e] | 1588±20 [h] | LPES | | 75KAS/HER2 |
| | | 0.74±0.05 | | | PD | | 70FEL |
| | | 2.6±0.3 | | | EIAP | From $CH_4$, $C_2H_2$, $C_2H_4$ | 70LOC/MOM |
| | 633 | | | | EIAP | From $CH_4$ | 63TRE/NEU |
| $CHBrN^-$ | | | | | | | |
| $HCN\cdot\cdot Br^-$ | | | | | | | |
| • | −145±9 [c] | | *67±8* | | Est | Extrapolated from other halide data | 84LAR/MCM3 |
| $CHClF_3^-$ | | | | | | | |
| $CHF_3\cdot\cdot Cl^-$ | | | | | | | |
| • | −992±12 [c] | | *70±10* [g] | *41±8* | IMRE | | 84LAR/MCM2 |
| $CHClN^-$ | | | | | | | |
| $HCN\cdot\cdot Cl^-$ | | | | | | | |
| • | −180±10 [c] | | *88±8* [g] | *58±8* | IMRE | | 84LAR/MCM2 |

Table 2. Negative Ion Table – Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CHCl_2^-$ | | | | | *$\Delta_f H(AH)$= −96±1* | *77PED/RYL* |
| $CHCl_2^-$ | | | | | *BDE(A−H)= 422±5* | *83WEI/BEN* |
| −59±17 [a] | 1.7±0.2 [d] | 1567±16 [g] | 1535±13 | IMRB | Comparable to DMSO | 72BOH/LEE |
| $CHCl_2F_2^-$ | | | | | | |
| $CHF_2Cl\cdot\cdot Cl^-$ | | | | | | |
| • −783±12 [c] | | *72±8* [g] | *43±8* | IMRE | | 84LAR/MCM2 |
| $CHCl_3^-$ | | | | | | |
| $CHCl_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −105±2* | *77PED/RYL* |
| −274±7 [b] | 1.76±0.05 | | | SI | | 66GAI/KAY |
| $CHCl_3F^-$ | | | | | | |
| $CHFCl_2\cdot\cdot Cl^-$ | | | | | | |
| • −582 [c] | | *74±8* [g] | *45±8* | IMRE | | 84LAR/MCM2 |
| $CHCl_3Si^-$ | | | | | | |
| $HCSiCl_3^{-\cdot}$ | | | | | | |
| 142±42 | | | | EIAP | From $MeSiCl_3$ | 68JAE/HEN |
| $CHCl_4^-$ | | | | | | |
| $CHCl_3\cdot\cdot Cl^-$ | | | | | | |
| • −396±12 [c] | | *64±8* | *45±8* | TDAs | | 71YAM/KEB |
| | | *76±8* [g] | *47±8* | IMRE | | 84LAR/MCM2 |
| −412±6 [c] | | *80±3* | *49±4* | TDEq | | 74DOU/DAL |
| | | | *43* | TDEq | | 82FRE/IKU |
| $CHF^-$ | | | | | | |
| $HCF^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 109±12* | *85LIA/KAR* |
| <116 | | | | IMRB | $O^-$ + $CH_3F$→ | 76DAW/JEN |
| $CHFN^-$ | | | | | | |
| $HCN\cdot\cdot F^-$ | | | | | | |
| • −279±11 [c] | | *165±8* [g] | *138±8* | IMRE | | 83LAR/MCM |
| $CHF_2^-$ | | | | | *$\Delta_f H(AH)$= −453±1* | *78KUD/KUD* |
| $HCF_2^-$ | | | | | *BDE(A−H)= 432±4* | *83PIC/ROD* |
| −364±28 [a] | 1.3±0.3 [d] | 1618±28 [g] | 1586±25 | IMRB | | 77SUL |
| $CHF_2O^-$ | | | | | | |
| $HCF{=}O\cdot\cdot F^-$ | | | | | | |
| <−703 [c] | | *>76* | | IMRB | $FCO^-$ + HCFO→ | 77KAR/KLE |
| $CHF_4^-$ | | | | | | |
| $CF_3H\cdot\cdot F^-$ | | | | | | |
| • −1057±12 [c] | | *113±8* [g] | *82±8* | IMRE | | 83LAR/MCM |
| $CHN^-$ | | | | | | |
| $HCN^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 135* | *82TN270* |
| <38 [b] | >1.0 | | | EIAP | From $CH_3CN$ | 71TSU/YOK |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$CHNO_2^-$** | | | | | | |
| $CHNO_2^{-\cdot}$ | | | | | | |
| < 59 | | | | IMRB | $O^- + CH_3NO_2 \rightarrow$ | 59HEN/MUC |
| **$CHN_2^-$** | | | | | *$\Delta_f H(AH)$= 230±17* | *78VOG/WIL* |
| $CHN_2^{-\cdot}$ | | | | | | |
| 262±38 [a] | | 1561±22 [g] | 1527±17 | IMRB | Near MeCN | 83DEP/SCH |
| **$CHO^-$** | | | | | *$\Delta_f H(AH)$= −109±1* | *77PED/RYL* |
| $HCO^-$ | | | | | *BDE(A−H)= 364±3* | *83MOO/SEI* |
| • 8±4 [a] | 0.313±0.005 | 1646±3 [c] | 1613±5 [h] | LPES | | 86MUR/MIL |
| | | | 1648±19 | IMRB | | 75KAR/KLE |
| **$CDO^-$** | | | | | | |
| $DCO^-$ | | | | | | |
| | 0.301±0.005 | | | LPES | | 86MUR/MIL |
| **$CHOS^-$** | | | | | *$\Delta_f H(AH)$= −182±8* | *85KAS/DEP* |
| $HCOS^-$ | | | | | | |
| | | | 1435±13 | IMRB | | 85KAS/DEP |
| **$CHO_2^-$** | | | | | *$\Delta_f H(AH)$= −379* | *77PED/RYL* |
| $HCO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −464±13 [a] | 3.23±0.21 [d] | 1444±12 [g] | 1415±8 | IMRE | | 78CUM/KEB |
| | | 1446±12 [g] | 1416±8 | IMRE | | 81FUJ/MCI |
| **$CHO_3^-$** | | | | | | |
| $CO_2\cdot\cdot OH^-$ | | | | | | |
| −897 [c] | | *367* | | Endo | | 84HIE/PAU |
| **$CHO_3^-$** | | | | *Est2* | *$\Delta_f H(AH)$= −280±42* | |
| $HC(=O)OO^-$ | | | | | | |
| −260±46 [a] | < 1.1 | 1551±4 [g] | < 1523 | IMRB | | 86BOW/DEP |
| **$CH_2^-$** | | | | | *$\Delta_f H(AH)$= 146±1* | *81HEN/KNO* |
| $CH_2^-$ | | | | | *BDE(A−H)= 462±2* | *82TN270* |
| • 327±1 [b] | 0.652±0.006 | 1712±2 [c] | 1679±3 [h] | LPES | Singlet−triplet splitting of $CH_2$ = 37.7 kJ | 85LEO/MUR |
| | 0.670 | | | LPES | | 85LEO/MUR |
| | 0.210±0.015 | | | LPES | Hot band problem | 81ENG/COR |
| | 0.208±0.031 | | | LPES | Hot band problem, singlet−triplet splitting = 81.6 kJ | 76ZIT/ELL |
| | < 0.60±0.03 | | | PD | | 77FEL/RAC |
| | > 0.9±0.4 | | | EIAP | From $CH_2=CH_2$ | 71THY/MAC |
| < 328±38 | | | | EIAP | From ketene | 70COL/LOC |
| < 290 | | | | EIAP | From $CH_4$ | 63TRE/NEU |
| **$CD_2^-$** | | | | | | |
| $CD_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 390±1* | *82TN270* |
| • | 0.645±0.006 | | | LPES | | 85LEO/MUR |
| | 1.043±0.010 | | | LPES | | 81ENG/COR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ / $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CH_2Br^-$ | | | | | $\Delta_f H(AH)$= -38±1 | 84BIC/MIN |
| $CH_2Br^-$ | | | | | BDE(A-H)= 427±8 | 82MCM/GOL |
| • 75±18 [a] | 1.0±0.3 [d] | 1643±16 [g] | 1614±13 | IMRB | | 85ING/NIB2 |
| | 1.9 | | | SI | | 69PAG/GOO |
| $CH_2Cl^-$ | | | | | $\Delta_f H(AH)$= -82±1 | 79KUD/KUD |
| $CH_2Cl^-$ | | | | | BDE(A-H)= 422±8 | 82MCM/GOL |
| • 45±16 [a] | 0.80±0.24 [d] | 1657±15 [g] | 1628±13 | IMRE | | 85ING/NIB2 |
| | | | 1641±17 | IMRB | | 85HEN/HIE |
| $CH_2ClO_2^-$ | | | | | | |
| $HCO_2H\cdot\cdot Cl^-$ | | | | | | |
| • -721±10 [c] | | *115±8* | *84±8* | TDAs | | 82FRE/IKU |
| | | *107±8* [g] | *77±8* | IMRE | | 84LAR/MCM2 |
| | | *156±8* | *106±8* | TDAs | | 71YAM/KEB |
| $CH_2Cl_3^-$ | | | | | | |
| $CH_2Cl_2\cdot\cdot Cl^-$ | | | | | | |
| • -389±10 [c] | | *66±8* [g] | *38±8* | IMRE | | 84LAR/MCM2 |
| | | *65±1* | *37±3* | TDEq | | 74DOU/DAL |
| $CH_2FO_2^-$ | | | | | | |
| $HCO_2H\cdot\cdot F^-$ | | | | | | |
| • -817±11 [c] | | *190±8* [g] | *159±8* | IMRE | | 83LAR/MCM |
| $CH_2I^-$ | | | | | $\Delta_f H(AH)$= 15±1 | 77PED/RYL |
| $CH_2I^-$ | | | | | | |
| 102±25 [a] | | 1617±24 [g] | 1587±20 | IMRB | | 85ING/NIB2 |
| $CH_2IO_2^-$ | | | | | | |
| $HCO_2H\cdot\cdot I^-$ | | | | | | |
| • -646±5 [c] | | *79±4* | *53±9* | TDAs | | 84CAL/KEB |
| $CH_2N^-$ | | | | | $\Delta_f H(AH)$= 135 | 78DEF/HEH |
| $CH_2{=}N^-$ | | | | | | |
| 230 [a] | 0.51±0.07 | 1625±22 [g] | 1594±21 | IMRB | EA: between $O_2$ and cyclooctatetraene | 85KAS/DEP |
| $CH_2NO^-$ | | | | *Est2* | $\Delta_f H(AH)$= 29±13 | |
| $CH_2{=}NO^-$ | | | | | | |
| <56 | | <1557 [f] | | EIAP | From $MeNO_2$ | 72DID/FRA |
| $CH_2NO^-$ | | | | | $\Delta_f H(AH)$= -186 | 69BEN/CRU |
| $HN{=}CHO^-$ | | | | | | |
| • -210 [a] | | 1506±11 [g] | 1476±8 | IMRE | | 86TAF |
| $CH_2NO^-$ | | | | | | |
| $HOH\cdot\cdot CN^-$ | | | | | | |
| • -225 [c] | | *58±8* | *33±8* | TDAs | | 71PAY/YAM |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CH_2NO_2^-$ | | | | | *$\Delta_f H(AH)$= -75±1* | *77PED/RYL* |
| $CH_2{=}NO_2^-$ | | | | | | |
| • -114±13 [a] | | 1491±12 [g] | 1463±8 | IMRE | | 79BAR/SCO |
| | | 1495±12 [g] | 1467±8 | IMRE | | 78CUM/KEB |
| | <2.36 | | 1467±8 | IMRE | EA: < $NO_2$ | 78MAC/BOH |
| 84 | 0.5 | | | EIAP | From $CH_3NO_2$ | 69TSU/YOK |
| | | | 1473±8 | IMRE[o] | | 79BAR/SCO |
| $CH_2NS^-$ | | | | | | |
| $CH_2{=}NS^-$ | | | | | | |
| | | | 1436±15 | IMRB | | 85KAS/DEP |
| $CH_2NS^-$ | | | | | | |
| $H_2S\cdot\cdot CN^-$ | | | | | | |
| • -29±24 [c] | | *83±15* [g] | *52±10* | IMRE | | 87LAR/MCM |
| $CH_2O_4^-$ | | | | | | |
| $HOH\cdot\cdot CO_3^{-\cdot}$ | | | | | | |
| • -793 [c] | | *48±4* [g] | *28±2* | IMRE | | 74FEH/FER |
| >-906 [c] | | *< 161* | | PDis | | 78SMI/LEE |
| | 1.9±0.2 | | | PD | | 72BUR |
| -792 | | | | PDis | | 76COS/LIN |
| $CH_2S^-$ | | | | | | |
| $CH_2{=}S^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 100±13* | *76BEN* |
| 56±15 [b] | 0.465±0.023 | | | LPES | | 87MOR/ELL |
| $CH_3^-$ | | | | | | |
| $CH_3^-$ | | | | | *$\Delta_f H(A)$= 147±5* | *82MCM/GOL* |
| • 139±8 [a] | 7.8±0.030 | 1744±7 [c] | 1710±7 [h] | LPES | | 78ELL/ENG |
| | <0.5 | | | PD | | 77FEL/RAC |
| | <0.6 [d] | >1691 [g] | >1657 | IMRB | | 72BOH/LEE |
| | 1.1 | | | SI | | 72PAG |
| | 1.0 | | | SI | | 69PAG/GOO |
| | 1.1 | | | SI | | 68GAI/PAG |
| $CH_3BF_3O^-$ | | | | | | |
| $BF_3\cdot\cdot MeO^-$ | | | | | | |
| <-1477±13 [c] | | *>92±8* | | IMRB | $MeOH\cdot\cdot MeO^- + BF_3 \rightarrow$ | 73BLA/ISO |
| $CH_3BrCl^-$ | | | | | | |
| $MeBr\cdot\cdot Cl^-$ | | | | | | |
| -311±4 [c] | | *46±2* | *30±5* | TDAs | | 74DOU/ROB |
| | | *51±13* | | IMRB | Anchored: 84LAR/MCM | 73RIV/BRE |
| $CH_3Br_2^-$ | | | | | | |
| $MeBr\cdot\cdot Br^-$ | | | | | | |
| -290±4 [c] | | *38±2* | *21±3* | TDAs | | 74DOU/ROB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CH_3ClF^-$ | | | | | | |
| $MeF\cdot\cdot Cl^-$ | | | | | | |
| • −522 [c] | | *48±8* | | IMRE | | 84LAR/MCM2 |
| $CH_3ClF_3Si^-$ | | | | | | |
| $MeSiF_3\cdot\cdot Cl^-$ | | | | | | |
| • −1532 [c] | | *67±8* [g] | *40±8* | IMRE | | 85LAR/MCM |
| $CH_3ClI^-$ | | | | | | |
| $MeI\cdot\cdot Cl^-$ | | | | | | |
| −253±3 [c] | | *41±1* | *29±5* | TDAs | | 74DOU/ROB |
| $CH_3ClNO_2^-$ | | | | | | |
| $MeNO_2\cdot\cdot Cl^-$ | | | | | | |
| −371±14 [c] | | *68±13* | | IMRB | Anchored: 84LAR/MCM | 73RIV/BRE |
| $CH_3Cl_2^-$ | | | | | | |
| $MeCl\cdot\cdot Cl^-$ | | | | | | |
| • −360±10 [c] | | *51±8* [g] | *26±8* | IMRE | | 84LAR/MCM2 |
| | | *36±1* | *17±2* | TDAs | | 74DOU/DAL |
| $CH_3Cl_2Si^-$ | | | | | *$\Delta_f H(AH)$= −402±4* | *77PED/RYL* |
| $MeSiCl_2^-$ | | | | | | |
| −105±21 | | 1828±25 [f] | | EIAP | From $MeSiCl_3$, probably ca. 300 kJ more stable | 68JAE/HEN |
| $CH_3F_4Si^-$ | | | | | | |
| $MeSiF_3\cdot\cdot F^-$ | | | | | | |
| • −1697 [c] | | *211±8* [g] | *180±8* | IMRE | | 85LAR/MCM |
| | | *257±21* | | IMRB | | 77MUR/BEA3 |
| $CH_3I^-$ | | | | | | |
| $CH_3I^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 15±1* | *77PED/RYL* |
| −13±20 [b] | 0.3±0.2 | | | NBIP | Vertical EA | 74MOU/ATE |
| $CH_3I_2^-$ | | | | | | |
| $MeI\cdot\cdot I^-$ | | | | | | |
| −210±10 [c] | | *38±8* | *17±1* | TDAs | | 74DOU/ROB |
| $CH_3NO_2^-$ | | | | | | |
| $CH_3NO_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −75±1* | *77PED/RYL* |
| • −121±11 [b] | 0.48±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.49±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.45±0.05 | | | ECD | | 83CHE/WEN |
| | 0.4±0.2 | | | NBIP | | 78COM/REI2 |
| $CH_3N_2O^-$ | | | | | *$\Delta_f H(AH)$= −246±2* | *77PED/RYL* |
| $HN=C(NH_2)O^-$ | | | | | | |
| • −259±15 [a] | | 1517±13 [g] | 1487±10 | IMRE | | 86TAF |

**Table 2. Negative Ion Table – Continued**

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $CH_3O^-$ | | | | | | *$\Delta_f H(AH)$= −202* | *77PED/RYL* |
| $MeO^-$ | | | | | | *BDE(A−H)= 437±4* | *82MCM/GOL* |
| • | −139±10 [a] | 1.62±0.14 [d] | 1592±9 [g] | 1565±8 | IMRE | | 79BAR/SCO |
| • | | 1.570±0.022 | 1597±6 [c] | | LPES | | 78ENG/ELL |
| | | 1.59±0.04 | | | PD | | 78JAN/ZIM |
| | | < 1.59±0.04 | | | PD | | 75REE/BRA |
| | | | 1595±2 | 1569±3 | TDEq | | 86MEO/SIE |
| | | 2.6 | | | EIAP | From MeOMe | 64TSU/HAM |
| | | 0.4 | | | SI | | 69PAG/GOO |
| | | | | 1559±8 | IMRE[o] | | 79BAR/SCO |
| $CD_3O^-$ | | | | | | | |
| $CD_3O^-$ | | | | | | | |
| | | 1.552±0.022 | | | LPES | | 78ENG/ELL |
| $CH_3O_3^-$ | | | | | | | |
| $HOH\cdot\cdot HCO_2^-$ | | | | | | | |
| | −773 [c] | | *67±4* | *38±7* | TDAs | | 86MEO/SIE2 |
| $CH_3S^-$ | | | | | | *$\Delta_f H(AH)$= −23* | *77PED/RYL* |
| $MeS^-$ | | | | | | *BDE(A−H)= 364±9* | *83SHU/BEN* |
| • | −60±13 [a] | 1.90±0.22 [d] | 1493±12 [g] | 1467±8 | IMRE | | 79BAR/SCO |
| • | | 1.882±0.022 | | | LPES | | 78ENG/ELL |
| | | 1.861±0.004 | | | LPD | | 80JAN/REE |
| | | 1.861±0.004 | | | LPD | | 80JAN/BRA |
| | | 1.4 | | | SI | | 69PAG/GOO |
| | | | | 1476±8 | IMRE[o] | | 79BAR/SCO |
| $CD_3S^-$ | | | | | | | |
| $CD_3S^-$ | | | | | | | |
| | | 1.858±0.006 | | | LPD | | 80JAN/BRA |
| $CH_4ClO^-$ | | | | | | | |
| $MeOH\cdot\cdot Cl^-$ | | | | | | | |
| • | −488±10 [c] | | *59±8* | *41±8* | TDAs | | 71YAM/KEB |
| | | | *70±8* [g] | *41±8* | IMRE | | 84LAR/MCM2 |
| | | | *73±8* | *43±11* | TDAs | | 86YAM/FUR |
| | | | | *41* | TDEq | | 82FRE/IKU |
| | | | *59* | *41* | TDAs | | 73YAM/PAY |
| $CH_4FO^-$ | | | | | | | |
| $MeOH\cdot\cdot F^-$ | | | | | | | |
| • | −574±11 [c] | | *124±8* [g] | *95±8* | IMRE | | 83LAR/MCM |
| $CH_4FS^-$ | | | | | | | |
| $MeSH\cdot\cdot F^-$ | | | | | | | |
| • | −415±11 [c] | | *143±8* [g] | *114±8* | IMRE | | 83LAR/MCM |
| $CH_4IO^-$ | | | | | | | |
| $MeOH\cdot\cdot I^-$ | | | | | | | |
| • | −437±5 [c] | | *47±4* | *25±9* | TDAs | | 84CAL/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $CH_4N^-$ | | | | | *$\Delta_f H(AH)$= -23* | *77PED/RYL* |
| $MeNH^-$ | | | | | *BDE(A-H)= 418±10* | *82MCM/GOL* |
| • 134±5 [a] | 0.45±0.16 [d] | 1687±5 [g] | 1656±3 | IMRE | | 76MAC/HEM |
| | <1.6 | | | EIAP | From $MeNH_2$ | 68COL/HUB |
| $CH_4O_3^-$ | | | | | | |
| $MeOH\cdot\cdot O_2^-$ | | | | | | |
| • −324±5 [c] | | *80±4* | *52±4* | TDAs | | 73YAM/PAY |
| $CH_5O_2^-$ | | | | | | |
| $HOH\cdot\cdot MeO^-$ | | | | | | |
| −481 [c] | | *100±1* | *71±1* | TDAs | | 86MEO/SIE |
| $C_2^-$ | | | | | *$\Delta_f H(AH)$= 565±4* | *82MCM/GOL* |
| $C_2^{-\cdot}$ | | | | | *BDE(A-H)= 485±5* | *79HUB/HER* |
| • 505±2 [b] | 3.391±0.017 | 1470±7 [e] | | LPD | | 80JON/MEA |
| | 3.54±0.05 | | | PD | | 70FEL |
| >596±18 [a] | | >1561±13 [g] | >1531±8 | IMRB | | 75SCH/BOH |
| | >2.9±0.5 | | | EIAP | From $C_2H_4$ | 71THY/MAC |
| | 3.3±0.2 | | | EIAP | From $C_2H_2$, $C_2H_4$ | 70LOC/MOM |
| <826±19 | | | | EIAP | From ketene | 70COL/LOC |
| | >2.9 | | | EIAP | From $C_2H_4$ | 63TRE/NEU |
| | 4.0 | | | EIAP | From graphite | 54HON |
| $C_2ClF_4O^-$ | | | | | | |
| $CF_3CF{=}O\cdot\cdot Cl^-$ | | | | | | |
| • −1339±30 [c] | | *70±8* [g] | *42±8* | IMRE | | 85LAR/MCM |
| $C_2Cl_2F_3O^-$ | | | | | | |
| $CF_3CCl{=}O\cdot\cdot Cl^-$ | | | | | | |
| • −1143±30 [c] | | *74±8* [g] | *47±8* | IMRE | | 85LAR/MCM |
| $C_2Cl_5^-$ | | | | | | |
| $C_2Cl_5^-$ | | | | | | |
| | 1.5 | | | SI | Correct value probably 1 eV larger | 66GAI/KAY |
| $C_2Cl_6^-$ | | | | | | |
| $C_2Cl_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −150±5* | *83KOL/PAP* |
| | 1.48±0.10 | | | SI | | 66GAI/KAY |
| $C_2F^-$ | | | | | *$\Delta_f H(AH)$= 109* | *80STA/VOG* |
| $FC{\equiv}C^-$ | | | | | *BDE(A-H)= 552±21* | |
| | >3.4±0.8 | <1536±98 [e] | <1504±100 [h] | EIAP | From $CH_2{=}CF_2$ | 71THY/MAC |
| $C_2F_2^-$ | | | | | | |
| $F_2C{=}C^{-\cdot}$ | | | | | | |
| <15 | | | | IMRB | $O^- + CH_2{=}CF_2 \rightarrow$ | 76DAW/JEN |
| −646±58 | 1.7±0.2 | | | EIAP | From $CF_3CHO$ | 75HAR/THY |

### Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2F_2O^-$ | | | | | | |
| $F_2C{=}C{=}O^{-\cdot}$ | | | | | | |
| −156±58 | 2.4±0.6 | | | EIAP | From $CF_3CHO$ | 75HAR/THY |
| $C_2F_3^-$ | | | | | *$\Delta_f H(AH)$= −490±8* | *77PED/RYL* |
| $C_2F_3^{-\cdot}$ | | | | | *BDE(A−H)= 516±17* | *83SPY/SAU* |
| −391±19 | 2.1±0.2 [i] | 1630±36 [c] | | EIAP | From $C_3F_8$ | 83SPY/SAU |
| | >1.6 | | | EIAP | From $CF_3CF{=}CFCF_3$ | 79SAU/CHR |
| −637±58 | | | | EIAP | From $CF_3CF_2CHO$ | 75HAR/THY |
| | 3.1±0.3 | | | EIAP | From $CF_3CHO$ | 75HAR/THY |
| −420±42 | 2.0±0.4 | | | EIAP | From $C_2F_4$ | 72LIF/GRA |
| | 2.0±0.4 | | | EIAP | From $C_2F_4$ | 70THY/MAC2 |
| $C_2F_3O^-$ | | | | *Est* | *$\Delta_f H(AH)$= −800±13* | |
| $CF_3CO^-$ | | | | | *BDE(A−H)= 368±17* | |
| >−707±29 [a] | <0.6 | >1623±17 [c] | | EIAP | From $(CF_3)_2CO$ | 70HAR/THY |
| $C_2F_3O_2^-$ | | | | | *$\Delta_f H(AH)$= −1031±1* | *77PED/RYL* |
| $CF_3CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −1210±18 [a] | 4.20±0.27 [d] | 1351±17 [g] | 1323±8 | IMRE | | 78CUM/KEB |
| | | 1351±17 [g] | 1324±8 | IMRE | | 86TAF |
| $C_2F_3O_2^-$ | | | | | | |
| $FCOCOF\cdot\cdot F^-$ | | | | | | |
| • −1170±31 [c] | | *191±8* [g] | *155±8* | IMRE | | 85LAR/MCM |
| $C_2F_4N^-$ | | | | | | |
| $CF_3CN\cdot\cdot F^-$ | | | | | | |
| • −871±8 [c] | | *122±8* [g] | *92±8* | IMRE | | 85LAR/MCM |
| $C_2F_5^-$ | | | | | *$\Delta_f H(AH)$= −1105±6* | *82MCM/GOL* |
| $C_2F_5^-$ | | | | | *BDE(A−H)= 430±2* | *82MCM/GOL* |
| • −1067±23 [a] | 1.8±0.2 [d] | 1567±17 [g] | 1535±13 | IMRB | Between $tBuO^-$, $F^-$ | 76SUL/BEA |
| | 2.2±0.3 | | | EIAP | From $n{-}C_4F_{10}$ | 73HAR/THY2 |
| | 2.1±0.2 | | | EIAP | From $C_3F_8$ | 72HAR/THY |
| | 2.4 | | | EIAP | From $C_2F_6$ | 69MAC/THY |
| | 2.3 | | | EIAP | From $C_3F_8$ | 69LIF/GRA |
| | >3.3 | | | EIAP | From $C_3F_8$ | 63BIB/CAR |
| | >2.2±0.3 | | | SI | | 69PAG/GOO |
| | | | 1524±11 | IMRB [o] | | 76SUL/BEA |
| $C_2F_5O^-$ | | | | | | |
| $CF_3CF{=}O\cdot\cdot F^-$ | | | | | | |
| • −1481±31 [c] | | *191±8* [g] | *156±8* | IMRE | | 85LAR/MCM |
| $C_2FeO_2^-$ | | | | | | |
| $Fe(CO)_2^-$ | | | | | | |
| • | 1.220±0.022 | | | LPES | | 79ENG/LIN2 |
| −256±25 | | | | NBAP | From $Fe(CO)_5$ | 76COM/STO |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_2N^-$ | | | | | | | |
| $C_2N^-$ | | | | | | | |
| | <290±19 | >2.3±0.2 | | | EIAP | From $CH_3CN$ | 71TSU/YOK |
| $C_2O^-$ | | | | | | | |
| $CCO^{-\cdot}$ | | | | | | | |
| • | 8±11 [b] | 1.848±0.027 | | | LPES | | 83OAK/JON |
| | <339 | | | | IMRB | $O^-$ + cis-CHF=CHF→ | 79DAW/NOE |
| | 26±19 | | | | EIAP | From ketene | 70COL/LOC |
| $C_2O_3^-$ | | | | | | | |
| $C_2O_3^-$ | | | | | | | |
| | -554 | | | | EIAP | From maleic anhydride | 73COO/COM |
| $C_2O_5^-$ | | | | | | | |
| $CO_2\cdot\cdot CO_3^-$ | | | | | | | |
| • | -926±7 [c] | | *30* | *3±1* | TDAs | | 80KEE/LEE |
| $C_2H^-$ | | | | | | *$\Delta_f H(AH)$= 228±1* | *77PED/RYL* |
| HC≡C⁻ | | | | | | *BDE(A-H)= 552±8* | *85WOD/LEE* |
| • | 274±10 [a] | 2.99±0.19 [d] | 1576±10 [g] | 1542±8 | IMRE | | 79BAR/SCO |
| • | | 2.940±0.100 | | | LPD | Adiabatic EA: 3.18±0.25 eV | 79JAN/BRA |
| | | | 1585±8 | 1546±8 | TDEq | | 87MEO |
| | | 3.73±0.05 | | | PD | | 70FEL |
| | | | 1589±2 | | TDEq | | 86MEO/SIE |
| | | | 1611±4 [g] | 1577±3 | IMRE | | 74BOH/MAC |
| | | | 1572±38 | | Endo | | 73HUG/LIF |
| | | | | | | | 72BOH/LEE |
| | | >2.3±0.7 | | | EIAP | From $C_2H_4$ | 71THY/MAC |
| | | 2.1±0.3 | | | EIAP | From $C_2H_2$, $C_2H_4$ | 70LOC/MOM |
| | <515±19 | | | | EIAP | From ketene | 70COL/LOC |
| | | >2.8 | | | EIAP | From $C_2H_4$ | 63TRE/NEU |
| | | 2.6 | | | SI | | 69PAG/GOO |
| | | | | 1536±8 | IMRE[o] | | 79BAR/SCO |
| $C_2HClF_5^-$ | | | | | | | |
| $CF_3CF_2H\cdot\cdot Cl^-$ | | | | | | | |
| • | -1411±16 [c] | | *79±8* [g] | *49±8* | IMRE | | 84LAR/MCM2 |
| $C_2HClF_5O^-$ | | | | | | | |
| $CF_3OCF_2H\cdot\cdot Cl^-$ | | | | | | | |
| • | | | | *51±8* | IMRE | | 84LAR/MCM |
| $C_2HCl_2FN^-$ | | | | | | | |
| $CHCl_2F\cdot\cdot CN^-$ | | | | | | | |
| • | -281 [c] | | *74±15* [g] | *44±10* | IMRE | | 87LAR/MCM |
| $C_2HCl_2O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -427±17* | |
| $CHCl_2CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -499±28 [a] | 3.96±0.20 [d] | 1374±11 [g] | 1347±8 | IMRE | | 78CUM/KEB |
| | -587±28 [a] | | 1369±11 [g] | 1342±8 | IMRE | | 81FUJ/MCI |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_2HCl_3N^-$ | | | | | | | |
| $CHCl_3\cdot\cdot CN^-$ | | | | | | | |
| • | −106±26 [c] | | *76±15* [g] | *45±10* | IMRE | | 87LAR/MCM |
| $C_2HCl_3NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −235±13* | |
| $HN{=}C(CCl_3)O^-$ | | | | | | | |
| • | −329±23 [a] | | 1436±11 [g] | 1406±8 | IMRE | | 86TAF |
| $C_2HF^-$ | | | | | | | |
| $FCH{=}C^{-}\cdot$ | | | | | | | |
| | −139 | | | | EIAP | $O^- + FCH{=}CH_2 \rightarrow$ | 76DAW/JEN |
| $C_2HFN^-$ | | | | | | | |
| $CHFCN^-$ | | | | | | | |
| • | | | 1544±11 [g] | 1513±8 | IMRE | | 86TAF |
| $C_2HF_2O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −824±17* | |
| $CHF_2CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −971±29 [a] | 3.85±0.21 [d] | 1384±12 [g] | 1354±8 | IMRE | | 78CUM/KEB |
| | | | 1385±12 [g] | 1355±8 | IMRE | | 81FUJ/MCI |
| $C_2HF_3N^-$ | | | | | | | |
| $CHF_3\cdot\cdot CN^-$ | | | | | | | |
| • | −692±25 [c] | | *71±15* [g] | *40±10* | IMRE | | 87LAR/MCM |
| $C_2HF_3NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −837±13* | |
| $HN{=}C(CF_3)O^-$ | | | | | | | |
| • | −928±23 [a] | | 1438±11 [g] | 1409±8 | IMRE | | 86TAF |
| $C_2HF_4^-$ | | | | | | | |
| $F_2C{=}CFH\cdot\cdot F^-$ | | | | | | | |
| • | −849±19 [c] | | *110±8* [g] | *78±8* | IMRE | | 83LAR/MCM |
| | −841±36 [c] | | *102±25* | | IMRB | | 76SUL/BEA |
| $C_2HF_6^-$ | | | | | | | |
| $C_2F_5H\cdot\cdot F^-$ | | | | | | | |
| • | −1480±17 [c] | | *127±8* [g] | *94±8* | IMRE | | 83LAR/MCM |
| $C_2HF_6O^-$ | | | | | | | |
| $CF_3OCF_2H\cdot\cdot F^-$ | | | | | | | |
| • | | | | *113±8* | IMRE | | 84LAR/MCM |
| $C_2HN^-$ | | | | | | | |
| $HCCN^{-}\cdot$ | | | | | | | |
| | | | 1569±18 [g] | 1539±13 | IMRB | Between $H_2O_2$ and mCl-toluene | 87GRA/MEL |
| | | 0.8±0.4 | | | EIAP | From $CH_3CN$ | 86HEN/ILL2 |
| | <422 | | | | IMRB | $O^- + CH_3CN \rightarrow$ | 76DAW/JEN |
| | 309±19 | >1.1 | | | EIAP | From $CH_3CN$ | 71TSU/YOK |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}$(AH) $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}$(AH) $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$C_2HNO^-$** | | | | | | |
| $HCCNO^{-\cdot}$ | | | | | | |
| 502 | | | | EIAP | From $CH_2=CHNO_2$ | 72SHI/YAM |
| **$C_2HN_2^-$** | | | | | | |
| $HCN\cdot\cdot CN^-$ | | | | | | |
| • 119±24 [c] | | *91±15* [g] | *57±10* | IMRE | | 87LAR/MCM |
| 126±18 [c] | | *84±8* | | Est | | 84LAR/MCM3 |
| **$C_2HO^-$** | | | | | *$\Delta_f H(AH)$= -48±3* | *77PED/RYL* |
| $HC{\equiv}CO^-$ | | | | *D-EA* | *BDE(A-H)= 441±9* | |
| • | 2.350±0.022 | | | LPES | | 83OAK/JON |
| • -51±13 [a] | | 1527±11 [g] | 1497±8 | IMRE | Acid: ketene | 83OAK/JON |
| < -54±19 | | | | EIAP | From ketene | 70COL/LOC |
| **$C_2H_2^-$** | | | | | | |
| $H_2C=C^{-\cdot}$ | | | | | | |
| • | 0.470±0.020 | | | LPES | | 83BUR/STE |
| 255±146 | | | | IMRB | | 78DAW/NIB |
| 255±146 | | | | IMRB | $O^- + C_2H_4 \rightarrow$, $C_2H_2^- + N_2O \rightarrow CH_2CN^-$ | 76DAW/JEN |
| | < 0.4 | | | IMRB | | 75LIN/ALB |
| **$C_2D_2^-$** | | | | | | |
| $D_2C=C^{-\cdot}$ | | | | | | |
| • | 0.490±0.020 | | | LPES | | 83BUR/STE |
| **$C_2H_2BrO_2^-$** | | | | *Est* | *$\Delta_f H(AH)$= -395±6* | |
| $BrCH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -528±19 [a] | 3.71±0.22 [d] | 1397±13 [g] | 1370±8 | IMRE | | 78CUM/KEB |
| **$C_2H_2ClF_4O^-$** | | | | | | |
| $(CF_2H)_2O\cdot\cdot Cl^-$ | | | | | | |
| • | | | *71±8* | IMRE | | 84LAR/MCM |
| **$C_2H_2ClO_2^-$** | | | | | *$\Delta_f H(AH)$= -435±8* | *77PED/RYL* |
| $ClCH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -558±21 [a] | 3.61±0.21 [d] | 1407±12 [g] | 1376±8 | IMRE | | 78CUM/KEB |
| | | 1407±12 [g] | 1376±8 | IMRE | | 81FUJ/MCI |
| **$C_2H_2Cl_2N^-$** | | | | | | |
| $CH_2Cl_2\cdot\cdot CN^-$ | | | | | | |
| • -90±24 [c] | | *68±15* [g] | *38±10* | IMRE | | 87LAR/MCM |
| **$C_2H_2FO^-$** | | | | | *$\Delta_f H(AH)$= -444±3* | *77PED/RYL* |
| $CH_2=CFO^-$ | | | | | *BDE(A-H)= 406±8* | |
| • -484±20 [a] | 2.4±0.3 [d] | *148±8* [k] | 1460±15 | IMRB | Between $MeCOCH_2F$, cyclopentadiene | 80FAR/MCM |
| • | 2.22±0.09 | | | PD | | 77ZIM/REE |
| | | *148±8* [g] | *115±8* | IMRE | | 83LAR/MCM |
| | | | 1459±13 | IMRB [o] | | 80FAR/MCM |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_2H_2FO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -586±8* | |
| $FCH_2CO_2^-$ | | | | | | *BDE(A–H)= 444±8* | |
| • | -700±21 [a] | 3.52±0.21 [d] | 1416±12 [g] | 1385±8 | IMRE | | 78CUM/KEB |
| | | | 1418±12 [g] | 1386±8 | IMRE | | 81FUJ/MCI |
| $C_2H_2F_2O_2P^-$ | | | | | | | |
| $C_2H_2F_2O_2P^-$ | | | | | | | |
| | <-1125 | | | | IMRB | $CH_2=CHO^- + PF_3O \rightarrow$ | 78SUL/BEA |
| $C_2H_2F_3^-$ | | | | | | | |
| $CF_2=CH_2\cdot\cdot F^-$ | | | | | | | |
| | -697±17 | | *112±21* [k] | | IMRB | | 76SUL/BEA |
| $C_2H_2F_3O^-$ | | | | | | *$\Delta_f H(AH)$= -888±5* | *77PED/RYL* |
| $CF_3CH_2O^-$ | | | | | | *BDE(A–H)= 436±4* | |
| • | -904±20 [a] | 2.42±0.20 [d] | 1514±15 [g] | 1482±8 | IMRE | | 79BAR/SCO |
| | | | | 1493±8 | IMRE [o] | | 79BAR/SCO |
| $C_2H_2F_3O_2S^-$ | | | | | | | |
| $CF_3SO_2CH_2^-$ | | | | | | | |
| • | | | 1452±11 [g] | 1422±8 | IMRE | | 86TAF |
| $C_2H_2F_3O_3^-$ | | | | | | | |
| $HOH\cdot\cdot CF_3CO_2^-$ | | | | | | | |
| | -1509 [c] | | *57±4* | *27±7* | TDAs | | 86MEO/SIE2 |
| $C_2H_2F_5O^-$ | | | | | | | |
| $(CHF_2)_2O\cdot\cdot F^-$ | | | | | | | |
| • | | | *151±8* [g] | *117±8* | IMRE | | 83LAR/MCM |
| $C_2H_2N^-$ | | | | | | *$\Delta_f H(AH)$= 75±1* | *83AN/MAN* |
| $CH_2CN^-$ | | | | | | *BDE(A–H)= 389±10* | *82MCM/GOL* |
| • | 105±12 [a] | 1.46±0.22 [d] | 1560±11 [g] | 1528±8 | IMRE | | 79BAR/SCO |
| • | | 1.543±0.014 | | | LPES | | 87MOR/ELL3 |
| | | | 1562±11 [g] | 1530±8 | IMRE | | 78CUM/KEB |
| | | 1.507±0.018 | 1556±12 [e] | 1523±15 [h] | LPD | | 77ZIM/BRA |
| | | 1.560±0.006 | | | LPD | | 86MAR/WET |
| | | | 1534±19 | | EIAP | From $CH_3CN$ | 86HEN/ILL2 |
| | 20±19 | >1.6±0.2 | | | EIAP | From $CH_3CN$, EtCN | 71TSU/YOK |
| | | | | 1525±8 | IMRE [o] | | 79BAR/SCO |
| $C_2H_2N^-$ | | | | | | *$\Delta_f H(AH)$= 173±1* | *77BAG/COL* |
| $CH_2NC^-$ | | | | | | | |
| | | 1.059±0.024 | | | LPES | | 87MOR/ELL2 |
| $C_2D_2N^-$ | | | | | | | |
| $CD_2CN^-$ | | | | | | | |
| | | 1.538±0.012 | | | LPES | | 87MOR/ELL3 |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ / $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2D_2N^-$ | | | | | | |
| $CD_2NC^-$ | | | | | | |
| | 1.070±0.024 | | | LPES | | 87MOR/ELL2 |
| $C_2H_2NO_2^-$ | | | | | | |
| $H_2C=C=NO_2^-$ | | | | | | |
| | | 1515±19 | | EIAP | From $CH_2=CHNO_2$ | 72SHI/YAM |
| | | <1563±3 [g] | <1531 | IMRB | | 80BAR |
| $C_2H_2O_2^-$ | | | | | | |
| $O=CH-CH=O^{-\cdot}$ | | | | | $\Delta_f H(A)=$ −212±1 | 77PED/RYL |
| −272±25 | | | | NBAP | From ethylene carbonate | 83COM/REI |
| $C_2H_3^-$ | | | | | $\Delta_f H(AH)=$ 52 | 77PED/RYL |
| $C_2H_3^-$ | | | | | BDE(A−H)= 460±8 | 82MCM/GOL |
| * 221±9 [a] | 0.8±0.2 [d] | 1699 | | Bran | | 84DEP/BIE |
| | >0.4 | | | IMRB | | 75LIN/ALB |
| | | | >1661 | IMRB | | 86FRO/FRE |
| $C_2H_3BrN^-$ | | | | | | |
| $MeCN\cdot\cdot Br^-$ | | | | | | |
| * −192±10 [c] | | *54±8* | *33±8* | TDAs | | 72YAM/KEB |
| $C_2H_3ClF_3^-$ | | | | | | |
| $CF_2HCH_2F\cdot\cdot Cl^-$ | | | | | | |
| * −1055±18 [c] | | *79±8* [g] | *59±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_3ClF_3O^-$ | | | | | | |
| $CF_3CH_2OH\cdot\cdot Cl^-$ | | | | | | |
| * −1216±15 [c] | | *100±8* [g] | *69±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_3ClN^-$ | | | | | | |
| $MeCN\cdot\cdot Cl^-$ | | | | | | |
| * −208±10 [c] | | *56±8* | *38±8* | TDAs | | 72YAM/KEB |
| | | *57±8* | *37±11* | TDAs | | 86YAM/FUR |
| | | *44±8* [g] | *19±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_3Cl_2O_2^-$ | | | | | | |
| $ClCO_2Me\cdot\cdot Cl^-$ | | | | | | |
| * | | *59±8* [g] | *33±8* | IMRE | | 85LAR/MCM |
| $C_2H_3FN^-$ | | | | | | |
| $MeCN\cdot\cdot F^-$ | | | | | | |
| * −240±11 [c] | | *67±8* | *50±8* | TDAs | | 72YAM/KEB |
| $C_2H_3F_2^-$ | | | | | | |
| $CHF=CH_2\cdot\cdot F^-$ | | | | | | |
| −453±27 [c] | | *65±17* | | IMRB | | 76SUL/BEA |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_2H_3F_2O^-$ | | | | | | | |
| $F_2CHCH_2O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -620±4* | |
| | | | | | | *BDE(A-H)= 436±4* | |
| • | -618±16 [a] | 2.23±0.17 [d] | 1533±12 [g] | 1503±8 | IMRE | | 79BAR/SCO |
| | | | | 1505±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_3F_4^-$ | | | | | | | |
| $CF_2HCH_2F\cdot\cdot F^-$ | | | | | | | |
| • | -1108±19 [c] | | *111±8* [g] | *79±8* | IMRE | | 83LAR/MCM |
| $C_2H_3F_4O^-$ | | | | | | | |
| $CF_3CH_2OH\cdot\cdot F^-$ | | | | | | | |
| • | -1300±16 [c] | | *164±8* [g] | *130±8* | IMRE | | 83LAR/MCM |
| $C_2H_3IN^-$ | | | | | | | |
| $MeCN\cdot\cdot I^-$ | | | | | | | |
| • | -163±10 [c] | | *50±8* | *27±8* | TDAs | | 72YAM/KEB |
| $C_2H_3NO_2^-$ | | | | | | | |
| $CH_2=CHNO_2^{-\cdot}$ | | | | | | | |
| | | >1.6 | | | IMRB | | 80BAR |
| $C_2H_3NO_2^-$ | | | | | | | |
| $MeCN\cdot\cdot O_2^-$ | | | | | | | |
| • | -36±6 [c] | | *69±4* | *47±4* | TDAs | | 73YAM/PAY |
| $C_2H_3O^-$ | | | | | | *$\Delta_f H(AH)$= -166* | *77PED/RYL* |
| $CH_2=CHO^-$ | | | | | *D-EA* | *BDE(A-H)= 394±15* | |
| • | -165±13 [a] | | 1531±12 [g] | 1502±8 | IMRE | | 79BAR/SCO |
| • | | 1.817±0.023 | | | LPES | | 82ELL/ENG |
| | | | 1533±12 [g] | 1505±8 | IMRE | | 78CUM/KEB |
| | | 1.81±0.06 | | | PD | | 77ZIM/REE |
| | | | | 1505±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_3O^-$ | | | | | | *$\Delta_f H(AH)$= -166* | *77PED/RYL* |
| $CH_3CO^-$ | | | | | | *BDE(A-H)= 360±3* | *82MCM/GOL* |
| • | -60±11 [a] | 0.4±0.1 [d] | 1636±11 [g] | 1604±8 | IMRB | | 85DEP/BIE |
| $C_2D_3O^-$ | | | | | | | |
| $CD_2=CDO^-$ | | | | | | | |
| • | | 1.817±0.029 | | | LPES | | 82ELL/ENG |
| $C_2H_3O_2^-$ | | | | | | *$\Delta_f H(AH)$= -356±1* | *77PED/RYL* |
| $HCO_2CH_2^-$ | | | | | | | |
| | -249±20 [a] | | 1637±19 [g] | 1607±17 | IMRB | | 85DEP/GRA |
| $C_2H_3O_2^-$ | | | | | | *$\Delta_f H(AH)$= -432* | *78CHA/ZWO* |
| $MeCO_2^-$ | | | | | | *BDE(A-H)= 443±8* | *82MCM/GOL* |
| • | -504±13 [a] | 3.07±0.21 [d] | 1459±12 [g] | 1429±8 | IMRE | | 78CUM/KEB |
| | | | 1457±12 [g] | 1427±8 | IMRE | | 86TAF |
| | | | 1459±12 [g] | 1430±8 | IMRE | | 81FUJ/MCI |
| | | 3.36±0.05 | | | ECD | | 68WEN/CHE |
| | | 3.3±0.2 | | | EIAP | From $MeCO_2Et$ | 64TSU/HAM |

Table 2. Negative Ion Table – Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2H_3O_4^-$ | | | | | | |
| $HCO_2H\cdot\cdot HCO_2^-$ | | | | | | |
| −997±17 [c] | | *154±4* | *105±7* | TDAs | | 86MEO/SIE2 |
| $C_2H_3Si^-$ | | | | | | |
| $H_3SiC\equiv C^-$ | | | | | | |
| <322 | | | | IMRB | $HC\equiv C^- + SiH_4 \rightarrow$ | 76PAY/TAN |
| $C_2H_4B_3^-$ | | | | | | |
| 1,5-$C_2B_3H_4^-$ | | | | | | |
| | | *<1795* | | EIAP | From closo-1,5-$C_2B_3H_5$ | 73ONA/HOW |
| $C_2H_4ClF_2^-$ | | | | | | |
| $MeCHF_2\cdot\cdot Cl^-$ | | | | | | |
| • −787±18 [c] | | *62±8* [g] | *34±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_4ClF_3N^-$ | | | | | | |
| $CF_3CH_2NH_2\cdot\cdot Cl^-$ | | | | | | |
| • −1004±14 [c] | | *75±8* [g] | *45±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_4ClO^-$ | | | | | | |
| $MeCHO\cdot\cdot Cl^-$ | | | | | | |
| • −453±10 [c] | | *60±8* [g] | *33±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_4ClO_2^-$ | | | | | | |
| $MeCO_2H\cdot\cdot Cl^-$ | | | | | | |
| • −750±10 [c] | | *90±8* | *66±8* | TDAs | | 71YAM/KEB |
| | | *100±8* [g] | *70±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_4Cl_2Si^-$ | | | | | | |
| $HCSiMeCl_2^{-\cdot}$ | | | | | | |
| 343±21 | | | | EIAP | From $Me_2SiCl_2$ | 68JAE/HEN |
| $C_2H_4F^-$ | | | | | | |
| $CH_2{=}CH_2\cdot\cdot F^-$ | | | | | | |
| −221±15 [c] | | *25±13* | | IMRB | Structure: 85ROY/MCM | 76SUL/BEA |
| $C_2H_4FO^-$ | | | | *Est* | *$\Delta_f H(AH)=$ −417±8* | |
| $FCH_2CH_2O^-$ | | | | | *BDE(A–H)= 436±4* | |
| −399±25 [a] | 2.1±0.2 [d] | 1548±16 [g] | 1521±15 | IMRB | Between HF, acetone | 80CLA/MCM |
| | | | 1527±14 | IMRB | | 77DAW/JEN |
| | | | 1520±17 | IMRB[o] | | 80CLA/MCM |
| $C_2H_4FO_2^-$ | | | | | | |
| $MeCO_2H\cdot\cdot F^-$ | | | | | | |
| • −865±11 [c] | | *185±8* [g] | *153±8* | IMRE | | 83LAR/MCM |
| $C_2H_4F_4N^-$ | | | | | | |
| $CF_3CH_2NH_2\cdot\cdot F^-$ | | | | | | |
| • −1067±19 [c] | | *118±8* [g] | *85±8* | IMRE | | 83LAR/MCM |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / *$\Delta H_{aff}(X\cdot\cdot Y^-)$* | $\Delta G_{acid}(AH)$ / *$\Delta G_{aff}(X\cdot\cdot Y^-)$* | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2H_4IO_2^-$ | | | | | | |
| $MeCO_2H\cdot\cdot I^-$ | | | | | | |
| • −691±5 [c] | | *71±4* | *44±9* | TDAs | | 84CAL/KEB |
| $C_2H_4N^-$ | | | | | *$\Delta_f H(AH)$= 71±8* | *69BEN/CRU* |
| $CH_2=NCH_2^-$ | | | | | | |
| 151±32 [a] | 0.8±0.3 | 1610±23 [g] | 1582±21 | IMRB | EA: between cyclooctatetraene, $SO_2$ | 85KAS/DEP |
| $C_2H_4NO^-$ | | | | | *$\Delta_f H(AH)$= −238±1* | *77PED/RYL* |
| $HN=C(Me)O^-$ | | | | | | |
| • −339±12 [a] | | 1429±11 [g] | 1400±8 | IMRE | | 86TAF |
| $C_2H_4NO^-$ | | | | | *$\Delta_f H(AH)$= −20±8* | *69BEN/CRU* |
| $MeCH=NO^-$ | | | | | | |
| • −20±21 [a] | | 1530±12 [g] | 1500±8 | IMRE | | 79BAR/SCO |
| | | | 1503±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_4NO^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −787±4* | |
| $MeN=CHO^-$ | | | | | | |
| • −809±15 [a] | | 1508±11 [g] | 1479±8 | IMRE | | 86TAF |
| $C_2H_4NO^-$ | | | | | | |
| $MeOH\cdot\cdot CN^-$ | | | | | | |
| • −196±24 [c] | | *69±15* [g] | *38±10* | IMRE | | 87LAR/MCM |
| $C_2H_4NO_2^-$ | | | | | *$\Delta_f H(AH)$= −391±5* | *77NGA/SAB* |
| $H_2NCH_2CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −488±15 [a] | 3.35±0.19 [d] | 1433±10 [g] | 1404±8 | IMRE | | 83LOC/MCI |
| $C_2H_4NO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −417±4* | |
| $HN=C(OMe)O^-$ | | | | | | |
| • −433±15 [a] | | 1514±11 [g] | 1485±8 | IMRE | | 86TAF |
| $C_2H_4NO_2^-$ | | | | | *$\Delta_f H(AH)$= −102* | *77PED/RYL* |
| $MeCH=NO_2^-$ | | | | | | |
| • −143±13 [a] | | 1490±12 [g] | 1462±8 | IMRE | | 79BAR/SCO |
| | | 1496±12 [g] | 1469±8 | IMRE | | 78CUM/KEB |
| | | | 1472±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_5^-$ | | | | | *$\Delta_f H(AH)$= −84* | *74SCO* |
| $MeCH_2^-$ | | | | | *BDE(A−H)= 421±2* | *86BRO/LIG* |
| • 147±9 [a] | | 1761±8 | 1725±10 [h] | Bran | | 84DEP/BIE |
| | 1.0 | | | SI | | 72PAG |
| | 0.9 | | | SI | | 69PAG/GOO |
| $C_2H_5B_4^-$ | | | | | | |
| 1,2-$C_2B_4H_5^-$ | | | | | | |
| | | < 1409±29 | | EIAP | From closo-1,2-$C_2B_4H_6$ | 73ONA/HOW |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_2H_5B_4^-$ | | | | | | | |
| 1,6-$C_2B_4H_5^-$ | | | | | | | |
| | | | <1891 | | EIAP | From closo-1,6-$C_2B_4H_6$ | 73ONA/HOW |
| $C_2H_5Br_2^-$ | | | | | | | |
| $EtBr\cdot\cdot Br^-$ | | | | | | | |
| * | −324 [c] | | *49* | *25* | TDAs | | 74DOU |
| $C_2H_5ClFO^-$ | | | | | | | |
| $FCH_2CH_2OH\cdot\cdot Cl^-$ | | | | | | | |
| * | −730±18 [c] | | *86±8* [g] | *54±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_5Cl_2^-$ | | | | | | | |
| $EtCl\cdot\cdot Cl^-$ | | | | | | | |
| | −400±20 [c] | | *61±19* | | IMRB | Anchored: 84LAR/MCM | 73RIV/BRE |
| $C_2H_5Cl_2O^-$ | | | | | | | |
| $ClCH_2CH_2OH\cdot\cdot Cl^-$ | | | | | | | |
| * | −579±14 [c] | | *90±8* [g] | *59±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_5F_2O^-$ | | | | | | | |
| $FCH_2CH_2OH\cdot\cdot F^-$ | | | | | | | |
| * | −811±19 [c] | | *146±8* [g] | *113±8* | IMRE | | 83LAR/MCM |
| $C_2H_5N^-$ | | | | | | | |
| $EtN^{-}\cdot$ | | | | | | | |
| * | | 1.9±0.2 | | | PD | | 74RIC/STE2 |
| $C_2H_5N_2O^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 49±8* | |
| $MeN(NO)CH_2^-$ | | | | | | | |
| * | 113±19 [a] | | 1594±11 [g] | 1564±8 | IMRE | | 85ING/NIB3 |
| | | | | 1567±8 | IMRE[o] | | 85ING/NIB3 |
| $C_2H_5O^-$ | | | | | | *$\Delta_f H(AH)$= −235* | *77PED/RYL* |
| $EtO^-$ | | | | | | *BDE(A−H)= 436±4* | *82MCM/GOL* |
| * | −186±10 [a] | 1.75±0.14 [d] | 1579±10 [g] | 1551±8 | IMRE | | 79BAR/SCO |
| * | | 1.726±0.033 | 1582±8 [e] | | LPES | | 82ELL/ENG |
| | | 1.7±0.1 | | | EIAP | From EtONO | 68WIL/HAM |
| | | >1.7 | | | EIAP | From EtOH | 63TRE/NEU |
| | | 0.6 | | | SI | | 69PAG/GOO |
| | | | | 1546±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_5O^-$ | | | | | | *$\Delta_f H(AH)$= −184* | *77PED/RYL* |
| $MeOCH_2^-$ | | | | | | *BDE(A−H)= 389±4* | *82MCM/GOL* |
| * | −11±9 [a] | | 1703±8 | 1666±12 [h] | Bran | | 84DEP/BIE |
| $C_2D_5O^-$ | | | | | | | |
| $CD_3CD_2O^-$ | | | | | | | |
| * | | 1.702±0.033 | | | LPES | | 82ELL/ENG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2H_5OS^-$ | | | | | *$\Delta_f H(AH)$= −151±1* | *77PED/RYL* |
| $MeSOCH_2^-$ | | | | | | |
| • −119±10 [a] | | 1563±10 [g] | 1533±8 | IMRE | | 79BAR/SCO |
| | | 1566±10 [g] | 1536±8 | IMRE | | 78CUM/KEB |
| | | | 1530±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_5O_2S^-$ | | | | | *$\Delta_f H(AH)$= −373±3* | *77PED/RYL* |
| $MeSO_2CH_2^-$ | | | | | | |
| • −373±15 [a] | | 1531±12 [g] | 1499±8 | IMRE | | 79BAR/SCO |
| −370±15 [a] | | 1533±12 [g] | 1502±8 | IMRE | | 78CUM/KEB |
| | | | 1502±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_5O_3^-$ | | | | | | |
| $HOH\cdot\cdot MeCO_2^-$ | | | | | | |
| • −813 [c] | | *67±4* | *39±7* | TDAs | | 86MEO/SIE2 |
| $C_2H_5O_3^-$ | | | | | | |
| $MeOH\cdot\cdot HCO_2^-$ | | | | | | |
| • −740±17 [c] | | *74±4* | *44±7* | TDAs | | 86MEO/SIE2 |
| $C_2H_5S^-$ | | | | | *$\Delta_f H(AH)$= −46* | *77PED/RYL* |
| $EtS^-$ | | | | | *BDE(A–H)= 364±9* | |
| • −90±13 [a] | 1.97±0.22 [d] | 1486±12 [g] | 1460±8 | IMRE | | 79BAR/SCO |
| • | 1.953±0.004 | 1488±9 [e] | | LPD | | 80JAN/REE |
| | 1.6 | | | SI | | 69PAG/GOO |
| | | | 1469±8 | IMRE[o] | | 79BAR/SCO |
| $C_2H_5S^-$ | | | | | *$\Delta_f H(AH)$= −38* | *77PED/RYL* |
| $MeSCH_2^-$ | | | | | | |
| • 77±11 [a] | | 1645±11 [g] | 1615±8 | IMRE | | 85ING/NIB |
| $C_2H_5Si^-$ | | | | | *$\Delta_f H(AH)$= 92±8* | *86WAL* |
| $MeSiCH_2^-$ | | | | | | |
| 155±32 [a] | | 1593±23 [g] | 1565±21 | IMRB | | 86DAM/DEP2 |
| $C_2H_6BF_2^-$ | | | | | | |
| $Me_2BF\cdot\cdot F^-$ | | | | | | |
| −773 [c] | | *259* | | IMRB | | 77MUR/BEA2 |
| | | | | | $F^-$A: $Et_3B > Me_2BF > MeSiF_3 > Me_3B > SF_4$ | |
| $C_2H_6BF_2O_2^-$ | | | | | | |
| $(MeO)_2BF\cdot\cdot F^-$ | | | | | | |
| • | | *218±21 [g]* | *190±21* | IMRE | | 85LAR/MCM |
| $C_2H_6B_5^-$ | | | | | | |
| $2,4\text{-}C_2B_5H_6^-$ | | | | | | |
| | | <1891 | | EIAP | From closo-2,4-$C_2B_4H_7$ | 73ONA/HOW |
| $C_2H_6BrOS^-$ | | | | | | |
| $Me_2SO\cdot\cdot Br^-$ | | | | | | |
| • −437±6 [c] | | *72±4* | *46±9* | TDAs | | 84MAG/CAL |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_2H_6ClO^-$ | | | | | | |
| $EtOH\cdot\cdot Cl^-$ | | | | | | |
| • −535±10 [c] | | *72±8* [g] | *44±8* | IMRE | | 84LAR/MCM2 |
| $C_2H_6ClOS^-$ | | | | | | |
| $Me_2SO\cdot\cdot Cl^-$ | | | | | | |
| • −457±6 [c] | | *78±4* | *52±9* | TDAs | | 84MAG/CAL |
| $C_2H_6ClSi^-$ | | | | | | |
| $Me_2SiCl^-$ | | | | | | |
| 67±21 | | | | EIAP | From $Me_2SiCl_2$ | 68JAE/HEN |
| $C_2H_6FO^-$ | | | | | | |
| $EtOH\cdot\cdot F^-$ | | | | | | |
| • −615±11 [c] | | *132±8* [g] | *101±8* | IMRE | | 83LAR/MCM |
| $C_2H_6F_3Si^-$ | | | | | | |
| $Me_2SiF_2\cdot\cdot F^-$ | | | | | | |
| | | *232±21* | | IMRB | $F^-A$: $SF_4 < Me_2SiF_2 < Me_3B$ | 77MUR/BEA3 |
| $C_2H_6IO^-$ | | | | | | |
| $EtOH\cdot\cdot I^-$ | | | | | | |
| • −474±5 [c] | | *51±4* | *27±9* | TDAs | | 84CAL/KEB |
| $C_2H_6IOS^-$ | | | | | | |
| $Me_2SO\cdot\cdot I^-$ | | | | | | |
| • −405±6 [c] | | *66±4* | *38±9* | TDAs | | 84MAG/CAL |
| $C_2H_6N^-$ | | | | | *$\Delta_f H(AH)$= −48±1* | *77PED/RYL* |
| $EtNH^-$ | | | | | *BDE(A−H)= 423±13* | *83MCM/GOL* |
| • 93±8 [a] | 0.66±0.20 [d] | 1671±7 [g] | 1639±3 | IMRE | | 76MAC/HEM |
| $C_2H_6N^-$ | | | | | *$\Delta_f H(AH)$= −18* | *77PED/RYL* |
| $Me_2N^-$ | | | | | *BDE(A−H)= 383±8* | *82MCM/GOL* |
| • 109±7 [a] | 0.39±0.15 [d] | 1658±6 [g] | 1628±3 | IMRE | | 76MAC/HEM |
| | 1.0 | | | SI | | 69PAG/GOO |
| $C_2H_6O_4P^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −1017±63* | |
| $(MeO)_2PO_2^-$ | | | | | | |
| −1084±149 [a] | | 1463±86 [g] | 1435±84 | IMRB | | 80HOD/SUL |
| $C_2H_7O_2^-$ | | | | | | |
| $MeOH\cdot\cdot MeO^-$ | | | | | | |
| −461±11 [c] | | *120±1* | *87±2* | TDAs | | 86MEO/SIE |
| −432±18 [c] | | *91±8* | *64±7* | TDAs | | 84CAL/ROZ |
| | | | The difference between 84CAL/ROZ and 86MEO/SIE2 has not been resolved. | | | |
| $C_3^-$ | | | | | | |
| $C_3^-$ | | | | | | |
| • | 1.981±0.020 | | | LPES | From propene discharge | 86OAK/ELL |
| | 2.5±1.0 | | | EIAP | From graphite | 54HON |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3ClF_6O^-$ | | | | | | |
| $(CF_3)_2CO\cdot\cdot Cl^-$ | | | | | | |
| • −1720±30 [c] | | *96±8* [g] | *68±8* | IMRE | | 85LAR/MCM |
| $C_3F_3^-$ | | | | | | |
| $C_3F_3^-$ | | | | | | |
| −425 | | | | EIAP | From $CF_2=CF-CF=CF_2$ | 79SAU/CHR |
| −941 | | | | EIAP | From $CF_3CF=CF_2$ | 72HAR/THY |
| $C_3F_3^-$ | | | | | *$\Delta_f H(AH)$= −414±13* | *86SMA* |
| $CF_3C\equiv C^-$ | | | | | *BDE(A−H)= 552±21* | |
| • −458±21 [a] | 3.92±0.31 [d] | 1486±9 [g] | 1454±8 | IMRE | | 86TAF |
| | <5.6 | | | EIAP | From $CF_3C\equiv CCF_3$ | 79SAU/CHR |
| $C_3F_4O^-$ | | | | | | |
| $CF_3CFCO^{-\cdot}$ | | | | | | |
| −926±58 | | | | EIAP | From $CF_3CF_2CHO$ | 75HAR/THY |
| $C_3F_5^-$ | | | | | | |
| $C_3F_5^-$ | | | | | | |
| | 2.7±0.2 | | | EIAP | From c−$C_4F_8$ | 72HAR/THY2 |
| −1052 | 3.0 | | | EIAP | From c−$C_4F_8$, 2−$C_4F_8$ | 79SAU/CHR |
| | >2.7±0.2 | | | EIAP | From $CF_3CF=CF_2$ | 72THY |
| −950±38 | 2.6±0.4 | | | EIAP | From $CF_3CF=CF_2$ | 72LIF/GRA |
| | 2.7±0.1 | | | EIAP | From $CF_3CF=CF_2$ | 72HAR/THY |
| $C_3F_5O^-$ | | | | *Est* | *$\Delta_f H(AH)$= −1201±21* | |
| $CF_2=C(CF_3)O^-$ | | | | | | |
| • −1318±42 [a] | | 1413±21 [g] | 1384±17 | IMRB | Between $FCH_2CO_2H$, HCl; nearer to HCl | 80FAR/MCM |
| | 2.1±0.3 | | | EIAP | From $(CF_3)_2CO$ | 70HAR/THY |
| | | | 1356±10 | IMRB[o] | | 80FAR/MCM |
| $C_3F_6^-$ | | | | | | |
| $(CF_3)_2C^{-\cdot}$ | | | | | | |
| • −1181±17 [a] | | 1527±17 [g] | 1498±17 | IMRB | | 84MCD/CHO |
| | 0.6 | | | EIAP | From $(CF_3)_2CO$ | 70HAR/THY |
| $C_3F_6N^-$ | | | | | | |
| $CF_3CF_2CN\cdot\cdot F^-$ | | | | | | |
| • | | *126±8* [g] | *97±8* | IMRE | | 83LAR/MCM |
| $C_3F_7^-$ | | | | | | |
| $(CF_3)_2CF^-$ | | | | | | |
| | >2.7±0.2 | | | EIAP | From i−$C_5F_{12}$ | 85SPY/HUN |
| | >2.6±0.2 | | | EIAP | From i−$C_4F_{10}$ | 83SPY/SAU |
| $C_3F_7^-$ | | | | | | |
| $C_3F_7^-$ | | | | | *$\Delta_f H(A)$= −1337±23* | *83EVA/WEE* |
| | >3.4±0.3 | | | EIAP | From neo−$C_5F_{12}$ | 85SPY/HUN |
| | >2.7±0.2 | | | EIAP | From i−$C_5F_{12}$ | 85SPY/HUN |
| | >2.6±0.1 | | | EIAP | From i−$C_4F_{10}$ | 85SPY/HUN |
| | >2.6±0.4 | | | EIAP | From $C_3F_8$ | 83SPY/SAU |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3F_7^-$ | | | | | | |
| $C_3F_7^-$ | | | | | *$\Delta_f H(A) = -1337\pm23$* | *83EVA/WEE* |
| | >2.8±0.1 | | | EIAP | From n-$C_6F_{14}$ | 83SPY/SAU |
| | >2.6±0.1 | | | EIAP | From n-$C_5F_{12}$ | 83SPY/SAU |
| | >2.5±0.4 | | | EIAP | From n-$C_4F_{10}$ | 83SPY/SAU |
| | >2.2±0.2 | | | EIAP | From n-$C_4F_{10}$ | 73HAR/THY2 |
| −1582±7 | >2.3±0.2 | | | EIAP | From $C_3F_8$ | 72HAR/THY |
| | >2.4 | | | EIAP | From $C_3F_8$ | 69LIF/GRA |
| $C_3F_7O^-$ | | | | | | |
| $(CF_3)_2CO\cdot\cdot F^-$ | | | | | | |
| * −1854±31 [c] | | *208±8* [g] | *174±8* | IMRE | | 85LAR/MCM |
| $C_3F_7O^-$ | | | | | | |
| $CF_3CF_2CFO\cdot\cdot F^-$ | | | | | | |
| * −1919±31 [c] | | *197±8* [g] | *162±8* | IMRE | | 85LAR/MCM |
| $C_3FeO_3^-$ | | | | | | |
| $Fe(CO)_3^-$ | | | | | | |
| * | 1.800±0.200 | | | LPES | | 79ENG/LIN2 |
| <−950 | | | | NBAP | From $Fe(CO)_5$ | 76COM/STO |
| $C_3N^-$ | | | | | *$\Delta_f H(AH) = 351$* | *85HAR* |
| $N\equiv CC\equiv C^-$ | | | | | *$BDE(A-H) = 552\pm21$* | |
| 289 [a] | 4.11±0.32 [d] | 1468±10 | 1438±10 | TDEq | | 87MEO |
| −365±19 | | | | EIAP | From $CH_2=CHCN$ | 86HEN/ILL2 |
| −512±21 | | | | EIAP | From TCNE | 72BRI/OLS |
| | 2.4 | | | EIAP | From EtCN | 71TSU/YOK |
| 318±29 | 2.4 | | | EIAP | From $HC\equiv C-C\equiv N$ | 61DIB/REE |
| $C_3O^-$ | | | | | | |
| $C_3O^{-\cdot}$ | | | | | | |
| | 1.340±0.150 | | | LPES | Large geometry change on detachment | 86OAK/ELL |
| $C_3O_2^-$ | | | | | | |
| $C_3O_2^-$ | | | | | | |
| | 0.850±0.150 | | | LPES | | 86OAK/ELL |
| $C_3H^-$ | | | | | | |
| $HC_3^-$ | | | | | | |
| | 1.858±0.027 | | | LPES | From propene discharge | 86OAK/ELL |
| $C_3HClF_5O^-$ | | | | | | |
| $CF_3COCF_2H\cdot\cdot Cl^-$ | | | | | | |
| * −1428 [c] | | | *68±8* | IMRE | | 84LAR/MCM |
| $C_3HCrO_3^-$ | | | | | | |
| $(CO)_3CrH^-$ | | | | | | |
| <−287 | | | | IMRB | | 85LAN/SQU |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$C_3HF_3^-$** | | | | | | |
| $CF_3CH=C^-$ | | | | | | |
| -614 | | | | EIAP | $O^- + CF_3CH=CH_2 \rightarrow$ | 76DAW/JEN |
| **$C_3HF_4O^-$** | | | | *Est* | *$\Delta_f H(AH)$= -971±17* | |
| $CF_2=C(CHF_2)O^-$ | | | | | | |
| • -1071±44 [a] | | 1430±27 [g] | 1401±23 | IMRB | Between $HCO_2H$, $FCH_2CO_2H$ | 80FAR/MCM |
| . | | | 1400±25 | IMRB[o] | | 80FAR/MCM |
| **$C_3HF_5NO^-$** | | | | | | |
| $CF_3OCF_2H\cdot\cdot CN^-$ | | | | | | |
| • | | *78±15* [g] | *47±10* | IMRE | | 87LAR/MCM |
| **$C_3HF_6^-$** | | | | | *$\Delta_f H(AH)$= -1406±8* | *86KOL/KOZ* |
| $(CF_3)_2CH^-$ | | | | | *BDE(A-H)= 452±33* | *84MCD/CHO* |
| • -1414±29 [a] | 2.5±0.6 [d] | 1522±21 [g] | 1490±17 | IMRB | | 84MCD/CHO |
| **$C_3HF_6O^-$** | | | | *Est* | *$\Delta_f H(AH)$= -1536±8* | |
| $(CF_3)_2CHO^-$ | | | | | *BDE(A-H)= 438±4* | |
| • -1623±19 [a] | 3.19±0.16 [d] | 1443±11 [g] | 1415±8 | IMRE | | 86TAF |
| | | | 1424 | IMRB | | 81KOP/PIK |
| **$C_3HN^-$** | | | | | | |
| $C=CHCN^{-\cdot}$ | | | | | | |
| <402 | | | | IMRB | $O^- + CH_2=CHCN \rightarrow$ | 76DAW/JEN |
| **$C_3HN^-$** | | | | | | |
| $HC{\equiv}C{-}CN^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 351* | *85HAR* |
| 134±19 | | | | EIAP | From $CH_2=CHCN$ | 86HEN/ILL2 |
| **$C_3HN_2^-$** | | | | | *$\Delta_f H(AH)$= 266±2* | *77PED/RYL* |
| $HC(CN)_2^-$ | | | | | | |
| | | 1405±11 [g] | 1373±8 | IMRE | | 81FUJ/MCI |
| • 141±13 [a] | | 1406±11 [g] | 1373±8 | IMRE | | 78CUM/KEB |
| **$C_3H_2^-$** | | | | | | |
| $H_2C=C=C^{-\cdot}$ | | | | | | |
| | 1.794±0.025 | | | LPES | From propene discharge | 86OAK/ELL |
| <191 | | | | IMRB | $O^-$ + allene $\rightarrow$ | 76DAW/JEN |
| **$C_3H_2Cl^-$** | | | | *Est* | *$\Delta_f H(AH)$= 169±13* | |
| $ClCH_2C{\equiv}C^-$ | | | | | *BDE(A-H)= 552±21* | |
| • 179±22 [a] | | 1540±10 [g] | 1507±8 | IMRE | | 86TAF |
| **$C_3H_2ClF_4O^-$** | | | | | | |
| $(CF_2H)_2CO\cdot\cdot Cl^-$ | | | | | | |
| • -1198 [c] | | | *76±8* | IMRE | | 84LAR/MCM |
| **$C_3H_2F_3O^-$** | | | | *Est* | *$\Delta_f H(AH)$= -811±13* | |
| $CH_2=C(CF_3)O^-$ | | | | *D-EA* | *BDE(A-H)= 398±22* | |
| • -880±22 [a] | | 1461±10 [g] | 1431±8 | IMRE | | 86TAF |
| • | 2.6±0.1 | | | PD | | 77ZIM/REE |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_3H_2F_3O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −811±13* | |
| $CH_2{=}C(CF_3)O^-$ | | | | | *D-EA* | *BDE(A−H)= 398±22* | |
| | | | 1466±15 [g] | 1436±8 | IMRE | | 78CUM/KEB |
| $C_3H_2F_3O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −1085±8* | |
| $CF_3CH_2CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −1215±19 [a] | 3.68±0.20 [d] | 1401±11 [g] | 1371±8 | IMRE | | 86TAF |
| $C_3H_2F_4NO^-$ | | | | | | | |
| $(CF_2H)_2O\cdot\cdot CN^-$ | | | | | | | |
| • | | | *92±15* [g] | *63±10* | IMRE | | 87LAR/MCM |
| $C_3H_2F_5O^-$ | | | | | | *$\Delta_f H(AH)$= −1310±3* | *77PED/RYL* |
| $CF_3CF_2CH_2O^-$ | | | | | | *BDE(A−H)= 435±8* | |
| | −1354±33 [a] | 2.7±0.4 [d] | 1487±30 [g] | 1459±25 | IMRB | Between $(CF_3)_2CHOH$, $CF_3CH_2OH$ | 77DAW/JEN |
| $C_3H_2F_7O^-$ | | | | | | | |
| $(CF_3)_2CHOH\cdot\cdot F^-$ | | | | | | | |
| • | −1889±19 [c] | | *105±8* [g] | *185±8* | IMRE | | 83LAR/MCM |
| $C_3H_2N^-$ | | | | | | *$\Delta_f H(AH)$= 184±2* | *82CHU/NGU* |
| $CH_2{=}CCN^-$ | | | | | | | |
| • | 207±14 [a] | | 1553±12 [g] | 1528±8 | IMRE | | 80BAR |
| | | | 1524±19 | | EIAP | From $CH_2{=}CHCN$ | 86HEN/ILL2 |
| | | | | 1523±8 | IMRE[o] | | 80BAR |
| $C_3H_2NO^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 22* | |
| $CH_2{=}C(CN)O^-$ | | | | | | *BDE(A−H)= 406±8* | |
| • | −67 [a] | 2.87±0.20 [d] | 1441±11 [g] | 1413±8 | IMRE | | 86TAF |
| | | | | 1432±21 | IMRB | | 68BRA/BLA |
| $C_3H_2NO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −297±21* | |
| $NCCH_2CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −445±32 [a] | 3.87±0.20 [d] | 1382±11 [g] | 1354±8 | IMRE | | 86TAF |
| $C_3H_2N_2^-$ | | | | | | | |
| pyrazolide$^-$ | | | | | | | |
| • | | | 1480±11 [g] | 1449±8 | IMRE | | 86TAF/ANV |
| $C_3H_3^-$ | | | | | | *$\Delta_f H(AH)$= 191±1* | *77PED/RYL* |
| $CH_2{=}C{=}CH^-$ | | | | | | *BDE(A−H)= 367±8* | *82MCM/GOL* |
| • | 253±12 [a] | 0.893±0.026 | 1592±11 [e] | 1556±13 [h] | LPES | | 83OAK/ELL |
| | | 2.3 | | | SI | | 69PAG/GOO |
| $C_3H_3^-$ | | | | | | *$\Delta_f H(AH)$= 187±2* | *77PED/RYL* |
| $MeC{\equiv}C^-$ | | | | | | *BDE(A−H)= 552±21* | |
| • | 251±12 [a] | 2.80±0.32 [d] | 1595±10 [g] | 1562±8 | IMRE | | 79BAR/SCO |
| • | | >2.602±0.043 | | | LPES | | 83OAK/ELL |
| | | | | 1556±8 | IMRE[o] | | 79BAR/SCO |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_3H_2D^-$ | | | | | | *$\Delta_f H(AH)$= 187±2* | *77PED/RYL* |
| $CH_2=C=CD^-$ | | | | | | *BDE(A–H)= 374±8* | |
| • | 258±25 [a] | 0.880±0.150 | 1601±23 [e] | | LPES | | 83OAK/ELL |
| $C_3HD_2^-$ | | | | | | | |
| $CD_2=C=CH^-$ | | | | | | | |
| • | | 0.907±0.023 | | | LPES | | 83OAK/ELL |
| $C_3H_3F_2O^-$ | | | | | | | |
| $CF_2=C(Me)O^-$ | | | | | | | |
| | | >1.0±0.3 | | | EIAP | From $CF_3COMe$ | 72THY |
| $C_3H_3F_2O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −561±21* | |
| $CHF=C(CH_2F)O^-$ | | | | | | | |
| • | −625±36 [a] | | 1466±15 [g] | 1436±13 | IMRB | Between $PhCH_2CN$, $CF_3COCH_3$ | 80FAR/MCM |
| | | | | 1433±10 | IMRB[o] | | 80FAR/MCM |
| $C_3H_3F_3N^-$ | | | | | | | |
| $CF_2HCH_2F\cdot\cdot CN^-$ | | | | | | | |
| • | | | *77±15* [g] | *46±10* | IMRE | | 87LAR/MCM |
| $C_3H_3F_3NO^-$ | | | | | | | |
| $CF_3CH_2OH\cdot\cdot CN^-$ | | | | | | | |
| • | −916±29 [c] | | *103±15* [g] | *69±10* | IMRE | | 87LAR/MCM |
| $C_3H_3N^-$ | | | | | | | |
| $MeCCN^{-\cdot}$ | | | | | | | |
| | <401 | | | | IMRB | $O^- + EtCN \rightarrow$ | 76DAW/JEN |
| $C_3H_3N_2^-$ | | | | | | | |
| $CH_2=CHCNN^-$ | | | | | | | |
| | <−435±21 | | | | IMRB | $N_2O + CH_2=CHCH_2^- \rightarrow$ | 77BIE/DEP |
| $C_3H_3N_2^-$ | | | | | | | |
| $MeCN\cdot\cdot CN^-$ | | | | | | | |
| • | 81±24 [c] | | *69±15* [g] | *38±10* | IMRE | | 87LAR/MCM |
| $C_3H_3N_2^-$ | | | | | | | |
| imidazolide$^-$ | | | | | | | |
| • | | | 1465±11 [g] | 1434±8 | IMRE | | 86TAF/ANV |
| $C_3H_3N_3^-$ | | | | | | | |
| sym-triazine$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 226±1* | *82BYS* |
| | 183 [b] | 0.5 | | | ETS | | 75NEN/SCH |
| $C_3H_4BrO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −432±8* | |
| $MeCHBrCO_2^-$ | | | | | | *BDE(A–H)= 444±8* | |
| • | −556±19 [a] | | 1407±11 [g] | 1377±8 | IMRE | | 85CAL/MCM |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_3H_4ClO_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −481±4* | |
| $ClCH_2CH_2CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −585±20 [a] | 3.41±0.25 [d] | 1426±16 [g] | 1397±8 | IMRE | | 78CUM/KEB |
| $C_3H_4ClO_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −472±13* | |
| $MeCHClCO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −594±22 [a] | 3.61±0.19 [d] | 1407±10 [g] | 1380±8 | IMRE | | 78CUM/KEB |
| $C_3H_4F^-$ | | | | | | | |
| $CH_2=CFCH_2^-$ | | | | | | | |
| • | | | 1586±14 [g] | 1559±13 | IMRB | | 84BAR/BUR |
| | | | 1579±10 [g] | 1551±8 | IMRB | | 78MCM/NOR |
| | | | | 1558±17 | IMRB[o] | | 84BAR/BUR |
| | | | *63±8* [k] | 1546±13 | IMRB[o] | | 78MCM/NOR |
| $C_3H_4FO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −383±21* | |
| $CH_2=C(CH_2F)O^-$ | | | | | | *BDE(A−H)= 389±8* | |
| | −381±41 [a] | 1.8±0.3 [d] | 1532±21 [g] | 1503±17 | IMRB | | 80CLA/MCM |
| $C_3H_4FO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −383±21* | |
| $CHF=C(Me)O^-$ | | | | | | | |
| • | −416±39 [a] | | 1497±18 [g] | 1465±15 | IMRB | Between pyrrole, $MeNO_2$ | 80FAR/MCM |
| | | | | 1469±10 | IMRB[o] | | 80FAR/MCM |
| $C_3H_4F_3O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −905±8* | |
| $CF_3CH(Me)O^-$ | | | | | | *BDE(A−H)= 438±4* | |
| • | −928±19 [a] | | 1507±11 [g] | 1480±8 | IMRE | | 85CAL/MCM |
| | | | | 1491±8 | IMRE[o] | | 85CAL/MCM |
| $C_3H_4N^-$ | | | | | | *$\Delta_f H(AH)$= 51* | *82CHU/NGU* |
| $MeCHCN^-$ | | | | | | *BDE(A−H)= 377±4* | *82MCM/GOL* |
| • | 90±11 [a] | 1.24±0.16 [d] | 1569±11 [g] | 1537±8 | IMRE | | 79BAR/SCO |
| | | | | 1532±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_4NO^-$ | | | | | | | |
| $CH_2=C(NO)CH_2^-$ | | | | | | | |
| | | | | 1586±21 | IMRB | | 86KAS/FIL |
| $C_3H_4NO^-$ | | | | | | | |
| $CH_2=CH-CH=NO^-$ | | | | | | | |
| | | | | 1504±13 | IMRB | | 86KAS/FIL |
| $C_3H_4NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −35±8* | |
| $MeOCHCN^-$ | | | | | | | |
| • | −10±23 [a] | | 1556±15 [g] | 1524±8 | IMRE | | 79BAR/SCO |
| | | | | 1522±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_4O^-$ | | | | | | | |
| $CH_2=C(CH_2.)O^-$ | | | | | | | |
| | | < 132 | | | IMRB | $O^- + Me_2CO \rightarrow$ | 79DAW/NOE2 |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_3H_5^-$ | | | | | | *$\Delta_f H(AH)$= 20* | *77PED/RYL* |
| $CH_2=CHCH_2^-$ | | | | | | *BDE(A-H)= 362±6* | *79ROS/GOL* |
| • | 125±10 [a] | 0.41±0.17 [d] | 1635±10 [g] | 1607±8 | IMRE | | 79BAR/SCO |
| • | | 0.362±0.020 | | | LPES | | 84OAK/ELL |
| | | 0.551±0.052 | | | LPD | | 77ZIM/BRA |
| • | | | 1633±4 [g] | 1605±2 | IMRE | | 78MAC/LIE |
| $C_3H_5^-$ | | | | | | *$\Delta_f H(AH)$= 20* | *77PED/RYL* |
| $CH_2=CMe^-$ | | | | | | | |
| | > 184±3 [a] | | > 1694±3 [g] | > 1661 | IMRB | | 86FRO/FRE |
| $C_3H_5^-$ | | | | | | *$\Delta_f H(AH)$= 20* | *77PED/RYL* |
| $MeCH=CH^-$ | | | | | | | |
| | > 184±4 [a] | | > 1694±4 [g] | > 1661 | IMRB | | 86FRO/FRE |
| $C_3H_5^-$ | | | | | | *$\Delta_f H(AH)$= 53±1* | *77PED/RYL* |
| cyclopropanide$^-$ | | | | | | *BDE(A-H)= 445±1* | *82MCM/GOL* |
| • | 247±9 [a] | 0.3±0.1 [d] | 1724±8 | 1687±11 [h] | Bran | | 84DEP/BIE |
| | > 213±3 [a] | | > 1690±3 [g] | > 1654 | IMRB | | 72BOH/LEE |
| | | | | > 1654 | IMRB | | 86FRO/FRE |
| $C_3H_4D^-$ | | | | | | | |
| $CH_2=CDCH_2^-$ | | | | | | | |
| | | 0.373±0.020 | | | LPES | | 83OAK/ELL |
| $C_3D_5^-$ | | | | | | | |
| $CD_2=CDCD_2^-$ | | | | | | | |
| | | 0.380±0.026 | | | LPES | | 83OAK/ELL |
| $C_3H_5ClNO^-$ | | | | | | | |
| $ClCH_2CH_2OH\cdot\cdot CN^-$ | | | | | | | |
| • | −275±28 [c] | | *88±15* [g] | *56±10* | IMRE | | 87LAR/MCM |
| $C_3H_5FNO^-$ | | | | | | | |
| $FCH_2CH_2OH\cdot\cdot CN^-$ | | | | | | | |
| • | −428±32 [c] | | *85±15* [g] | *54±10* | IMRE | | 87LAR/MCM |
| $C_3H_5F_2O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −620±4* | |
| $(FCH_2)_2CHO^-$ | | | | | | *BDE(A-H)= 436±4* | |
| • | −628±25 [a] | | 1521±21 [g] | 1492±17 | IMRB | Between MeCHO, PhCOMe | 80CLA/MCM |
| | | | | 1498±17 | IMRB [o] | | 80CLA/MCM |
| $C_3H_5F_2O^-$ | | | | | | | |
| $c\text{-}CH_2(O)CHCH_2F\cdot\cdot F^-$ | | | | | | | |
| • | −610±15 [c] | | *107±8* [g] | *77±8* | IMRE | | 83LAR/MCM |
| $C_3H_5N_2O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −441±8* | |
| $H_2NCON=C(Me)O^-$ | | | | | | | |
| • | | | 1458±12 [g] | 1427±8 | IMRE | Acid: acetylurea | 78CUM/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}$(AH) $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}$(AH) $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3H_5O^-$ | | | | | *$\Delta_f H$(AH)= -217* | *76CHA/ZWO* |
| $CH_2{=}C(Me)O^-$ | | | | | *BDE(A-H)= 411±11* | *70SOL/GOL* |
| • -203±11 [a] | 1.86±0.23 [d] | 1544±11 [g] | 1514±8 | IMRE | | 79BAR/SCO |
| • | 1.757±0.033 | | | LPES | | 82ELL/ENG |
| | | 1546±11 [g] | 1516±8 | IMRE | | 78CUM/KEB |
| | 1.76±0.06 | | | PD | | 77ZIM/REE |
| | | | 1513±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_5O^-$ | | | | | *$\Delta_f H$(AH)= -187±2* | *77PED/RYL* |
| MeCH=CHO$^-$ | | | | *D-EA* | *BDE(A-H)= 372±12* | |
| • -189±12 [a] | | 1528±10 [g] | 1501±8 | IMRE | | 79BAR/SCO |
| • | 1.611±0.023 | | | LPES | | 82ELL/ENG |
| | | 1531±10 [g] | 1504±8 | IMRE | | 78CUM/KEB |
| | 1.69±0.06 | | | PD | | 77ZIM/REE |
| | | | 1503±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_5O_2^-$ | | | | | *$\Delta_f H$(AH)= -410±1* | *77PED/RYL* |
| $CH_2{=}C(OMe)O^-$ | | | | *D-EA* | *BDE(A-H)= 418±15* | |
| • -384±10 [a] | | 1556±10 [g] | 1528±8 | IMRE | | 79BAR/SCO |
| • | 1.80±0.06 | | | PD | | 77ZIM/REE |
| | | | 1524±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_5O_2^-$ | | | | | *$\Delta_f H$(AH)= -448±2* | *77PED/RYL* |
| $EtCO_2^-$ | | | | | *BDE(A-H)= 445±8* | *82MCM/GOL* |
| • -525±14 [a] | 3.15±0.21 [d] | 1454±12 [g] | 1424±8 | IMRE | | 78CUM/KEB |
| $C_3H_5O_3^-$ | | | | *Est2* | *$\Delta_f H$(AH)= -556±17* | |
| $MeOCH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -657±28 [a] | 3.38±0.20 [d] | 1429±11 [g] | 1402±8 | IMRE | | 86TAF |
| $C_3H_6ClF_2O^-$ | | | | | | |
| $(FCH_2)_2CHOH\cdot\cdot Cl^-$ | | | | | | |
| • -946±14 [c] | | *99±8* [g] | *67±8* | IMRE | | 84LAR/MCM2 |
| $C_3H_6ClO^-$ | | | | | | |
| $Me_2CO\cdot\cdot Cl^-$ | | | | | | |
| • -504±10 [c] | | *59±8* [g] | *34±8* | IMRE | | 84LAR/MCM2 |
| | | *57±8* | *33±8* | TDAs | | 82FRE/IKU |
| $C_3H_6F_3O^-$ | | | | | | |
| $(FCH_2)_2CHOH\cdot\cdot F^-$ | | | | | | |
| • -1026±15 [c] | | *158±8* [g] | *125±8* | IMRE | | 83LAR/MCM |
| $C_3H_6IO_2^-$ | | | | | | |
| $EtCO_2H\cdot\cdot I^-$ | | | | | | |
| • -706±7 [c] | | *69±4* | *44±9* | TDAs | | 84CAL/KEB |
| $C_3H_6NO^-$ | | | | | | |
| $EtOH\cdot\cdot CN^-$ | | | | | | |
| • -233±24 [c] | | *73±15* [g] | *42±10* | IMRE | | 87LAR/MCM |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}$(AH) $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}$(AH) $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3H_6NO^-$ | | | | | *$\Delta_f H(AH)$= −192±2* | *77PED/RYL* |
| $HCON(Me)CH_2^-$ | | | | | | |
| • −52±21 [a] | | 1670±19 [g] | 1640±17 | IMRB | | 85DEP/GRA |
| $C_3H_6NO^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −63±13* | |
| $Me_2C=NO^-$ | | | | | | |
| • −61±25 [a] | | 1532±12 [g] | 1502±8 | IMRE | | 79BAR/SCO |
| | | | 1505±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_6NO^-$ | | | | | | |
| $Me_2CO\cdot\cdot CN^-$ | | | | | | |
| • −204±24 [c] | | *62±15* [g] | *33±10* | IMRE | | 87LAR/MCM |
| $C_3H_6NO_2^-$ | | | | | *$\Delta_f H(AH)$= −414±4* | *77NGA/SAB* |
| $H_2NCH(Me)CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −519±14 [a] | 3.42±0.19 [d] | 1425±10 [g] | 1396±8 | IMRE | | 83LOC/MCI |
| $C_3H_6NO_2^-$ | | | | | *$\Delta_f H(AH)$= −446±8* | *75BER/BOU* |
| $HN=C(OEt)O^-$ | | | | | | |
| • −462±20 [a] | | 1514±12 [g] | 1485±9 | IMRE | | 86TAF |
| $C_3H_6NO_2^-$ | | | | | *$\Delta_f H(AH)$= −139±1* | *77PED/RYL* |
| $Me_2C=NO_2^-$ | | | | | | |
| • −179±13 [a] | | 1490±12 [g] | 1464±8 | IMRE | | 79BAR/SCO |
| | | 1491±12 [g] | 1466±8 | IMRE | | 78CUM/KEB |
| | | | 1474±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_6NO_2^-$ | | | | | *$\Delta_f H(AH)$= −368±1* | *77SAB/LAF* |
| $MeNHCH_2CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −469±10 [a] | 3.39±0.19 [d] | 1429±10 [g] | 1400±8 | IMRE | | 83LOC/MCI |
| $C_3H_6NS^-$ | | | | | | |
| $HCSN(Me)CH_2^-$ | | | | | | |
| • | | 1587±11 [g] | 1558±8 | IMRE | | 85ING/NIB3 |
| | | | 1561±8 | IMRE[o] | | 85ING/NIB3 |
| $C_3H_7^-$ | | | | | *$\Delta_f H(AH)$= −105* | *74SCO* |
| $Me_2CH^-$ | | | | | *BDE(A−H)= 398±4* | *82MCM/GOL* |
| • 118±9 [a] | | 1753±8 | 1719±10 [h] | Bran | | 84DEP/BIE |
| | 0.7 | | | SI | | 69PAG/GOO |
| $C_3H_7Br_2^-$ | | | | | | |
| $iPrBr\cdot\cdot Br^-$ | | | | | | |
| | | *51* | *26* | TDAs | | 74DOU |
| $C_3H_7Br_2^-$ | | | | | | |
| $nPrBr\cdot\cdot Br^-$ | | | | | | |
| | | *49* | *24* | TDAs | | 74DOU |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3H_7ClSi^-$ | | | | | | |
| $HCSiMe_2Cl^{-\cdot}$ | | | | | | |
| −93±21 | | | | EIAP | From $Me_3SiCl$ | 68JAE/HEN |
| $C_3H_7N_2O^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −243±13* | |
| $HN=C(NMe_2)O^-$ | | | | | | |
| • −259±25 [a] | | 1514±13 [g] | 1484±10 | IMRE | | 86TAF |
| $C_3H_7O^-$ | | | | | *$\Delta_f H(AH)$= −273* | *77PED/RYL* |
| iPrO⁻ | | | | | *BDE(A−H)= 438±4* | *82MCM/GOL* |
| • −232±10 [a] | 1.86±0.14 [d] | 1571±10 [g] | 1543±8 | IMRE | | 79BAR/SCO |
| • | 1.839±0.029 | | | LPES | | 82ELL/ENG |
| | 1.7±0.1 | | | EIAP | From iPrONO | 68WIL/HAM |
| | >1.7 | | | EIAP | From iPrOH | 63TRE/NEU |
| | 0.7 | | | SI | | 69PAG/GOO |
| | | | 1538±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_7O^-$ | | | | | *$\Delta_f H(AH)$= −255±1* | *77PED/RYL* |
| nPrO⁻ | | | | | *BDE(A−H)= 433±4* | *82MCM/GOL* |
| • −212±10 [a] | 1.78±0.14 [d] | 1573±9 [g] | 1546±8 | IMRE | | 79BAR/SCO |
| • | 1.789±0.033 | | | LPES | | 82ELL/ENG |
| | 1.9±0.1 | | | EIAP | From nPrONO | 68WIL/HAM |
| | >1.8 | | | EIAP | From nPrOH | 63TRE/NEU |
| | | | 1540±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −366±4* | |
| $MeOCH_2CH_2O^-$ | | | | | *BDE(A−H)= 436±4* | |
| • −332±16 [a] | 1.90±0.17 [d] | 1564±12 [g] | 1535±8 | IMRE | | 79BAR/SCO |
| | | | 1530±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_7S^-$ | | | | | *$\Delta_f H(AH)$= −76±1* | *77PED/RYL* |
| iPrS⁻ | | | | | *BDE(A−H)= 364±9* | |
| • −128±13 [a] | 2.05±0.22 [d] | 1479±12 [g] | 1452±8 | IMRE | | 79BAR/SCO |
| • | 2.020±0.020 | | | LPD | | 80JAN/REE |
| | | | 1461±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_7S^-$ | | | | | *$\Delta_f H(AH)$= −68* | *77PED/RYL* |
| nPrS⁻ | | | | | *BDE(A−H)= 364±9* | |
| • −116±13 [a] | 2.02±0.22 [d] | 1482±12 [g] | 1456±8 | IMRE | | 79BAR/SCO |
| • | 2.000±0.020 | | | LPD | | 80JAN/REE |
| | | | 1465±8 | IMRE[o] | | 79BAR/SCO |
| $C_3H_7Si^-$ | | | | | *$\Delta_f H(AH)$= 21±17* | *86WAL* |
| $CH_2=Si(Me)CH_2^-$ | | | | | | |
| • 104±41 [a] | | 1613±25 [g] | 1586±21 | IMRB | | 86DAM/DEP |
| $C_3H_8B^-$ | | | | | *$\Delta_f H(AH)$= −123±10* | *77PED/RYL* |
| $Me_2BCH_2^-$ | | | | | *BDE(A−H)= 397±21* | *71BEL/PLA* |
| −120±39 [a] | 1.8±0.5 [d] | 1532±29 [g] | 1502±25 | IMRB | Between $AsH_3$, $PH_3$ | 76MUR/BEA |
| | | | 1492±20 | IMRB[o] | | 76MUR/BEA |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ *$\Delta H_{aff}(X\cdot\cdot Y^-)$* | $\Delta G_{acid}(AH)$ *$\Delta G_{aff}(X\cdot\cdot Y^-)$* | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3H_8ClO^-$ iPrOH··Cl$^-$ | | | | | | |
| • −574±10 [c] | | *74±8* [g] | *45±8* | IMRE | | 84LAR/MCM2 |
| $C_3H_8ClO^-$ nPrOH··Cl$^-$ | | | | | | |
| • −556±10 [c] | | *74±8* [g] | *45±8* | IMRE | | 84LAR/MCM2 |
| $C_3H_8FO^-$ iPrOH··F$^-$ | | | | | | |
| • −657±11 [c] | | *135±8* [g] | *103±8* | IMRE | | 83LAR/MCM |
| $C_3H_8FO^-$ nPrOH··F$^-$ | | | | | | |
| • −639±11 [c] | | *135±8* [g] | *103±8* | IMRE | | 83LAR/MCM |
| $C_3H_8IO^-$ iPrOH··I$^-$ | | | | | | |
| • −512±5 [c] | | *51±4* | *27±9* | TDAs | | 84CAL/KEB |
| $C_3H_8N^-$ | | | | *Est* | *$\Delta_f H(AH)$= −46±4* | |
| Et(Me)N$^-$ | | | | | *BDE(A−H)= 383±8* | *82MCM/GOL* |
| • 77±15 [a] | 0.43±0.20 [d] | 1653±11 [g] | 1621±8 | IMRE | | 85ING/NIB2 |
| $C_3H_8N^-$ | | | | | *$\Delta_f H(AH)$= −24* | *77PED/RYL* |
| $Me_2NCH_2^-$ | | | | | *BDE(A−H)= 351±8* | *82MCM/GOL* |
| | | >1700 [g] | >1665 | IMRB | | 78MAC/BOH2 |
| $C_3H_8N^-$ | | | | | *$\Delta_f H(AH)$= −84±1* | *77PED/RYL* |
| iPrNH$^-$ | | | | | *BDE(A−H)= 423±13* | |
| 49±17 [a] | 0.8±0.3 [d] | 1662±16 [g] | 1631±13 | IMRB | | 71BRA/BLA |
| $C_3H_8N^-$ | | | | | *$\Delta_f H(AH)$= −70* | *77PED/RYL* |
| nPrNH$^-$ | | | | | *BDE(A−H)= 423±13* | |
| 67±17 [a] | 0.7±0.3 [d] | 1667±16 [g] | 1636±13 | IMRB | | 71BRA/BLA |
| $C_3H_8NO^-$ iPrOH··CN$^-$ | | | | | | |
| • −274±24 [c] | | *76±15* [g] | *45±10* | IMRE | | 87LAR/MCM |
| $C_3H_8P^-$ | | | | | *$\Delta_f H(AH)$= −101±5* | *77PED/RYL* |
| $Me_2PCH_2^-$ | | | | | | |
| • 5±16 [a] | | 1636±11 [g] | 1606±8 | IMRE | | 85ING/NIB2 |
| $C_3H_9BF^-$ $Me_3B$··F$^-$ | | | | | | |
| • −569±21 [c] | | *197±8* [g] | *166±8* | IMRE | | 85LAR/MCM |
| −616 [c] | | *245* | | IMRB | F$^-$A: $MeSiF_3$ > $Me_3B$ > $SF_4$ | 77MUR/BEA2 |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_3H_9BFO_3^-$ | | | | | | |
| $(MeO)_3B\cdot\cdot F^-$ | | | | | | |
| * −1324±21 [c] | | *176±17* [g] | *142±13* | IMRB | | 85LAR/MCM |
| $C_3H_9F_2Si^-$ | | | | | | |
| $Me_3SiF\cdot\cdot F^-$ | | | | | | |
| * | | *160±8* [g] | *132±8* | IMRE | | 85LAR/MCM |
| | | *< 226±42* | | IMRB | | 77MUR/BEA3 |
| $C_3H_9O_2^-$ | | | | | | |
| $EtOH\cdot\cdot MeO^-$ | | | | | | |
| −459±20 [c] | | *85±10* [g] | *57±8* | IMRE | | 84CAL/ROZ |
| $C_3H_9Si^-$ | | | | | *$\Delta_f H(AH)$= −163±8* | *81WAL* |
| $Me_3Si^-$ | | | | | *BDE(A−H)= 378±17* | *81WAL* |
| −98±23 [a] | 1.0±0.3 [d] | 1595±15 [g] | 1565±13 | IMRB | | 87THO/BAR |
| $C_3H_{10}NSi^-$ | | | | | | |
| $Me_3SiNH^-$ | | | | | | |
| | | 1585±15 [g] | 1552±13 | IMRB | | 87THO/BAR |
| $C_4CoO_4^-$ | | | | | | |
| $Co(CO)_4^-$ | | | | | | |
| | | | < 1294±8 | IMRB | | 87STE/BEA |
| $C_4F_4O_3^-$ | | | | | | |
| tetrafluorosuccinic anhydride$^{-\cdot}$ | | | | | | |
| | 0.5±0.2 | | | NBIP | | 74COO/COM |
| $C_4F_5^-$ | | | | | | |
| $C_4F_5^-$ | | | | | | |
| −685 | 2.0 | | | EIAP | From c−$C_4F_6$ | 79SAU/CHR |
| $C_4F_6O^-$ | | | | | | |
| $CF_3CF_2CFCO^{-\cdot}$ | | | | | | |
| −1331±58 | | | | EIAP | From $CF_3CF_2\check{C}F_2CHO$ | 75HAR/THY |
| $C_4F_7^-$ | | | | | | |
| $C_4F_7^-$ | | | | | *$\Delta_f H(A)$= −1167±29* | *83SPY/SAU* |
| −1457±73 [b] | 3.0±0.5 | | | EIAP | From n−$C_6F_{14}$ | 83SPY/SAU |
| | 0.9±0.2 | | | EIAP | From $CF_3CF{=}CFCF_3$ | 72LIF/GRA |
| | 2.7 | | | SI | | 69PAG/GOO |
| $C_4F_8^-$ | | | | | | |
| $C_4F_8^{-\cdot}$ | | | | | | |
| | > 0.7±0.4 | | | EIAP | From n−$C_5F_{12}$ | 83SPY/SAU |
| $C_4F_8^-$ | | | | | | |
| $CF_3CF{=}CFCF_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1602* | *70BEN/O'N* |
| < −1670 [b] | > 0.7±0.3 | | | EnCT | | 73LIF/TIE |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}$(AH) $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}$(AH) $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4F_8^-$ | | | | | | |
| c–$C_4F_8^{-\cdot}$ | | | | | $\Delta_f H(A)= -1543\pm10$ | 77PED/RYL |
| <–1581±39 [b] | >0.4±0.3 | | | EnCT | | 73LIF/TIE |
| $C_4F_8N^-$ | | | | | | |
| $CF_3CF_2CF_2CN\cdot\cdot F^-$ | | | | | | |
| • | | *129±8* [g] | *99±8* | IMRE | | 85LAR/MCM |
| $C_4F_9^-$ | | | | | | |
| $\cdot(CF_3)_2CFCF_2^-$ | | | | | | |
| | 3.5±0.5 | | | EIAP | From i–$C_4F_{10}$ | 85SPY/HUN |
| | 3.5±0.5 | | | EIAP | From i–$C_4F_{10}$ | 83SPY/SAU |
| $C_4F_9^-$ | | | | | | |
| $(CF_3)_3C^-$ | | | | *Est* | $\Delta_f H(A)= -1820$ | |
| | 3.4±0.1 | | | EIAP | From $(CF_3)_3CF$ | 85SPY/HUN |
| | 3.4±0.2 | | | EIAP | From $(CF_3)_3CF$ | 83SPY/SAU |
| $C_4F_9^-$ | | | | | | |
| $C_4F_9^-$ | | | | | | |
| | >4.0±0.2 | | | EIAP | From n–$C_4F_{10}$ | 83SPY/SAU |
| | >2.9±0.1 | | | EIAP | From n–$C_5F_{12}$ | 83SPY/SAU |
| | 3.2±0.3 | | | EIAP | From n–$C_4F_{10}$ | 73HAR/THY2 |
| $C_4F_9^-$ | | | | | | |
| $CF_3CF_2CF(CF_3)^-$ | | | | | | |
| | >3.2±0.1 | | | EIAP | From i–$C_5F_{12}$ | 85SPY/HUN |
| $C_4F_9O^-$ | | | | *Est2* | $\Delta_f H(AH)= -2297\pm21$ | |
| $(CF_3)_3CO^-$ | | | | | *BDE(A–H)= 439±8* | |
| • –2439±33 [a] | 3.77±0.21 [d] | 1388±12 [g] | 1356±8 | IMRE | | 86TAF |
| –2442 [a] | | | 1352±21 | IMRB | | 81KOP/PIK |
| –2451 [a] | | | 1345±21 | IMRB | | 80CLA/MCM |
| $C_4FeO_4^-$ | | | | | | |
| $Fe(CO)_4^-$ | | | | | $\Delta_f H(A)= -414\pm23$ | *81SMI/LAI* |
| • –646±52 [b] | 2.398±0.300 | | | LPES | | 79ENG/LIN2 |
| | 2.1±0.3 | | | EIAP | | 76COM/STO |
| | | | | | $Fe(CO)_5 + e^- \rightarrow Fe(CO)_4^- + CO$ "near thermoneutral". BDE from 81SMI/LAI | |
| $C_4O^-$ | | | | | | |
| $C_4O^{-\cdot}$ | | | | | | |
| | 2.050±0.150 | | | LPES | | 86OAK/ELL |
| $C_4HF_5NO^-$ | | | | | | |
| $CF_3COCF_2H\cdot\cdot CN^-$ | | | | | | |
| • –1234±44 [c] | | *108±15* [g] | *75±10* | IMRE | | 87LAR/MCM |
| $C_4HF_{10}O^-$ | | | | | | |
| $(CF_3)_3COH\cdot\cdot F^-$ | | | | | | |
| • –2617±31 [c] | | *71±8* [g] | *151±8* | IMRE | | 83LAR/MCM |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_4HFeO_4^-$ | | | | | | | |
| $Fe(CO)_4H^-$ | | | | | | | |
| | | | | 1313±23 | IMRB | | 87STE/BEA |
| $C_4H_2F_6NO^-$ | | | | | | | |
| $(CF_3)_2CHOH\cdot\cdot CN^-$ | | | | | | | |
| • | -1566±32 [c] | | *105±15* [g] | *70±10* | IMRE | | 87LAR/MCM |
| $C_4H_2F_7O^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -1561±21* | |
| $CF_3CF_2CF_2CH_2O^-$ | | | | | | *BDE(A-H)= 435±8* | |
| | -1626±51 [a] | 2.9±0.4 [d] | 1465±30 [g] | 1437±25 | IMRB | Between $(CF_3)_2CHOH$, $CF_3CH_2OH$ | 77DAW/JEN |
| $C_4H_2NO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -287±8* | |
| maleimidate$^-$ | | | | | | | |
| | | | 1360±19 | | EIAP | From maleimide | 73COO/COM |
| $C_4H_2N_2^-$ | | | | | | | |
| fumaronitrile$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 339* | *82CHU/NGU* |
| • | 219 [b] | 1.24±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.25±0.09 | | | TDEq | | 86CHO/KEB |
| | | 0.8±0.1 | | | SI | | 67FAR/PAG |
| $C_4H_2O_3^-$ | | | | | | | |
| maleic anhydride$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -397±4* | *77PED/RYL* |
| • | -536±14 [b] | 1.44±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.41±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.38±0.05 | | | IMRE | | 85FUK/MCI |
| | | 1.4±0.2 | | | NBIP | | 74COM/REI |
| $C_4H_3F_3NO^-$ | | | | | | | |
| $CH_3COCF_3\cdot\cdot CN^-$ | | | | | | | |
| • | -822±36 [c] | | *85±15* [g] | *54±10* | IMRE | | 87LAR/MCM |
| $C_4H_3F_6O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -1576±4* | |
| $(CF_3)_2C(Me)O^-$ | | | | | | *BDE(A-H)= 440±4* | |
| • | -1648±14 [a] | | 1457±10 [g] | 1425±8 | IMRE | - | 85CAL/MCM |
| | | | | 1431±8 | IMRE[o] | | 85CAL/MCM |
| $C_4H_3N_2^-$ | | | | | | *$\Delta_f H(AH)$= 197±1* | *77PED/RYL* |
| pyrimidinide$^-$ | | | | | | | |
| • | 272±9 [a] | | 1606±8 | 1569±8 | TDEq | | 87MEO |
| $C_4H_3N_2O_3^-$ | | | | | | *$\Delta_f H(AH)$= -554±8* | *72DOM* |
| barbiturate$^-$ | | | | | | | |
| • | -680±12 [a] | | 1402±12 [g] | 1369±8 | IMRE | Acid: barbituric acid | 78CUM/KEB |
| $C_4H_3O^-$ | | | | | | | |
| $CH_2{=}CHC{\equiv}CO^-$ | | | | | | | |
| | <35 | | | | IMRB | $CH_2{=}CHCH_2^- + CF_2{=}O \rightarrow$ | 79DAW/NOE |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_4H_3O^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 67±13* | |
| $MeCOC{\equiv}C^-$ | | | | | | *BDE(A–H)= 552±21* | |
| • | 44±23 [a] | | 1507±10 [g] | 1474±9 | IMRE | | 86TAF |
| $C_4H_3O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −142±13* | |
| $MeOCOC{\equiv}C^-$ | | | | | | *BDE(A–H)= 552±21* | |
| • | −171±22 [a] | | 1501±10 [g] | 1469±8 | IMRE | | 86TAF |
| $C_4H_4F_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −649±13* | |
| $CH_2{=}C(CF_3)CH_2^-$ | | | | | | | |
| • | −615±23 [a] | | 1565±10 [g] | 1537±8 | IMRE | | 84BAR/BUR |
| | | | | 1532±8 | IMRE[o] | | 84BAR/BUR |
| $C_4H_4F_3O_2S^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −929±13* | |
| $CF_3SO_2CH{=}CHCH_2^-$ | | | | | | | |
| • | −1023±23 [a] | | 1436±11 [g] | 1407±8 | IMRE | | 86TAF |
| $C_4H_4F_7O^-$ | | | | | | | |
| $(CF_3)_2C(Me)OH\cdot\cdot F^-$ | | | | | | | |
| • | −1933±15 [c] | | *109±8* [g] | *189±8* | IMRE | | 83LAR/MCM |
| $C_4H_4N^-$ | | | | | | *$\Delta_f H(AH)$= 130* | *80WIL/BAE* |
| $CH_2{=}C(CN)CH_2^-$ | | | | | | | |
| • | 151 [a] | | 1551±10 [g] | 1523±8 | IMRE | | 84BAR/BUR |
| | | | | 1523±8 | IMRE[o] | | 84BAR/BUR |
| $C_4H_4N^-$ | | | | | | | |
| $CH_2{=}CHCH{=}C{=}N^-$ | | | | | | | |
| | | | | <1527±8 | IMRB | Acid: $CH_2{=}CHCH_2CN$ | 80DAW/NIB |
| $C_4H_4N^-$ | | | | | | *$\Delta_f H(AH)$= 184±1* | *82FUC/HAL* |
| $c\text{-}(CH_2)_2CCN^-$ | | | | | | | |
| • | 225±13 [a] | | 1571±12 [g] | 1539±8 | IMRE | Acid:cyanocyclopropane | 79BAR/SCO |
| | | | | 1533±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_4N^-$ | | | | | | *$\Delta_f H(AH)$= 108* | *77PED/RYL* |
| pyrrolide$^-$ | | | | | *D–EA* | *BDE(A–H)= 419±25* | |
| • | 79±13 [a] | | 1501±12 [g] | 1468±8 | IMRE | | 79BAR/SCO |
| • | | 2.4±0.1 | | | PD | | 75RIC/STE3 |
| | 83±13 [a] | | 1505±12 [g] | 1472±8 | IMRE | | 78CUM/KEB |
| | | | | 1477±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_4NO_2^-$ | | | | | | *$\Delta_f H(AH)$= −360±8* | *69BEN/CRU* |
| succinimidate$^-$ | | | | | | | |
| • | −445±18 [a] | | 1445±10 [g] | 1414±8 | IMRE | | 78CUM/KEB |
| | | | 1379±19 | | EIAP | | 73COO/COM |
| $C_4H_4NS^-$ | | | | | | | |
| 2-(thiofuryl)-NH$^-$ | | | | | | | |
| • | | | 1472±11 [g] | 1441±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4H_4N_2^-$ | | | | | | |
| pyrazine$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 196±1* | *77PED/RYL* |
| 157 [b] | 0.4 | | | ETS | | 75NEN/SCH |
| $C_4H_4N_2^-$ | | | | | | |
| pyridazine$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 278±1* | *77PED/RYL* |
| 254 [b] | 0.3 | | | ETS | | 75NEN/SCH |
| $C_4H_4N_2^-$ | | | | | | |
| pyrimidine$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 197±1* | *77PED/RYL* |
| | 0.0 | | | ETS | | 75NEN/SCH |
| $C_4H_5ClN^-$ | | | | | | |
| pyrrole··$Cl^-$ | | | | | | |
| • −198±10 [c] | | *79±8* [g] | *49±8* | IMRE | | 84LAR/MCM2 |
| | | | *59* | TDEq | | 82FRE/IKU |
| $C_4H_5FN^-$ | | | | | | |
| pyrrole··$F^-$ | | | | | | |
| • −283±11 [c] | | *143±8* [g] | *111±8* | IMRE | | 83LAR/MCM |
| $C_4H_5N^-$ | | | | | | |
| EtCCN$^{-\cdot}$ | | | | | | |
| <381 | | | | IMRB | $O^-$ + nPrCN→ | 76DAW/JEN |
| $C_4H_5N_2^-$ | | | | | | |
| 3-Me-pyrazolide$^-$ | | | | | | |
| • | | 1485±11 [g] | 1452±8 | IMRE | | 86TAF |
| $C_4H_5N_2^-$ | | | | | | |
| 4-Me-pyrazolide$^-$ | | | | | | |
| • | | 1484±11 [g] | 1454±8 | IMRE | | 86TAF |
| $C_4H_5O^-$ | | | | | *$\Delta_f H(AH)$= −138±8* | *79VAJ/HAR* |
| $CH_2{=}C(CH{=}CH_2)O^-$ | | | | | | |
| • −148±19 [a] | | 1520±11 [g] | 1492±8 | IMRE | | 86BAR/KIP |
| | | | 1500±10 | IMRE[o] | | 86BAR/KIP |
| $C_4H_5O^-$ | | | | | | |
| $CH_2{=}C(CHO)CH_2^-$ | | | | | | |
| • | | 1578±16 [g] | 1549±13 | IMRB | | 84BAR/BUR |
| $C_4H_5O^-$ | | | | | *$\Delta_f H(AH)$= −104±2* | *77PED/RYL* |
| $CH_2{=}CHCH{=}CHO^-$ | | | | | | |
| • −149±11 [a] | | 1484±10 [g] | 1456±8 | IMRE | | 86BAR/KIP |
| | | | 1466±10 | IMRE[o] | | 86BAR/KIP |
| $C_4H_5O^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −88±4* | |
| cyclobutanone enolate$^-$ | | | | | | |
| • | 1.84±0.07 | | | PD | | 78ZIM/JAC |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4H_6BrO_2^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −477±13* | |
| $EtCHBrCO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −600±23 [a] | | 1407±11 [g] | 1378±8 | IMRE | | 85CAL/MCM |
| $C_4H_6ClO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −501±4* | |
| $Cl(CH_2)_3CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −586±20 [a] | 3.22±0.25 [d] | 1445±16 [g] | 1416±8 | IMRE | | 78CUM/KEB |
| $C_4H_6ClO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −492±13* | |
| $EtCHClCO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −610±22 [a] | 3.56±0.19 [d] | 1412±10 [g] | 1384±8 | IMRE | | 78CUM/KEB |
| $C_4H_6ClO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −516±4* | |
| $MeCHClCH_2CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −616±20 [a] | 3.37±0.25 [d] | 1431±16 [g] | 1401±8 | IMRE | - | 78CUM/KEB |
| $C_4H_6F_2NO^-$ | | | | | | |
| $(CH_2F)_2CHOH\cdot\cdot CN^-$ | | | | | | |
| • −654±28 [c] | | *109±15* [g] | *66±10* | IMRE | | 87LAR/MCM |
| $C_4H_6F_3O^-$ | | | | *Est* | *$\Delta_f H(AH)$= −905±4* | |
| $CF_3C(Me)_2O^-$ | | | | | *BDE(A−H)= 440±4* | |
| • −928±14 [a] | 2.54±0.14 [d] | 1507±10 [g] | 1479±8 | IMRE | | 85CAL/MCM |
| | | | 1490±8 | IMRE[o] | | 85CAL/MCM |
| $C_4H_6N^-$ | | | | | *$\Delta_f H(AH)$= 25±1* | *77PED/RYL* |
| $Me_2CCN^-$ | | | | | *BDE(A−H)= 362±8* | *82MCM/GOL* |
| • 64±13 [a] | 1.08±0.21 [d] | 1570±12 [g] | 1539±8 | IMRE | | 79BAR/SCO |
| | | | 1534±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_6NO_2^-$ | | | | | *$\Delta_f H(AH)$= −430±4* | *69BEN/CRU* |
| $MeCON{=}C(Me)O^-$ | | | | | | |
| • −509±19 [a] | | 1451±15 [g] | 1422±8 | IMRE | | 78CUM/KEB |
| $C_4H_6NO_3^-$ | | | | | | |
| $HN{=}C(CO_2Et)O^-$ | | | | | | |
| • | | 1472±11 [g] | 1442±8 | IMRE | | 86TAF |
| $C_4H_6O_2^-$ | | | | | | |
| 2,3−butanedione$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −327±1* | *77PED/RYL* |
| • −394±11 [b] | 0.69±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.70±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.1 | | | ES | | 66COM/CHR |
| $C_4H_7^-$ | | | | | *$\Delta_f H(AH)$= −17±1* | *77PED/RYL* |
| $CH_2{=}C(Me)CH_2^-$ | | | | | *BDE(A−H)= 356±1* | *77LIA/AUS* |
| • 86±11 [a] | 0.36±0.12 [d] | 1633±10 [g] | 1602±9 | IMRE | | 84BAR/BUR |
| $C_4H_7O^-$ | | | | | *$\Delta_f H(AH)$= −241* | *77PED/RYL* |
| $CH_2{=}C(Et)O^-$ | | | | | *BDE(A−H)= 406±8* | |
| • −222±14 [a] | 1.75±0.06 | 1549±14 [c] | 1520±18 [h] | PD | | 77ZIM/REE |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4H_7O^-$ | | | | *Est* | *$\Delta_f H(AH)$= −144±4* | |
| $CH_2=C(OMe)CH_2^-$ | | | | | | |
| −60±30 [a] | | 1614±26 [g] | 1586±23 | IMRB | | 84BAR/BUR |
| $C_4H_7O^-$ | | | | | *$\Delta_f H(AH)$= −208±2* | *77PED/RYL* |
| $EtCH=CHO^-$ | | | | | *BDE(A−H)= 381±13* | |
| • −206±19 [a] | 1.67±0.05 | 1532±18 [c] | 1504±22 [h] | PD | | 77ZIM/REE |
| $C_4H_7O^-$ | | | | | *$\Delta_f H(AH)$= −241* | *77PED/RYL* |
| $MeCH=C(Me)O^-$ | | | | | *BDE(A−H)= 386±6* | *82MCM/GOL* |
| −231±13 [a] | 1.64±0.19 [d] | 1540±12 [g] | 1512±8 | IMRE | | 78CUM/KEB |
| • | 1.67±0.05 | | | PD | | 77ZIM/REE |
| $C_4H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −482±4* | |
| $iPrCO_2^-$ | | | | | *BDE(A−H)= 444±13* | |
| • −562±15 [a] | 3.17±0.24 [d] | 1449±11 [g] | 1420±8 | IMRE | | 86TAF |
| $C_4H_7O_2^-$ | | | | | *$\Delta_f H(AH)$= −473±4* | *82BUT/FRA* |
| $nPrCO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −553±16 [a] | 3.17±0.21 [d] | 1450±12 [g] | 1420±8 | IMRE | | 78CUM/KEB |
| $C_4H_7O_4^-$ | | | | | | |
| $MeCO_2H\cdot\cdot MeCO_2^-$ | | | | | | |
| −1059±17 [c] | | *123±4* | *85±7* | TDAs | | 86MEO/SIE2 |
| $C_4H_8ClO^-$ | | | | | | |
| $EtCOMe\cdot\cdot Cl^-$ | | | | | | |
| • −530±10 [c] | | *62±8* [g] | *36±8* | IMRE | | 84LAR/MCM2 |
| $C_4H_8IO_2^-$ | | | | | | |
| $iPrCO_2H\cdot\cdot I^-$ | | | | | | |
| • −740±9 [c] | | *70±4* | *44±9* | TDAs | | 84CAL/KEB |
| $C_4H_8NO^-$ | | | | | *$\Delta_f H(AH)$= −234* | *78BEA/LEE* |
| $CH_2=C(NMe_2)O^-$ | | | | | | |
| • −196 [a] | | 1569±21 [g] | 1540±8 | IMRE | | 79BAR/SCO |
| | | | 1535±8 | IMRE [o] | | 79BAR/SCO |
| $C_4H_8NO^-$ | | | | | *$\Delta_f H(AH)$= −43±6* | *74CHO/MEN* |
| $Me_2C(NO)CH_2^-$ | | | | | | |
| 40±34 [a] | | 1613±28 [g] | 1586±25 | IMRB | | 80NOE/NIB |
| $C_4H_9^-$ | | | | | *$\Delta_f H(AH)$= −135* | *74SCO* |
| $Me_3C^-$ | | | | | *BDE(A−H)= 390±8* | *82MCM/GOL* |
| • 67±9 [a] | | 1732±8 | 1701±10 [h] | Bran | | 84DEP/BIE |
| | 0.7 | | | SI | | 72PAG |
| | 0.6 | | | SI | | 69PAG/GOO |
| $C_4H_9Br_2^-$ | | | | | | |
| $iBuBr\cdot\cdot Br^-$ | | | | | | |
| −374 [c] | | *54* | *27* | TDAs | | 74DOU |

Table 2. Negative Ion Table – Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4H_9Br_2^-$ | | | | | | |
| tBuBr··Br⁻ | | | | | | |
| −397 [c] | | *52* | *28* | TDAs | | 74DOU |
| $C_4H_9ClF^-$ | | | | | | |
| tBuF··Cl⁻ | | | | | | |
| • −614±18 [c] | | *56±8* [g] | *30±8* | IMRE | | 84LAR/MCM2 |
| $C_4H_9Cl_2^-$ | | | | | | |
| tBuCl··Cl⁻ | | | | | | |
| • −469±11 [c] | | *60±8* [g] | *33±8* | IMRE | | 84LAR/MCM2 |
| $C_4H_9F_2^-$ | | | | | | |
| tBuF··F⁻ | | | | | | |
| • −673±15 [c] | | *93±8* [g] | *64±8* | IMRE | | 83LAR/MCM |
| $C_4H_9O^-$ | | | | | *$\Delta_f H(AH)$= −284±2* | *77PED/RYL* |
| iBuO⁻ | | | | | *BDE(A−H)= 436±6* | |
| • −246±11 [a] | 1.87±0.16 [d] | 1568±9 [g] | 1540±8 | IMRE | | 79BAR/SCO |
| | | | 1535±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_9O^-$ | | | | | *$\Delta_f H(AH)$= −275* | *77PED/RYL* |
| nBuO⁻ | | | | | *BDE(A−H)= 431±5* | *82MCM/GOL* |
| • −234±10 [a] | 1.78±0.15 [d] | 1571±10 [g] | 1543±8 | IMRE | | 79BAR/SCO |
| | | 1569±12 | 1541±13 [h] | CIDC | | 83BOA/HOU |
| | 1.9±0.1 | | | EIAP | From nBuONO | 68WIL/HAM |
| | 0.9 | | | SI | | 69PAG/GOO |
| | | | 1537±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_9O^-$ | | | | | *$\Delta_f H(AH)$= −295* | *77PED/RYL* |
| sBuO⁻ | | | | | *BDE(A−H)= 441±4* | *82MCM/GOL* |
| • −259±10 [a] | 1.95±0.14 [d] | 1566±10 [g] | 1538±8 | IMRE | | 86TAF |
| | | 1565±11 | 1538±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1533±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_9O^-$ | | | | | *$\Delta_f H(AH)$= −313±3* | *77PED/RYL* |
| tBuO⁻ | | | | | *BDE(A−H)= 440±4* | *82MCM/GOL* |
| • −275±12 [a] | 1.91±0.14 [d] | 1567±9 [g] | 1540±8 | IMRE | | 79BAR/SCO |
| • | 1.912±0.054 | | | LPES | | 82ELL/ENG |
| | 1.87±0.01 | | | PD | | 78JAN/ZIM |
| | <1.87±0.04 | | | PD | | 75REE/BRA |
| | | | 1534±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_9O_3^-$ | | | | | | |
| EtOH··$MeCO_2^-$ | | | | | | |
| | | *87±4* | *50±7* | TDAs | | 86MEO/SIE2 |
| $C_4H_9O_3^-$ | | | | | | |
| HOH··$iPrCO_2^-$ | | | | | | |
| | | *66±4* | *37±7* | TDAs | | 86MEO/SIE2 |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_4H_9S^-$ | | | | | | *$\Delta_f H(AH)$= -97±1* | *77PED/RYL* |
| iBuS⁻ | | | | | | *BDE(A-H)= 364±10* | |
| • | −149±13 [a] | 2.06±0.23 [d] | 1477±12 [g] | 1451±8 | IMRE | | 86TAF |
| $C_4H_9S^-$ | | | | | | *$\Delta_f H(AH)$= -88±1* | *77PED/RYL* |
| nBuS⁻ | | | | | | *BDE(A-H)= 364±10* | |
| • | −138±13 [a] | 2.04±0.23 [d] | 1480±12 [g] | 1454±8 | IMRE | | 86TAF |
| • | | 2.030±0.020 | | | LPD | | 80JAN/REE |
| $C_4H_9S^-$ | | | | | | *$\Delta_f H(AH)$= -110±1* | *77PED/RYL* |
| tBuS⁻ | | | | | | *BDE(A-H)= 364±9* | |
| • | −165±13 [a] | 2.09±0.22 [d] | 1475±12 [g] | 1449±8 | IMRE | | 79BAR/SCO |
| • | | 2.070±0.020 | | | LPD | | 80JAN/REE |
| | | | | 1458±8 | IMRE[o] | | 79BAR/SCO |
| $C_4H_{10}BF_2^-$ | | | | | | | |
| $Et_2BF\cdot\cdot F^-$ | | | | | | | |
| • | −740±44 [c] | | *243±21* [g] | *215±21* | IMRE | | 85LAR/MCM |
| | −765 [c] | | *268* | | IMRB | $F^-$: $iPr_3B > Et_2BF > Et_3B$ | 77MUR/BEA2 |
| $C_4H_{10}ClO^-$ | | | | | | | |
| nBuOH··Cl⁻ | | | | | | | |
| • | −576±10 [c] | | *74±8* [g] | *45±8* | IMRE | | 84LAR/MCM2 |
| $C_4H_{10}ClO^-$ | | | | | | | |
| tBuOH··Cl⁻ | | | | | | | |
| • | −599±12 [c] | | *59±8* | *46±8* | TDAs | | 71YAM/KEB |
| | | | *76±8* [g] | *46±8* | IMRE | | 84LAR/MCM2 |
| $C_4H_{10}FO^-$ | | | | | | | |
| nBuOH··F⁻ | | | | | | | |
| • | −658±11 [c] | | *135±8* [g] | *103±8* | IMRE | | 83LAR/MCM |
| $C_4H_{10}FO^-$ | | | | | | | |
| tBuOH··F⁻ | | | | | | | |
| • | −701±13 [c] | | *139±8* [g] | *107±8* | IMRE | | 83LAR/MCM |
| $C_4H_{10}IO^-$ | | | | | | | |
| tBuOH··I⁻ | | | | | | | |
| • | | | *51±4* | *27±9* | TDAs | | 84CAL/KEB |
| $C_4H_{10}NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -36±13* | |
| $Et_2NO^-$ | | | | | | *BDE(A-H)= 291±8* | *78CAC/LIS* |
| • | −15±23 [a] | 0.54±0.20 [d] | 1551±11 [g] | 1523±8 | IMRE | | 83BAR/BAS |
| | | | | 1520±8 | IMRE[o] | | 83BAR/BAS |
| $C_4H_{11}O_2^-$ | | | | | | | |
| EtOH··EtO⁻ | | | | | | | |
| | | | *115±4* | *82±7* | TDEq | | 86MEO/SIE2 |
| | −507±21 [c] | | *86±10* [g] | *59±7* | IMRE | | 84CAL/ROZ |

The difference between 84CAL/ROZ and 86MEO/SIE2 has not been resolved.

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_4H_{11}O_2^-$ | | | | | | |
| $MeOH\cdot\cdot nPrO^-$ | | | | | | |
| −496±21 [c] | | *83±10* [g] | *55±8* | IMRE | | 84CAL/ROZ |
| $C_4H_{11}Si^-$ | | | | | | |
| $Me_3SiCH_2^-$ | | | | | *$\Delta_f H(AH)$= −233±3* | *83STE* |
| | | | | | *BDE(A−H)= 415±8* | *83STE2* |
| −102±26 [a] | 0.7±0.3 [d] | 1661±23 [g] | 1635±21 | IMRB | | 84DEP/DAM |
| $C_4H_{12}FSi^-$ | | | | | | |
| $Me_4Si\cdot\cdot F^-$ | | | | | | |
| • −607±13 [c] | | *125±8* [g] | *99±8* | IMRE | | 85LAR/MCM |
| $C_5ClFeO_5^-$ | | | | | | |
| $Fe(CO)_5\cdot\cdot Cl^-$ | | | | | | |
| −1053±16 [c] | | *58±13* [g] | *33±13* | IMRB | | 85LAN/SAL |
| $C_5CrO_5^-$ | | | | | | |
| $Cr(CO)_5^-$ | | | | | | |
| | >2.3 | | | IMRB | | 85SAL/LAN |
| $C_5FFeO_5^-$ | | | | | | |
| $Fe(CO)_5\cdot\cdot F^-$ | | | | | | |
| −1188±13 [c] | | *171±8* [g] | *144±8* | IMRE | | 85LAN/SAL |
| $C_5F_6O_3^-$ | | | | | | |
| hexafluoroglutaric anhydride$^{-\cdot}$ | | | | | | |
| | 1.5±0.2 | | | NBIP | | 74COO/COM |
| $C_5F_9^-$ | | | | | | |
| $C_5F_9^-$ | | | | | *$\Delta_f H(A)$= −1573±29* | *83SPY/SAU* |
| −2017±73 [b] | 4.6±0.5 | | | EIAP | From n−$C_6F_{14}$ | 83SPY/SAU |
| | >3.1±0.3 | | | EIAP | From c−$C_4F_6(CF_3)_2$ | 72THY |
| | 3.1 | | | EIAP | From c−$C_4F_6(CF_3)_2$ | 70LIF/PEE |
| $C_5F_9O_2^-$ | | | | | | |
| $FCOCF_2CF_2CF_2CFO\cdot\cdot F^-$ | | | | | | |
| • | | | *192±19* | IMRE | | 84LAR/MCM |
| $C_5F_{10}^-$ | | | | | | |
| $C_5F_{10}^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −2007±21* | *83SPY/SAU* |
| <−2508±64 [b] | >5.2±0.5 | | | EIAP | From n−$C_5F_{12}$ | 83SPY/SAU |
| $C_5F_{11}^-$ | | | | | | |
| $(CF_3)_3CCF_2^-$ | | | | | | |
| | 4.7±0.3 | | | EIAP | From neo−$C_5F_{12}$ | 85SPY/HUN |
| $C_5F_{11}^-$ | | | | | | |
| $C_2F_5(CF_3)_2C^-$ | | | | | | |
| | >4.2±0.3 | | | EIAP | From i−$C_5F_{12}$ | 85SPY/HUN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_5F_{11}^-$ | | | | | | |
| $C_5F_{11}^-$ | | | | | | |
| | >4.5±0.2 | | | EIAP | From n-$C_5F_{12}$ | 83SPY/SAU |
| $C_5MnO_5^-$ | | | | | | |
| $Mn(CO)_5^-$ | | | | | *$\Delta_f H(A)$= −740±10* | *82CON/ZAF* |
| | | | 1309±17 | IMRB | | 87STE/BEA |
| $C_5N^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 577±21* | |
| N≡CC≡CC≡C⁻ | | | | | *BDE(A−H)= 552±21* | |
| 682 | 2.3 | 1643±21 [c] | | EIAP | From HC≡C−$(C≡C)_2$−C≡N | 61DIB/REE |
| $C_5N_3^-$ | | | | | | |
| $(NC)_2C$=CCN⁻ | | | | | | |
| | 3.8±0.5 | | | EIAP | From tetracyanoethylene | 72BRI/OLS |
| $C_5HFeO_5^-$ | | | | | | |
| $Fe(CO)_5\cdot\cdot H^-$ | | | | | | |
| −858 [c] | | *235±13* | | IMRB | | 85LAN/SAL |
| $C_5HFeO_6^-$ | | | | | | |
| $Fe(CO)_5\cdot\cdot OH^-$ | | | | | | |
| −1142 [c] | | *237±17* [g] | *196±17* | IMRB | | 85LAN/SAL |
| <−1075 | | | | IMRB | | 84LAN/LEE |
| $C_5H_3F_2^-$ | | | | | | |
| difluorocyclopentadienide⁻ | | | | | | |
| <9 | | | | IMRB | $CH_2$=$CHCH_2^-$ + $C_2F_4$ → | 79DAW/NOE |
| $C_5H_4^-$ | | | | | *$\Delta_f H(AH)$= 217±10* | *82MCM/GOL* |
| cyclopentadienylide⁻· | | | | *D-EA* | *BDE(A−H)= 466±46* | |
| 274±27 [a] | | 1587±16 [g] | 1556±13 | IMRB | | 80MCD/CHO |
| <243±19 | | | | EIAP | | 72DID/HAR |
| | | | 1546±13 | IMRB[o] | | 80MCD/CHO |
| $C_5H_4F_3O_2^-$ | | | | | *$\Delta_f H(AH)$= −1003±4* | *84ERA/KOL* |
| $CF_3COCH$=C(Me)O⁻ | | | | | | |
| | | 1374±17 [g] | 1347±8 | IMRE | | 81FUJ/MCI |
| −1130±21 [a] | | 1374±17 [g] | 1348±8 | IMRE | | 78CUM/KEB |
| $C_5H_4F_6NO^-$ | | | | | | |
| $(CF_3)_2C(Me)OH\cdot\cdot CN^-$ | | | | | | |
| • −1609±28 [c] | | *108±15* [g] | *74±10* | IMRE | | 87LAR/MCM |
| $C_5H_4N^-$ | | | | | *$\Delta_f H(AH)$= 140±1* | *79KUD/KUD* |
| pyridinide⁻ | | | | | | |
| • 250±3 [a] | | 1640±2 | 1602±2 | TDEq | | 87MEO |
| | | | <1574±8 | IMRB | O⁻ deprotonates | 78BRU/FER |
| | 2.41±0.03 | | | SI | | 76FAI/JOY |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$C_5H_4O^-$** | | | | | | | |
| $C_5H_4O^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −35±35* | |
| | 84±21 | | | | NBAP | | 75COO/NAF |
| | | | | | | From benzoquinone. Possibly cyclopentadienone$^{-\cdot}$? | |
| **$C_5H_5^-$** | | | | | | *$\Delta_f H(AH)$= 131±4* | *77PED/RYL* |
| cyclopentadienide$^-$ | | | | | | *BDE(A−H)= 329±8* | *82MCM/GOL* |
| • | 82±16 [a] | 1.67±0.21 [d] | 1481±12 [g] | 1455±8 | IMRE | | 79BAR/SCO |
| • | | 1.786±0.020 | | | LPES | | 77ENG/LIN2 |
| | | | 1485±12 [g] | 1459±8 | IMRE | | 78CUM/KEB |
| | | 1.839±0.030 | | | LPD | | 73RIC/STE |
| | 79±8 | <2.2±0.3 | | | EIAP | From cyclopentadiene | 72DID/HAR |
| | | | | 1464±8 | IMRE[o] | | 79BAR/SCO |
| **$C_5H_5N_2^-$** | | | | | | | |
| pyrrole··CN$^-$ | | | | | | | |
| • | 101±24 [c] | | *82±15* [g] | *51±10* | IMRE | | 87LAR/MCM |
| **$C_5H_5N_2O_2^-$** | | | | | | | |
| EtOCOCN··CN$^-$ | | | | | | | |
| • | | | *73±15* [g] | *42±10* | IMRE | | 87LAR/MCM |
| **$C_5H_6Cl^-$** | | | | | | | |
| cyclopentadiene··Cl$^-$ | | | | | | | |
| | | | | *<10* | TDEq | | 82FRE/IKU |
| **$C_5H_6NO^-$** | | | | | *Est2* | *$\Delta_f H(AH)$= 21±13* | |
| Me$_2$NCOC≡C$^-$ | | | | | | *BDE(A−H)= 552±21* | |
| • | 8±22 [a] | | 1517±10 [g] | 1484±8 | IMRE | | 86TAF |
| **$C_5H_7^-$** | | | | | | *$\Delta_f H(AH)$= 75±1* | *77PED/RYL* |
| CH$_2$=C(CH=CH$_2$)CH$_2^-$ | | | | | | | |
| | 159±24 [a] | | 1614±23 [g] | 1586±21 | IMRB | Acid: isoprene | 79BAR/MCI |
| **$C_5H_7^-$** | | | | | | *$\Delta_f H(AH)$= 144±4* | *79ROG/DAG* |
| nPrC≡C$^-$ | | | | | | *BDE(A−H)= 552±21* | |
| • | 203±19 [a] | 2.85±0.37 [d] | 1589±15 [g] | 1556±8 | IMRE | | 79BAR/SCO |
| | | | | 1551±8 | IMRE[o] | | 79BAR/SCO |
| **$C_5H_7^-$** | | | | | | *$\Delta_f H(AH)$= 106* | *77PED/RYL* |
| pentadienide$^-$ | | | | | | *BDE(A−H)= 318±13* | *82MCM/GOL* |
| • | 118±16 [a] | 0.91±0.03 | 1542±15 [e] | 1522±22 [h] | PD | Acid: 1,4-pentadiene | 78ZIM/GYG |
| **$C_5H_7N_2^-$** | | | | | | | |
| 3,5-diMe-pyrazolide$^-$ | | | | | | | |
| • | | | 1481±11 [g] | 1450±8 | IMRE | | 86TAF |
| **$C_5H_7O^-$** | | | | | | *$\Delta_f H(AH)$= −194±2* | *77PED/RYL* |
| cyclopentanone enolate$^-$ | | | | | | | |
| • | | 1.62±0.06 | | | PD | | 78ZIM/JAC |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_5H_7O_2^-$ | | | | | *$\Delta_f H(AH)$= -384±2* | *79HAC/PIL* |
| $MeCOCH=C(Me)O^-$ | | | | | | |
| • -472±11 [a] | | 1438±10 [g] | 1408±8 | IMRE | | 78CUM/KEB |
| | | 1438±10 [g] | 1409±8 | IMRE | | 86TAF |
| $C_5H_7O_3^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -573±13* | |
| $MeCO_2CH=C(Me)O^-$ | | | | | *BDE(A-H)= 377±8* | |
| • -638±25 [a] | | 1466±12 [g] | 1436±8 | IMRE | | 78CUM/KEB |
| $C_5H_8Cl^-$ | | | | | | |
| $CH_2=CHCH_2CH=CH_2\cdot\cdot Cl^-$ | | | | | | |
| | | | *15* | TDEq | | 82FRE/IKU |
| $C_5H_8ClO_2^-$ | | | | | | |
| $MeCOCH_2COMe\cdot\cdot Cl^-$ | | | | | | |
| | | | *56* | TDEq | | 82FRE/IKU |
| $C_5H_9O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -244±4* | |
| $Me_2C(CHO)CH_2^-$ | | | | | | |
| -153±25 [a] | | 1621±21 [g] | 1594±17 | IMRB | | 80NOE/NIB |
| $C_5H_9O^-$ | | | | | *$\Delta_f H(AH)$= -262±1* | *77PED/RYL* |
| $Me_2C=C(Me)O^-$ | | | | | *BDE(A-H)= 364±13* | |
| • -257±13 [a] | 1.46±0.26 [d] | 1535±12 [g] | 1508±8 | IMRE | | 78CUM/KEB |
| $C_5H_9O^-$ | | | | | *$\Delta_f H(AH)$= -259±1* | *77PED/RYL* |
| $MeCH=C(Et)O^-$ | | | | | *BDE(A-H)= 390±17* | |
| • -246±13 [a] | 1.65±0.30 [d] | 1542±12 [g] | 1512±8 | IMRE | | 78CUM/KEB |
| • | 1.68±0.05 | | | PD | | 77ZIM/REE |
| $C_5H_9O_2^-$ | | | | | *$\Delta_f H(AH)$= -515±6* | *77PED/RYL* |
| $iBuCO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -596±17 [a] | 3.17±0.20 [d] | 1449±11 [g] | 1420±8 | IMRE | | 86TAF |
| $C_5H_9O_2^-$ | | | | | *$\Delta_f H(AH)$= -490±2* | *77PED/RYL* |
| $nBuCO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -572±11 [a] | 3.2±0.2 [d] | 1449±10 | 1419±12 [h] | CIDC | | 81MCL/CAM |
| $C_5H_9O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -512±4* | |
| $tBuCO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -600±15 [a] | 3.25±0.20 [d] | 1442±11 [g] | 1412±8 | IMRE | | 86TAF |
| $C_5H_{10}ClO^-$ | | | | | | |
| $Et_2CO\cdot\cdot Cl^-$ | | | | | | |
| • -545±10 [c] | | *59±8* [g] | *34±8* | IMRE | | 84LAR/MCM2 |
| $C_5H_{10}ClO^-$ | | | | | | |
| $tBuCHO\cdot\cdot Cl^-$ | | | | | | |
| • -534±14 [c] | | *63±8* [g] | *35±8* | IMRE | | 84LAR/MCM2 |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_5H_{10}FO^-$ | | | | | | | |
| $tBuCHO\cdot\cdot F^-$ | | | | | | | |
| • | −596±15 [c] | | *103±8* [g] | *70±8* | IMRE | | 83LAR/MCM |
| $C_5H_{10}IO_2^-$ | | | | | | | |
| $tBuCO_2H\cdot\cdot I^-$ | | | | | | | |
| • | −765±9 [c] | | *64±4* | *37±9* | TDAs | | 84CAL/KEB |
| $C_5H_{10}NO^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −322±13* | |
| $HN{=}C(tBu)O^-$ | | | | | | | |
| • | −354±23 [a] | | 1499±11 [g] | 1469±8 | IMRE | | 86TAF |
| $C_5H_{10}NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −135±8* | |
| $tBuCH{=}NO^-$ | | | | | | | |
| • | −147±23 [a] | | 1518±14 [g] | 1489±10 | IMRE | | 79BAR/SCO |
| | | | | 1497±8 | IMRE[o] | | 79BAR/SCO |
| $C_5H_{10}NO^-$ | | | | | | | |
| $tBuOH\cdot\cdot CN^-$ | | | | | | | |
| • | −314±26 [c] | | *76±15* [g] | *45±10* | IMRE | | 87LAR/MCM |
| $C_5H_{10}NO_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −189±4* | |
| $tBuCH{=}NO_2^-$ | | | | | | | |
| • | −233±16 [a] | | 1486±12 [g] | 1458±8 | IMRE | | 79BAR/SCO |
| | | | | 1467±8 | IMRE[o] | | 79BAR/SCO |
| $C_5H_{11}Br_2^-$ | | | | | | | |
| $tBuCH_2Br\cdot\cdot Br^-$ | | | | | | | |
| | −418 [c] | | *60* | *29* | TDAs | | 74DOU |
| $C_5H_{11}O^-$ | | | | | | *$\Delta_f H(AH)$= −316±1* | *77PED/RYL* |
| $Et_2CHO^-$ | | | | | | *BDE(A−H)= 438±4* | |
| • | −286±12 [a] | 2.0±0.2 [d] | 1559±11 | 1532±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1556±10 | | CIDC[o] | | 83BOA/HOU |
| $C_5H_{11}O^-$ | | | | | | *$\Delta_f H(AH)$= −316±1* | *77PED/RYL* |
| $iPrCH(Me)O^-$ | | | | | | *BDE(A−H)= 438±4* | |
| • | −285±13 [a] | 2.0±0.2 [d] | 1561±11 | 1533±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1556±10 | | CIDC[o] | | 83BOA/HOU |
| $C_5H_{11}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −306±4* | |
| $iPrCH_2CH_2O^-$ | | | | | | *BDE(A−H)= 436±4* | |
| • | −274±15 [a] | 1.9±0.2 [d] | 1563±11 | 1535±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1559±10 | 1531±12 [h] | CIDC[o] | | 83BOA/HOU |
| $C_5H_{11}O^-$ | | | | | | *$\Delta_f H(AH)$= −297±2* | *77PED/RYL* |
| $nC_5H_{11}O^-$ | | | | | | *BDE(A−H)= 436±4* | |
| • | −262±13 [a] | 1.9±0.2 [d] | 1564±11 | 1537±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1560±10 | | CIDC[o] | | 83BOA/HOU |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_5H_{11}O^-$ | | | | | Est | $\Delta_f H(AH)=$ −318±2 | |
| $tBuCH_2O^-$ | | | | | | BDE(A−H)= 428±6 | 82MCM/GOL |
| • | −290±14 [a] | 1.88±0.19 [d] | 1559±12 [g] | 1531±8 | IMRE | | 79BAR/SCO |
| • | | 1.93±0.05 | | | PD | | 78JAN/ZIM |
| | | < 1.93±0.06 | | | PD | | 75REE/BRA |
| | | | | 1528±8 | IMRE[o] | | 79BAR/SCO |
| $C_5H_{11}O^-$ | | | | | | $\Delta_f H(AH)=$ −331±1 | 77PED/RYL |
| $tPnO^-$ | | | | | | BDE(A−H)= 440±4 | |
| • | −300±13 [a] | 2.0±0.2 [d] | 1561±11 | 1533±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1556±10 | | CIDC[o] | | 83BOA/HOU |
| $C_5H_{11}S^-$ | | | | | | $\Delta_f H(AH)=$ −110±1 | 77PED/RYL |
| $nC_5H_{11}S^-$ | | | | | | BDE(A−H)= 364±10 | |
| • | −165±13 [a] | 2.090±0.020 | 1475 [e] | | LPD | | 80JAN/REE |
| $C_5H_{11}S^-$ | | | | | | $\Delta_f H(AH)=$ −129±1 | 77PED/RYL |
| $tBuCH_2S^-$ | | | | | | BDE(A−H)= 364±10 | |
| • | −188±13 [a] | 2.13±0.23 [d] | 1472±12 [g] | 1445±8 | IMRE | | 86TAF |
| $C_5H_{12}FSi^-$ | | | | | | | |
| $c\text{-}(CH_2)_3Si(Me)_2\cdot\cdot F^-$ | | | | | | | |
| | −544±23 [c] | | *158±9* [g] | *130±9* | IMRE | | 81SUL/DEP |
| $C_5H_{13}O_2^-$ | | | | | | | |
| $EtOH\cdot\cdot nPrO^-$ | | | | | | | |
| | −531±21 [c] | | *85±10* [g] | *57±8* | IMRE | | 84CAL/ROZ |
| $C_5H_{13}O_2^-$ | | | | | | | |
| $MeOH\cdot\cdot tBuO^-$ | | | | | | | |
| | | | *107±4* | *72±7* | TDEq | | 86MEO/SIE2 |
| | −556±23 [c] | | *79±10* [g] | *51±7* | IMRE | | 84CAL/ROZ |
| $C_5H_{15}Si^-$ | | | | | | | |
| $nPnSiH_3\cdot\cdot H^-$ | | | | | | | |
| | | | *45±23* | | IMRB | | 86HAJ/SQU |
| $C_6Br_4O_2^-$ | | | | | | | |
| bromanil$^{-\cdot}$ | | | | | Est | $\Delta_f H(A)=$ 18±21 | |
| | −218±40 [b] | 2.4±0.2 | | | NBIP | | 78COO/FRE |
| $C_6Cl_4O_2^-$ | | | | | | | |
| chloranil$^{-\cdot}$ | | | | | | $\Delta_f H(A)=$ −186±12 | 77PED/RYL |
| • | −454±21 [b] | 2.78±0.10 | | | TDEq | | 87KEB/CHO |
| | | 2.68±0.11 | | | IMRE | | 85GRI/CAL |
| | | 2.67±0.05 | | | IMRE | | 85FUK/MCI |
| | | 2.8±0.2 | | | NBIP | | 78COO/FRE |
| | | 2.5±0.3 | | | SI | | 66FAR/PAG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6Cl_5^-$ | | | | | | |
| $C_6Cl_5^-$ | | | | | *$\Delta_f H(AH)$= -40±9* | *85PLA/SIM2* |
| | | | | | *BDE(A-H)= 464±13* | |
| | 2.8 | 1510±13 [c] | | SI | | 69PAG/GOO |
| $C_6F_4O_2^-$ | | | | | | |
| fluoranil$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -816±41* | |
| • -1076±51 [b] | 2.70±0.10 | | | TDEq | | 87KEB/CHO |
| -1043±46 [b] | 2.36±0.05 | | | IMRE | | 85FUK/MCI |
| | 2.9±0.2 | | | NBIP | | 78COO/FRE |
| | 2.3 | | | SI | | 69PAG/GOO |
| $C_6F_5^-$ | | | | | *$\Delta_f H(AH)$= -806±7* | *77PED/RYL* |
| $C_6F_5^-$ | | | | | *BDE(A-H)= 487±8* | *82MCM/GOL* |
| -797±34 [b] | 2.7±0.2 | 1539±28 [e] | 1506±29 [h] | NBAP | From perfluorobenzene | 82COM/REI |
| -464 | | | | Endo | $I^- + C_6F_6 \rightarrow$ | 73LIF/TIE |
| | 2.7 | | | SI | | 69PAG/GOO |
| $C_6F_5O^-$ | | | | | *$\Delta_f H(AH)$= -957±2* | *77PED/RYL* |
| pentafluorophenoxide$^-$ | | | | | | |
| | 3.06±0.09 | | | ECD | | 84HER/WEN |
| <-857±8 | | <1630±10 [f] | | IMRB | $HO^- + C_6F_6 \rightarrow$, acidity probably ca. 1340 kJ | 75BRI/RIV |
| $C_6F_6^-$ | | | | | | |
| $C_6F_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -946±8* | *79PRI/SAP* |
| • -996±18 [b] | 0.52±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.52±0.10 | | | TDEq | | 86CHO/GRI |
| | 1.8±0.3 | | | EnCT | | 73LIF/TIE |
| | 1.20±0.07 | | | SI | | 69PAG/GOO |
| $C_6F_{10}^-$ | | | | | | |
| perfluorocyclohexene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -2369±8* | *79PRI/SAP* |
| <-2504±37 [b] | >1.4±0.3 | | | EnCT | | 73LIF/TIE |
| $C_6F_{11}^-$ | | | | | | |
| $C_6F_{11}^-$ | | | | | | |
| | >4.2±0.2 | | | EIAP | From c-$C_4F_6(CF_3)_2$ | 72THY |
| | 3.5 | | | EIAP | From c-$C_6F_{12}$ | 70LIF/PEE |
| $C_6F_{13}^-$ | | | | | | |
| $C_6F_{13}^-$ | | | | | | |
| | >4.6±0.2 | | | EIAP | From n-$C_6F_{14}$ | 83SPY/SAU |
| $C_6N_4^-$ | | | | | | |
| tetracyanoethylene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 705±6* | *77PED/RYL* |
| • 400±25 [b] | 3.17±0.20 | | | TDEq | | 87KEB/CHO |
| | 3.17±0.20 | | | TDEq | | 86CHO/KEB |
| | 2.300±0.300 | | | LPD | | 76LYO/PAL |
| | 2.03±0.05 | | | PD | | 73LYO/PAL |
| | 1.700±0.300 | | | LPD | | 75LYO/PAL |
| | 2.88±0.06 | | | SI | | 67FAR/PAG |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_6HCl_3O_2^-$ | | | | | | | |
| triCl-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −180±13* | |
| • | −423±17 [b] | 2.52±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6HF_4O^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −764±13* | |
| 2,3,5,6-tetrafluorophenoxide$^-$ | | | | | | *BDE(A-H)= 385±17* | |
| | | 2.75±0.09 | | | ECD | | 84HER/WEN |
| $C_6H_2Cl_2O_2^-$ | | | | | | | |
| 2,5-diCl-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −174±13* | |
| • | −409±22 [b] | 2.43±0.10 | | | TDEq | | 87KEB/CHO |
| | | 2.29±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_2Cl_2O_2^-$ | | | | | | | |
| 2,6-diCl-benzoquinone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −174±12* | *77PED/RYL* |
| • | −414±21 [b] | 2.48±0.10 | | | TDEq | | 87KEB/CHO |
| | | 2.39±0.11 | | | IMRE | | 85GRI/CAL |
| | | 2.40±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_2Cl_3O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −164±8* | |
| 3,4,5-triCl-phenoxide$^-$ | | | | | | *BDE(A-H)= 362±13* | |
| • | −310±21 [a] | 3.00±0.26 [d] | 1384±12 [g] | 1355±8 | IMRE | | 81FUJ/MCI |
| $C_6H_2FO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −387±13* | |
| fluorobenzoquinonide$^-$ | | | | | | | |
| | | 2.4±0.1 | | | SI | | 66FAR/PAG |
| $C_6H_2N_3O_7^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −159±21* | |
| 2,4,6-triNO$_2$-phenoxide$^-$ | | | | | | *BDE(A-H)= 381±17* | |
| | < −365±25 [a] | | < 1324±4 [g] | < 1293 | IMRB | $I^-$ deprotonates | 74DZI/CAR |
| $C_6H_3ClNO_3^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −151±17* | |
| 2-Cl-4-NO$_2$-phenoxide$^-$ | | | | | | *BDE(A-H)= 381±17* | |
| • | −328±28 [a] | | 1353±11 [g] | 1323±8 | IMRE | | 86TAF |
| $C_6H_3Cl_2NO_2^-$ | | | | | | | |
| 2,3-diCl-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 3±8* | |
| • | −116±13 [b] | 1.23±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_3Cl_2NO_2^-$ | | | | | | | |
| 3,4-diCl-nitrobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 8±8* | |
| • | −125±13 [b] | 1.38±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_3Cl_2O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −153±8* | |
| 3,5-diCl-phenoxide$^-$ | | | | | | *BDE(A-H)= 362±13* | |
| • | −284±19 [a] | 2.85±0.24 [d] | 1399±11 [g] | 1370±8 | IMRE | | 81FUJ/MCI |
| $C_6H_3FO_2^-$ | | | | | | | |
| fluorobenzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −387±13* | |
| | | 1.5±0.2 | | | SI | | 66FAR/PAG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_3F_2^-$ | | | | | *$\Delta_f H(AH)$= -309±1* | *77PED/RYL* |
| m-difluorophenide⁻ | | | | | | |
| <-264±3 [a] | | <1576±1 [g] | <1543 | IMRB | < iPrOH | 75BRI/RIV |
| $C_6H_3F_2^-$ | | | | | *$\Delta_f H(AH)$= -294±1* | *77PED/RYL* |
| o-difluorophenide⁻ | | | | | *BDE(A-H)= 460±13* | |
| -242±18 [a] | 2.0±0.3 [d] | 1582±16 [g] | 1547±13 | IMRB | Between EtO⁻, iPrO⁻ | 75BRI/RIV |
| $C_6H_3F_2^-$ | | | | | *$\Delta_f H(AH)$= -307±1* | *77PED/RYL* |
| p-difluorophenide⁻ | | | | | *BDE(A-H)= 460±13* | |
| -247±16 [a] | 1.9±0.3 [d] | 1590±15 [g] | 1555±13 | IMRB | < MeOH, ≤ EtOH | 75BRI/RIV |
| $C_6H_3FeO_6^-$ | | | | | | |
| $Fe(CO)_5\cdot\cdot OMe^-$ | | | | | | |
| -1095±37 [c] | | *188±25 [g]* | *149±25* | IMRB | | 85LAN/SAL |
| $C_6H_3N_3O_6^-$ | | | | | | |
| 1,3,5-trinitrobenzene⁻· | | | | | *$\Delta_f H(A)$= 62±2* | *77PED/RYL* |
| -191 [b] | 2.6 | | | SI | | 69PAG/GOO |
| $C_6H_3O_2^-$ | | | | | *$\Delta_f H(AH)$= -123±3* | *77PED/RYL* |
| benzoquinonide⁻ | | | | | | |
| | | | <1607 | IMRB | | 87JOH/SPE |
| | 2.00±0.04 | | | SI | | 66FAR/PAG |
| $C_6H_4^-$ | | | | | | |
| o-benzyne⁻· | | | | | *$\Delta_f H(A)$= 494±21* | *80POL/HEH* |
| • 440±22 [b] | 0.560±0.010 | | | LPES | | 86LEO/MIL |
| <433 | | | | IMRB | $O^-$ + $C_6H_6$ →, D label indicates ortho loss | 78BRU/FER |
| $C_6D_4^-$ | | | | | | |
| o-benzyne-$d_4$⁻· | | | | | | |
| • | 0.551±0.010 | | | LPES | | 86LEO/MIL |
| $C_6H_4BrNO_2^-$ | | | | | | |
| mBr-nitrobenzene⁻· | | | | *Est* | *$\Delta_f H(A)$= 90±4* | |
| • -38±14 [b] | 1.32±0.10 | | | TDEq | | 87KEB/CHO |
| $C_6H_4BrNO_2^-$ | | | | | | |
| oBr-nitrobenzene⁻· | | | | *Est2* | *$\Delta_f H(A)$= 92±8* | |
| • -21±18 [b] | 1.17±0.10 | | | TDEq | | 87KEB/CHO |
| $C_6H_4BrNO_2^-$ | | | | | | |
| pBr-nitrobenzene⁻· | | | | *Est* | *$\Delta_f H(A)$= 90±4* | |
| • -35±14 [b] | 1.29±0.10 | | | TDEq | | 87KEB/CHO |
| $C_6H_4Cl^-$ | | | | | *$\Delta_f H(AH)$= 54±1* | *85PLA/SIM* |
| chlorophenide⁻ | | | | | *BDE(A-H)= 460±13* | |
| 144±24 [a] | 1.6±0.4 [d] | 1620±23 [g] | 1586±21 | IMRB | | 79BAR/MCI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_4ClF_2^-$ | | | | | | |
| m-$C_6H_4F_2\cdot\cdot Cl^-$ | | | | | | |
| • −598±11 [c] | | *61±8* [g] | *33±8* | IMRE | | 84LAR/MCM2 |
| | | | *32±4* | TDEq | | 82FRE/IKU |
| $C_6H_4ClF_2^-$ | | | | | | |
| o-$C_6H_4F_2\cdot\cdot Cl^-$ | | | | | | |
| • −581±11 [c] | | *60±8* [g] | *33±8* | IMRE | | 84LAR/MCM2 |
| $C_6H_4ClF_2^-$ | | | | | | |
| p-$C_6H_4F_2\cdot\cdot Cl^-$ | | | | | | |
| • −592±11 [c] | | *58±8* [g] | *31±8* | IMRE | | 84LAR/MCM2 |
| $C_6H_4ClNO_2^-$ | | | | | | |
| mCl-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 38±8* | |
| • −85±18 [b] | 1.28±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.22±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.20±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4ClNO_2^-$ | | | | | | |
| oCl-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 42±4* | |
| • −68±14 [b] | 1.14±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.08±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.05±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4ClNO_2^-$ | | | | | | |
| pCl-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 38±8* | |
| • −84±18 [b] | 1.26±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.19±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.17±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4ClO^-$ | | | | | *$\Delta_f H(AH)$= −146±8* | *77PED/RYL* |
| mCl-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −245±29 [a] | 2.52±0.30 [d] | 1431±21 [g] | 1402±8 | IMRE | | 81FUJ/MCI |
| | | 1433±21 [g] | 1404±8 | IMRE | | 77MCM/KEB |
| $C_6H_4ClO^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −173±17* | |
| oCl-phenoxide$^-$ | | | | | *BDE(A−H)= 402±17* | |
| • −266±30 [a] | 2.87±0.31 [d] | 1437±13 [g] | 1410±8 | IMRE | | 77MCM/KEB |
| • | <2.58±0.08 | | | PD | | 75RIC/STE2 |
| $C_6H_4ClO^-$ | | | | | *$\Delta_f H(AH)$= −153±8* | *77PED/RYL* |
| pCl-phenoxide$^-$ | | | | | *BDE(A−H)= 362±13* | |
| • −248±18 [a] | 2.47±0.23 [d] | 1436±10 [g] | 1407±8 | IMRE | | 81FUJ/MCI |
| | | 1438±10 [g] | 1409±8 | IMRE | | 77MCM/KEB |
| $C_6H_4Cl_2^-$ | | | | | | |
| o-dichlorobenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 33±2* | *85PLA/SIM* |
| 24 [b] | 9.4 | | | ECD | | 69STE/WEN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_4F^-$ | | | | | $\Delta_f H(AH)$= -116±1 | 77PED/RYL |
| fluorophenide$^-$ | | | | | BDE(A-H)= 460±13 | |
| -26±26 [a] | 1.6±0.4 [d] | 1620±25 [g] | 1586±22 | IMRB | | 75BRI/RIV |
| $C_6H_4FNO_2^-$ | | | | | | |
| mF-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -126±8 | |
| • · -245±18 [b] | 1.23±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.18±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.15±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4FNO_2^-$ | | | | | | |
| oF-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -118±8 | |
| • -221±18 [b] | 1.07±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.02±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.04±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4FNO_2^-$ | | | | | | |
| pF-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -131±8 | |
| • -239±18 [b] | 1.12±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.05±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.04±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4FO^-$ | | | | Est | $\Delta_f H(AH)$= -297±8 | |
| mF-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • -389±18 [a] | 2.45±0.19 [d] | 1438±10 [g] | 1409±8 | IMRE | | 81FUJ/MCI |
| | | 1441±10 [g] | 1413±8 | IMRE | | 77MCM/KEB |
| | 2.61±0.09 | 1422±17 [e] | 1393±18 [h] | ECD | | 84HER/WEN |
| $C_6H_4FO^-$ | | | | Est2 | $\Delta_f H(AH)$= -285 | |
| oF-phenoxide$^-$ | | | | | | |
| • | | 1445±12 [g] | 1418±8 | IMRE | | 81FUJ/MCI |
| | | 1447±12 [g] | 1420±8 | IMRE | | 77MCM/KEB |
| $C_6H_4FO^-$ | | | | Est | $\Delta_f H(AH)$= -291±8 | |
| pF-phenoxide$^-$ | | | | | BDE(A-H)= 362±13 | |
| • -370±18 [a] | 2.31±0.23 [d] | 1451±10 [g] | 1422±8 | IMRE | | 81FUJ/MCI |
| | | 1455±10 [g] | 1426±8 | IMRE | | 77MCM/KEB |
| $C_6H_4F_2N^-$ | | | | Est | $\Delta_f H(AH)$= -478±13 | |
| 2,4-diF-anilide$^-$ | | | | | | |
| • -497±25 [a] | | 1510±12 [g] | 1480±8 | IMRE | | 79BAR/SCO |
| | | | 1480±8 | IMRE [o] | | 79BAR/SCO |
| $C_6H_4NO_2^-$ | | | | Est | $\Delta_f H(AH)$= -91±8 | |
| pNO-phenoxide$^-$ | | | | | | |
| • -246±19 [a] | | 1376±11 [g] | 1345±8 | IMRE | | 86TAF |
| $C_6H_4NO_3^-$ | | | | Est | $\Delta_f H(AH)$= -113±8 | |
| $mNO_2$-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • -244±19 [a] | 2.85±0.20 [d] | 1399±11 [g] | 1370±8 | IMRE | | 81FUJ/MCI |
| | | 1400±11 [g] | 1371±8 | IMRE | | 77MCM/KEB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / *$\Delta H_{aff}(X\cdot\cdot Y^-)$* | $\Delta G_{acid}(AH)$ / *$\Delta G_{aff}(X\cdot\cdot Y^-)$* | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_6H_4NO_3^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −105±13* | |
| $oNO_2$-phenoxide$^-$ | | | | | | | |
| * | | | | 1379±8 | IMRE | | 77MCM/KEB |
| $C_6H_4NO_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −117±8* | |
| $pNO_2$-phenoxide$^-$ | | | | | | | |
| * | −276±19 [a] | | 1372±11 [g] | 1343±8 | IMRE | | 81FUJ/MCI |
| $C_6H_4N_2O_4^-$ | | | | | | | |
| $mNO_2$-nitrobenzene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 59±1* | *76FER/PIA* |
| * | −101±11 [b] | 1.65±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.57±0.11 | | | IMRE | | 85GRI/CAL |
| | −93±5 [b] | 1.57±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4N_2O_4^-$ | | | | | | | |
| $oNO_2$-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 84±8* | |
| * | −76±18 [b] | 1.65±0.10 | | | TDEq | | 87KEB/CHO |
| $C_6H_4N_2O_4^-$ | | | | | | | |
| $pNO_2$-nitrobenzene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 57±3* | *76FER/PIA* |
| * | −136±13 [b] | 2.00±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.89±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.89±0.05 | | | IMRE | | 85FUK/MCI |
| $C_6H_4N_3^-$ | | | | | | | |
| benzotriazolide$^-$ | | | | | | | |
| * | | | 1413±11 [g] | 1382±8 | IMRE | | 86TAF |
| $C_6H_4O_2^-$ | | | | | | | |
| o-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −121±21* | |
| * | | 1.620±0.048 | | | LPD | | 85MAR/COM |
| $C_6H_4O_2^-$ | | | | | | | |
| p-benzoquinone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −123±3* | *77PED/RYL* |
| * | −307±13 [b] | 1.91±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.81±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.990±0.048 | | | LPD | | 85MAR/COM |
| | | 1.83±0.05 | | | IMRE | | 85FUK/MCI |
| | | 1.9±0.3 | | | NBIP | | 75COO/NAF |
| | | >0.0 | | | ES | | 70COL/CHR |
| | | 1.37±0.08 | | | SI | | 66FAR/PAG |
| $C_6H_5^-$ | | | | | | *$\Delta_f H(AH)$= 83* | *77PED/RYL* |
| phenide$^-$ | | | | | | *BDE(A−H)= 464±8* | *82MCM/GOL* |
| * | 229±3 [a] | 1.03±0.11 [d] | 1677±2 | 1636±3 | TDEq | | 86MEO/SIE |
| | | | | 1632±27 | IMRB | | 79BAR/MCI |
| | 341±29 | | | | EIAP | From benzonitrile | 86HEN/ILL2 |
| | | 1.1±0.3 [d] | 1665±25 [g] | 1628±23 | IMRB | | 71BOH/YOU |
| | | 2.36±0.04 | | | SI | | 76FAI/JOY |
| | | 2.2 | | | SI | | 72PAG |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_5BrCl^-$ | | | | | | |
| $PhBr\cdot\cdot Cl^-$ | | | | | | |
| | | | *28* | TDEq | | 82FRE/IKU |
| $C_6H_5ClF^-$ | | | | | | |
| $PhF\cdot\cdot Cl^-$ | | | | | | |
| | | | *25* | TDEq | | 82FRE/IKU |
| $C_6H_5ClFO^-$ | | | | | | |
| $pF\text{–}C_6H_4OH\cdot\cdot Cl^-$ | | | | | | |
| • −629±18 [c] | | *110±8* | *81±8* | TDEq | | 77CUM/FRE |
| $C_6H_5ClI^-$ | | | | | | |
| $PhI\cdot\cdot Cl^-$ | | | | | | |
| | | | *30* | TDEq | | 82FRE/IKU |
| $C_6H_5ClN^-$ | | | | *Est* | *$\Delta_f H(AH)$= 55±8* | |
| mCl–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • 26±18 [a] | | 1502±10 [g] | 1471±8 | IMRE | | 79BAR/SCO |
| | | | 1480±8 | IMRE$^o$ | | 79BAR/SCO |
| $C_6H_5ClN^-$ | | | | *Est* | *$\Delta_f H(AH)$= 55±8* | |
| pCl–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • 33±18 [a] | | 1508±10 [g] | 1477±8 | IMRE | | 79BAR/SCO |
| | | | 1482±8 | IMRE$^o$ | | 79BAR/SCO |
| $C_6H_5ClNO_2^-$ | | | | | | |
| $PhNO_2\cdot\cdot Cl^-$ | | | | | | |
| | | | *30* | TDEq | | 82FRE/IKU |
| $C_6H_5Cl_2^-$ | | | | | | |
| $PhCl\cdot\cdot Cl^-$ | | | | | | |
| • −230±10 [c] | | *57±8* [g] | *29±8* | IMRE | | 84LAR/MCM2 |
| | | *57±4* [g] | *29±4* | IMRE | | 84LAR/MCM4 |
| | | | *27* | TDEq | | 82FRE/IKU |
| $C_6H_5Cl_2O^-$ | | | | | | |
| $pCl\text{–}C_6H_4OH\cdot\cdot Cl^-$ | | | | | | |
| • −498±18 [c] | | *118±8* | *87±8* | TDEq | | 77CUM/FRE |
| $C_6H_5FN^-$ | | | | *Est* | *$\Delta_f H(AH)$= −113±8* | |
| mF–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • −132±19 [a] | | 1511±11 [g] | 1481±8 | IMRE | | 79BAR/SCO |
| | | | 1489±8 | IMRE$^o$ | | 79BAR/SCO |
| $C_6H_5FN^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −130±17* | |
| oF–anilide$^-$ | | | | | *BDE(A–H)= 389±17* | |
| • −143±29 [a] | 1.91±0.30 [d] | 1517±12 [g] | 1487±8 | IMRE | | 79BAR/SCO |
| | | | 1495±8 | IMRE$^o$ | | 79BAR/SCO |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_6H_5FN^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −109±8* | |
| pF–anilide$^-$ | | | | | | *BDE(A–H)= 368±13* | |
| • | −115±19 [a] | 1.62±0.24 [d] | 1524±11 [g] | 1494±8 | IMRE | | 79BAR/SCO |
| | | | | 1499±8 | IMRE[o] | | 79BAR/SCO |
| $C_6H_5F_5NS^-$ | | | | | | | |
| mSF$_5$–anilide$^-$ | | | | | | *BDE(A–H)= 368±13* | |
| • | | 2.76±0.24 [d] | 1414±11 [g] | 1383±8 | IMRE | | 86TAF |
| $C_6H_5F_5NS^-$ | | | | | | | |
| pSF$_5$–anilide$^-$ | | | | | | *BDE(A–H)= 368±13* | |
| • | | 2.92±0.24 [d] | 1399±11 [g] | 1368±8 | IMRE | | 86TAF |
| $C_6H_5N^-$ | | | | | | | |
| PhN$^{-\cdot}$ | | | | | | | |
| • | 263±26 [a] | | 1556±16 [g] | 1527±13 | IMRB | Acidity near MeCN | 81MCD/CHO |
| • | | 1.461±0.013 | | | LPD | | 84DRZ/BRA |
| | | | | 1532±13 | IMRB[o] | | 81MCD/CHO |
| $C_6H_5NO_2^-$ | | | | | | | |
| nitrobenzene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 67±1* | *77PED/RYL* |
| • | −30±11 [b] | 1.01±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.96±0.11 | | | IMRE | | 85GRI/CAL |
| | | 0.97±0.05 | | | IMRE | | 85FUK/MCI |
| | | >0.7±0.2 | | | EnCT | | 73LIF/TIE |
| | | >0.4 | | | ES | | 66COM/CHR |
| | | <1.1 | | | IMRB | EA: < $SO_2$ | 59HEN/MUC |
| $C_6H_5N_2O^-$ | | | | | | | |
| PhN=NO$^-$ | | | | | | | |
| | <308±25 | | | | IMRB | $Ph^-$ + $N_2O$ →; thermochemical limit | 77BIE/DEP |
| $C_6H_5N_2O_2^-$ | | | | | | *$\Delta_f H(AH)$= 62±2* | *83NIS/SAK* |
| mNO$_2$–anilide$^-$ | | | | | | *BDE(A–H)= 368±13* | |
| • | 6±13 [a] | 2.14±0.24 [d] | 1474±11 [g] | 1443±8 | IMRE | | 86TAF |
| $C_6H_5N_2O_2^-$ | | | | | | *$\Delta_f H(AH)$= 55±2* | *83NIS/SAK* |
| pNO$_2$–anilide$^-$ | | | | | | | |
| • | −38±13 [a] | | 1437±11 [g] | 1407±8 | IMRE | | 86TAF |
| $C_6H_5O^-$ | | | | | | *$\Delta_f H(AH)$= −96±1* | *77PED/RYL* |
| phenoxide$^-$ | | | | | | *BDE(A–H)= 362±8* | *82MCM/GOL* |
| • | −165±10 [a] | 2.21±0.19 [d] | 1461±10 [g] | 1432±8 | IMRE | | 81FUJ/MCI |
| • | | <2.36±0.06 | | | PD | | 75RIC/STE2 |
| | | | 1466±10 [g] | 1437±8 | IMRE | | 78CUM/KEB |
| | | | | 86SHI/VOR: tautomer acidities $\Delta_{acid}H$(ortho) = 1439±13 kJ, (para) = 1423±8 kJ | | | |
| | | | | 1441±8 | IMRE[o] | | 79BAR/SCO |
| $C_6H_5O_2^-$ | | | | | | *$\Delta_f H(AH)$= −274±2* | *79KUD/KUD* |
| mOH–phenoxide$^-$ | | | | | | *BDE(A–H)= 362±8* | |
| • | −354±13 [a] | 2.32±0.20 [d] | 1451±11 [g] | 1422±8 | IMRE | | 81FUJ/MCI |
| | | | 1444±11 [g] | 1415±8 | IMRE | | 77MCM/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_5O_2^-$ | | | | | *$\Delta_f H(AH)$= −272±4* | *79KUD/KUD* |
| oOH-phenoxide$^-$ | | | | | | |
| • | | 1421±11 [g] | 1392±8 | IMRE | | 81FUJ/MCI |
| | | 1422±11 [g] | 1393±8 | IMRE | | 77MCM/KEB |
| $C_6H_5O_2^-$ | | | | | *$\Delta_f H(AH)$= −264±2* | *79KUD/KUD* |
| pOH-phenoxide$^-$ | | | | | | |
| • −328±13 [a] | | 1466±11 [g] | 1436±8 | IMRE | | 81FUJ/MCI |
| $C_6H_5S^-$ | | | | | *$\Delta_f H(AH)$= 113±1* | *77PED/RYL* |
| thiophenoxide$^-$ | | | | | *BDE(A−H)= 335±9* | *82MCM/GOL* |
| • | <2.47±0.06 | >1409±15 [e] | | PD | | 75RIC/STE2 |
| $C_6H_6Cl^-$ | | | | | | |
| $C_6H_6\cdot\cdot Cl^-$ | | | | | | |
| • | | *41* [g] | *20±8* | IMRE | | 84LAR/MCM2 |
| | | | *16* | TDEq | | 82FRE/IKU |
| $C_6H_6ClO^-$ | | | | | | |
| PhOH··Cl$^-$ | | | | | | |
| −432 [c] | | *109* | *72* | TDAs | | 82FRE/IKU |
| −426±10 [c] | | *103±8* | *83±8* | TDEq | | 77CUM/FRE |
| | | *81±8* | *62±8* | TDAs | | 71YAM/KEB |
| $C_6H_6FO^-$ | | | | | | |
| PhOH··F$^-$ | | | | | | |
| • −518±11 [c] | | *173±8* [g] | *140±8* | IMRE | | 83LAR/MCM |
| $C_6H_6N^-$ | | | | | *$\Delta_f H(AH)$= 87±1* | *77PED/RYL* |
| anilide$^-$ | | | | | *BDE(A−H)= 368±8* | *82MCM/GOL* |
| • 90±12 [a] | 1.53±0.20 [d] | 1533±11 [g] | 1502±8 | IMRE | | 79BAR/SCO |
| • | 1.704±0.030 | | | LPD | | 84DRZ/BRA2 |
| | | | 1505±8 | IMRE [o] | | 79BAR/SCO |
| $C_6H_6NO^-$ | | | | | *$\Delta_f H(AH)$= −90±2* | *86NUN/BAR* |
| mNH$_2$-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −153±11 [a] | 2.15±0.19 [d] | 1467±10 [g] | 1438±8 | IMRE | | 81FUJ/MCI |
| | | 1469±10 [g] | 1441±8 | IMRE | | 77MCM/KEB |
| $C_6H_6NO^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −105±17* | |
| oNH$_2$-phenoxide$^-$ | | | | | *BDE(A−H)= 391±17* | |
| • | | | 1428±8 | IMRE | | 77MCM/KEB |
| $C_6H_6NO^-$ | | | | | *$\Delta_f H(AH)$= −82±2* | *86NUN/BAR* |
| pNH$_2$-phenoxide$^-$ | | | | | *BDE(A−H)= 368±13* | |
| • −137±11 [a] | | 1475±10 [g] | 1446±8 | IMRE | | 81FUJ/MCI |
| | | 1483±10 [g] | 1454±8 | IMRE | | 77MCM/KEB |
| $C_6H_6N_2O_2^-$ | | | | | | |
| mNH$_2$-nitrobenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 59±1* | *77PED/RYL* |
| • −33±11 [b] | 0.95±0.10 | | | TDEq | | 87KEB/CHO |

Table 2. Negative Ion Table - Continued

| Ion<br>$\Delta_f H(A^-)$<br>$\Delta_f H(X\cdot\cdot Y^-)$ | EA(A)<br>eV | $\Delta H_{acid}(AH)$<br>$\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$<br>$\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_7^-$ | | | | | *$\Delta_f H(AH)$= 106* | *77PED/RYL* |
| 1,3-cyclohexadienide$^-$ | | | | | *BDE(A-H)= 305±21* | *82MCM/GOL* |
| 138±21 [a] | 0.6±0.4 [d] | 1562±21 [g] | 1531±17 | IMRB | Between $SiH_4$, tBuOH | 86LEE/SQU |
| 134±75 | | | | IMRB | | 78DEP/BIE |
| $C_6H_7^-$ | | | | *Est* | *$\Delta_f H(AH)$= 96±4* | |
| 1-methylcyclopentadienide$^-$ | | | | | | |
| • | 1.670±0.039 | | | LPD | | 73RIC/STE |
| $C_6H_7FN^-$ | | | | | | |
| $PhNH_2\cdot\cdot F^-$ | | | | | | |
| • -292±11 [c] | | *131±8* [g] | *98±8* | IMRE | | 83LAR/MCM |
| $C_6H_7O^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -116±13* | |
| cyclohexenone-4-enolate$^-$ | | | | | | |
| • -150±22 [a] | | 1496±10 [g] | 1464±8 | IMRE | | 86BAR/KIP |
| | | | 1473±8 | IMRE° | | 86BAR/KIP |
| $C_6H_7O_2^-$ | | | | | | |
| $HOH\cdot\cdot PhO^-$ | | | | | | |
| -471±14 [c] | | *64±4* | *34±7* | TDAs | | 86MEO/SIE2 |
| $C_6H_8B^-$ | | | | *Est* | *$\Delta_f H(AH)$= 146±13* | |
| $MeB(CH=CH)_2CH^-$ | | | | | | |
| 17±31 [a] | | 1402±18 [g] | 1370±17 | IMRB | Acid: 3-methyl-3-bora-1,4-cyclohexadiene | 77SUL |
| $C_6H_9^-$ | | | | | *$\Delta_f H(AH)$= -5* | *77PED/RYL* |
| cyclohexenide$^-$ | | | | | | |
| 82±25 [a] | | 1617±25 [g] | 1586±21 | IMRB | | 86LEE/SQU |
| $C_6H_9^-$ | | | | | *$\Delta_f H(AH)$= 106±3* | *77KUP/SHI* |
| tBuC≡C$^-$ | | | | | *BDE(A-H)= 552±21* | |
| • 157±15 [a] | 2.93±0.34 [d] | 1582±12 [g] | 1549±8 | IMRE | | 79BAR/SCO |
| | | | 1544±8 | IMRE° | | 79BAR/SCO |
| $C_6H_9O^-$ | | | | | *$\Delta_f H(AH)$= -226±2* | *77PED/RYL* |
| cyclohexanone enolate$^-$ | | | | | | |
| • | 1.55±0.05 | | | PD | | 78ZIM/JAC |
| $C_6H_{11}^-$ | | | | | *$\Delta_f H(AH)$= -123* | *77PED/RYL* |
| cyclohexanide$^-$ | | | | | *BDE(A-H)= 400±4* | *82MCM/GOL* |
| >37±4 [a] | | 1690±4 [g] | >1665 | IMRB | | 72BOH/LEE |
| $C_6H_{11}O^-$ | | | | | *$\Delta_f H(AH)$= -290±1* | *77PED/RYL* |
| $CH_2=C(tBu)O^-$ | | | | | *BDE(A-H)= 406±8* | |
| • -280±15 [a] | 1.84±0.07 | 1540±15 [e] | 1512±18 [h] | PD | | 77ZIM/REE |
| $C_6H_{11}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -269±2* | |
| tBuCH=CHO$^-$ | | | | | *BDE(A-H)= 381±13* | |
| • -282±21 [a] | 1.82±0.06 | 1517±18 [e] | 1490±23 [h] | PD | | 77ZIM/REE |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X \cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{afl}(X \cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{afl}(X \cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_6H_{11}O_2^-$ | | | | | *$\Delta_f H(AH)$= -514±2* | *77PED/RYL* |
| $nPnCO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -597±11 [a] | 3.2±0.2 [d] | 1447±10 | 1418±12 [h] | CIDC | | 81MCL/CAM |
| $C_6H_{11}O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -538±4* | |
| $tBuCH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| •• -623±15 [a] | | 1444±11 [g] | 1415±8 | IMRE | | 86TAF |
| $C_6H_{11}S_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -59±17* | |
| 5,5-dimethyl-1,3-dithianide$^-$ | | | | | | |
| • -24±28 [a] | | 1566±11 [g] | 1535±8 | IMRE | | 81BAR/HAY |
| | | | 1530±8 | IMRE[o] | | 81BAR/HAY |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -356±4* | |
| $Et_2C(Me)O^-$ | | | | | *BDE(A-H)= 440±4* | |
| • -330±15 [a] | 2.0±0.2 [d] | 1556±11 | 1528±13 [h] | CIDC | | 83BOA/HOU |
| | | 1553±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -342±4* | |
| $iPrCH(Et)O^-$ | | | | | *BDE(A-H)= 438±4* | |
| • -318±15 [a] | 2.0±0.2 [d] | 1554±11 | 1527±13 [h] | CIDC | | 83BOA/HOU |
| | | 1551±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -327±4* | |
| $iPrCH_2CH_2CH_2O^-$ | | | | | *BDE(A-H)= 436±4* | |
| • -296±14 [a] | 1.9±0.1 [d] | 1561±10 | 1533±11 [h] | CIDC | | 83BOA/HOU |
| | | 1557±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O^-$ | | | | | *$\Delta_f H(AH)$= -315±1* | *77PED/RYL* |
| $nC_6H_{13}O^-$ | | | | | *BDE(A-H)= 436±4* | |
| • -284±12 [a] | 1.9±0.2 [d] | 1561±11 | 1533±13 [h] | CIDC | | 83BOA/HOU |
| | | 1557±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -352±4* | |
| $nPrC(Me)_2O^-$ | | | | | *BDE(A-H)= 440±4* | |
| • -326±15 [a] | 2.0±0.2 [d] | 1557±11 | 1529±13 [h] | CIDC | | 83BOA/HOU |
| | | 1554±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -351±4* | |
| $tBuCH(Me)O^-$ | | | | | *BDE(A-H)= 438±4* | |
| • -328±16 [a] | 2.05±0.17 [d] | 1553±12 [g] | 1525±8 | IMRE | | 79BAR/SCO |
| | | | 1523±8 | IMRE[o] | | 79BAR/SCO |
| $C_6H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -332±4* | |
| $tBuCH_2CH_2O^-$ | | | | | *BDE(A-H)= 436±4* | |
| • -304±15 [a] | 2.0±0.2 [d] | 1559±11 | 1531±13 [h] | CIDC | | 83BOA/HOU |
| | | 1555±10 | | CIDC[o] | | 83BOA/HOU |
| $C_6H_{13}O_2^-$ | | | | | | |
| $nPrOH \cdot\cdot CH_2{=}C(Me)O^-$ | | | | | | |
| -518±23 [c] | | *61±10* [g] | *33±8* | IMRE | | 84CAL/ROZ |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$C_6H_{14}BF_2^-$** | | | | | | |
| $iPr_2BF\cdot\cdot F^-$ | | | | | | |
| $<-817$[c] | | *278* | | IMRB | $F^-A$: $SiF_4 > iPr_2BF > iPr_3B$ | 77MUR/BEA2 |
| **$C_6H_{15}BCl^-$** | | | | | | |
| $Et_3B\cdot\cdot Cl^-$ | | | | | | |
| • $-476\pm15$[c] | | *100±8*[g] | *72±8* | IMRE | | 85LAR/MCM |
| **$C_6H_{15}BF^-$** | | | | | | |
| $Et_3B\cdot\cdot F^-$ | | | | | | |
| • $-611\pm16$[c] | | *213±8*[g] | *182±8* | IMRE | | 85LAR/MCM |
| | | *259* | | IMRB | $F^-A$: $iPr_3B > Et_3B > MeSiF_3$ | 77MUR/BEA2 |
| **$C_6H_{15}BFO_3^-$** | | | | | | |
| $(EtO)_3B\cdot\cdot F^-$ | | | | | | |
| • $-1434\pm17$[c] | | *184±13*[g] | *153±8* | IMRB | | 85LAR/MCM |
| **$C_6H_{15}OSi^-$** | | | | *Est2* | *$\Delta_f H(AH)= -559\pm8$* | |
| $Et_3SiO^-$ | | | | | | |
| $-580\pm19$[a] | | 1508±11[g] | 1479±8 | IMRE | | 87THO/BAR |
| **$C_6H_{15}O_2^-$** | | | | | | |
| $EtOH\cdot\cdot tBuO^-$ | | | | | | |
| $-592\pm23$[c] | | *82±10*[g] | *54±8* | IMRE | | 84CAL/ROZ |
| **$C_6H_{15}O_2^-$** | | | | | | |
| $MeOH\cdot\cdot tBuCH_2O^-$ | | | | | | |
| $-569\pm25$[c] | | *78±10*[g] | *50±8* | IMRE | | 84CAL/ROZ |
| **$C_6H_{15}O_2^-$** | | | | | | |
| $nPrOH\cdot\cdot nPrO^-$ | | | | | | |
| $-554\pm21$[c] | | *88±10*[g] | *60±8* | IMRE | | 84CAL/ROZ |
| **$C_6H_{17}Si^-$** | | | | | | |
| $Et_3SiH\cdot\cdot H^-$ | | | | | | |
| $-98$[c] | | *43±23* | | IMRB | | 86HAJ/SQU |
| **$C_6H_{18}NSi_2^-$** | | | | | *$\Delta_f H(AH)= -477\pm6$* | *77PED/RYL* |
| $(Me_3Si)_2N^-$ | | | | | *BDE(A-H)= >421* | *78ROB/WIN* |
| $-497\pm15$[a] | 2.32[d] | 1509±10[g] | 1477±8 | IMRE | | 87THO/BAR |
| **$C_7F_5N^-$** | | | | | | |
| $C_6F_5CN^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)= -746\pm13$* | |
| • $-852\pm22$[b] | 1.10±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.10±0.10 | | | TDEq | | 86CHO/GRI |
| **$C_7F_8^-$** | | | | | | |
| perfluorotoluene$^{-\cdot}$ | | | | | *$\Delta_f H(A)= -1187\pm8$* | *77PED/RYL* |
| • $-1278\pm17$[b] | 0.94±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.91±0.10 | | | IMRE | | 86CHO/GRI |
| | >1.7±0.3 | | | EnCT | | 73LIF/TIE |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7F_{13}^-$ | | | | *Est* | *$\Delta_f H(AH)$= -2705±21* | |
| perfluoromethylcyclohexanide$^-$ | | | | | | |
| -3063 [b] | 3.9 | | | EIAP | From c-$C_6F_{11}(CF_3)$ | 70LIF/PEE |
| $C_7F_{14}^-$ | | | | | | |
| perfluoromethylcyclohexane$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -2900±1* | *77PED/RYL* |
| • -3002±11 [b] | 1.06±0.10 | | | TDEq | | 85GRI/CHO |
| | <1.6 | | | IMRB | | 85GRI/CAL |
| $C_7H_3Cl_2N^-$ | | | | | | |
| 2,6-diCl-benzonitrile$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= 156±13* | |
| • 87±22 [b] | 0.72±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.70±0.09 | | | TDEq | | 86CHO/KEB |
| $C_7H_3Cl_3O_2^-$ | | | | | | |
| Me-triCl-benzoquinone$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -212±17* | |
| • -449±21 [b] | 2.46±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_3F_5O^-$ | | | | | | |
| pentafluoroanisole$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -937±8* | |
| -990±17 [b] | 0.54±0.09 | | | ECD | | 84HER/WEN |
| $C_7H_3N_3O_4^-$ | | | | | | |
| 3-$NO_2$-5-CN-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 188±4* | |
| • -20±14 [b] | 2.16±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_4ClO_2^-$ | | | | | *$\Delta_f H(AH)$= -342±4* | *77PED/RYL* |
| mCl-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -473±15 [a] | 3.69±0.24 [d] | 1400±11 [g] | 1368±8 | IMRE | | 77MCM/KEB |
| $C_7H_4ClO_2^-$ | | | | | *$\Delta_f H(AH)$= -325±3* | *77PED/RYL* |
| oCl-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -454±14 [a] | 3.67±0.24 [d] | 1401±11 [g] | 1372±8 | IMRE | | 77MCM/KEB |
| $C_7H_4ClO_2^-$ | | | | | *$\Delta_f H(AH)$= -341±3* | *77PED/RYL* |
| pCl-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -472±14 [a] | 3.69±0.24 [d] | 1399±11 [g] | 1369±8 | IMRE | | 77MCM/KEB |
| $C_7H_4FO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -490±4* | |
| mF-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -617±15 [a] | 3.65±0.24 [d] | 1403±11 [g] | 1372±8 | IMRE | | 77MCM/KEB |
| $C_7H_4FO_2^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -502±13* | |
| oF-benzoate$^-$ | | | | | *BDE(A-H)= 460±17* | |
| • -623±25 [a] | 3.76±0.30 [d] | 1410±12 [g] | 1378±8 | IMRE | | 77MCM/KEB |
| $C_7H_4FO_2^-$ | | | | | *$\Delta_f H(AH)$= -495±3* | *77PED/RYL* |
| pF-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -620±14 [a] | 3.63±0.24 [d] | 1405±11 [g] | 1376±8 | IMRE | | 77MCM/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_4F_3^-$ | | | | | $\Delta_f H(AH)$= -599±1 | 77PED/RYL |
| $CF_3$-phenide$^-$ | | | | | BDE(A-H)= 460±13 | |
| -511±24 [a] | 1.6±0.4 [d] | 1618±23 [g] | 1586±21 | IMRB | | 79BAR/MCI |
| $C_7H_4F_3NO_2^-$ | | | | | | |
| m$CF_3$-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -604±8 | |
| • -740±18 [b] | 1.41±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.34±0.11 | | | IMRE | | 85GRI/CAL |
| | 1.33±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_4F_3NO_2^-$ | | | | | | |
| o$CF_3$-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -604±4 | |
| • -732±14 [b] | 1.33±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_4F_3NO_2^-$ | | | | | | |
| p$CF_3$-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -604±4 | |
| • -746±14 [b] | 1.47±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_4F_3O^-$ | | | | Est | $\Delta_f H(AH)$= -765±8 | |
| m$CF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • -875±18 [a] | 2.64±0.19 [d] | 1420±10 [g] | 1391±8 | IMRE | | 81FUJ/MCI |
| $C_7H_4F_3O^-$ | | | | Est | $\Delta_f H(AH)$= -765±8 | |
| p$CF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±13 | |
| • -885±19 [a] | 2.74±0.24 [d] | 1410±11 [g] | 1381±8 | IMRE | | 81FUJ/MCI |
| $C_7H_4F_3OS^-$ | | | | | | |
| m$SCF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • | 2.72±0.20 [d] | 1411±11 [g] | 1382±8 | IMRE | | 86TAF |
| $C_7H_4F_3OS^-$ | | | | | | |
| p$SCF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±13 | |
| • | 2.81±0.23 [d] | 1403±10 [g] | 1374±8 | IMRE | | 86TAF |
| $C_7H_4F_3O_3S^-$ | | | | | | |
| m$SO_2CF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • | 3.06±0.20 [d] | 1379±11 [g] | 1350±8 | IMRE | | 86TAF |
| $C_7H_4F_3O_3S^-$ | | | | | | |
| p$SO_2CF_3$-phenoxide$^-$ | | | | | BDE(A-H)= 362±13 | |
| • | 3.36±0.24 [d] | 1350±11 [g] | 1321±8 | IMRE | | 86TAF |
| $C_7H_4F_4O^-$ | | | | | | |
| 2,3,5,6-tetrafluoroanisole$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= -845±4 | |
| -866±13 [b] | 0.22±0.09 | | | ECD | | 84HER/WEN |
| $C_7H_4NO^-$ | | | | Est | $\Delta_f H(AH)$= 43±8 | |
| mCN-phenoxide$^-$ | | | | | BDE(A-H)= 362±8 | |
| • -82±18 [a] | 2.79±0.19 [d] | 1405±10 [g] | 1376±8 | IMRE | | 81FUJ/MCI |
| | | 1405±10 [g] | 1377±8 | IMRE | | 77MCM/KEB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_7H_4NO^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 25±13* | |
| oCN-phenoxide$^-$ | | | | | | *BDE(A-H)= 378±17* | |
| • | -105±25 [a] | 3.00±0.30 [d] | 1400±12 [g] | 1369±8 | IMRE | | 81FUJ/MCI |
| | | | 1400±12 [g] | 1369±8 | IMRE | | 77MCM/KEB |
| $C_7\dot{H}_4NO^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 43±8* | |
| pCN-phenoxide$^-$ | | | | | | | |
| • | -97±19 [a] | | 1390±11 [g] | 1361±8 | IMRE | | 81FUJ/MCI |
| | | | 1392±11 [g] | 1363±8 | IMRE | | 77MCM/KEB |
| $C_7H_4NO_4^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -310±8* | |
| $mNO_2$-benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | -458±19 [a] | 3.88±0.24 [d] | 1382±11 [g] | 1350±8 | IMRE | | 77MCM/KEB |
| | | | 1379±11 [g] | 1347±8 | IMRE | | 86TAF |
| $C_7H_4N_2O_2^-$ | | | | | | | |
| mCN-nitrobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 204±8* | |
| • | 53±18 [b] | 1.56±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.48±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.49±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_4N_2O_2^-$ | | | | | | | |
| oCN-nitrobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 204±4* | |
| • | 48±14 [b] | 1.61±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_4N_2O_2^-$ | | | | | | | |
| pCN-nitrobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 202±4* | |
| • | 36±14 [b] | 1.72±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.65±0.11 | | | IMRE | | 85GRI/CAL |
| $C_7H_4N_3O_6^-$ | | | | | | *$\Delta_f H(AH)$= 39±2* | *77PEL* |
| 2,4,6-tri$NO_2$-$C_6H_2CH_2^-$ | | | | | | | |
| | -112±27 [a] | | 1379±25 [g] | 1351±21 | IMRB | | 74DZI/CAR |
| $C_7H_5ClNO^-$ | | | | | | | |
| pCN-$C_6H_4OH\cdot\cdot Cl^-$ | | | | | | | |
| | | | *141±8* | *109±8* | TDEq | | 77CUM/FRE |
| $C_7H_5ClO_2^-$ | | | | | | | |
| 2-Cl-5-Me-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -180±17* | |
| • | -375±21 [b] | 2.02±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_5FO^-$ | | | | | | | |
| mF-benzaldehyde$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -230±8* | |
| | -295±13 [b] | 0.67±0.05 | | | ECD | | 75WEN/KAO |
| $C_7H_5FO^-$ | | | | | | | |
| oF-benzaldehyde$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -230±21* | |
| | -292±25 [b] | 0.64±0.04 | | | ECD | | 75WEN/KAO |

Table 2. Negative Ion Table – Continued

| Ion $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_5FO^-$ | | | | | | |
| pF–benzaldehyde$^{-\cdot}$ | | | | *Est* | *$\Delta_fH(A)$= −226±8* | |
| −273±10 [b] | 0.49±0.02 | | | ECD | | 75WEN/KAO |
| $C_7H_5F_3N^-$ | | | | *Est* | *$\Delta_fH(AH)$= −585±8* | |
| m$CF_3$–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • −621±18 [a] | | 1493±10 [g] | 1463±8 | IMRE | | 79BAR/SCO |
| | | | 1472±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_5F_3N^-$ | | | | *Est* | *$\Delta_fH(AH)$= −585±10* | |
| p$CF_3$–anilide$^-$ | | | | | | |
| • −636±19 [a] | | 1479±10 [g] | 1448±8 | IMRE | | 79BAR/SCO |
| | | | 1457±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_5F_3NO_2S^-$ | | | | | | |
| m$SO_2CF_3$–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • | 2.37±0.24 [d] | 1451±11 [g] | 1421±8 | IMRE | | 86TAF |
| $C_7H_5F_3NO_2S^-$ | | | | | | |
| p$SO_2CF_3$–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • | 2.73±0.24 [d] | 1417±11 [g] | 1386±8 | IMRE | | 86TAF |
| $C_7H_5F_3NS^-$ | | | | | | |
| m$SCF_3$–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • | 2.01±0.24 [d] | 1487±11 [g] | 1456±8 | IMRE | | 86TAF |
| $C_7H_5F_3NS^-$ | | | | | | |
| p$SCF_3$–anilide$^-$ | | | | | *BDE(A–H)= 368±13* | |
| • | 2.19±0.24 [d] | 1469±11 [g] | 1438±8 | IMRE | | 86TAF |
| $C_7H_5N^-$ | | | | | | |
| benzonitrile$^{-\cdot}$ | | | | | *$\Delta_fH(A)$= 219±2* | *82CHU/NGU* |
| 194±4 [b] | 0.26±0.02 | | | ECD | | 75WEN/KAO |
| | 0.3±0.1 | | | ECD | | 83ZLA/LEE |
| $C_7H_5NO_3^-$ | | | | | | |
| mCHO–nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_fH(A)$= −52±4* | |
| • −188±14 [b] | 1.41±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_5NO_3^-$ | | | | | | |
| oCHO–nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_fH(A)$= −52±4* | |
| • −198±14 [b] | 1.51±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_5NO_3^-$ | | | | | | |
| pCHO–nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_fH(A)$= −52±4* | |
| • −213±14 [b] | 1.67±0.10 | | | TDEq | | 87KEB/CHO |
| $C_7H_5N_2^-$ | | | | | | |
| indazolide$^-$ | | | | | | |
| • | | 1456±11 [g] | 1424±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_7H_5N_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 223±4* | |
| mCN-anilide$^-$ | | | | | | *BDE(A-H)= 368±13* | |
| • | 170±14 [a] | 2.11±0.23 [d] | 1477±10 [g] | 1446±8 | IMRE | | 86TAF |
| $C_7H_5N_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 216±4* | |
| pCN-anilide$^-$ | | | | | | | |
| • | 146±14 [a] | | 1460±10 [g] | 1429±8 | IMRE | | 86TAF |
| $C_7H_5O_2^-$ | | | | | | *$\Delta_f H(AH)$= −294±2* | *77PED/RYL* |
| benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | −407±14 [a] | | 1418±12 [g] | 1388±8 | IMRE | | 78CUM/KEB |
| | | | 1423±12 [g] | 1393±8 | IMRE | | 81FUJ/MCI |
| $C_7H_5O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −213±8* | |
| mCHO-phenoxide$^-$ | | | | | | *BDE(A-H)= 362±8* | |
| • | −319±18 [a] | 2.58±0.19 [d] | 1425±10 [g] | 1396±8 | IMRE | | 81FUJ/MCI |
| $C_7H_5O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −213±8* | |
| pCHO-phenoxide$^-$ | | | | | | | |
| • | −350±19 [a] | | 1393±11 [g] | 1364±8 | IMRE | | 81FUJ/MCI |
| $C_7H_5O_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −470±8* | |
| mOH-benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | −587±19 [a] | 3.54±0.24 [d] | 1414±11 [g] | 1382±8 | IMRE | | 77MCM/KEB |
| $C_7H_5O_3^-$ | | | | | | *$\Delta_f H(AH)$= −495* | *77PED/RYL* |
| oOH-benzoate$^-$ | | | | | | | |
| • | −660±13 [a] | | 1365±12 [g] | 1332±8 | IMRE | | 77MCM/KEB |
| $C_7H_5O_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −470±8* | |
| pOH-benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | −598±19 [a] | 3.66±0.24 [d] | 1402±11 [g] | 1371±8 | IMRE | | 77MCM/KEB |
| $C_7H_6Cl^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 18±8* | |
| mCl-$C_6H_4CH_2^-$ | | | | | | *BDE(A-H)= 356±8* | *80PRY* |
| • | 53±19 [a] | 1.07±0.20 [d] | 1565±11 [g] | 1535±8 | IMRE | | 83CAL/BAR |
| $C_7H_6Cl^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 18±8* | |
| pCl-$C_6H_4CH_2^-$ | | | | | | *BDE(A-H)= 360±8* | *80PRY* |
| • | 53±19 [a] | 1.11±0.20 [d] | 1565±11 [g] | 1535±8 | IMRE | | 83CAL/BAR |
| $C_7H_6F^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −150±8* | |
| mF-$C_6H_4CH_2^-$ | | | | | | *BDE(A-H)= 358±8* | |
| • | −109±19 [a] | 1.03±0.20 [d] | 1571±11 [g] | 1541±8 | IMRE | | 83CAL/BAR |
| $C_7H_6F^-$ | | | | | | *$\Delta_f H(AH)$= −148±1* | *77PED/RYL* |
| pF-$C_6H_4CH_2^-$ | | | | | | *BDE(A-H)= 360±13* | |
| • | −90±12 [a] | 0.87±0.24 [d] | 1588±11 [g] | 1558±8 | IMRE | | 83CAL/BAR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$C_7H_6FNO_2^-$** | | | | | | |
| 2-Me-4-F-nitrobenzene$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= −155±17* | |
| • −246±21 [b] | 0.95±0.05 | | | IMRE | | 85FUK/MCI |
| **$C_7H_6FO^-$** | | | | *Est* | *$\Delta_f H(AH)$= −267±8* | |
| mF-$C_6H_3$OMe$^-$ | | | | | | |
| • −208±23 [a] | | 1589±15 [g] | 1556±13 | IMRB | | 83ING/NIB |
| **$C_7H_6FO^-$** | | | | *Est* | *$\Delta_f H(AH)$= −264±8* | |
| oF-$C_6H_3$OMe$^-$ | | | | | | |
| −175±32 [a] | | 1618±23 [g] | 1586±21 | IMRB | | 83ING/NIB |
| **$C_7H_6FO^-$** | | | | *Est* | *$\Delta_f H(AH)$= −267±8* | |
| pF-$C_6H_3$OMe$^-$ | | | | | | |
| −178±32 [a] | | 1618±23 [g] | 1586±21 | IMRB | | 83ING/NIB |
| **$C_7H_6NO^-$** | | | | | *$\Delta_f H(AH)$= −101±13* | *82TOR/SAB2* |
| HN=C(Ph)O$^-$ | | | | | | |
| • −149±23 [a] | | 1482±11 [g] | 1452±8 | IMRE | | 86TAF |
| **$C_7H_6NO^-$** | | | | *Est* | *$\Delta_f H(AH)$= 108±8* | |
| PhCH=NO$^-$ | | | | | | |
| • 54±28 [a] | | 1477±20 [g] | 1447±8 | IMRE | | 79BAR/SCO |
| | | | 1453±8 | IMRE[o] | | 79BAR/SCO |
| **$C_7H_6NO^-$** | | | | *Est* | *$\Delta_f H(AH)$= 55±4* | |
| mNO-$C_6H_4CH_2^-$ | | | | | *BDE(A−H)= 360±13* | |
| • 64±15 [a] | 1.38±0.24 [d] | 1539±11 [g] | 1511±8 | IMRE | | 86TAF |
| **$C_7H_6NO^-$** | | | | *Est* | *$\Delta_f H(AH)$= −34±4* | |
| pCHO-anilide$^-$ | | | | | | |
| • −101±15 [a] | | 1463±11 [g] | 1432±8 | IMRE | | 86TAF |
| **$C_7H_6NO^-$** | | | | *Est* | *$\Delta_f H(AH)$= 55±4* | |
| pNO-$C_6H_4CH_2^-$ | | | | | | |
| • −3±15 [a] | | 1472±11 [g] | 1444±8 | IMRE | | 86TAF |
| **$C_7H_6NO_2^-$** | | | | | *$\Delta_f H(AH)$= −289±4* | *77NAB/SAB* |
| mNH$_2$-benzoate$^-$ | | | | | *BDE(A−H)= 444±13* | |
| • −393±15 [a] | 3.42±0.24 [d] | 1426±11 [g] | 1395±8 | IMRE | | 77MCM/KEB |
| **$C_7H_6NO_2^-$** | | | | | *$\Delta_f H(AH)$= 31±4* | *77PED/RYL* |
| mNO$_2$-$C_6H_4CH_2^-$ | | | | | *BDE(A−H)= 360±13* | |
| • 19±15 [a] | | 1518±11 [g] | 1488±8 | IMRE | | 83CAL/BAR |
| **$C_7H_6NO_2^-$** | | | | | *$\Delta_f H(AH)$= −298±2* | *77NAB/SAB* |
| oNH$_2$-benzoate$^-$ | | | | | | |
| • −422±14 [a] | | 1406±12 [g] | 1377±8 | IMRE | | 77MCM/KEB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_7H_6NO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 53±13* | |
| $oNO_2-C_6H_4CH_2^-$ | | | | | | | |
| • | 13±23 [a] | | 1490±11 [g] | 1459±8 | IMRE | | 86TAF |
| $C_7H_6NO_2^-$ | | | | | | *$\Delta_f H(AH)$= -294±4* | *77NAB/SAB* |
| $pNH_2$-benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | -397±15 [a] | 3.40±0.24 [d] | 1427±11 [g] | 1397±8 | IMRE | | 77MCM/KEB |
| $C_7H_6NO_2^-$ | | | | | | *$\Delta_f H(AH)$= 30±4* | *77PED/RYL* |
| $pNO_2-C_6H_4CH_2^-$ | | | | | | | |
| • | -25±14 [a] | | 1475±10 [g] | 1445±8 | IMRE | | 86TAF |
| | -23±14 [a] | | 1477±10 [g] | 1447±8 | IMRE | | 78CUM/KEB |
| $C_7H_6NO_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -142±8* | |
| 2-Me-4-$NO_2$-phenoxide$^-$ | | | | | | | |
| • | -297±21 [a] | | 1375±12 [g] | 1343±8 | IMRE | | 81FUJ/MCI |
| $C_7H_6N_2O_4^-$ | | | | | | | |
| 2-Me-3-$NO_2$-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 203±13* | |
| • | 69±17 [b] | 1.39±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_6O^-$ | | | | | | | |
| benzaldehyde$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -37±2* | *77PED/RYL* |
| | -78±3 [b] | 0.429±0.009 | | | ECD | | 75WEN/KAO |
| | | 0.39±0.05 | | | ECD | | 83ZLA/LEE |
| | | 0.42±0.01 | | | ECD | | 67WEN/CHE |
| $C_7H_6O_2^-$ | | | | | | | |
| methylbenzoquinone$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -155±8* | |
| • | -334±18 [b] | 1.85±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.75±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.76±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_7^-$ | | | | | | *$\Delta_f H(AH)$= 50* | *77PED/RYL* |
| $PhCH_2^-$ | | | | | | *BDE(A-H)= 368±4* | *82MCM/GOL* |
| • | 113±10 [a] | 0.90±0.15 [d] | 1593±10 [g] | 1564±8 | IMRE | | 79BAR/SCO |
| • | | 0.863±0.013 | | | LPD | | 84DRZ/BRA2 |
| | | 0.885±0.065 | | | LPD | | 75RIC/STE |
| | | | 1609±31 [g] | 1579±29 | IMRB | | 71BOH/YOU |
| | | 2.35±0.07 | | | SI | | 76FAI/JOY |
| | | 1.1 | | | SI | | 72PAG |
| | | 0.8 | | | SI | | 69PAG/GOO |
| | | 0.8 | | | SI | | 68GAI/PAG |
| | | | | 1558±8 | IMRE [o] | | 79BAR/SCO |
| $C_7H_7^-$ | | | | | | *$\Delta_f H(AH)$= 183±1* | *77PED/RYL* |
| cycloheptatrienide$^-$ | | | | | | *BDE(A-H)= 305±8* | *82MCM/GOL* |
| • | 223±13 [a] | 0.49±0.21 [d] | 1570±12 [g] | 1545±8 | IMRE | | 79BAR/SCO |
| | | | | 1539±8 | IMRE [o] | | 79BAR/SCO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_7^-$ | | | | | *$\Delta_f H(AH)$= 238±4* | *80ROG/CHO* |
| norbornadienide$^-$ | | | | | | |
| • 380±14 [a] | | 1672±10 [g] | 1637±6 | IMRB | Between $EtNH_2$, $nPrNH_2$ | 86LEE/SQU |
| | | | 1628±21 | IMRB | | 81WRI/BEA |
| $C_7H_7ClNO_2^-$ | | | | | | |
| $pNO_2-C_6H_4CH_3\cdot\cdot Cl^-$ | | | | | | |
| | | | *31* | TDEq | | 82FRE/IKU |
| $C_7H_7F_2^-$ | | | | | | |
| $PhCH_2F\cdot\cdot F^-$ | | | | | | |
| • −230 [c] | | *102±8* [g] | *69±8* | IMRE | | 83LAR/MCM |
| $C_7H_7NO_2^-$ | | | | | | |
| mMe-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 31±4* | |
| • −65±14 [b] | 0.99±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.93±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.92±0.05 | | | IMRE | | 85FUK/MCI |
| | 0.8±0.1 | | | ECD | | 83ZLA/LEE |
| $C_7H_7NO_2^-$ | | | | | | |
| oMe-nitrobenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 53±8* | *77PED/RYL* |
| • −36±18 [b] | 0.92±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.87±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.89±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_7NO_2^-$ | | | | | | |
| pMe-nitrobenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 31±4* | *77PED/RYL* |
| • −61±13 [b] | 0.95±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.89±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.91±0.05 | | | IMRE | | 85FUK/MCI |
| $C_7H_7NO_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= −142±17* | |
| 3-Me-4-$NO_2$-phenoxide$^-$ | | | | | | |
| • −292±28 [a] | | 1380±11 [g] | 1350±8 | IMRE | | 81FUJ/MCI |
| $C_7H_7NO_3^-$ | | | | | | |
| mOMe-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −90±4* | |
| • −191±14 [b] | 1.04±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.98±0.11 | | | IMRE | | 85GRI/CAL |
| $C_7H_7NO_3^-$ | | | | | | |
| pOMe-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −90±4* | |
| • −178±14 [b] | 0.91±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.85±0.11 | | | IMRE | | 85GRI/CAL |
| $C_7H_7O^-$ | | | | | *$\Delta_f H(AH)$= −100±1* | *77PED/RYL* |
| $PhCH_2O^-$ | | | | | *BDE(A-H)= 436±4* | |
| • −82±13 [a] | 2.07±0.17 [d] | 1548±12 [g] | 1520±8 | IMRE | | 79BAR/SCO |
| • | 2.142±0.013 | | | LPD | | 85MOY/DOD |
| | | | 1519±8 | IMRE [o] | | 79BAR/SCO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_7O^-$ | | | | | *$\Delta_f H(AH)$= −132±1* | *79KUD/KUD* |
| mMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −200±11 [a] | 2.19±0.19 [d] | 1463±10 [g] | 1434±8 | IMRE | | 81FUJ/MCI |
| | | 1467±10 [g] | 1438±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O^-$ | | | | | *$\Delta_f H(AH)$= −124±1* | *79KUD/KUD* |
| oMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±13* | |
| • −192±13 [a] | 2.19±0.26 [d] | 1462±12 [g] | 1431±8 | IMRE | | 81FUJ/MCI |
| • | <2.36±0.06 | | | PD | | 75RIC/STE2 |
| | | 1465±12 [g] | 1434±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O^-$ | | | | | *$\Delta_f H(AH)$= −125±2* | *79KUD/KUD* |
| pMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±13* | |
| • −190±11 [a] | 2.16±0.23 [d] | 1466±10 [g] | 1437±8 | IMRE | | 81FUJ/MCI |
| | | 1466±10 [g] | 1437±8 | IMRE | | 79BAR/SCO |
| | | 1471±10 [g] | 1442±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −250±8* | |
| mOMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −324±18 [a] | 2.26±0.19 [d] | 1456±10 [g] | 1427±8 | IMRE | | 81FUJ/MCI |
| | | 1459±10 [g] | 1431±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O_2^-$ | | | | *Est2* | *$\Delta_f H(AH)$= −264±17* | |
| oOMe-phenoxide$^-$ | | | | | | |
| • | | | 1433±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −242±8* | |
| pOMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±13* | |
| • −306±18 [a] | 2.15±0.23 [d] | 1466±10 [g] | 1437±8 | IMRE | | 81FUJ/MCI |
| | | 1469±10 [g] | 1440±8 | IMRE | | 77MCM/KEB |
| $C_7H_7O_2S^-$ | | | | | *$\Delta_f H(AH)$= −254±3* | *77PED/RYL* |
| $PhSO_2CH_2^-$ | | | | | | |
| • −266±13 [a] | | 1518±10 [g] | 1487±8 | IMRE | | 78CUM/KEB |
| $C_7H_7O_2S^-$ | | | | *Est* | *$\Delta_f H(AH)$= −194±8* | |
| mSOMe-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −297±18 [a] | 2.55±0.19 [d] | 1428±10 [g] | 1399±8 | IMRE | | 81FUJ/MCI |
| $C_7H_7O_2S^-$ | | | | *Est* | *$\Delta_f H(AH)$= −194±8* | |
| pSOMe-phenoxide$^-$ | | | | | | |
| • −312±19 [a] | | 1412±11 [g] | 1383±8 | IMRE | | 81FUJ/MCI |
| $C_7H_7O_3S^-$ | | | | *Est* | *$\Delta_f H(AH)$= −443±8* | |
| $mSO_2Me$-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −567±18 [a] | 2.77±0.19 [d] | 1406±10 [g] | 1377±8 | IMRE | | 81FUJ/MCI |
| $C_7H_7O_3S^-$ | | | | *Est* | *$\Delta_f H(AH)$= −443±8* | |
| $pSO_2Me$-phenoxide$^-$ | | | | | | |
| • −587±19 [a] | | 1385±11 [g] | 1356±8 | IMRE | | 81FUJ/MCI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_7S^-$ | | | | | $\Delta_f H(AH)=$ 98±1 | 77PED/RYL |
| $MeSC_6H_4^-$ | | | | | $BDE(A-H)=$ 460±13 | |
| 185±25 [a] | | 1617±23 [g] | 1586±21 | IMRB | | 85ING/NIB |
| | | | 1583±33 | IMRB[o] | | 85ING/NIB |
| $C_7H_7S^-$ | | | | | $\Delta_f H(AH)=$ 98±1 | 77PED/RYL |
| $PhSCH_2^-$ | | | | | | |
| • 164±12 [a] | | 1597±11 [g] | 1566±8 | IMRE | | 85ING/NIB |
| | | | 1560±8 | IMRE[o] | | 85ING/NIB |
| $C_7H_8Cl^-$ | | | | | | |
| $PhMe\cdot\cdot Cl^-$ | | | | | | |
| | | | *17* | TDEq | | 82FRE/IKU |
| $C_7H_8ClO^-$ | | | | | | |
| $PhOMe\cdot\cdot Cl^-$ | | | | | | |
| | | | *31* | TDEq | | 82FRE/IKU |
| $C_7H_8ClO^-$ | | | | | | |
| $pMe-C_6H_4OH\cdot\cdot Cl^-$ | | | | | | |
| • −453±11 [c] | | *101±8* | *69±8* | TDEq | | 77CUM/FRE |
| $C_7H_8N^-$ | | | | | $\Delta_f H(AH)=$ 85±4 | 78COL/BEN |
| $PhNMe^-$ | | | | | $BDE(A-H)=$ 366±8 | 82MCM/GOL |
| • 81±15 [a] | 1.57±0.20 [d] | 1526±11 [g] | 1496±8 | IMRE | | 86TAF |
| $C_7H_8N^-$ | | | | *Est* | $\Delta_f H(AH)=$ 54±8 | |
| mMe–anilide$^-$ | | | | | $BDE(A-H)=$ 368±13 | |
| • 59±18 [a] | 1.51±0.23 [d] | 1535±10 [g] | 1505±8 | IMRE | | 79BAR/SCO |
| | | | 1507±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_8N^-$ | | | | *Est* | $\Delta_f H(AH)=$ 59±4 | |
| pMe–anilide$^-$ | | | | | $BDE(A-H)=$ 368±13 | |
| • 65±15 [a] | 1.49±0.24 [d] | 1537±11 [g] | 1507±8 | IMRE | | 79BAR/SCO |
| | | | 1510±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_8NO^-$ | | | | *Est* | $\Delta_f H(AH)=$ −59±8 | |
| pOMe–anilide$^-$ | | | | | $BDE(A-H)=$ 368±13 | |
| • −53±18 [a] | 1.50±0.23 [d] | 1536±10 [g] | 1505±8 | IMRE | | 79BAR/SCO |
| | | | 1509±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_8NO_2S^-$ | | | | *Est* | $\Delta_f H(AH)=$ −236±4 | |
| $mSO_2Me$–anilide$^-$ | | | | | $BDE(A-H)=$ 368±13 | |
| • −291±15 [a] | 2.13±0.24 [d] | 1475±11 [g] | 1445±8 | IMRE | | 86TAF |
| $C_7H_8NO_2S^-$ | | | | *Est* | $\Delta_f H(AH)=$ −236±4 | |
| $pSO_2Me$–anilide$^-$ | | | | | $BDE(A-H)=$ 368±13 | |
| • −312±15 [a] | 2.34±0.24 [d] | 1455±11 [g] | 1424±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_7H_8NS^-$ | | | | *Est* | *$\Delta_f H(AH)$= 104±8* | |
| mSMe-anilide$^-$ | | | | | *BDE(A-H)= 368±13* | |
| • 89±18 [a] | 1.71±0.23 [d] | 1515±10 [g] | 1484±8 | IMRE | | 79BAR/SCO |
| | | | 1492±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_9^-$ | | | | *Est* | *$\Delta_f H(AH)$= 133±4* | |
| heptatrienide$^-$ | | | | | | |
| • | 1.27±0.03 | | | PD | | 78ZIM/GYG |
| $C_7H_9^-$ | | | | | *$\Delta_f H(AH)$= 90±4* | *80ROG/CHO* |
| norbornenide$^-$ | | | | | | |
| 242±19 [a] | | 1682±15 [g] | 1648±13 | IMRB | between $NH_3$, $EtNH_2$ | 86LEE/SQU |
| $C_7H_9O^-$ | | | | | *$\Delta_f H(AH)$= -168±3* | *78STE* |
| 2-norbornanone enolate$^-$ | | | | | | |
| • | 1.61±0.05 | | | PD | | 78ZIM/JAC |
| $C_7H_{11}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -272±4* | |
| 2,5-diMe-cyclopentanone enolate$^-$ | | | | | | |
| • | 1.49±0.04 | | | PD | | 78ZIM/JAC |
| $C_7H_{11}O^-$ | | | | | *$\Delta_f H(AH)$= -248±2* | *77PED/RYL* |
| cycloheptanone enolate$^-$ | | | | | | |
| • | 1.48±0.04 | | | PD | | 78ZIM/JAC |
| $C_7H_{11}O_4^-$ | | | | *Est* | *$\Delta_f H(AH)$= -839±2* | |
| $HC(CO_2Et)_2^-$ | | | | | | |
| • -912±12 [a] | | 1457±10 [g] | 1432±8 | IMRE | | 78CUM/KEB |
| $C_7H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -301±4* | |
| $EtCH=C(nPr)O^-$ | | | | | *BDE(A-H)= 389±8* | |
| • -296±18 [a] | 1.72±0.06 | 1535±14 [e] | | PD | | 77ZIM/REE |
| $C_7H_{13}O^-$ | | | | | *$\Delta_f H(AH)$= -311±1* | *77PED/RYL* |
| $Me_2C=C(iPr)O^-$ | | | | | *BDE(A-H)= 364±13* | |
| • -307±19 [a] | 1.47±0.05 | 1535±18 [e] | 1505±23 [h] | PD | | 77ZIM/REE |
| $C_7H_{13}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -305±4* | |
| $c-C_6H_{11}-CH_2O^-$ | | | | | *BDE(A-H)= 435±8* | |
| • -271±14 [a] | 1.90±0.19 [d] | 1564±10 [g] | 1536±8 | IMRE | | 86TAF |
| $C_7H_{13}S^-$ | | | | *Est* | *$\Delta_f H(AH)$= -116±4* | |
| $c-C_6H_{11}-CH_2S^-$ | | | | | *BDE(A-H)= 364±10* | |
| • -171±16 [a] | 2.09±0.23 [d] | 1475±12 [g] | 1449±8 | IMRE | | 86TAF |
| $C_7H_{15}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -369±4* | |
| $(iPr)_2CHO^-$ | | | | | *BDE(A-H)= 438±4* | |
| • -348±15 [a] | 2.1±0.2 [d] | 1551±11 | 1523±13 [h] | CIDC | | 83BOA/HOU |
| | | 1549±10 | | CIDC[o] | | 83BOA/HOU |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_7H_{15}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -366±4* | |
| $Et_3CO^-$ | | | | | | *BDE(A-H)= 440±4* | |
| • | -344±15 [a] | 2.1±0.2 [d] | 1552±11 | 1524±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1549±10 | | CIDC[o] | | 83BOA/HOU |
| $C_7H_{15}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -373±4* | |
| $nBuC(Me)_2O^-$ | | | | | | *BDE(A-H)= 440±4* | |
| • | -348±15 [a] | 2.0±0.2 [d] | 1555±11 | 1527±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1552±10 | | CIDC[o] | | 83BOA/HOU |
| $C_7H_{15}O^-$ | | | | | | *$\Delta_f H(AH)$= -336±2* | *77PED/RYL* |
| $nC_7H_{15}O^-$ | | | | | | *BDE(A-H)= 436±4* | |
| • | -307±13 [a] | 2.0±0.2 [d] | 1559±11 | 1531±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1555±10 | | CIDC[o] | | 83BOA/HOU |
| $C_7H_{15}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -371±4* | |
| $tBuCH(Et)O^-$ | | | | | | *BDE(A-H)= 438±4* | |
| • | -353±16 [a] | 2.10±0.17 [d] | 1548±12 [g] | 1520±8 | IMRE | | 79BAR/SCO |
| | | | | 1519±8 | IMRE[o] | | 79BAR/SCO |
| $C_7H_{15}OS_2^-$ | | | | | | | |
| MeOH··5,5-diMe-1,3-dithianide$^-$ | | | | | | | |
| | -287±38 [c] | | *62±10* [g] | *34±7* | IMRE | | 84CAL/ROZ |
| $C_7H_{17}O_2^-$ | | | | | | | |
| $EtOH\cdot\cdot tBuCH_2O^-$ | | | | | | | |
| | -605±24 [c] | | *80±10* [g] | *53±8* | IMRE | | 84CAL/ROZ |
| $C_7H_{17}O_2^-$ | | | | | | | |
| $nPrOH\cdot\cdot tBuO^-$ | | | | | | | |
| | -615±23 [c] | | *85±10* [g] | *57±8* | IMRE | | 84CAL/ROZ |
| $C_8F_4N_2^-$ | | | | | | | |
| pCN-perfluorobenzonitrile$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -417±17* | |
| • | -599±26 [b] | 1.89±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.89±0.10 | | | IMRE | | 86CHO/GRI |
| $C_8HN_2O_2^-$ | | | | | | | |
| 2,3-diCN-benzoquinonide$^-$ | | | | | | | |
| | | 1.82±0.09 | | | SI | | 66FAR/PAG |
| $C_8H_3F_5O^-$ | | | | | | | |
| $C_6F_5COCH_3^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -1052±17* | |
| • | -1143±26 [b] | 0.94±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.94±0.10 | | | IMRE | | 86CHO/GRI |
| $C_8H_3F_6NO_2^-$ | | | | | | | |
| 3,5-di$CF_3$-nitrobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -1276±4* | |
| • | -1449±14 [b] | 1.79±0.10 | | | TDEq | | 87KEB/CHO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_3F_6O^-$ | | | | Est | $\Delta_f H(AH)$= −1485±17 | |
| 3,5-diCF$_3$-phenoxide$^-$ | | | | | BDE(A−H)= 362±13 | |
| • −1636±28 [a] | 3.05±0.24 [d] | 1380±11 [g] | 1351±8 | IMRE | | 86TAF |
| $C_8H_4F_3N^-$ | | | | | | |
| mCF$_3$-benzonitrile$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= −434±8 | |
| • . −499±18 [b] | 0.67±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.67±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_4F_3N^-$ | | | | | | |
| oCF$_3$-benzonitrile$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= −452±4 | |
| • −519±14 [b] | 0.70±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_4F_3N^-$ | | | | | | |
| pCF$_3$-benzonitrile$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= −452±4 | |
| • −525±14 [b] | 0.76±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_4F_3O_2^-$ | | | | Est | $\Delta_f H(AH)$= −976±8 | |
| mCF$_3$-benzoate$^-$ | | | | | BDE(A−H)= 444±13 | |
| • −1114±19 [a] | 3.77±0.24 [d] | 1392±11 [g] | 1361±8 | IMRE | | 86TAF |
| $C_8H_4F_3O_2^-$ | | | | Est | $\Delta_f H(AH)$= −976±8 | |
| pCF$_3$-benzoate$^-$ | | | | | BDE(A−H)= 444±13 | |
| • −1115±19 [a] | 3.78±0.24 [d] | 1391±11 [g] | 1361±8 | IMRE | | 86TAF |
| $C_8H_4F_6N^-$ | | | | Est | $\Delta_f H(AH)$= −1302±8 | |
| 3,5-diCF$_3$-anilide$^-$ | | | | | BDE(A−H)= 368±13 | |
| • −1377±19 [a] | 2.33±0.24 [d] | 1456±11 [g] | 1425±8 | IMRE | | 86TAF |
| $C_8H_4NO_2^-$ | | | | Est | $\Delta_f H(AH)$= −158±13 | |
| mCN-benzoate$^-$ | | | | | BDE(A−H)= 444±13 | |
| • −309±23 [a] | 3.90±0.24 [d] | 1379±11 [g] | 1348±8 | IMRE | | 77MCM/KEB |
| $C_8H_4NO_2^-$ | | | | Est | $\Delta_f H(AH)$= −158±13 | |
| pCN-benzoate$^-$ | | | | | BDE(A−H)= 444±13 | |
| • −314±23 [a] | 3.95±0.24 [d] | 1374±11 [g] | 1345±8 | IMRE | | 77MCM/KEB |
| $C_8H_4N_2^-$ | | | | | | |
| mCN-benzonitrile$^{-\cdot}$ | | | | | $\Delta_f H(A)$= 363±2 | 80SAT/SAK |
| • 275±12 [b] | 0.91±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.91±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_4N_2^-$ | | | | | | |
| o-CN-benzonitrile$^{-\cdot}$ | | | | Est2 | $\Delta_f H(A)$= 363±13 | |
| • 271±22 [b] | 0.95±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.95±0.09 | | | TDEq | | 86CHO/KEB |
| | 1.1±0.1 | | | SI | | 67FAR/PAG |
| $C_8H_4N_2^-$ | | | | | | |
| p-CN-benzonitrile$^{-\cdot}$ | | | | Est2 | $\Delta_f H(A)$= 363±8 | |
| • 257±18 [b] | 1.10±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.10±0.09 | | | TDEq | | 86CHO/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_4O_3^-$ | | | | | | |
| phthalic anhydride$^{-\cdot}$ | | | | | | |
| • −487±12 [b] | 1.21±0.10 | | | TDEq | | 87KEB/CHO |
| • | 1.20±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_5^-$ | | | | | $\Delta_f H(AH)$= 306±2 | 85DAV/ALL |
| PhC≡C$^-$ | | | | | BDE(A−H)= 552±21 | |
| • 327±15 [a] | 3.25±0.36 [d] | 1551±13 [g] | 1518±8 | IMRE | | 79BAR/SCO |
| | | | 1518±8 | IMRE[o] | | 79BAR/SCO |
| $C_8H_5ClN^-$ | | | | Est | $\Delta_f H(AH)$= 156±4 | |
| mCl−$C_6H_4CHCN^-$ | | | | | | |
| • 68±18 [a] | | 1441±13 [g] | 1412±8 | IMRE | | 81FUJ/MCI |
| $C_8H_5ClN^-$ | | | | Est | $\Delta_f H(AH)$= 156±4 | |
| pCl−$C_6H_4CHCN^-$ | | | | | | |
| • 70±18 [a] | | 1444±13 [g] | 1416±8 | IMRE | | 81FUJ/MCI |
| $C_8H_5FN^-$ | | | | Est | $\Delta_f H(AH)$= −7±4 | |
| mF−$C_6H_4CHCN^-$ | | | | | | |
| • −70±19 [a] | | 1467±15 [g] | 1439±8 | IMRE | | 86TAF |
| $C_8H_5FN^-$ | | | | Est | $\Delta_f H(AH)$= −7±4 | |
| pF−$C_6H_4CHCN^-$ | | | | | | |
| • −77±15 [a] | | 1460±11 [g] | 1433±8 | IMRE | | 86TAF |
| $C_8H_5F_3NO^-$ | | | | Est2 | $\Delta_f H(AH)$= −706±13 | |
| PhN=C($CF_3$)O$^-$ | | | | | | |
| • −841±23 [a] | | 1395±11 [g] | 1366±8 | IMRE | | 86TAF |
| $C_8H_5NO^-$ | | | | | | |
| mCHO−benzonitrile$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= 99±4 | |
| • 2±14 [b] | 1.00±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.01±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_5NO^-$ | | | | | | |
| pCHO−benzonitrile$^{-\cdot}$ | | | | Est | $\Delta_f H(A)$= 99±4 | |
| • −19±14 [b] | 1.22±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.22±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_5N_2O_2^-$ | | | | Est | $\Delta_f H(AH)$= 171±4 | |
| $mNO_2$−$C_6H_4CHCN^-$ | | | | | | |
| • 53±19 [a] | | 1412±15 [g] | 1384±8 | IMRE | | 86TAF |
| $C_8H_5N_2O_2^-$ | | | | Est | $\Delta_f H(AH)$= 171±4 | |
| $pNO_2$−$C_6H_4CHCN^-$ | | | | | | |
| • 19±18 [a] | | 1378±13 [g] | 1350±8 | IMRE | | 81FUJ/MCI |
| $C_8H_5O_3^-$ | | | | Est | $\Delta_f H(AH)$= −414±8 | |
| pCHO−benzoate$^-$ | | | | | BDE(A−H)= 444±13 | |
| • −550±19 [a] | 3.74±0.24 [d] | 1395±11 [g] | 1363±8 | IMRE | | 86TAF |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_6ClO^-$ | | | | *Est* | *$\Delta_f H(AH)$= −116±8* | |
| $mCl-C_6H_4C(=CH_2)O^-$ | | | | | | |
| • −152±18 [a] | | 1495±10 [g] | 1466±8 | IMRE | | 79BAR/SCO |
| $C_8H_6Cl_2O_2^-$ | | | | | | |
| 2,5-diCl-3,6-diMe-benzoquinone$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= −230±17* | |
| • −437±21 [b] | 2.14±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_6F_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= −622±8* | |
| $mCF_3-C_6H_4CH_2^-$ | | | | | | |
| • −608±18 [a] | | 1545±10 [g] | 1515±8 | IMRE | | 83CAL/BAR |
| $C_8H_6F_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= −622±8* | |
| $pCF_3-C_6H_4CH_2^-$ | | | | | | |
| • −617±18 [a] | | 1536±10 [g] | 1505±8 | IMRE | | 83CAL/BAR |
| $C_8H_6F_3O_2^-$ | | | | | | |
| $pSO_2CF_3-C_6H_4CH_2^-$ | | | | | | |
| • | | 1454±11 [g] | 1425±8 | IMRE | | 86TAF |
| $C_8H_6N^-$ | | | | *Est* | *$\Delta_f H(AH)$= 186±4* | |
| $PhCHCN^-$ | | | | | | |
| • 123±18 [a] | | 1467±13 [g] | 1440±8 | IMRE | | 81FUJ/MCI |
| | | 1471±13 [g] | 1443±8 | IMRE | | 78CUM/KEB |
| | | | 1451±8 | IMRE[o] | | 79BAR/SCO |
| $C_8H_6N^-$ | | | | | *$\Delta_f H(AH)$= 157±5* | *77PED/RYL* |
| indolide$^-$ | | | | | | |
| • 89±15 [a] | | 1461±11 [g] | 1431±8 | IMRE | | 86TAF |
| $C_8H_6N^-$ | | | | *Est* | *$\Delta_f H(AH)$= 183±8* | |
| $mCN-C_6H_4CH_2^-$ | | | | | | |
| • 198±18 [a] | | 1545±10 [g] | 1515±8 | IMRE | | 83CAL/BAR |
| $C_8H_6N^-$ | | | | *Est* | *$\Delta_f H(AH)$= 182±8* | |
| $pCN-C_6H_4CH_2^-$ | | | | | | |
| • 162±19 [a] | | 1510±11 [g] | 1479±10 | IMRE | | 83CAL/BAR |
| $C_8H_6O_2^-$ | | | | | | |
| p-CHO-benzaldehyde$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −157±8* | |
| −211 [b] | 0.6 | | | ECD | | 68KUH/LEV |
| $C_8H_7ClO^-$ | | | | | | |
| mCl-acetophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −117±8* | |
| −173±9 [b] | 0.583±0.006 | | | ECD | | 69STE/WEN |
| $C_8H_7ClO^-$ | | | | | | |
| pCl-acetophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −117±8* | |
| −172±9 [b] | 0.567±0.005 | | | ECD | | 69STE/WEN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_7ClO_2^-$ | | | | | | |
| 2-Cl-3,6-diMe-benzoquinone$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -212±17* | |
| • -398±21 [b] | 1.93±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_7FO^-$ | | | | | | |
| mF-acetophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -280±8* | |
| -336±11 [b] | 0.58±0.03 | | | ECD | | 75WEN/KAO |
| $C_8H_7FO^-$ | | | | | | |
| oF-acetophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -280±21* | |
| -323±22 [b] | 0.442±0.009 | | | ECD | | 75WEN/KAO |
| $C_8H_7FO^-$ | | | | | | |
| pF-acetophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -280±8* | |
| -318±10 [b] | 0.40±0.01 | | | ECD | | 75WEN/KAO |
| $C_8H_7N^-$ | | | | | | |
| oMe-benzonitrile$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 178±1* | |
| • 110±11 [b] | 0.70±0.10 | | | TDEq | | 87KEB/CHO |
| 110±9 [b] | 0.70±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_7N^-$ | | | | | | |
| pMe-benzonitrile$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 182±1* | |
| • 109±9 [b] | 0.76±0.09 | | | TDEq | | 86CHO/KEB |
| $C_8H_7NO_3^-$ | | | | | | |
| mCOMe-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -103±4* | |
| • -229±14 [b] | 1.31±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_7NO_3^-$ | | | | | | |
| oCOMe-nitrobenzene$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -84±8* | |
| • -217±18 [b] | 1.38±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_7NO_3^-$ | | | | | | |
| pCOMe-nitrobenzene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -103±4* | |
| • -252±14 [b] | 1.55±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_7O^-$ | | | | | *$\Delta_f H(AH)$= -87±2* | *77PED/RYL* |
| $CH_2$=C(Ph)$O^-$ | | | | *D-EA* | *BDE(A-H)= 399±18* | |
| • -105±13 [a] | | 1512±11 [g] | 1483±8 | IMRE | | 79BAR/SCO |
| • | 2.06±0.08 | | | PD | | 77ZIM/REE |
| -101±13 [a] | | 1516±11 [g] | 1487±8 | IMRE | | 78CUM/KEB |
| | | | 1491±8 | IMRE[o] | | 79BAR/SCO |
| $C_8H_7O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -53±4* | |
| PhCH=$CHO^-$ | | | | | | |
| • | 2.10±0.08 | | | PD | | 77ZIM/REE |
| $C_8H_7O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -71±8* | |
| mCHO-$C_6H_4CH_2^-$ | | | | | | |
| • -47±19 [a] | | 1554±11 [g] | 1524±8 | IMRE | | 83CAL/BAR |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_7O^-$ | | | | *Est* | *$\Delta_f H(AH)$= -75±8* | |
| $pCHO\text{-}C_6H_4CH_2^-$ | | | | | | |
| • -100±21 [a] | | 1505±12 [g] | 1475±10 | IMRE | | 86TAF |
| $C_8H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -320±4* | |
| $PhCH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -423±15 [a] | 3.40±0.20 [d] | 1428±11 [g] | 1398±8 | IMRE | | 86TAF |
| $C_8H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -264±8* | |
| mCOMe-phenoxide$^-$ | | | | | *BDE(A-H)= 362±8* | |
| • -361±18 [a] | 2.50±0.19 [d] | 1433±10 [g] | 1404±8 | IMRE | | 81FUJ/MCI |
| $C_8H_7O_2^-$ | | | | | *$\Delta_f H(AH)$= -329±1* | *76COL/JIM* |
| mMe-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -437±12 [a] | 3.46±0.24 [d] | 1422±11 [g] | 1391±8 | IMRE | | 77MCM/KEB |
| $C_8H_7O_2^-$ | | | | | *$\Delta_f H(AH)$= -320±1* | *76COL/JIM* |
| oMe-benzoate$^-$ | | | | | | |
| • -436±13 [a] | | 1415±12 [g] | 1384±8 | IMRE | | 77MCM/KEB |
| $C_8H_7O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -264±8* | |
| pCOMe-phenoxide$^-$ | | | | | | |
| • -390±19 [a] | | 1404±11 [g] | 1375±8 | IMRE | | 81FUJ/MCI |
| $C_8H_7O_2^-$ | | | | | *$\Delta_f H(AH)$= -332±1* | *76COL/JIM* |
| pMe-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -440±12 [a] | 3.46±0.24 [d] | 1422±11 [g] | 1392±8 | IMRE | | 77MCM/KEB |
| $C_8H_7O_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= -468±8* | |
| $mCO_2Me$-phenoxide$^-$ | | | | | *BDE(A-H)= 362±8* | |
| • -559±18 [a] | 2.44±0.19 [d] | 1439±10 [g] | 1410±8 | IMRE | | 81FUJ/MCI |
| $C_8H_7O_3^-$ | | | | | *$\Delta_f H(AH)$= -446±1* | *78COL/JIM* |
| mOMe-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -559±12 [a] | 3.51±0.24 [d] | 1417±11 [g] | 1386±8 | IMRE | | 77MCM/KEB |
| $C_8H_7O_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= -452±8* | |
| oOMe-benzoate$^-$ | | | | | | |
| • -567±19 [a] | | 1415±11 [g] | 1386±8 | IMRE | | 77MCM/KEB |
| $C_8H_7O_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= -468±8* | |
| $pCO_2Me$-phenoxide$^-$ | | | | | | |
| • -587±19 [a] | | 1411±11 [g] | 1382±8 | IMRE | | 81FUJ/MCI |
| $C_8H_8^-$ | | | | | | |
| cyclooctatetraene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 297±1* | *77PED/RYL* |
| 242±5 [b] | 0.58±0.04 | | | ECD | | 69WEN/RIS |
| | <0.8 | | | PD | | 79GYG/PET |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_8ClO^-$ | | | | | | |
| PhCOMe··Cl$^-$ | | | | | | |
| | | | *40* | TDEq | | 82FRE/IKU |
| $C_8H_8NO^-$ | | | | | *$\Delta_f H(AH)$= -129±1* | *77PED/RYL* |
| PhN=C(Me)O$^-$ | | | | | | |
| • -205±11 [a] | | 1454±10 [g] | 1425±8 | IMRE | | 86TAF |
| | | 1476±10 [g] | 1447±8 | IMRE | | 78CUM/KEB |
| $C_8H_8NO^-$ | | | | *Est* | *$\Delta_f H(AH)$= -100±4* | |
| mCOMe-anilide$^-$ | | | | | *BDE(A-H)= 368±13* | |
| • -125±15 [a] | 1.82±0.24 [d] | 1505±11 [g] | 1474±8 | IMRE | | 86TAF |
| $C_8H_8NO^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -88±4* | |
| pCOMe-anilide$^-$ | | | | | | |
| • -148±15 [a] | | 1470±11 [g] | 1439±8 | IMRE | | 86TAF |
| $C_8H_8NO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -300±4* | |
| mCO$_2$Me-anilide$^-$ | | | | | *BDE(A-H)= 368±13* | |
| • -322±15 [a] | 1.78±0.24 [d] | 1509±11 [g] | 1478±8 | IMRE | | 86TAF |
| $C_8H_8NO_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -300±4* | |
| pCO$_2$Me-anilide$^-$ | | | | | | |
| • -356±15 [a] | | 1475±11 [g] | 1444±8 | IMRE | | 86TAF |
| $C_8H_8O^-$ | | | | | | |
| acetophenone$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -87±2* | *77PED/RYL* |
| -119±2 [b] | 0.334±0.004 | | | ECD | | 75WEN/KAO |
| | 0.334±0.004 | | | ECD | | 67WEN/CHE |
| $C_8H_8O^-$ | | | | | | |
| mMe-benzaldehyde$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -71±8* | |
| -110±10 [b] | 0.41±0.01 | | | ECD | | 75WEN/KAO |
| $C_8H_8O^-$ | | | | | | |
| pMe-benzaldehyde$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -75±8* | |
| -111±10 [b] | 0.37±0.02 | | | ECD | | 75WEN/KAO |
| $C_8H_8O_2^-$ | | | | | | |
| 2,5-diMe-benzoquinone$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -187±8* | |
| • -358±18 [b] | 1.77±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.72±0.11 | | | IMRE | | 85GRI/CAL |
| $C_8H_8O_2^-$ | | | | | | |
| 2,6-diMe-benzoquinone$^-$ | | | | *Est* | *$\Delta_f H(A)$= -187±8* | |
| • -359±18 [b] | 1.78±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.67±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_8O_2^-$ | | | | | | |
| mOMe-benzaldehyde$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -182±8* | |
| -224±13 [b] | 0.43±0.04 | | | ECD | | 75WEN/KAO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_8O_2^-$ | | | | | | |
| methyl benzoate$^{-\cdot}$ | | | | | $\Delta_f H(A)=$ -288±7 | 77PED/RYL |
| -305 [b] | 0.2 | | | ECD | | 68KUH/LEV |
| $C_8H_8O_2^-$ | | | | | | |
| oOH-acetophenone$^{-\cdot}$ | | | | Est2 | $\Delta_f H(A)=$ -100±13 | |
| • -184±17 [b] | 0.86±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_8O_4^-$ | | | | | | |
| 2,6-diMeO-benzoquinone$^{-\cdot}$ | | | | | | |
| • | 1.73±0.10 | | | TDEq | | 87KEB/CHO |
| $C_8H_9^-$ | | | | | | |
| 2-methylenenorborn-5-en-3-ide$^-$ | | | | | | |
| • | | 1632±10 [g] | 1603±8 | IMRB | | 86LEE/SQU |
| $C_8H_9^-$ | | | | | $\Delta_f H(AH)=$ 29 | 77PED/RYL |
| PhCHMe$^-$ | | | | | BDE(A-H)= 354±8 | 81ROB/STE |
| • 88±10 [a] | 0.80±0.19 [d] | 1589±10 [g] | 1562±8 | IMRE | | 79BAR/SCO |
| | | | 1556±8 | IMRE[o] | | 79BAR/SCO |
| $C_8H_9^-$ | | | | | | |
| bicyclo[3.2.1]octa-2,6-dien-4-ide$^-$ | | | | | | |
| • | | 1588±11 [g] | 1559±8 | IMRE | | 86LEE/SQU |
| $C_8H_9^-$ | | | | | $\Delta_f H(AH)=$ 17 | 77PED/RYL |
| mMe-$C_6H_4CH_2^-$ | | | | | BDE(A-H)= 368±9 | 86HAY/KRU |
| • 82±12 [a] | 0.89±0.22 [d] | 1595±12 [g] | 1564±10 | IMRE | | 83CAL/BAR |
| $C_8H_9^-$ | | | | | $\Delta_f H(AH)=$ 18±1 | 77PED/RYL |
| pMe-$C_6H_4CH_2^-$ | | | | | BDE(A-H)= 367±10 | 86HAY/KRU |
| • 86±12 [a] | 0.84±0.22 [d] | 1598±11 [g] | 1568±10 | IMRE | | 79BAR/SCO |
| $C_8H_9NO_2^-$ | | | | | | |
| 1,2-diMe-3-nitrobenzene$^{-\cdot}$ | | | | Est2 | $\Delta_f H(A)=$ 13±13 | |
| • -70±22 [b] | 0.86±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.81±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.86±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_9NO_2^-$ | | | | | | |
| 1,2-diMe-4-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)=$ -1±8 | |
| • -85±13 [b] | 0.87±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_9NO_2^-$ | | | | | | |
| 1,3-diMe-2-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)=$ 40±13 | |
| • -33±17 [b] | 0.76±0.05 | | | IMRE | | 85FUK/MCI |
| $C_8H_9NO_2^-$ | | | | | | |
| 1,3-diMe-4-nitrobenzene$^{-\cdot}$ | | | | Est | $\Delta_f H(A)=$ 20±8 | |
| • -60±13 [b] | 0.83±0.05 | | | IMRE | | 85FUK/MCI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_9O^-$ | | | | | *$\Delta_f H(AH)$= -146±2* | *77PED/RYL* |
| mEt-phenoxide$^-$ | | | | | *BDE(A-H)= 362±8* | |
| • -215±11 [a] | 2.20±0.19 [d] | 1461±10 [g] | 1433±8 | IMRE | | 81FUJ/MCI |
| $C_8H_9O^-$ | | | | | *$\Delta_f H(AH)$= -144±1* | *77PED/RYL* |
| pEt-phenoxide$^-$ | | | | | *BDE(A-H)= 362±8* | |
| • -210±10 [a] | 2.18±0.19 [d] | 1464±10 [g] | 1435±8 | IMRE | | 81FUJ/MCI |
| $C_8H_9OS^-$ | | | | *Est* | *$\Delta_f H(AH)$= -32±8* | |
| pSOMe-$C_6H_4CH_2^-$ | | | | | | |
| • -31±19 [a] | | 1531±11 [g] | 1503±8 | IMRE | | 86TAF |
| $C_8H_9O_2S^-$ | | | | *Est* | *$\Delta_f H(AH)$= -280±4* | |
| $PhSO_2CHMe^-$ | | | | | | |
| • -283±13 [a] | | 1527±8 [g] | 1495±8 | IMRE | | 78CUM/KEB |
| $C_8H_9O_2S^-$ | | | | | *$\Delta_f H(AH)$= -273±3* | *77PED/RYL* |
| $pSO_2Me$-$C_6H_4CH_2^-$ | | | | | | |
| • -302±14 [a] | | 1501±11 [g] | 1473±8 | IMRE | | 86TAF |
| $C_8H_9O_3^-$ | | | | | | |
| $PhOH\cdot\cdot MeCO_2^-$ | | | | | | |
| | | *109±4* | *79±7* | TDAs | | 86MEO/SIE2 |
| $C_8H_{10}Cl^-$ | | | | | | |
| $PhEt\cdot\cdot Cl^-$ | | | | | | |
| | | | *21* | TDEq | | 82FRE/IKU |
| $C_8H_{10}Cl^-$ | | | | | | |
| m-xylene$\cdot\cdot Cl^-$ | | | | | | |
| | | | *16* | TDEq | | 82FRE/IKU |
| $C_8H_{10}Cl^-$ | | | | | | |
| p-xylene$\cdot\cdot Cl^-$ | | | | | | |
| | | | *16* | TDEq | | 82FRE/IKU |
| $C_8H_{10}N^-$ | | | | | *$\Delta_f H(AH)$= -56±6* | *77PED/RYL* |
| $PhNEt^-$ | | | | | *BDE(A-H)= 366±8* | |
| • 50±17 [a] | 1.60±0.20 [d] | 1523±11 [g] | 1493±8 | IMRE | | 86TAF |
| $C_8H_{10}NO^-$ | | | | *Est* | *$\Delta_f H(AH)$= -84±8* | |
| $mNMe_2$-phenoxide$^-$ | | | | | *BDE(A-H)= 362±8* | |
| • -148±18 [a] | 2.15±0.19 [d] | 1466±10 [g] | 1437±8 | IMRE | | 81FUJ/MCI |
| $C_8H_{10}NO^-$ | | | | *Est* | *$\Delta_f H(AH)$= -84±8* | |
| $pNMe_2$-phenoxide$^-$ | | | | | | |
| • -144±18 [a] | | 1470±10 [g] | 1441±8 | IMRE | | 81FUJ/MCI |
| $C_8H_{10}N_2O_2^-$ | | | | | | |
| $mNMe_2$-nitrobenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 67±2* | *84FUR/MUR* |
| • -21±6 [b] | 0.92±0.05 | | | IMRE | | 85FUK/MCI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_8H_{11}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 39±13* | |
| 2-methylenenorbornan-3-ide$^-$ | | | | | | |
| • 138±18 [a] | | 1629±5 [g] | 1600±3 | IMRE | | 86LEE/SQU |
| $C_8H_{11}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 13±17* | |
| bicyclo[3.2.1]oct-2-en-4-ide$^-$ | | | | | | |
| • 117±22 [a] | | 1635±5 [g] | 1604±3 | IMRE | | 86LEE/SQU |
| $C_8H_{11}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 42±13* | |
| cyclooctadienide$^-$ | | | | | | |
| 88±29 [a] | | 1576±16 [g] | 1548±13 | IMRB | between EtOH, nPrOH | 86LEE/SQU |
| $C_8H_{11}O^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -180±13* | |
| 4,4-diMe-cyclohexenone-6-enolate$^-$ | | | | | | |
| • -181±22 [a] | | 1529±10 [g] | 1497±8 | IMRE | | 86BAR/KIP |
| | | | 1500±8 | IMRE[o] | | 86BAR/KIP |
| $C_8H_{11}O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -287±13* | |
| 5,5-diMe-1,3-cyclohexandion-2-ide$^-$ | | | | | | |
| • -399±22 [a] | | 1418±10 [g] | 1385±8 | IMRE | Acid: dimedone | 78CUM/KEB |
| $C_8H_{11}O_2^-$ | | | | | | |
| EtOH··PhO$^-$ | | | | | | |
| | | *81±4* | *47±7* | TDAs | | 86MEO/SIE2 |
| $C_8H_{12}B^-$ | | | | *Est* | *$\Delta_f H(AH)$= 86±13* | |
| $Me_2C(CH=CH)_2BCH_2^-$ | | | | | | |
| 100±32 [a] | | 1544±19 [g] | 1515±17 | IMRB | | 77SUL |
| $C_8H_{13}^-$ | | | | | *$\Delta_f H(AH)$= -27±1* | *77PED/RYL* |
| cyclooctenide$^-$ | | | | | | |
| 60±26 [a] | | 1617±25 [g] | 1586±21 | IMRB | Between EtOH, nPrOH | 86LEE/SQU |
| $C_8H_{13}O^-$ | | | | | *$\Delta_f H(AH)$= -272±5* | *77PED/RYL* |
| cycloctanone enolate$^-$ | | | | | | |
| • | 1.63±0.06 | | | PD | | 78ZIM/JAC |
| $C_8H_{13}O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -523±8* | |
| $cC_6H_{11}-CH_2CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • -609±19 [a] | 3.23±0.20 [d] | 1444±11 [g] | 1415±8 | IMRE | | 86TAF |
| $C_8H_{15}O_4^-$ | | | | | | |
| $iPrCO_2H\cdot\cdot iPrCO_2^-$ | | | | | | |
| | | *125±4* | *83±7* | TDAs | | 86MEO/SIE2 |
| $C_8H_{17}O^-$ | | | | | *$\Delta_f H(AH)$= -355±1* | *77PED/RYL* |
| $nC_8H_{17}O^-$ | | | | | *BDE(A-H)= 436±4* | |
| • -330±12 [a] | 2.0±0.2 [d] | 1556±11 | 1528±13 [h] | CIDC | | 83BOA/HOU |
| | | 1553±10 | | CIDC[o] | | 83BOA/HOU |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_8H_{17}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -392±4* | |
| tBuCH(iPr)$O^-$ | | | | | | *BDE(A-H)= 438±4* | |
| • | -379±16 [a] | 2.15±0.17 [d] | 1543±12 [g] | 1515±8 | IMRE | | 79BAR/SCO |
| | | | | 1514±8 | IMRE[o] | | 79BAR/SCO |
| $C_8H_{17}O_5^-$ | | | | | | | |
| $MeO(CH_2CH_2O)_2Me\cdot\cdot MeCO_2^-$ | | | | | | | |
| | | | *63±4* | *40±7* | TDAs | | 86MEO/SIE2 |
| $C_8H_{19}O_2^-$ | | | | | | | |
| nPrOH··tBu$CH_2O^-$ | | | | | | | |
| | -627±25 [c] | | *83±10* [g] | *55±8* | IMRE | | 84CAL/ROZ |
| $C_8H_{19}O_2^-$ | | | | | | | |
| tBuOH··tBu$O^-$ | | | | | | | |
| | -673±26 [c] | | *85±10* [g] | *58±8* | IMRE | | 84CAL/ROZ |
| $C_9HN_5^-$ | | | | | | | |
| 2,3,5,6-tetracyanopyridine$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 669±17* | |
| | | 2.17±0.07 | | | SI | | 67FAR/PAG |
| $C_9H_3F_6N^-$ | | | | | | | |
| 3,5-di$CF_3$-benzonitrile$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -1125±4* | |
| • | -1235±14 [b] | 1.14±0.10 | | | TDEq | | 87KEB/CHO |
| $C_9H_3F_6O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -1637±8* | |
| 3,5-di$CF_3$-benzoate$^-$ | | | | | | *BDE(A-H)= 444±13* | |
| • | -1810±19 [a] | 4.13±0.24 [d] | 1357±11 [g] | 1328±8 | IMRE | | 86TAF |
| $C_9H_4N^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 443±8* | |
| pCN-$C_6H_4C\equiv C^-$ | | | | | | *BDE(A-H)= 552±21* | |
| • | 383±18 [a] | 4.08±0.32 [d] | 1471±10 [g] | 1438±8 | IMRE | | 86TAF |
| $C_9H_5CrO_3^-$ | | | | | | *$\Delta_f H(AH)$= -350±9* | *77PED/RYL* |
| $(CO)_3CrC_6H_5^-$ | | | | | | | |
| | -326±30 [a] | | 1554±21 | | IMRB | | 85LAN/SQU |
| $C_9H_5F_3N^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -485±4* | |
| m$CF_3$-$C_6H_4$CHC$N^-$ | | | | | | | |
| • | -585±19 [a] | | 1431±15 [g] | 1403±8 | IMRE | | 86TAF |
| $C_9H_5F_3N^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -485±4* | |
| p$CF_3$-$C_6H_4$CHC$N^-$ | | | | | | | |
| • | -595±19 [a] | | 1420±15 [g] | 1393±8 | IMRE | | 86TAF |
| $C_9H_5F_6^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -1320±8* | |
| 3,5-di$CF_3$-$C_6H_3CH_2^-$ | | | | | | *BDE(A-H)= 368±13* | |
| • | -1340±19 [a] | 1.76±0.24 [d] | 1510±11 [g] | 1482±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_9H_5N_2^-$ | | | | | | | |
| Ph-$C(CN)_2^-$ | | | | | | | |
| • | | | 1348±11 [g] | 1317±8 | IMRE | | 86TAF |
| $C_9H_5N_2^-$ | | | | | *Est* | $\Delta_f H(AH)=$ 322±4 | |
| mCN-$C_6H_4$CHCN$^-$ | | | | | | | |
| • | 211±18 [a] | | 1419±13 [g] | 1390±8 | IMRE | | 81FUJ/MCI |
| $C_9H_5N_2^-$ | | | | | *Est* | $\Delta_f H(AH)=$ 322±4 | |
| pCN-$C_6H_4$CHCN$^-$ | | | | | | | |
| • | 192±18 [a] | | 1400±13 [g] | 1372±8 | IMRE | | 81FUJ/MCI |
| $C_9H_6BrO_2^-$ | | | | | | | |
| 4-Br-cubyl-$CO_2^-$ | | | | | - | BDE(A-H)= 444±8 | |
| • | | 3.61±0.21 [d] | 1407±12 [g] | 1378±8 | IMRE | | 86TAF |
| $C_9H_6F_3O^-$ | | | | | *Est* | $\Delta_f H(AH)=$ -715±4 | |
| p$COCF_3$-$C_6H_4CH_2^-$ | | | | | | | |
| • | -776±15 [a] | | 1470±11 [g] | 1439±8 | IMRE | | 86TAF |
| $C_9H_6N^-$ | | | | | | $\Delta_f H(AH)=$ 211±1 | *79VIS* |
| quinolinide$^-$ | | | | | | | |
| • | 289±9 [a] | | 1608±8 | 1572±8 | TDEq | | 87MEO |
| $C_9H_6NO^-$ | | | | | *Est2* | $\Delta_f H(AH)=$ 15±13 | |
| pCOCN-$C_6H_4CH_2^-$ | | | | | | | |
| • | -69±23 [a] | | 1446±11 [g] | 1418±8 | IMRE | | 86TAF |
| $C_9H_7^-$ | | | | | | $\Delta_f H(AH)=$ 163±1 | *80KUD/KUD* |
| indenide$^-$ | | | | | | BDE(A-H)= 351±13 | *82MCM/GOL* |
| • | 106±12 [a] | 1.98±0.24 [d] | 1473±11 [g] | 1442±8 | IMRE | | 86TAF |
| $C_9H_7F_3O^-$ | | | | | | | |
| m$CF_3$-acetophenone$^{-\cdot}$ | | | | | *Est* | $\Delta_f H(A)=$ -805±8 | |
| | -869±9 [b] | 0.663±0.009 | | | ECD | | 75WEN/KAO |
| $C_9H_7F_3O^-$ | | | | | | | |
| o$CF_3$-acetophenone$^{-\cdot}$ | | | | | *Est* | $\Delta_f H(A)=$ -805±8 | |
| | -867±9 [b] | 0.642±0.009 | | | ECD | | 75WEN/KAO |
| $C_9H_7F_3O^-$ | | | | | | | |
| p$CF_3$-acetophenone$^{-\cdot}$ | | | | | *Est* | $\Delta_f H(A)=$ -805±8 | |
| | -867±9 [b] | 0.642±0.009 | | | ECD | | 75WEN/KAO |
| $C_9H_7NO^-$ | | | | | | | |
| pCOMe-benzonitrile$^{-\cdot}$ | | | | | *Est* | $\Delta_f H(A)=$ 49±4 | |
| • | -61±14 [b] | 1.13±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.12±0.09 | | | TDEq | | 86CHO/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_9H_7O_2^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 238±21* | |
| cubyl-$CO_2^-$ | | | | | *BDE(A-H)= 444±8* | |
| • 136±33 [a] | 3.40±0.21 [d] | 1428±12 [g] | 1398±8 | IMRE | | 86TAF |
| $C_9H_7O_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= -464±4* | |
| pCOMe-benzoate$^-$ | | | | | *BDE(A-H)= 444±13* | |
| • -595±15 [a] | 3.69±0.24 [d] | 1399±11 [g] | 1369±8 | IMRE | | 86TAF |
| $C_9H_8^-$ | | | | | | |
| indene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 163±1* | *80KUD/KUD* |
| 146±3 [b] | 0.17±0.03 | | | ECD | | 81WOJ/FOL |
| $C_9H_8N^-$ | | | | *Est* | *$\Delta_f H(AH)$= 153±8* | |
| pMe-$C_6H_4CHCN^-$ | | | | | | |
| • 94±23 [a] | | 1471±15 [g] | 1443±8 | IMRE | | 86TAF |
| $C_9H_8NO^-$ | | | | *Est* | *$\Delta_f H(AH)$= 30±4* | |
| pOMe-$C_6H_4CHCN^-$ | | | | | | |
| • -29±19 [a] | | 1471±15 [g] | 1443±8 | IMRE | | 86TAF |
| $C_9H_8O^-$ | | | | | | |
| PhCH=CHCHO$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 21±8* | |
| -59±13 [b] | 0.82±0.04 | | | ECD | | 67WEN/CHE |
| $C_9H_9^-$ | | | | | *$\Delta_f H(AH)$= 151±1* | *82FUC/HAL* |
| 1-phenylcyclopropanide$^-$ | | | | | | |
| 260±17 [a] | | 1639±16 [g] | 1607±13 | IMRB | | 84AND/DEP |
| $C_9H_9^-$ | | | | | *$\Delta_f H(AH)$= 113±4* | *69BEN/CRU* |
| $CH_2$=C(Ph)$CH_2^-$ | | | | | | |
| 196±31 [a] | | 1613±27 [g] | 1586±23 | IMRB | | 84BAR/BUR |
| $C_9H_9ClO_2^-$ | | | | | | |
| Cl-triMe-benzoquinone$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= -243±17* | |
| • -423±21 [b] | 1.86±0.05 | | | IMRE | | 85FUK/MCI |
| $C_9H_9N^-$ | | | | | | |
| 3,5-diMe-benzonitrile$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= 149±13* | |
| • 39±21 [b] | 1.14±0.09 | | | TDEq | | 86CHO/KEB |
| $C_9H_9O^-$ | | | | | *$\Delta_f H(AH)$= -109±2* | *77PED/RYL* |
| MeCH=C(Ph)$O^-$ | | | | | *BDE(A-H)= 389±8* | |
| • -131±23 [a] | | 1508±21 [g] | 1481±8 | IMRE | | 79BAR/SCO |
| | | 1509±21 [g] | 1482±8 | IMRE | | 78CUM/KEB |
| | | | 1483±8 | IMRE[o] | | 79BAR/SCO |
| $C_9H_9O^-$ | | | | | | |
| MeOH··PhC≡C$^-$ | | | | | | |
| 70±26 [c] | | *56±10* [g] | *32±8* | IMRE | | 84CAL/ROZ |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_9H_9O^-$ | | | | | | *$\Delta_f H(AH)$= -98±2* | *77PED/RYL* |
| $PhCH=C(Me)O^-$ | | | | | | | |
| • | -163±16 [a] | | 1465±15 [g] | 1441±8 | IMRE | | 79BAR/SCO |
| | | | 1469±15 [g] | 1445±8 | IMRE | | 78CUM/KEB |
| | | | | 1451±8 | IMRE[o] | | 79BAR/SCO |
| $C_9H_9O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -119±4* | |
| $pCOMe-C_6H_4CH_2^-$ | | | | | | | |
| • | -136±15 [a] | | 1513±11 [g] | 1485±8 | IMRE | | 86TAF |
| $C_9H_9O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -244±4* | |
| $mOMe-C_6H_4C(=CH_2)O^-$ | | | | | | | |
| • | -264±15 [a] | | 1509±11 [g] | 1481±8 | IMRE | | 79BAR/SCO |
| | | | | 1490±8 | IMRE[o] | | 79BAR/SCO |
| $C_9H_9O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -320±4* | |
| $pCO_2Me-C_6H_4CH_2^-$ | | | | | | | |
| • | -336±15 [a] | | 1515±11 [g] | 1487±8 | IMRE | | 86TAF |
| $C_9H_9O_2S^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -161±4* | |
| $PhSO_2$-cyclopropanide$^-$ | | | | | | | |
| • | -179±14 [a] | | 1512±10 [g] | 1485±8 | IMRE | | 78CUM/KEB |
| $C_9H_9O_3^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -502±4* | |
| $mCO_2Et$-phenoxide$^-$ | | | | | | *BDE(A-H)= 362±8* | |
| • | -593±14 [a] | 2.44±0.19 [d] | 1439±10 [g] | 1410±8 | IMRE | | 81FUJ/MCI |
| $C_9H_{10}ClO^-$ | | | | | | | |
| $PhCH_2COMe\cdot\cdot Cl^-$ | | | | | | | |
| | | | | *45* | TDEq | | 82FRE/IKU |
| $C_9H_{10}ClO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -410±13* | |
| 4-Cl-bicyclo[2.2.2]octene-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -535±25 [a] | 3.63±0.21 [d] | 1405±12 [g] | 1376±8 | IMRE | | 86TAF |
| $C_9H_{10}O^-$ | | | | | | | |
| propiophenone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -109±2* | *77PED/RYL* |
| | -143±3 [b] | 0.351±0.004 | | | ECD | | 75WEN/KAO |
| $C_9H_{10}O_2^-$ | | | | | | | |
| benzyl acetate$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -313±8* | |
| | -328±18 [b] | 0.1±0.1 | | | ECD | | 83ZLA/LEE |
| $C_9H_{10}O_2^-$ | | | | | | | |
| triMe-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -220±8* | |
| • | -374±13 [b] | 1.60±0.05 | | | IMRE | | 85FUK/MCI |
| $C_9H_{10}O_4^-$ | | | | | | | |
| 2,3-diMeO-5-Me-benzoquinone$^{-\cdot}$ | | | | | | | |
| • | | 1.86±0.10 | | | TDEq | | 87KEB/CHO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_9H_{11}^-$ | | | | | $\Delta_f H(AH)=$ 4±1 | 77PED/RYL |
| $PhCMe_2^-$ | | | | | BDE(A−H)= 350±7 | 81ROB/STE |
| • 59±11 [a] | 0.79±0.18 [d] | 1586±10 [g] | 1560±8 | IMRE | | 79BAR/SCO |
| | | | 1554±8 | IMRE[o] | | 79BAR/SCO |
| $C_9H_{11}NO_2^-$ | | | | | | |
| 2,4,6-triMe-nitrobenzene$^{-\cdot}$ | | | | Est2 | $\Delta_f H(A)=$ −17±13 | |
| • −84±22 [b] | 0.70±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.67±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.72±0.05 | | | IMRE | | 85FUK/MCI |
| $C_9H_{11}O^-$ | | | | | $\Delta_f H(AH)=$ −195±13 | 77PED/RYL |
| miPr-phenoxide$^-$ | | | | | BDE(A−H)= 362±8 | |
| • −264±22 [a] | 2.21±0.19 [d] | 1461±10 [g] | 1432±8 | IMRE | | 81FUJ/MCI |
| $C_9H_{11}O^-$ | | | | | $\Delta_f H(AH)=$ −182±13 | 77PED/RYL |
| oiPr-phenoxide$^-$ | | | | | | |
| • −258±25 [a] | | 1454±12 [g] | 1423±8 | IMRE | | 81FUJ/MCI |
| $C_9H_{11}O^-$ | | | | | $\Delta_f H(AH)=$ −209±13 | 77PED/RYL |
| piPr-phenoxide$^-$ | | | | | BDE(A−H)= 362±13 | |
| • −278±22 [a] | 2.20±0.23 [d] | 1461±10 [g] | 1433±8 | IMRE | | 81FUJ/MCI |
| $C_9H_{11}O_2^-$ | | | | Est2 | $\Delta_f H(AH)=$ −363±13 | |
| bicyclo[2.2.2]octene-$CO_2^-$ | | | | | BDE(A−H)= 444±8 | |
| • −460±25 [a] | 3.35±0.21 [d] | 1433±12 [g] | 1403±8 | IMRE | | 86TAF |
| $C_9H_{11}O_2S^-$ | | | | Est | $\Delta_f H(AH)=$ −319±2 | |
| $PhSO_2CHEt^-$ | | | | | | |
| • −326±10 [a] | | 1523±8 [g] | 1491±8 | IMRE | | 78CUM/KEB |
| $C_9H_{12}BrO_2^-$ | | | | Est2 | $\Delta_f H(AH)=$ −480±13 | |
| 4-Br-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | BDE(A−H)= 444±8 | |
| • −598±25 [a] | 3.56±0.21 [d] | 1412±12 [g] | 1382±8 | IMRE | | 86TAF |
| $C_9H_{12}Cl^-$ | | | | | | |
| 1,3,5-triMe-benzene··$Cl^-$ | | | | | | |
| | | | *19* | TDEq | | 82FRE/IKU |
| $C_9H_{12}Cl^-$ | | | | | | |
| PhiPr··$Cl^-$ | | | | | | |
| | | | *23* | TDEq | | 82FRE/IKU |
| $C_9H_{12}Cl^-$ | | | | | | |
| PhnPr··$Cl^-$ | | | | | | |
| | | | *21* | TDEq | | 82FRE/IKU |
| $C_9H_{12}ClO_2^-$ | | | | Est2 | $\Delta_f H(AH)=$ −523±13 | |
| 3-Cl-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | BDE(A−H)= 444±8 | |
| • −629±25 [a] | 3.44±0.21 [d] | 1423±12 [g] | 1394±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_9H_{12}ClO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −530±13* | |
| 4-Cl-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −645±25 [a] | 3.53±0.21 [d] | 1415±12 [g] | 1385±8 | IMRE | | 86TAF |
| $C_9H_{12}FO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −677±13* | |
| 4-F-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −790±25 [a] | 3.51±0.21 [d] | 1417±12 [g] | 1387±8 | IMRE | | 86TAF |
| $C_9H_{12}N^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 67±8* | |
| mNMe$_2$-$C_6H_4CH_2^-$ | | | | | | | |
| | 134±32 [a] | | 1597±23 [g] | 1569±21 | IMRB | | 83CAL/BAR |
| $C_9H_{12}N^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 71±8* | |
| pNMe$_2$-$C_6H_4CH_2^-$ | | | | | | | |
| | 155±32 [a] | | 1614±23 [g] | 1586±21 | IMRB | | 83CAL/BAR |
| $C_9H_{12}NO_4^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −537±13* | |
| 4-$NO_2$-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −664±25 [a] | 3.65±0.21 [d] | 1403±12 [g] | 1374±8 | IMRE | | 86TAF |
| $C_9H_{13}O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 8±13* | |
| bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −82±23 [a] | 3.27±0.20 [d] | 1440±11 [g] | 1411±8 | IMRE | | 86TAF |
| $C_9H_{15}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −279±8* | |
| cyclononanone enolate$^-$ | | | | | | | |
| • | | 1.69±0.06 | | | PD | | 78ZIM/JAC |
| $C_9H_{19}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −415±4* | |
| $(tBu)_2CHO^-$ | | | | | | *BDE(A−H)= 438±4* | |
| • | −412±16 [a] | 2.25±0.17 [d] | 1533±12 [g] | 1505±8 | IMRE | | 79BAR/SCO |
| | | | | 1509±8 | IMRE[o] | | 79BAR/SCO |
| $C_9H_{19}O^-$ | | | | | | *$\Delta_f H(AH)$= −376±2* | *77PED/RYL* |
| $nC_9H_{19}O^-$ | | | | | | *BDE(A−H)= 436±4* | |
| • | −353±13 [a] | 2.0±0.2 [d] | 1553±11 | 1525±13 [h] | CIDC | | 83BOA/HOU |
| | | | 1551±10 | | CIDC[o] | | 83BOA/HOU |
| $C_9H_{21}BF^-$ | | | | | | | |
| $iPr_3B\cdot\cdot F^-$ | | | | | | | |
| | −773 [c] | | *272* | | IMRB | $F^-A$: $iPr_2BF > iPr_3B > Et_2BF > Et_3B$ | 77MUR/BEA2 |
| $C_9H_{21}O_2^-$ | | | | | | | |
| $tBuOH\cdot\cdot tBuCH_2O^-$ | | | | | | | |
| | −687±27 [c] | | *85±10* [g] | *57±8* | IMRE | | 84CAL/ROZ |
| $C_{10}N_6^-$ | | | | | | | |
| hexacyanobutadiene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 586±42* | |
| | | 3.3±0.1 | | | SI | | 69PAG/GOO |
| | | 3.3±0.1 | | | SI | | 67FAR/PAG |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{10}HN_4^-$ | | | | | | | |
| 2,3,5,6-tetracyanophenide$^-$ | | | | | | | |
| | | 2.41±0.04 | | | SI | | 67FAR/PAG |
| $C_{10}H_2F_{12}O_6U^-$ | | | | | | | |
| $UO_2$.(hexafluoroAcAc)$_2^-$ | | | | | | | |
| | | 1.9±0.3 | | | NBIP | | 82YOK/QUI |
| $C_{10}H_2N_4^-$ | | | | | | | |
| 1,2,4,5-tetracyanobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 627±13* | |
| | | 2.2±0.2 | | | SI | | 67FAR/PAG |
| $C_{10}H_4Cl_2O_2^-$ | | | | | | | |
| 2,3-diCl-1,4-naphthoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −162±10* | |
| • | −374±20 [b] | 2.19±0.10 | | | TDEq | | 87KEB/CHO |
| | | 2.08±0.11 | | | IMRE | | 85GRI/CAL |
| $C_{10}H_5O_2^-$ | | | | | | *$\Delta_f H(AH)$= −111±4* | *77PED/RYL* |
| 1,4-naphthoquinonide$^-$ | | | | | | | |
| | | | 1641±3 [g] | <1607 | IMRB | | 87JOH/SPE |
| $C_{10}H_6Cl_4O_4^-$ | | | | | | | |
| dimethyl tetrachloroterephthalate$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 785±13* | |
| | 711 [b] | 0.8 | | | ECD | | 68KUH/LEV |
| $C_{10}H_6N_2O_4^-$ | | | | | | | |
| 1,3-diNO$_2$-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 120±4* | |
| • | −52±14 [b] | 1.78±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{10}H_6N_2O_4^-$ | | | | | | | |
| 1,5-diNO$_2$-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 120±4* | |
| • | −51±14 [b] | 1.77±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{10}H_6O_2^-$ | | | | | | | |
| 1,4-naphthoquinone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −111±4* | *77PED/RYL* |
| • | −286±14 [b] | 1.81±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.71±0.11 | | | IMRE | | 85GRI/CAL |
| | | 1.71±0.05 | | | IMRE | | 85FUK/MCI |
| | | >0.8 | | | ECD | | 83CHE/WEN |
| | | >0.6 | | | ES | | 70COL/CHR |
| $C_{10}H_7^-$ | | | | | | *$\Delta_f H(AH)$= 150±1* | *82COL/JIM* |
| naphthalenide$^-$ | | | | | | | |
| • | 272±6 [a] | | 1651±5 | 1611±5 | TDEq | | 87MEO |
| $C_{10}H_7Cl^-$ | | | | | | | |
| 1-Cl-naphthalene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 120±10* | *77PED/RYL* |
| | 93±10 [b] | 0.277±0.003 | | | ECD | | 69STE/WEN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{10}H_7NO_2^-$ | | | | | | |
| 1-$NO_2$-naphthalene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 150±2* | *77PED/RYL* |
| • 31±12 [b] | 1.23±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{10}H_7NO_2^-$ | | | | | | |
| 2-$NO_2$-naphthalene$^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= 150±8* | |
| • 36±18 [b] | 1.18±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{10}H_7N_2^-$ | | | | | | |
| pMe-$C_6H_4$-$C(CN)_2^-$ | | | | | | |
| • | | 1354±12 [g] | 1323±8 | IMRE | | 86TAF |
| $C_{10}H_7O^-$ | | | | | *$\Delta_f H(AH)$= -30±1* | *77PED/RYL* |
| 2-naphthoxide$^-$ | | | | | | |
| • -122±11 [a] | | 1438±10 [g] | 1408±8 | IMRE | | 86TAF |
| $C_{10}H_8^-$ | | | | | | |
| azulene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 289±3* | *77PED/RYL* |
| • 223±13 [b] | 0.69±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.75±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.68±0.04 | | | Kine | | 85GRI/CHO2 |
| | 0.52±0.01 | | | ECD | | 81WOJ/FOL |
| | >0.5 | | | ES | | 70CHA/CHR |
| | 0.656±0.008 | | | ECD | | 66BEC/CHE |
| $C_{10}H_8^-$ | | | | | | |
| naphthalene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 150±1* | *82COL/JIM* |
| 137±6 [b] | 0.14±0.05 | | | ECD | | 83ZLA/LEE |
| | 0.13±0.04 | | | ECD | | 81WOJ/FOL |
| | 0.148±0.006 | | | ECD | | 66BEC/CHE |
| $C_{10}H_9BrCl_2O_2^-$ | | | | | | |
| 2,6-diCl-Br-tBu-benzoquinone$^{-\cdot}$ | | | | | | |
| • | 2.42±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{10}H_9N_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= 164±13* | |
| 1,5-diaminonaphthalenide$^-$ | | | | | | |
| • 127±22 [a] | | 1493±10 [g] | 1463±8 | IMRE | | 82ARN/VEN |
| | | | 1472±8 | IMRE[o] | | 82ARN/VEN |
| $C_{10}H_9N_2^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 192±8* | |
| 1,8-diaminonaphthalenide$^-$ | | | | | | |
| • | | | 1441±8 | IMRE | | 82ARN/VEN |
| | | | 1450±8 | IMRE[o] | | 82ARN/VEN |
| $C_{10}H_9O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= -250±2* | |
| PhCOCH=C(Me)O$^-$ | | | | | | |
| • -358±12 [a] | | 1422±10 [g] | 1393±8 | IMRE | | 78CUM/KEB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{10}Cl_2O_2^-$ | | | | | | | |
| 2,3-diCl-tBu-benzoquinone$^{-\cdot}$ | | | | | | | |
| * | | 2.25±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{10}H_{10}F_3O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -1028±13* | |
| 4-$CF_3$-bicyclo[2.2.2]octene-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| * | -1153±25 [a] | 3.63±0.21 [d] | 1405±12 [g] | 1376±8 | IMRE | | 86TAF |
| $C_{10}H_{10}NO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -231±13* | |
| 4-CN-bicyclo[2.2.2]octene-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| * | -367±25 [a] | 3.75±0.21 [d] | 1394±12 [g] | 1365±8 | IMRE | | 86TAF |
| $C_{10}H_{10}O_4^-$ | | | | | | | |
| dimethyl isophthalate$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -681±8* | |
| | -734 [b] | 0.6 | | | ECD | | 68KUH/LEV |
| $C_{10}H_{10}O_4^-$ | | | | | | | |
| dimethyl phthalate$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -654±17* | |
| | -707 [b] | 0.6 | | | ECD | | 68KUH/LEV |
| $C_{10}H_{10}O_4^-$ | | | | | | | |
| dimethyl terephthalate$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -681±8* | |
| | -743 [b] | 0.6 | | | ECD | | 68KUH/LEV |
| $C_{10}H_{11}ClO_2^-$ | | | | | | | |
| 2-Cl-5-tBu-benzoquinone$^{-\cdot}$ | | | | | | | |
| * | | 2.06±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{10}H_{11}N_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= 195±8* | |
| p$NMe_2$-$C_6H_4CHCN^-$ | | | | | | | |
| * | 143±23 [a] | | 1478±15 [g] | 1450±8 | IMRE | | 86TAF |
| $C_{10}H_{11}O_2^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -252±8* | |
| triMe-benzoquinone-$CH_2^-$ | | | | | | | |
| | | 0.80±0.09 | | | SI | | 67FAR/PAG |
| $C_{10}H_{12}F_3O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -1148±13* | |
| 4-$CF_3$-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| * | -1264±25 [a] | 3.55±0.21 [d] | 1413±12 [g] | 1384±8 | IMRE | | 86TAF |
| $C_{10}H_{12}NO^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -130±8* | |
| m$CONMe_2$-$C_6H_4CH_2^-$ | | | | | | | |
| * | -95±19 [a] | | 1564±11 [g] | 1536±8 | IMRE | | 86TAF |
| $C_{10}H_{12}NO^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -130±8* | |
| p$CONMe_2$-$C_6H_4CH_2^-$ | | | | | | | |
| * | -131±19 [a] | | 1529±11 [g] | 1501±8 | IMRE | | 86TAF |
| $C_{10}H_{12}NO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -354±13* | |
| 2-CN-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| * | -478±25 [a] | 3.63±0.21 [d] | 1405±12 [g] | 1376±8 | IMRE | | 86TAF |

**Table 2. Negative Ion Table - Continued**

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{10}H_{12}NO_2^-$ | | | | Est2 | *$\Delta_f H(AH)$= −354±13* | |
| 3-CN-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −470±25 [a] | 3.55±0.21 [d] | 1413±12 [g] | 1384±8 | IMRE | | 86TAF |
| $C_{10}H_{12}NO_2^-$ | | | | Est2 | *$\Delta_f H(AH)$= −350±13* | |
| 4-CN-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −476±25 [a] | 3.64±0.21 [d] | 1405±12 [g] | 1375±8 | IMRE | | 86TAF |
| $C_{10}H_{12}O^-$ | | | | | | |
| 2,4,6-triMe-benzaldehyde$^{-\cdot}$ | | | | Est2 | *$\Delta_f H(A)$= −138±13* | |
| −180±17 [b] | 0.44±0.04 | | | ECD | | 69WEN/RIS |
| $C_{10}H_{12}O_2^-$ | | | | | | |
| 2-iPr-5-Me-benzoquinone$^{-\cdot}$ | | | | | | |
| • | 1.79±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{10}H_{12}O_2^-$ | | | | | | |
| tetraMe-benzoquinone$^{-\cdot}$ | | | | Est | *$\Delta_f H(A)$= −252±8* | |
| • −405±18 [b] | 1.59±0.10 | | | TDEq | | 87KEB/CHO |
| | 1.52±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{10}H_{13}O^-$ | | | | Est | *$\Delta_f H(AH)$= −202±8* | |
| mtBu-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| • −274±18 [a] | 2.23±0.19 [d] | 1459±10 [g] | 1430±8 | IMRE | | 81FUJ/MCI |
| $C_{10}H_{13}O^-$ | | | | Est2 | *$\Delta_f H(AH)$= −186±13* | |
| otBu-phenoxide$^-$ | | | | | | |
| • −270±25 [a] | | 1447±12 [g] | 1415±8 | IMRE | | 81FUJ/MCI |
| $C_{10}H_{13}O^-$ | | | | Est | *$\Delta_f H(AH)$= −202±8* | |
| ptBu-phenoxide$^-$ | | | | | *BDE(A−H)= 362±13* | |
| • −274±18 [a] | 2.24±0.23 [d] | 1458±10 [g] | 1429±8 | IMRE | | 81FUJ/MCI |
| $C_{10}H_{13}O_2^-$ | | | | Est2 | *$\Delta_f H(AH)$= −395±13* | |
| 4-Me-bicyclo[2.2.2]octene-$CO_2^-$ | | | | | *BDE(A−H)= 444±8* | |
| • −497±25 [a] | 3.39±0.21 [d] | 1428±12 [g] | 1399±8 | IMRE | | 86TAF |
| $C_{10}H_{13}O_2S^-$ | | | | Est | *$\Delta_f H(AH)$= −349±2* | |
| $PhSO_2CHiPr^-$ | | | | | | |
| • −362±12 [a] | | 1517±10 [g] | 1487±8 | IMRE | | 78CUM/KEB |
| $C_{10}H_{14}^-$ | | | | | | |
| 1,2,3,5-tetramethylbenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −42±8* | *75GOO* |
| −52±10 [b] | 0.11±0.01 | | | ECD | | 81WOJ/FOL |
| $C_{10}H_{14}^-$ | | | | | | |
| 1,2,4,5-tetramethylbenzene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −46±8* | *75GOO* |
| −51±10 [b] | 4.80±0.02 | | | ECD | | 81WOJ/FOL |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{10}H_{15}^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -33±17* | |
| pentaMe-cyclopentadienide$^-$ | | | | | | | |
| • | -54±29 [a] | | 1510±12 [g] | 1485±8 | IMRE | | 86TAF |
| $C_{10}H_{15}O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -515±13* | |
| 4-Me-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -609±25 [a] | 3.31±0.21 [d] | 1436±12 [g] | 1407±8 | IMRE | | 86TAF |
| $C_{10}H_{15}O_3^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -628±13* | |
| 3-OMe-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -720±25 [a] | 3.30±0.21 [d] | 1438±12 [g] | 1408±8 | IMRE | | 86TAF |
| $C_{10}H_{15}O_3^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -631±13* | |
| 4-OMe-bicyclo[2.2.2]octane-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -732±25 [a] | 3.38±0.21 [d] | 1430±12 [g] | 1400±8 | IMRE | | 86TAF |
| $C_{10}H_{17}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= -304±4* | |
| cyclodecanone enolate$^-$ | | | | | | | |
| • | | 1.83±0.07 | | | PD | | 78ZIM/JAC |
| $C_{10}H_{23}O_2^-$ | | | | | | | |
| $tBuCH_2OH\cdot\cdot tBuCH_2O^-$ | | | | | | | |
| | -698±26 [c] | | *90±10 [g]* | *62±8* | IMRE | | 84CAL/ROZ |
| $C_{11}H_7N^-$ | | | | | | | |
| 1-naphthonitrile$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 286±13* | |
| • | 221±22 [b] | 0.68±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.68±0.09 | | | TDEq | | 86CHO/KEB |
| $C_{11}H_7N^-$ | | | | | | | |
| 2-naphthonitrile$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 286±13* | |
| • | 223±22 [b] | 0.65±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.65±0.09 | | | TDEq | | 86CHO/KEB |
| $C_{11}H_8O^-$ | | | | | | | |
| 1-naphthaldehyde$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 31±8* | |
| • | -37±18 [b] | 0.70±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.68±0.02 | | | ECD | | 75WEN/KAO |
| | | 0.74±0.07 | | | ECD | | 67WEN/CHE |
| $C_{11}H_8O^-$ | | | | | | | |
| 2-naphthaldehyde$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 31±8* | |
| • | -32±18 [b] | 0.65±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.62±0.02 | | | ECD | | 75WEN/KAO |
| | | 0.62±0.04 | | | ECD | | 67WEN/CHE |
| $C_{11}H_8O_2^-$ | | | | | | | |
| 2-Me-1,4-naphthoquinone$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -127±8* | |
| • | -295±18 [b] | 1.74±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.66±0.05 | | | IMRE | | 85FUK/MCI |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{11}H_9NO_2^-$ | | | | | | | |
| 2-Me-1-$NO_2$-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 117±4* | |
| • | 18±14 [b] | 1.03±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{11}H_9NO_3^-$ | | | | | | | |
| 4-MeO-1-$NO_2$-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -21±4* | |
| •. | -127±14 [b] | 1.10±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{11}H_9O_4^-$ | | | | | | | |
| 4-$CO_2$Me-cubyl-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | | 3.55±0.21 [d] | 1413±12 [g] | 1384±8 | IMRE | | 86TAF |
| $C_{11}H_{10}^-$ | | | | | | | |
| 1-Me-naphthalene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 113±2* | *74SAB/CHA* |
| | 97±13 [b] | 0.2±0.1 | | | ECD | | 81WOJ/FOL |
| $C_{11}H_{10}^-$ | | | | | | | |
| 2-Me-naphthalene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 111±2* | *74SAB/CHA* |
| | 97±9 [b] | 0.14±0.07 | | | ECD | | 81WOJ/FOL |
| $C_{11}H_{13}O^-$ | | | | | | | |
| nPrOH··PhC≡C$^-$ | | | | | | | |
| | 8±26 [c] | | *64±10 [g]* | *37±8* | IMRE | | 84CAL/ROZ |
| $C_{11}H_{14}ClO_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -577±13* | |
| 3-Cl-1-adamantyl-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -692±23 [a] | | 1416±11 [g] | 1387±8 | IMRE | | 86TAF |
| $C_{11}H_{14}O^-$ | | | | | | | |
| 2,4,6-triMe-acetophenone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -205±4* | *77PED/RYL* |
| | -252±8 [b] | 0.49±0.04 | | | ECD | | 69WEN/RIS |
| $C_{11}H_{15}NO_2^-$ | | | | | | | |
| p-t-amyl-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -97±13* | |
| | -306±29 [b] | 2.2±0.2 | | | CIDC | | 84BUR/FUK |
| $C_{11}H_{15}O_2^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= -532±13* | |
| 1-adamantyl-$CO_2^-$ | | | | | | *BDE(A-H)= 444±8* | |
| • | -624±23 [a] | | 1438±11 [g] | 1408±8 | IMRE | | 86TAF |
| $C_{11}H_{16}^-$ | | | | | | | |
| pentamethylbenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -75±8* | |
| | -93±10 [b] | 0.18±0.01 | | | ECD | | 81WOJ/FOL |
| $C_{11}H_{25}O_2^-$ | | | | | | | |
| tBu$CH_2$OH··tBuCH(Me)O$^-$ | | | | | | | |
| | -736±28 [c] | | *89±10 [g]* | *62±8* | IMRE | | 84CAL/ROZ |
| $C_{12}F_{10}^-$ | | | | | | | |
| $C_6F_5$-$C_6F_5^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -785±13* | |
| • | -873±22 [b] | 0.91±0.10 | | | TDEq | | 87KEB/CHO |
| | | 0.91±0.10 | | | IMRE | | 86CHO/GRI |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{12}N_6^-$ | | | | | | | |
| hexacyanobenzene$^{-\cdot}$ | | | | | *Est* | *$\Delta_fH(A)$= 900±21* | |
| | | 2.5±0.1 | | | SI | | 67FAR/PAG |
| $C_{12}H_4N_4^-$ | | | | | | | |
| tetracyanoquinodimethane$^{-\cdot}$ | | | | | | *$\Delta_fH(A)$= 770±10* | *77PED/RYL* |
| | • 500±19 [b] | 2.8±0.1 | | | NBIP | | 74KLO/COM |
| | | 2.8±0.3 | | | NBIP | | 77COM/COO |
| | | 2.8±0.1 | | | SI | | 79NAZ/POK |
| | | 2.9±0.2 | | | SI | | 67FAR/PAG |
| $C_{12}H_8^-$ | | | | | | | |
| acenaphthylene$^{-\cdot}$ | | | | | | *$\Delta_fH(A)$= 260* | *81KUD/KUD* |
| | 221±3 [b] | 0.40±0.03 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_8N^-$ | | | | | | *$\Delta_fH(AH)$= 229±4* | *81KUD/KUD2* |
| carbazolide$^-$ | | | | | | | |
| | • 143±15 [a] | | 1444±11 [g] | 1412±8 | IMRE | | 86TAF |
| $C_{12}H_8O_2^-$ | | | | | | | |
| 2-Ph-benzoquinone$^{-\cdot}$ | | | | | | | |
| | • | 2.04±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{12}H_9NO_2^-$ | | | | | | | |
| mPh-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_fH(A)$= 167±8* | |
| | • 58±18 [b] | 1.13±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{12}H_9NO_2^-$ | | | | | | | |
| oPh-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_fH(A)$= 188±8* | |
| | • 85±18 [b] | 1.07±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{12}H_9NO_2^-$ | | | | | | | |
| pPh-nitrobenzene$^{-\cdot}$ | | | | | *Est2* | *$\Delta_fH(A)$= 167±8* | |
| | • 52±18 [b] | 1.20±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{12}H_{10}^-$ | | | | | | | |
| biphenyl$^{-\cdot}$ | | | | | | *$\Delta_fH(A)$= 182±1* | *77PED/RYL* |
| | 170±5 [b] | 0.13±0.04 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{10}N^-$ | | | | | | *$\Delta_fH(AH)$= 219±3* | *78STE* |
| $Ph_2N^-$ | | | | | | | |
| | • 157±14 [a] | | 1468±11 [g] | 1438±8 | IMRE | | 86TAF |
| $C_{12}H_{10}O^-$ | | | | | | | |
| 1-acetonaphthone$^{-\cdot}$ | | | | | *Est* | *$\Delta_fH(A)$= -21±8* | |
| | -79±11 [b] | 0.60±0.03 | | | ECD | | 75WEN/KAO |
| $C_{12}H_{12}^-$ | | | | | | | |
| 1,4-diMe-naphthalene$^{-\cdot}$ | | | | | | *$\Delta_fH(A)$= 83±8* | *69STU/WES* |
| | 59±16 [b] | 0.25±0.08 | | | ECD | | 81WOJ/FOL |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X \cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X \cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X \cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{12}H_{12}^-$ | | | | | | | |
| 1-Et-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 96±8* | |
| | 82±14 [b] | 0.15±0.06 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{12}^-$ | | | | | | | |
| 2,3-diMe-naphthalene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 84±8* | *69STU/WES* |
| | 67±21 [b] | 0.2±0.1 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{12}^-$ | | | | | | | |
| 2,6-diMe-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 84±4* | |
| | 68±11 [b] | 0.16±0.07 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{12}^-$ | | | | | | | |
| 2-Et-naphthalene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 86±8* | |
| | 67±14 [b] | 0.20±0.06 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{14}O_4^-$ | | | | | | | |
| diethyl phthalate$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −688±12* | *77PED/RYL* |
| | −740 [b] | 0.5 | | | ECD | | 68KUH/LEV |
| $C_{12}H_{15}O_4^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −753±17* | |
| 4-$CO_2$Et-bicyclo[2.2.2]octene-$CO_2^-$ | | | | | | *BDE(A−H)= 444±8* | |
| • | −865±28 [a] | 3.50±0.20 [d] | 1418±11 [g] | 1389±8 | IMRE | | 86TAF |
| $C_{12}H_{18}^-$ | | | | | | | |
| hexamethylbenzene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −87±3* | *77PED/RYL* |
| | −98±4 [b] | 0.12±0.02 | | | ECD | | 81WOJ/FOL |
| $C_{12}H_{21}O^-$ | | | | | *Est* | *$\Delta_f H(AH)$= −350±8* | |
| cyclododecanone enolate$^-$ | | | | | | | |
| • | | 1.90±0.07 | | | PD | | 78ZIM/JAC |
| $C_{12}H_{27}O_2^-$ | | | | | | | |
| tBuCH(Me)OH··tBuCH(Me)O$^-$ | | | | | | | |
| | −768±31 [c] | | *90±10* [g] | *62±8* | IMRE | | 84CAL/ROZ |
| $C_{13}F_{10}O^-$ | | | | | | | |
| $(C_6F_5)_2CO^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= −1868±21* | |
| • | −2023±31 [b] | 1.61±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.61±0.10 | | | IMRE | | 85GRI/CAL |
| $C_{13}H_8F_2O^-$ | | | | | | | |
| p,p'-diF-benzophenone$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= −327±8* | |
| • | −403±13 [b] | 0.79±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{13}H_9^-$ | | | | | | *$\Delta_f H(AH)$= 187±1* | *81KUD/KUD* |
| fluorenide$^-$ | | | | | | *BDE(A−H)= 339±13* | *70TRO/BAZ* |
| • | 129±12 [a] | 1.86±0.24 [d] | 1472±11 [g] | 1439±8 | IMRE | | 86TAF |
| | | | 1478±11 [g] | 1446±8 | IMRE | | 78CUM/KEB |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{13}H_9^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 226±13* | |
| perinaphthalenide$^-$ | | | | | | |
| * | 1.1±0.1 | | | PD | | 79GYG/PET |
| $C_{13}H_9ClO^-$ | | | | | | |
| pCl-benzophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 29±8* | |
| * −53±13 [b] | 0.85±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{13}H_9FO^-$ | | | | | | |
| pF-benzophenone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −134±8* | |
| * −196±18 [b] | 0.64±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.74±0.05 | | | IMRE | | 85FUK/MCI |
| $C_{13}H_9O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −131±8* | |
| mCOPh-phenoxide$^-$ | | | | | *BDE(A−H)= 362±8* | |
| * −232±18 [a] | 2.54±0.19 [d] | 1428±10 [g] | 1400±8 | IMRE | | 81FUJ/MCI |
| $C_{13}H_9O_2^-$ | | | | *Est* | *$\Delta_f H(AH)$= −131±8* | |
| pCOPh-phenoxide$^-$ | | | | | | |
| * −268±19 [a] | | 1393±11 [g] | 1364±8 | IMRE | | 81FUJ/MCI |
| $C_{13}H_{10}^-$ | | | | | | |
| fluorene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 188±1* | *81KUD/KUD* |
| 162±3 [b] | 0.28±0.03 | | | ECD | | 81WOJ/FOL |
| $C_{13}H_{10}Cl^-$ | | | | *Est* | *$\Delta_f H(AH)$= 110±4* | |
| mCl-$C_6H_4$-CH(Ph)$^-$ | | | | | | |
| * 85±16 [a] | | 1505±12 [g] | 1482±8 | IMRE | | 86TAF |
| $C_{13}H_{10}F^-$ | | | | *Est* | *$\Delta_f H(AH)$= −53±8* | |
| mF-$C_6H_4$CH(Ph)$^-$ | | | | | | |
| * −76±21 [a] | | 1507±12 [g] | 1479±8 | IMRE | | 86TAF |
| $C_{13}H_{10}O^-$ | | | | | | |
| benzophenone$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 50±3* | *78SAB/LAF3* |
| * −10±13 [b] | 0.62±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.61±0.11 | | | IMRE | | 85GRI/CAL |
| | 0.69±0.05 | | | IMRE | | 85FUK/MCI |
| | 0.64±0.05 | | | ECD | | 83CHE/WEN |
| $C_{13}H_{11}^-$ | | | | | *$\Delta_f H(AH)$= 140±3* | *77PED/RYL* |
| $Ph_2CH^-$ | | | | | *BDE(A−H)= 351±4* | *82MCM/GOL* |
| * 131±13 [a] | 1.47±0.14 [d] | 1521±10 [g] | 1499±8 | IMRE | | 79BAR/SCO |
| | | 1512±10 [g] | 1489±8 | IMRE | | 78CUM/KEB |
| | 0.8±0.3 | | | SI | | 68GAI/PAG |
| | | | 1502±8 | IMRE[o] | | 79BAR/SCO |
| $C_{13}H_{11}FO^-$ | | | | | | |
| mF-$C_6H_4CH_2$OPh$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= −166±4* | |
| | 0.28±0.09 | | | ECD | | 84HER/WEN |

**Table 2. Negative Ion Table - Continued**

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{13}H_{11}F_{12}PUO_{10}^-$ | | | | | | | |
| $UO_2$.(hexafluoroAcAc)$_2$.OP(OMe)$_3^-$ | | | | | | | |
| | | 1.5±0.3 | | | NBIP | | 82YOK/QUI |
| $C_{13}H_{11}O_2S^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= −160±13* | |
| $pSO_2Ph-C_6H_4CH_2^-$ | | | | | | | |
| | • −187±23 [a] | | 1504±11 [g] | 1473±8 | IMRE | | 86TAF |
| $C_{13}H_{12}^-$ | | | | | | | |
| $Ph_2CH_2^{-\cdot}$ | | | | | | | |
| | 125±7 [b] | 0.16±0.04 | | | ECD | | 81WOJ/FOL |
| $C_{13}H_{12}Cl^-$ | | | | | | | |
| $Ph_2CH_2\cdot\cdot Cl^-$ | | | | | | | |
| | | | | *31* | TDEq | | 82FRE/IKU |
| $C_{13}H_{15}O^-$ | | | | | | | |
| tBuOH··PhC≡C$^-$ | | | | | | | |
| | −57±28 [c] | | *72±10* [g] | *44±8* | IMRE | | 84CAL/ROZ |
| $C_{13}H_{21}O_2^-$ | | | | | | | |
| tBuCH(Me)OH··$PhCH_2O^-$ | | | | | | | |
| | −523±27 [c] | | *90±10* [g] | *63±8* | IMRE | | 84CAL/ROZ |
| $C_{14}H_7ClO_2^-$ | | | | | | | |
| 1–Cl–9,10–anthraquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= −125±13* | |
| | • −290±22 [b] | 1.71±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{14}H_7O_2^-$ | | | | | | *$\Delta_f H(AH)$= −95±7* | *77PED/RYL* |
| 9,10–anthraquinonide$^-$ | | | | | | | |
| | | | | 1607±17 | IMRB | | 87JOH/SPE |
| $C_{14}H_8O_2^-$ | | | | | | | |
| 9,10–anthraquinone$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −95±7* | *77PED/RYL* |
| | −249±16 [b] | 1.59±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.1±0.1 | | | SI | | 69PAG/GOO |
| $C_{14}H_9Cl^-$ | | | | | | | |
| 1–Cl–anthracene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 201±4* | |
| | • 126±14 [b] | 0.78±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{14}H_9Cl^-$ | | | | | | | |
| 2–Cl–anthracene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 201±4* | |
| | • 128±14 [b] | 0.75±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{14}H_9Cl^-$ | | | | | | | |
| 9–Cl–anthracene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 201±4* | |
| | • 118±14 [b] | 0.86±0.10 | | | TDEq | | 87KEB/CHO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{14}H_9NO_2^-$ | | | | | | |
| 9-$NO_2$-anthracene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 213±4* | |
| • 75±14 [b] | 1.43±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{14}H_{10}^-$ | | | | | | |
| PhC≡CPh$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 402±4* | *82CHI/LIE* |
| 371±11 [b] | 0.32±0.07 | | | ECD | | 81WOJ/FOL |
| $C_{14}H_{10}^-$ | | | | | | |
| anthracene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 230±1* | *79KUD/KUD4* |
| • 172±11 [b] | 0.60±0.10 | | | TDEq | | 87KEB/CHO |
| | 0.48±0.04 | | | ECD | | 81WOJ/FOL |
| | 0.57±0.02 | | | ECD | | 68LYO/MOR |
| | 0.556±0.008 | | | ECD | | 66BEC/CHE |
| $C_{14}H_{10}^-$ | | | | | | |
| phenanthrene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 207±1* | *79KUD/KUD4* |
| 181±4 [b] | 0.27±0.04 | | | ECD | | 81WOJ/FOL |
| | 0.307±0.007 | | | ECD | | 66BEC/CHE |
| $C_{14}H_{10}F_3^-$ | | | | *Est* | *$\Delta_f H(AH)$= -528±4* | |
| mCF$_3$-C$_6$H$_4$-CH(Ph)$^-$ | | | | | | |
| • -574±14 [a] | | 1484±10 [g] | 1462±8 | IMRE | | 86TAF |
| $C_{14}H_{10}F_{12}O_7U^-$ | | | | | | |
| UO$_2$.(hexafluoroAcAc)$_2$.THF$^-$ | | | | | | |
| | 1.6±0.2 | | | NBIP | | 82YOK/QUI |
| $C_{14}H_{10}N^-$ | | | | *Est* | *$\Delta_f H(AH)$= 276±4* | |
| mCN-C$_6$H$_4$-CH(Ph)$^-$ | | | | | | |
| • 216±14 [a] | | 1470±10 [g] | 1448±8 | IMRE | | 86TAF |
| $C_{14}H_{11}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 155±8* | |
| 2-Me-fluorenide$^-$ | | | | | | |
| • 100±21 [a] | | 1475±12 [g] | 1443±8 | IMRE | | 86TAF |
| $C_{14}H_{11}^-$ | | | | *Est2* | *$\Delta_f H(AH)$=` 109±13* | |
| 9-Me-fluorenide$^-$ | | | | | | |
| • 47±23 [a] | | 1468±11 [g] | 1437±8 | IMRE | | 86TAF |
| $C_{14}H_{11}O^-$ | | | | *Est* | *$\Delta_f H(AH)$= 26±4* | |
| pCOPh-C$_6$H$_4$CH$_2^-$ | | | | | | |
| • 3±15 [a] | | 1507±11 [g] | 1479±8 | IMRE | | 86TAF |
| $C_{14}H_{11}O_2S^-$ | | | | *Est2* | *$\Delta_f H(AH)$= -141±13* | |
| 9-SO$_2$Me-fluorenide$^-$ | | | | | | |
| • -287±23 [a] | | 1384±11 [g] | 1351±8 | IMRE | | 86TAF |
| $C_{14}H_{12}^-$ | | | | | | |
| (E)-PhCH=CHPh$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 235±3* | *77PED/RYL* |
| 197±9 [b] | 0.39±0.06 | | | ECD | | 81WOJ/FOL |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $C_{14}H_{12}^-$ | | | | | | | |
| $Ph_2C=CH_2^{-\cdot}$ | | | | | | | |
| | 208±10 [b] | 0.39±0.06 | | | ECD | | 81WOJ/FOL |
| $C_{14}H_{15}O_2^-$ | | | | | | | |
| $PhCH_2OH\cdot\cdot PhCH_2O^-$ | | | | | | | |
| | -276±18 [c] | | *93±4* | *66±7* | TDAs | | 84CAL/ROZ |
| $C_{14}H_{20}O_2^-$ | | | | | | | |
| 2,6-di-tBu-benzoquinone$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= -335±13* | |
| • | -516±22 [b] | 1.88±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{15}H_9N^-$ | | | | | | | |
| 9-CN-anthracene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 366±4* | |
| • | 244±14 [b] | 1.27±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{15}H_{10}O^-$ | | | | | | | |
| 9-anthraldehyde$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 110±8* | |
| • | -16±18 [b] | 1.31±0.10 | | | TDEq | | 87KEB/CHO |
| | | 1.0±0.1 | | | ECD | | 67WEN/CHE |
| $C_{15}H_{10}O^-$ | | | | | | | |
| 9-phenanthraldehyde$^{-\cdot}$ | | | | | *Est2* | *$\Delta_f H(A)$= 70±8* | |
| | 0±9 [b] | 0.724±0.009 | | | ECD | | 75WEN/KAO |
| | | 0.7±0.1 | | | ECD | | 67WEN/CHE |
| $C_{15}H_{13}^-$ | | | | | *Est2* | *$\Delta_f H(AH)$= 88±13* | |
| 9-Et-fluorenide$^-$ | | | | | | | |
| • | 27±23 [a] | | 1469±11 [g] | 1437±8 | IMRE | | 86TAF |
| $C_{15}H_{13}O^-$ | | | | | | | |
| $PhCH_2OH\cdot\cdot PhC\equiv C^-$ | | | | | | | |
| | 145±26 [c] | | *82±10* [g] | *54±8* | IMRE | | 84CAL/ROZ |
| $C_{16}H_{10}^-$ | | | | | | | |
| fluoranthene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 289±1* | *81KUD/KUD* |
| | 228 [b] | 0.6 | | | ECD | | 69MIC |
| $C_{16}H_{10}^-$ | | | | | | | |
| pyrene$^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 216±1* | *79KUD/KUD2* |
| | 168±4 [b] | 0.50±0.03 | | | ECD | | 68LYO/MOR |
| | | 0.591±0.008 | | | ECD | | 66BEC/CHE |
| $C_{16}H_{12}O^-$ | | | | | | | |
| 9-COMe-anthracene$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= 60±4* | |
| • | -34±14 [b] | 0.97±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{16}H_{12}O_2^-$ | | | | | | | |
| 2-Et-9,10-anthraquinone$^{-\cdot}$ | | | | | *Est* | *$\Delta_f H(A)$= -149±4* | |
| • | -299±14 [b] | 1.56±0.10 | | | TDEq | | 87KEB/CHO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{16}H_{15}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 59±13* | |
| 9-iPr-fluorenide$^-$ | | | | | | |
| * -2±23 [a] | | 1470±11 [g] | 1437±8 | IMRE | | 86TAF |
| $C_{17}H_{12}Cl^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 293±13* | |
| 2-Ph-5-pCl-$C_6H_4$-cyclopentadienide$^-$ | | | | | | |
| * 170±23 [a] | | 1407±11 [g] | 1376±8 | IMRE | | 86TAF |
| $C_{17}H_{13}^-$ | | | | *Est* | *$\Delta_f H(AH)$= 322±8* | |
| 1,4-diphenylcyclopentadienide$^-$ | | | | | | |
| * 205±18 [a] | | 1413±10 [g] | 1383±8 | IMRE | | 86TAF |
| $C_{17}H_{17}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 42±13* | |
| 9-iBu-fluorenide$^-$ | | | | | | |
| * -21±23 [a] | | 1468±11 [g] | 1435±8 | IMRE | | 86TAF |
| $C_{17}H_{17}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 25±17* | |
| 9-tBu-fluorenide$^-$ | | | | | | |
| * -36±28 [a] | | 1469±11 [g] | 1438±8 | IMRE | | 86TAF |
| $C_{18}H_{12}^-$ | | | | | | |
| benz[a]anthracene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 285±1* | *79KUD/KUD2* |
| 224±2 [b] | 0.630±0.008 | | | ECD | | 66BEC/CHE |
| $C_{18}H_{12}^-$ | | | | | | |
| benzo[c]phenanthrene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 293±1* | *79KUD/KUD2* |
| 240±2 [b] | 0.545±0.008 | | | ECD | | 66BEC/CHE |
| $C_{18}H_{12}^-$ | | | | | | |
| chrysene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 284±1* | *79KUD/KUD2* |
| 246±2 [b] | 0.397±0.008 | | | ECD | | 66BEC/CHE |
| $C_{18}H_{12}^-$ | | | | | | |
| naphthacene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 284±1* | *79KUD/KUD2* |
| 199±5 [b] | 0.88±0.04 | | | ECD | | 68LYO/MOR |
| $C_{18}H_{12}^-$ | | | | | | |
| triphenylene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 270±1* | *79KUD/KUD2* |
| 242±2 [b] | 0.285±0.008 | | | ECD | | 66BEC/CHE |
| $C_{18}H_{15}^-$ | | | | *Est* | *$\Delta_f H(AH)$= 288±8* | |
| 2-Ph-5-p-tolyl-cyclopentadienide$^-$ | | | | | | |
| * 171±19 [a] | | 1413±11 [g] | 1381±8 | IMRE | | 86TAF |
| $C_{18}H_{16}O_2^-$ | | | | | | |
| 2-tBu-9,10-anthraquinone$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= -202±4* | |
| * -353±14 [b] | 1.56±0.10 | | | TDEq | | 87KEB/CHO |
| $C_{18}H_{19}^-$ | | | | *Est* | *$\Delta_f H(AH)$= 4±17* | |
| 9-tBuCH$_2$-fluorenide$^-$ | | | | | | |
| * -74±28 [a] | | 1452±11 [g] | 1419±8 | IMRE | | 86TAF |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $C_{19}H_{11}^-$ | | | | | | |
| fluoradenide$^-$ | | | | | | |
| • | | 1391±10 [g] | 1359±8 | IMRE | | 86TAF |
| $C_{19}H_{13}^-$ | | | | *Est2* | *$\Delta_f H(AH)$= 318±13* | |
| 9-Ph-fluorenide$^-$ | | | | | | |
| • 224±23 [a] | | 1436±11 [g] | 1404±8 | IMRE | | 86TAF |
| $C_{19}H_{15}^-$ | | | | | *$\Delta_f H(AH)$= 271±4* | *77PED/RYL* |
| $Ph_3C^-$ | | | | | | |
| 242±16 [a] | | 1501±12 [g] | 1467±8 | IMRE | | 86TAF |
| | | 1510±13 [g] | 1476±10 | IMRE | | 84BAR |
| | 2.56 | | | IMRE | Solution equilibrium + solvation cycle | 30BEN |
| | 0.8 | | | SI | From hexaphenylethane | 68GAI/PAG |
| $C_{19}H_{16}Cl^-$ | | | | | | |
| $Ph_3CH\cdot\cdot Cl^-$ | | | | | | |
| | | | *17* | TDEq | | 82FRE/IKU |
| $C_{20}H_{12}^-$ | | | | | | |
| benz[a]pyrene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 289±4* | *77STE/GOL* |
| | 0.680±0.008 | | | ECD | | 66BEC/CHE |
| $C_{20}H_{12}^-$ | | | | | | |
| benz[e]pyrene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 261±4* | |
| 210±5 [b] | 0.534±0.008 | | | ECD | | 66BEC/CHE |
| $C_{21}H_{15}^-$ | | | | *Est* | *$\Delta_f H(AH)$= 371±8* | |
| 1,3-diphenylindenide$^-$ | | | | | | |
| • 244±18 [a] | | 1403±10 [g] | 1376±8 | IMRE | | 86TAF |
| $C_{22}H_{14}^-$ | | | | | | |
| dibenz[a,h]anthracene$^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 336±4* | *77STE/GOL* |
| 279±5 [b] | 0.595±0.008 | | | ECD | | 66BEC/CHE |
| $C_{22}H_{14}^-$ | | | | | | |
| dibenz[a,j]anthracene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 336±4* | |
| 279±5 [b] | 0.591±0.008 | | | ECD | | 66BEC/CHE |
| $C_{22}H_{14}^-$ | | | | | | |
| picene$^{-\cdot}$ | | | | *Est* | *$\Delta_f H(A)$= 326±8* | |
| 274±9 [b] | 0.542±0.008 | | | ECD | | 66BEC/CHE |
| $C_{27}H_{19}^-$ | | | | | | |
| 1,2,3-triPh-indenide$^-$ | | | | | | |
| • | | 1404±11 [g] | 1373±8 | IMRE | | 86TAF |
| $CaH^-$ | | | | | | |
| $CaH^-$ | | | | | *$\Delta_f H(A)$= 229±42* | *82TN270* |
| • 139±47 [b] | 0.93±0.05 | | | PD | | 77RAC/FEL |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$CeF_4^-$** | | | | | | |
| $CeF_3\cdot\cdot F^-$ | | | | | | |
| −2005±29 | 3.60±0.30 [i] | *459±29* [k] | | TDEq | | 81SID/SOR |
| **$CeI^-$** | | | | | | |
| $CeI^{-\cdot}$ | | | | | | |
| | >0.3±0.3 | | | EIAP | From $CeI_3$ | 76CHA |
| **$CeI_2^-$** | | | | | | |
| $CeI_2^-$ | | | | | *$\Delta_f H(A)$= −192* | *76CHA* |
| <−221 [b] | >0.3±0.2 | | | EIAP | From $CeI_3$ | 76CHA |
| **$CeI_3^-$** | | | | | | |
| $CeI_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −339* | *76CHA* |
| <−368 [b] | >0.3 | | | IMRB | $CeI_2^- + CeI_3 \rightarrow$ | 76CHA |
| **$CeI_4^-$** | | | | | | |
| $CeI_4^-$ | | | | | | |
| −808 [c] | | *280±33* | *245±42* | TDEq | | 76CHA |
| **$Cl^-$** | | | | | | |
| $Cl^-$ | | | | | *$\Delta_f H(A)$= 122* | *85JANAF* |
| * −227±1 [a] | 3.617±0.003 | 1395±1 [e] | 1372±1 [h] | LOG | | 85HOT/LIN |
| | | 1396±9 [g] | 1374±8 | IMRE | | 81FUJ/MCI |
| **$ClCrO^-$** | | | | | | |
| $CrOCl^-$ | | | | | *$\Delta_f H(A)$= −116±48* | *69FLE/WHI* |
| −231±48 | 1.2±0.1 | | | EIAP | From $CrO_2Cl_2$ | 69FLE/WHI |
| **$ClCrO_2^-$** | | | | | | |
| $CrO_2Cl^-$ | | | | | *$\Delta_f H(A)$= −309±48* | *69FLE/WHI* |
| −531±48 | 2.4±0.4 | | | EIAP | From $CrO_2Cl_2$ | 69FLE/WHI |
| **$ClF^-$** | | | | | | |
| $ClF^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −50* | *85JANAF* |
| −195±29 [b] | 1.5±0.3 | | | NBIP | From $CF_2Cl_2$ | 78DIS/LAC |
| | >1.5±0.2 | | | EIAP | From $CFCl_3$ | 79ILL/SCH |
| | 2.9±0.2 | | | EIAP | From $ClF_3$ | 79DUD/GOR |
| | >1.5±0.4 | | | EIAP | From $SF_5Cl$ | 72THY |
| **$ClFH^-$** | | | | | | |
| $HF\cdot\cdot Cl^-$ | | | | | | |
| * −591±10 [c] | | *91±8* [g] | *63±8* | IMRE | | 84LAR/MCM2 |
| **$ClFO^-$** | | | | | | |
| $ClOF^{-\cdot}$ | | | | *Est2* | *$\Delta_f H(A)$= 54±21* | |
| | >2.0±0.2 | | | EIAP | | 80BAL/NIK2 |
| **$ClFO_2^-$** | | | | | | |
| $ClO_2F^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −33* | *73BAR* |
| −255 [b] | >2.3 | | | EIAP | From $ClO_3F$ | 83ALE/FED |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $ClF_2^-$ | | | | | | |
| $ClF_2^-$ | | | | | | |
| | >3.2±0.2 | | | EIAP | From $ClF_5$ | 80BAL/NIK |
| | >0.9±0.2 | | | EIAP | From $ClF_3$ | 79DUD/GOR |
| $ClF_2OS^-$ | | | | | | |
| $F_2SO\cdot\cdot Cl^-$ | | | | | | |
| • −851±30 [c] | | *72±8* [g] | *43±8* | IMRE | | 85LAR/MCM |
| $ClF_3^-$ | | | | | | |
| $ClF_3^-$ | | | | | *$\Delta_f H(A)$= −163±2* | *82BAU/COX* |
| | >2.4±0.1 | | | EIAP | From $ClF_5$ | 80BAL/NIK |
| $ClF_3OP^-$ | | | | | | |
| $PF_3O\cdot\cdot Cl^-$ | | | | | | |
| • −1497±12 [c] | | *58±8* [g] | *32±8* | IMRE | | 85LAR/MCM |
| $ClF_3P^-$ | | | | | | |
| $PF_3\cdot\cdot Cl^-$ | | | | | | |
| • −1211±12 [c] | | *65±8* [g] | *38±8* | IMRE | | 85LAR/MCM |
| $ClF_4Si^-$ | | | | | | |
| $SiF_4\cdot\cdot Cl^-$ | | | | | | |
| • −1940±12 [c] | | *98±8* [g] | *70±8* | IMRE | | 85LAR/MCM |
| $ClHI^-$ | | | | | | |
| $HCl\cdot\cdot I^-$ | | | | | | |
| • −343±9 [c] | | *62±8* | *37±11* | TDAs | | 85CAL/KEB |
| $ClH_2O^-$ | | | | | | |
| $HOH\cdot\cdot Cl^-$ | | | | | | |
| • −532 [c] | | *62±1* | *38±6* | TDAs | | 80KEE/CAS2 |
| | | *62±8* | *38±11* | TDAs | | 86YAM/FUR |
| | | *60±8* [g] | *35±8* | IMRE | | 84LAR/MCM2 |
| | | *62* | *37* | TDAs | | 82BUR/HAY |
| | | *55±8* | *30±8* | TDAs | | 71YAM/KEB |
| $ClH_2O_2^-$ | | | | | | |
| $HOOH\cdot\cdot Cl^-$ | | | | | | |
| −456±6 [c] | | *92±4* | *65±4* | TDEq | Relative to $HOH\cdot\cdot Cl^-$, 80KEE/LEE | 84BOH/FAH |
| $ClH_2O_4S^-$ | | | | | | |
| $HCl\cdot\cdot HSO_4^-$ | | | | | | |
| | | *66±4* | *47±4* | TDEq | Relative to $HOH\cdot\cdot HSO_4^-$, 84BOH/FAH | 84BOH/FAH |
| $ClH_3N^-$ | | | | | | |
| $NH_3\cdot\cdot Cl^-$ | | | | | | |
| • −317±18 [c] | | *44±17* [g] | *19±8* | IMRE | | 84LAR/MCM2 |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $ClI^-$ | | | | | | | |
| $ICl^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 18* | *85JANAF* |
| | −215±10 [b] | 2.4±0.1 | | | NBIP | | 73AUE/HUB |
| | −155 | 1.8 [i] | | | Endo | $I^-$ + NOCl → | 77REF/FRA |
| | | 1.48±0.05 | | | NBIP | Vertical EA | 76HUB/KLE |
| $ClK^-$ | | | | | | | |
| $KCl^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −215* | *85JANAF* |
| | −276 [b] | 0.6 | | | Scat | | 79DEV/WIJ |
| | | >1.3 | | | EIAP | From $(KCl)_2$ | 64EBI |
| $ClLi^-$ | | | | | | | |
| $LiCl^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −196±8* | *85JANAF* |
| | −255±10 [b] | 0.610±0.020 | | | LPES | | 76CAR/PET |
| | | >1.3 | | | EIAP | From $(LiCl)_2$ | 64EBI |
| $ClNa^-$ | | | | | | | |
| $NaCl^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −181±8* | *85JANAF* |
| | −255 [b] | 0.8 | | | Scat | | 79DEV/WIJ |
| | | >1.3 | | | EIAP | From $(NaCl)_2$ | 64EBI |
| $ClO^-$ | | | | | | *$\Delta_f H(AH)$= −79±8* | *82BAU/COX* |
| $ClO^-$ | | | | | | *BDE(A−H)= 399±9* | *82TN270* |
| • | −108±18 [a] | 2.170 | 1502±9 [c] | 1474±10 [h] | LPD | | 79LEE/SMI |
| | | 2.4±0.2 | | | EIAP | From $Cl_2O$ | 80BAL/NIK2 |
| | | 1.9±0.3 | | | IMRB | | 78DOT/ALB |
| | <−54±21 | >1.6±0.2 [i] | | | Endo | $Cl^-$ + $O_2$ → | 77VOG/DRE |
| $ClOV^-$ | | | | | | | |
| $VOCl^-$ | | | | | | | |
| | −310±48 | 1.4±0.4 | | | EIAP | From $VOCl_3$ | 75FLE/SVE |
| $ClO_2^-$ | | | | | | | |
| $OClO^-$ | | | | | | *$\Delta_f H(A)$= 97±8* | *82BAU/COX* |
| | −29±50 [b] | 1.3±0.4 | | | ECD | | 81WEC/CHR |
| | | 1.8±0.2 | | | EIAP | From $FClO_3$ | 80BAL/NIK2 |
| $ClO_2S^-$ | | | | | | | |
| $SO_2\cdot\cdot Cl^-$ | | | | | | | |
| • | −617±11 [c] | | *93±8* | *66±8* | TDAs | | 85CAL/KEB |
| | | | *93±8* | *63±7* | TDEq | Relative to $HOH\cdot\cdot Cl^-$ in 80KEE/LEE | 84BOH/FAH |
| | | | *91±1* | *62±1* | TDAs | | 80KEE/LEE |
| | | | *87±8* [g] | *62±8* | IMRE | | 85LAR/MCM |
| | <−565 | | | | IMRB | | 79ROB/FRA |
| | −326 | | | | IMRB | | 78SUL/BEA2 |
| $ClO_3^-$ | | | | | | | |
| $ClO_3^-$ | | | | | | *$\Delta_f H(A)$= 126±21* | *82TN270* |
| | −183±21 [b] | >3.2 | | | EIAP | From $ClO_3F$ | 83ALE/FED |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$ClO_3S^-$** | | | | | | |
| $SO_3\cdot\cdot Cl^-$ | | | | | | |
| | | <1312±8 | | EIAP | From $ClSO_3H$ (Appearance Potential = 0 eV) | 86ADA/SMI |
| **$ClO_4S_2^-$** | | | | | | |
| $SO_2\cdot\cdot SO_2Cl^-$ | | | | | | |
| −982 | | | | IMRE | | 80KEE/CAS |
| <−920 | | | | IMRB | | 79ROB/FRA |
| **$ClPb^-$** | | | | | | |
| $PbCl^-$ | | | | | | |
| | 1.0±0.2 | | | EIAP | From $PbCl_2$ | 67HAS/BLO |
| **$ClRb^-$** | | | | | | |
| $RbCl^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −229* | *82TN270* |
| | >1.5 | | | EIAP | From $(RbCl)_2$ | 64EBI |
| **$ClXe^-$** | | | | | | |
| $Xe\cdot\cdot Cl^-$ | | | | | | |
| | | *13* | | Mobl | | 84GAT |
| | | *13* | | Mobl | | 80THA/EIS |
| | | *<13* | | Mobl | | 79DEV/WIJ2 |
| **$Cl_2^-$** | | | | | | |
| $Cl_2^{-\cdot}$ | | | | | | |
| • −232±19 [b] | 2.4±0.2 | | | NBIP | | 77DIS/LAC2 |
| | 2.3 | | | ECD | Vertical EA: 1.02 eV | 81AYA/WEN |
| | 2.3±0.1 | | | EnCT | | 73HUG/LIF |
| | 2.5±0.1 | | | IMRB | | 72DUN/FEH |
| | 2.5±0.1 | | | NBIP | | 72BAE |
| | 2.5±0.2 | | | EIAP | From $CCl_4$ | 71DEC/FRA |
| | 1.02±0.05 | | | NBIP | Vertical EA | 76HUB/KLE |
| | 2.4±0.1 | | | EnCT | | 71CHU/BER |
| | 3.2±0.2 | | | NBIP | | 70LAC/HER |
| **$Cl_2CrO^-$** | | | | | | |
| $CrOCl_2^-$ | | | | | *$\Delta_f H(A)$= −309±48* | *69FLE/WHI* |
| −550±48 | 2.5±0.1 | | | EIAP | From $CrO_2Cl_2$ | 69FLE/WHI |
| **$Cl_2Ge^-$** | | | | | | |
| $GeCl_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −172±4* | *79TPIS* |
| −418 [b] | 2.6 | | | EIAP | From $GeCl_4$ | 77PAB/MAR |
| **$Cl_2H^-$** | | | | | | |
| $HCl\cdot\cdot Cl^-$ | | | | | | |
| • −419±10 [c] | | *100±8* | *72±11* | TDAs | | 85CAL/KEB |
| | | *97±8* [g] | *67±8* | IMRE | | 84LAR/MCM2 |
| | | *99±1* | *70±1* | TDAs | | 74YAM/KEB |
| <−521±48 | | | | EIAP | From $CHCl_3$ | 80SCH/ILL |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$Cl_2I^-$** | | | | | | |
| $ICl_2^-$ | | | | | | |
| −605 | | *377* [k] | | Latt | | 77FIN/GAT |
| **$Cl_2O^-$** | | | | | | |
| $Cl_2O^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 105±2* | *82TN270* |
| <−109 [b] | >2.2 | | | ECD | | 81WEC/CHR |
| **$Cl_2OP^-$** | | | | | | |
| $Cl_2PO^-$ | | | | | | |
| | 3.8±0.3 | | | NBAP | From $POCl_3$ | 76MAT/ROT |
| **$Cl_2OV^-$** | | | | | | |
| $VOCl_2^-$ | | | | | | |
| −590±48 | 3.2±0.5 | | | EIAP | From $VOCl_3$ | 75FLE/SVE |
| **$Cl_2O_2S^-$** | | | | | | |
| $SO_2Cl_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −364±2* | *82TN270* |
| <−598 [b] | >2.4 | | | IMRB | EA: > $Cl_2^-$ | 79ROB/FRA |
| **$Cl_2P^-$** | | | | | | |
| $PCl_2^-$ | | | | | | |
| | 0.9±0.1 | | | EIAP | From $PCl_3$ | 78PAB/MAR |
| <−891±19 | | | | EIAP | From $POCl_3$ | 74HAL/KLE |
| **$Cl_2Si^-$** | | | | | | |
| $SiCl_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −166* | *82TN270* |
| | 0.8±0.1 | | | EIAP | From $SiCl_4$ | 77PAB/MAR |
| −228±21 | >2.5 | | | EIAP | From $SiCl_4$ | 68JAE/HEN |
| **$Cl_2Sn^-$** | | | | | | |
| $SnCl_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −203±4* | *82TPIS* |
| −95 | 1.0 | | | EIAP | From $SnCl_4$ | 77PAB/PER |
| **$Cl_2V^-$** | | | | | | |
| $VCl_2^-$ | | | | | *$\Delta_f H(A)$= −1073±8* | *82TN270* |
| −1189±28 [b] | 1.2±0.2 | | | EIAP | From $VOCl_3$ | 75FLE/SVE |
| **$Cl_3^-$** | | | | | | |
| $Cl_3^-$ | | | | | | |
| −300 | | *70* [k] | | IMRE | | 79ROB/FRA2 |
| −300±21 | >4.3±0.2 [i] | | | IMRB | | 79ROB/FRA |
| >−410 [c] | | *<182* | | PDis | | 79LEE/SMI |
| **$Cl_3Ge^-$** | | | | | | |
| $GeCl_3^-$ | | | | | | |
| | >2.6 | | | NBAP | From $GeCl_4$ | 79MAT/ROT |
| | 1.8±0.1 | | | EIAP | From $GeCl_4$ | 78PAB/MAR |
| | 1.8 | | | EIAP | From $GeCl_4$ | 77PAB/MAR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$Cl_3OP^-$** | | | | | | |
| $Cl_3PO^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −558±1* | *82TN270* |
| −694±20 [b] | 1.4±0.2 | | | NBIP | | 76MAT/ROT |
| **$Cl_3OV^-$** | | | | | | |
| $VOCl_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −696* | *82TN270* |
| < −1043±49 [b] | > 3.6±0.5 | | | IMRB | EA: > $Cl^-$ | 75FLE/SVE |
| **$Cl_3O_2S^-$** | | | | | | |
| $SO_2Cl_2\cdot\cdot Cl^-$ | | | | | | |
| < −644±21 | | | | IMRB | $Cl^-$A: > $Cl_2$, $SO_2$ | 79ROB/FRA |
| **$Cl_3P^-$** | | | | | | |
| $PCl_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −289±2* | *85JANAF* |
| −368±12 [b] | 0.8±0.1 | | | NBIP | | 76MAT/ROT |
| | > 3.6 | | | IMRB | From $PCl_5$ | 74HAL/KLE |
| **$Cl_3Si^-$** | | | | | *$\Delta_f H(AH)$= −481±8* | *81BEU/PER* |
| $SiCl_3^-$ | | | | | *BDE(A−H)= 382±4* | *81WAL* |
| < −510±13 [a] | > 2.0 | < 1501 [c] | | EIAP | From $SiCl_4$ | 77PAB/MAR |
| −589±21 | 3.5±0.4 | | | EIAP | From $SiCl_4$ | 68JAE/HEN |
| **$Cl_3Sn^-$** | | | | | | |
| $SnCl_3^-$ | | | | | | |
| | 3.4±0.2 | | | NBAP | From $SnCl_4$ | 83LAC/MAN |
| | 3.7±0.5 | | | NBAP | From $SnCl_4$ | 79MAT/ROT |
| | 2.53±0.01 | | | EIAP | From $SnCl_4$ | 78PAB/MAR |
| −583 | 2.5 | | | EIAP | From $SnCl_4$ | 77PAB/PER |
| **$Cl_3Ti^-$** | | | | | | |
| $TiCl_3^-$ | | | | | *$\Delta_f H(A)$= −542±2* | *82TN270* |
| −601±18 [b] | 0.6±0.2 | | | NBAP | From $TiCl_4$ | 79MAT/ROT |
| | 0.6±0.1 | | | EIAP | From $TiCl_4$ | 78PAB/MAR |
| −597±13 | 0.6±0.2 | | | EIAP | From $TiCl_4$ | 74BEN/PAB |
| **$Cl_3V^-$** | | | | | | |
| $VCl_3^-$ | | | | | | |
| −569±48 | 2.2±0.5 | | | EIAP | From $VOCl_3$ | 75FLE/SVE |
| **$Cl_4I^-$** | | | | | | |
| $ICl_4^-$ | | | | | | |
| −631 | | | | Latt | | 77FIN/GAT |
| **$Cl_4Nb^-$** | | | | | | |
| $NbCl_4^-$ | | | | | *$\Delta_f H(A)$= −561±2* | *82TN270* |
| < −696 [b] | > 1.4 | | | EIAP | From $NbCl_5$ | 75BEN/MAR |
| **$Cl_4Sn^-$** | | | | | | |
| $SnCl_4^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −472±2* | *82TN270* |
| −684±21 [b] | 2.2±0.2 | | | NBIP | | 83LAC/MAN |
| | 2.5±0.2 | | | NBIP | | 79MAT/ROT |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $Cl_4Ta^-$ | | | | | | | |
| $TaCl_4^-$ | | | | | | *$\Delta_f H(A)$= −561±2* | *82TN270* |
| | <−696 [b] | >1.4 | | | EIAP | From $TaCl_5$ | 75BEN/MAR |
| $Cl_4Ti^-$ | | | | | | | |
| $TiCl_4^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −763±2* | *85JANAF* |
| | −1041±17 [b] | 2.9±0.2 | | | NBIP | | 79MAT/ROT |
| $Cl_5Si^-$ | | | | | | | |
| $SiCl_4\cdot\cdot Cl^-$ | | | | | | | |
| * | −986±12 [c] | | *101±8* [g] | *74±8* | IMRE | | 85LAR/MCM |
| $Co^-$ | | | | | | | |
| $Co^-$ | | | | | | *$\Delta_f H(A)$= 425±2* | *82TN270* |
| * | 361±2 [b] | 0.662±0.003 | 1437±5 [c] | | LPES | | 86LEO/LIN |
| | 372 [a] | | | 1395±13 | IMRB | | 85SAL/LAN |
| $CoH^-$ | | | | | | | |
| $CoH^-$ | | | | | | *$\Delta_f H(A)$= 477±13* | *81ARM/BEA* |
| * | 412±14 [b] | 0.671±0.010 | | | LPES | | 87MIL/FEI |
| $CoH_2^-$ | | | | | | | |
| $CoH_2^-$ | | | | | | | |
| * | | 1.450±0.014 | | | LPES | | 86MIL/FEI |
| $CoD_2^-$ | | | | | | | |
| $CoD_2^-$ | | | | | | | |
| * | | 1.465±0.013 | | | LPES | | 86MIL/FEI |
| $Co_2^-$ | | | | | | | |
| $Co_2^-$ | | | | | | *$\Delta_f H(A)$= 683±8* | *82TN270* |
| * | 576±9 [b] | 1.110±0.008 | | | LPES | | 86LEO/LIN |
| $Cr^-$ | | | | | | | |
| $Cr^-$ | | | | | | *$\Delta_f H(A)$= 397±2* | *82TN270* |
| * | 332±3 [b] | 0.666±0.012 | | | LPES | | 85HOT/LIN |
| | | | | 1389±13 | IMRB | | 85SAL/LAN |
| $CrCl^-$ | | | | | | | |
| $CrCl^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 48±48* | *69FLE/WHI* |
| | −145±48 | 1.1±0.2 | | | EIAP | From $CrO_2Cl_2$ | 69FLE/WHI |
| $CrCl_2^-$ | | | | | | | |
| $CrCl_2^-$ | | | | | | *$\Delta_f H(A)$= −128±2* | *82TN270* |
| | −309±48 | 1.7±0.2 | | | EIAP | From $CrO_2Cl_2$ | 69FLE/WHI |
| $CrF^-$ | | | | | | | |
| $CrF^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 21* | *81WOO* |
| | −67±48 | 1.0±0.4 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$CrFO^-$** | | | | | | |
| $CrOF^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −309±48* | *69FLE/WHI* |
| −367±48 | 0.7±0.2 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrFO_2^-$** | | | | | | |
| $CrO_2F^-$ | | | | | *$\Delta_f H(A)$= −473±48* | *69FLE/WHI* |
| −724±48 | 2.5±0.2 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrF_2^-$** | | | | | | |
| $CrF_2^-$ | | | | | *$\Delta_f H(A)$= −216* | *81WOO* |
| −540±48 | 1.5±0.4 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrF_2O^-$** | | | | | | |
| $CrOF_2^-$ | | | | | *$\Delta_f H(A)$= −618±48* | *69FLE/WHI* |
| −820±48 | 2.1±0.1 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrH^-$** | | | | | | |
| $CrH^-$ | | | | | | |
| * | 0.563±0.010 | | | LPES | | 87MIL/FEI |
| **$CrHO_3^-$** | | | | | | |
| $HCrO_3^-$ | | | | | | |
| −1132±40 | 2.37±0.42 [i] | | | TDEq | | 72MIL |
| **$CrH_2^-$** | | | | | | |
| $CrH_2^-$ | | | | | | |
| | >2.500 | | | LPES | | 86MIL/FEI |
| **$CrKO_4^-$** | | | | | | |
| $KCrO_4^-$ | | | | | | |
| −1000±16 | | | | TDEq | | 85RUD/SID |
| **$CrO^-$** | | | | | | |
| $CrO^-$ | | | | | *$\Delta_f H(A)$= 218±29* | *83PED/MAR* |
| 183±48 | 1.3±0.7 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrO_2^-$** | | | | | | |
| $CrO_2^-$ | | | | | *$\Delta_f H(A)$= −59±21* | *82TN270* |
| <−594±42 | | | | IMRB | | 72MIL |
| −280±48 | 2.3±0.7 | | | EIAP | From $CrO_2F_2$ | 69FLE/WHI |
| **$CrO_3^-$** | | | | | | |
| $CrO_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −386±2* | *82TN270* |
| −674±27 | 3.70±0.30 [i] | | | TDEq | | 85RUD/SID |
| −838±82 [a] | 4.04±0.42 [i] | 1437±40 | | TDEq | | 72MIL |
| **$CrO_4^-$** | | | | | | |
| $CrO_4^-$ | | | | | | |
| −785±30 | | | | TDEq | | 85RUD/SID |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $Cr_2O_6^-$ | | | | | | |
| $Cr_2O_6^{-\cdot}$ | | | | | | |
| | 1.6±0.3 | | | EIAP | From $(CrO_3)_3$ | 75WAN/MAR |
| $Cr_3O_9^-$ | | | | | | |
| $Cr_3O_9^{-\cdot}$ | | | | | | |
| | 1.8 | | | EIAP | From $(CrO_3)_5$ | 75WAN/MAR |
| $Cs^-$ | | | | | | |
| $Cs^-$ | | | | | *$\Delta_f H(A)$= 76* | *82TN270* |
| * 31±5 [a] | 0.472 | 1445±3 [c] | | LPD | | 85HOT/LIN |
| $CsI_2^-$ | | | | | | |
| $CsI\cdot\cdot I^-$ | | | | | | |
| −492±5 [c] | | *151±5* | | TDAs | | 79GUS/GOR |
| $Cs_2I_3^-$ | | | | | | |
| $Cs_2I_2\cdot\cdot I^-$ | | | | | | |
| −766±13 | | *115±13* [k] | | TDAs | | 79GUS/GOR |
| $Cu^-$ | | | | | | |
| $Cu^-$ | | | | | *$\Delta_f H(A)$= 338* | *82TN270* |
| * 220±1 [b] | 1.228±0.010 | 1459±22 [f] | | LPES | | 85HOT/LIN |
| $Cu_7^-$ | | | | | | |
| $Cu_7^-$ | | | | | | |
| | 1.870±0.080 | | | LPES | | 86ZHE/KAR |
| $Cu_8^-$ | | | | | | |
| $Cu_8^-$ | | | | | | |
| | < 1.440 | | | LPES | | 86ZHE/KAR |
| $Cu_9^-$ | | | | | | |
| $Cu_9^-$ | | | | | | |
| | 2.270±0.060 | | | LPES | | 86ZHE/KAR |
| $Cu_{10}^-$ | | | | | | |
| $Cu_{10}^-$ | | | | | | |
| | 2.010±0.060 | | | LPES | | 86ZHE/KAR |
| $Cu_{11}^-$ | | | | | | |
| $Cu_{11}^-$ | | | | | | |
| | 2.380±0.060 | | | LPES | | 86ZHE/KAR |
| $Cu_{12}^-$ | | | | | | |
| $Cu_{12}^-$ | | | | | | |
| | 2.140±0.070 | | | LPES | | 86ZHE/KAR |
| $Cu_{13}^-$ | | | | | | |
| $Cu_{13}^-$ | | | | | | |
| | 2.605±0.175 | | | LPES | | 86ZHE/KAR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $Cu_{14}^-$ | | | | | | |
| $Cu_{14}^-$ | | | | | | |
| | 2.075±0.025 | | | LPES | | 86ZHE/KAR |
| $Cu_{15}^-$ | | | | | | |
| $Cu_{15}^-$ | | | | | | |
| . | 2.575±0.135 | | | LPES | | 86ZHE/KAR |
| $Cu_{16}^-$ | | | | | | |
| $Cu_{16}^-$ | | | | | | |
| | 2.325±0.115 | | | LPES | | 86ZHE/KAR |
| $Cu_{17}^-$ | | | | | | |
| $Cu_{17}^-$ | | | | | | |
| | <2.720 | | | LPES | | 86ZHE/KAR |
| $Cu_{18}^-$ | | | | | | |
| $Cu_{18}^-$ | | | | | | |
| | 2.570±0.130 | | | LPES | | 86ZHE/KAR |
| $Cu_{19}^-$ | | | | | | |
| $Cu_{19}^-$ | | | | | | |
| | 2.705±0.265 | | | LPES | | 86ZHE/KAR |
| $F^-$ | | | | | | |
| $F^-$ | | | | | *$\Delta_f H(A)$= 79* | *85JANAF* |
| • −249±2 [a] | 3.399±0.003 | 1554±1 [c] | 1530±2 [h] | PLA | | 85HOT/LIN |
| | | | 1530±8 | IMRE[o] | | 79BAR/SCO |
| $FHI^-$ | | | | | | |
| $HF\cdot\cdot I^-$ | | | | | | |
| • −524±10 [c] | | *63±8* | | Est | Extrapolated from other bihalide data | 84LAR/MCM3 |
| $FH_2O^-$ | | | | | | |
| $HOH\cdot\cdot F^-$ | | | | | | |
| −588 [c] | | *97±8* | *76±8* | TDAs | | 70ARS/YAM |
| $FH_2S^-$ | | | | | | |
| $HSH\cdot\cdot F^-$ | | | | | | |
| • −414±11 [c] | | *145±8* [g] | *121±8* | IMRE | | 83LAR/MCM |
| $FK^-$ | | | | | | |
| $KF^{-}\cdot$ | | | | | *$\Delta_f H(A)$= −327±2* | *85JANAF* |
| −427±22 [b] | 1.0±0.2 | | | EIAP | From $K_2BO_2F$ | 76SHE/ILJ |
| | <1.50 | | | IMRE | | 80SID/SKO |
| | 0.2 | | | Scat | | 79DEV/WIJ |
| | >1.3 | | | EIAP | From $(KF)_2$ | 64EBI |
| $FLi^-$ | | | | | | |
| $LiF^{-}\cdot$ | | | | | *$\Delta_f H(A)$= −340* | *82TN270* |
| | >1.4 | | | EIAP | From $(LiF)_2$ | 64EBI |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$FN^-$** | | | | | | | |
| $FN^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 232±2* | *84BER/GRE* |
| | 184±2 [b] | 0.5 | | | EIAP | | 82SID |
| **$FNP^-$** | | | | | | | |
| $NPF^-$ | | | | | | | |
| | <−285 | | | | IMRB | $NH_2^- + PF_3 \rightarrow$ | 78SUL/BEA |
| **$FNa^-$** | | | | | | | |
| $NaF^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −291* | *82TN270* |
| | −399±20 [b] | 1.1±0.2 | | | EIAP | From $Na_2BO_2F$ | 76SHE/ILJ |
| | | 0.4 | | | Scat | | 79DEV/WIJ |
| | | >1.4 | | | EIAP | From $(NaF)_2$ | 64EBI |
| **$FNa_2^-$** | | | | | | | |
| $Na_2F^-$ | | | | | | | |
| | −300±42 | | | | EIAP | From $Na_2BO_2F$ | 76SHE/ILJ |
| **$FO^-$** | | | | | | | |
| $FO^-$ | | | | | | *$\Delta_f H(AH)$= −96±4* | *82BAU/COX* |
| | | | | | | *BDE(A–H)= 412±13* | *82BAU/COX* |
| | −89±13 [b] | 2.05±0.08 | | | EIAP | From $F_2O$ | 84ALE/VOL |
| | | >1.4±0.5 | | | EIAP | From $CF_3OF$ | 70THY/MAC |
| **$FOV^-$** | | | | | | | |
| $VOF^-$ | | | | | | | |
| | −473±48 | 1.2±0.4 | | | EIAP | From $VOF_3$ | 75FLE/SVE |
| **$FO_2S^-$** | | | | | | | |
| $SO_2\cdot\cdot F^-$ | | | | | | | |
| | * −729±12 [c] | | *183±8 [g]* | *154±8* | IMRE | | 83LAR/MCM |
| | <−595 | | | | EIAP | From $SO_2F_2$ | 80WAN/FRA |
| | −511 | | | | IMRB | | 78SUL/BEA2 |
| | | 2.8 | | | SI | | 69PAG/GOO |
| | −715 | | | | EIAP | From $SO_2F_2$ | 58REE/DIB |
| **$FO_3S^-$** | | | | | | | |
| $SO_3\cdot\cdot F^-$ | | | | | | | |
| | * −971±45 [c] | 4.6±0.6 [d] | *326±42 [g]* | *297±42* | IMRB | | 85LAR/MCM |
| | <−971±13 [a] | | <1312±8 | | EIAP | From $FSO_3H$ (Appearance Potential = 0 eV) | 86ADA/SMI |
| **$FS^-$** | | | | | | | |
| $FS^-$ | | | | | | *$\Delta_f H(A)$= 13±6* | *85JANAF* |
| | −180±55 [b] | 2.0±0.5 | | | Est | From trends in EA of $SF_x$ | 82JANAF |
| **$FXe^-$** | | | | | | | |
| $Xe\cdot\cdot F^-$ | | | | | | | |
| | −276 [c] | | *27±4* | | Mobl | | 79DEV/WIJ2 |
| **$F_2^-$** | | | | | | | |
| $F_2^{-\cdot}$ | | | | | | | |
| | −297 [b] | 3.1 | | | ECD | Vertical EA: 1.24 eV | 81AYA/WEN |
| | | 2.9±0.2 | | | EIAP | From $NF_3$ | 74HAR/FRA |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / *$\Delta H_{aff}(X\cdot\cdot Y^-)$* | $\Delta G_{acid}(AH)$ / *$\Delta G_{aff}(X\cdot\cdot Y^-)$* | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$F_2^-$** | | | | | | | |
| $F_2^{-\cdot}$ | | | | | | | |
| | | 2.9±0.2 | | | EIAP | From $BF_3$ | 71DEC/FRA |
| | | 3.2 | | | EIAP | From $SO_2F_2$ | 80WAN/FRA |
| • | | >2.8±0.3 | | | EIAP | From $CF_2O$ | 72THY |
| | | 3.1±0.1 | | | EnCT | | 71CHU/BER |
| | | >3.0 | | | EIAP | From $SO_2F_2$ | 58REE/DIB |
| **$F_2Ge^-$** | | | | | | | |
| $GeF_2^{-\cdot}$ | | | | | | *$\Delta_f H(A) = -573$* | *81WOO* |
| | −695±29 | >1.3±0.3 | | | EIAP | From $GeF_4$ | 72HAR/CRA |
| **$F_2H^-$** | | | | | | | |
| $FH\cdot\cdot F^-$ | | | | | | | |
| • | −683±11 [c] | | *162±8* [g] | *134±8* | IMRE | | 83LAR/MCM |
| | <−666±19 | | *>145±19* [k] | | EIAP | From CHF=CHF | 85HEN/ILL |
| **$F_2HNOP^-$** | | | | | | | |
| $HNOPF_2^-$ | | | | | | | |
| | <−1079 | | | | IMRB | | 78SUL/BEA |
| | | | | | | $NH_2^- + OPF_3 \rightarrow HNOPF_2^- + HF$; $HNOPF_2^- + OPF_3 \rightarrow (F_3PO)_2N^- + HF$ | |
| **$F_2HNP^-$** | | | | | | | |
| $HNPF_2^-$ | | | | | | | |
| | <−556 | | | | IMRB | $NH_2^- + PF_3 \rightarrow$ | 78SUL/BEA |
| **$F_2K^-$** | | | | | | | |
| $KF\cdot\cdot F^-$ | | | | | | | |
| | −806±11 [c] | | *224±3* | | TDAs | | 81NIK/SID |
| | −790±6 [c] | | *200±4* | | TDEq | $F^-A$: 1100K; $\Delta Hf(KF_2^-)$: 298K | 80SID/NIK |
| | <−803±21 | | | | | | 79GUS/GOR |
| **$F_2Mn^-$** | | | | | | | |
| $MnF_2^{-\cdot}$ | | | | | | *$\Delta_f H(A) = -525$* | *81WOO* |
| | −943±15 [b] | 4.36±0.15 | | | TDEq | | 82SID/GUB |
| **$F_2N^-$** | | | | | | *$\Delta_f H(AH) = -65±6$* | *69PAN/ZER* |
| $NF_2^-$ | | | | | | *BDE(A−H) = 314±10* | *84BER/GRE* |
| • | −93±15 [a] | 1.28±0.20 [d] | 1502±10 [g] | 1473±8 | IMRE | | 86TAF |
| | | | | 1477 | IMRE | | 81KOP/PIK |
| | −123±31 | 1.7±0.2 | | | EIAP | From $NF_3$ | 74HAR/FRA |
| | <−45±19 | >0.7±0.2 | | | EIAP | From $NF_3$ | 79DUD/BAL |
| | | >0.4±0.1 | | | EIAP | From $N_2F_4$ | 78DUD/BAL |
| | | 3.0 | | | SI | | 69PAG/GOO |
| **$F_2NOP^-$** | | | | | | | |
| $ONPF_2^{-\cdot}$ | | | | | | | |
| | <−582 | | | | IMRB | $HNO^- + PF_3 \rightarrow NOPF_2^- + HF$ | 78SUL/BEA |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_2OP^-$ | | | | | | |
| $F_2PO^-$ | | | | | | |
| <−962 | | | | IMRB | $HNO^- + OPF_3 \rightarrow$ | 78SUL/BEA |
| −448±19 | 3.4±0.2 | | | EIAP | From $F_3PO$ | 71RHY/DIL |
| $F_2OPS^-$ | | | | | | |
| $F_2POS^-$ | | | | | | |
| <−1033 | | | | IMRB | $HS^- + OPF_3 \rightarrow$ | 78SUL/BEA |
| $F_2OV^-$ | | | | | | |
| $VOF_2^-$ | | | | | | |
| −925±48 | 2.8±0.5 | | | EIAP | From $VOF_3$ | 75FLE/SVE |
| $F_2O_2P^-$ | | | | | | |
| $F_2PO_2^-$ | | | | | | |
| <−1167 | | | | IMRB | $HO^-$ or $EtO^- + OPF_3 \rightarrow$ | 78SUL/BEA |
| $F_2O_2S^-$ | | | | | | |
| $SO_2F_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −759±8* | *87HER* |
| | <3.1 | | | IMRB | EA: < $F_2$ | 78GAL/FAI |
| $F_2O_2U^-$ | | | | | | |
| $UO_2F_2^-$ | | | | | | |
| | 3.36±0.52 | | | TDEq | | 84GOR/PYA |
| $F_2P^-$ | | | | | | |
| $PF_2^-$ | | | | | *$\Delta_f H(A)$= −482±2* | *84BER/GRE* |
| −636±51 [b] | 1.6±0.5 | | | EIAP | From $PF_2NCS$ | 72THY |
| | >1.6±0.5 | | | SI | | 69PAG/GOO |
| | 1.5±0.5 | | | Est2 | | 82JANAF |
| $F_2PS^-$ | | | | | | |
| $F_2PS^-$ | | | | | | |
| | 2.6±1.0 | | | EIAP | From $PF_3S$ | 71RHY/DIL |
| $F_2V^-$ | | | | | | |
| $VF_2^-$ | | | | | | |
| −703±48 | 0.4±0.5 | | | EIAP | From $VOF_3$ | 75FLE/SVE |
| $F_3Cr^-$ | | | | | | |
| $CrF_2\cdot\cdot F^-$ | | | | | | |
| −1124±15 | | | | TDEq | | 83IGO |
| $F_3Cu^-$ | | | | | | |
| $CuF_2\cdot\cdot F^-$ | | | | | | |
| | >5.26 [i] | *351±17* | | TDEq | Anchor: $F^-A(FeF_3)$ 84CHI/KOR | 86KUZ/KOR |
| $F_3Fe^-$ | | | | | | |
| $FeF_2\cdot\cdot F^-$ | | | | | | |
| −1069±12 [c] | 3.62±0.13 [i] | *359±9* | | TDEq | | 86SID/BOR |
| | | | | | Corrections to 81SOR/SID, better neutral pressure determination | |
| | | *374±17* | | TDEq | | 86KUZ/KOR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_3Fe^-$ | | | | | | |
| $FeF_2\cdot\cdot F^-$ | | | | | | |
| −1138±14 [c] | 4.30±0.20 [i] | *441±14* | | TDEq | $F^-A$: 64±5 kJ < $AlF_3$ | 81SOR/SID |
| $F_3Ge^-$ | | | | | | |
| $GeF_3^-$ | | | | | | |
| −860±21 | 1.1±0.4 | | | EIAP | From $GeF_4$ | 74WAN/MAR |
| −858 | 1.6 | | | EIAP | From $GeF_4$ | 74FRA/WAN |
| | 3.1±0.1 | | | EIAP | From $GeF_4$ | 72HAR/CRA |
| $F_3Mn^-$ | | | | | | |
| $MnF_2\cdot\cdot F^-$ | | | | | | |
| −1213 [c] | 4.36 [i] | *430* | | TDEq | | 81SID/SOR |
| $F_3Ni^-$ | | | | | | |
| $NiF_2\cdot\cdot F^-$ | | | | | | |
| | | *338±15* | | TDEq | Reanalyzed literature data, 150 kJ < $AlF_3$ | 86NIK/IGO |
| $F_3OS^-$ | | | | | | |
| $F_2SO\cdot\cdot F^-$ | | | | | | |
| • −904±42 [c] | | *156±8* [g] | *126±8* | IMRE | | 83LAR/MCM |
| $F_3OV^-$ | | | | | | |
| $VOF_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1234±29* | *75FLE/SVE* |
| | 3.1±0.4 | | | IMRB | EA: > $VOF_2^-$, < $F^-$ | 75FLE/SVE |
| $F_3OW^-$ | | | | | | |
| $WOF_3^{-\cdot}$ | | | | | | |
| | >0.3 | | | EIAP | From $WOF_4$ | 77HIL |
| $F_3O_2S^-$ | | | | | | |
| $SO_2F_2\cdot\cdot F^-$ | | | | | | |
| • −1157±19 [c] | | *150±8* [g] | *115±8* | IMRE | | 83LAR/MCM |
| −1284±21 | | | | IMRB | | 78GAL/FAI |
| $F_3Pb^-$ | | | | | | |
| $PbF_3^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −510±54* | *75BEN/WAN* |
| −867±54 | 3.7 | | | EIAP | From $PbF_4$ | 75BEN/WAN |
| −887 | 4.3 | | | EIAP | From $PbF_4$ | 74FRA/WAN |
| $F_3S^-$ | | | | | | |
| $SF_3^-$ | | | | | *$\Delta_f H(A)$= −488±25* | *87HER* |
| −785±44 [b] | 3.1±0.2 | | | NBAP | From $SF_6$ | 78COM/REI |
| | 2.9±0.1 | | | EIAP | From $SF_4$ | 71HAR/THY |
| | 2.7±0.7 | | | Est | Reanalysis: 71HAR/THY | 82JANAF |
| | 2.7 | | | SI | | 69PAG/GOO |
| $F_3Se^-$ | | | | | | |
| $SeF_3^-$ | | | | | | |
| −774 | | | | EIAP | From $SeF_6$ | 69BRI |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X \cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X \cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X \cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_3Si^-$ | | | | | *$\Delta_f H(AH)$= -1201±21* | *85JANAF* |
| $SiF_3^-$ | | | | | *BDE(A-H)= 419±4* | *81WAL* |
| • -1284±35 [a] | 2.9±0.1 | 1446±14 [c] | 1414±15 [h] | PD | | 75RIC/STE4 |
| -1176 | 2.0 | | | EIAP | From $SiF_4$ | 74FRA/WAN |
| -1176 | 2.0 | | | EIAP | From $SiF_4$ | 73WAN/MAR |
| | 3.7 | | | EIAP | From $SiF_4$ | 70MAC/THY |
| | 3.4 | | | SI | | 69PAG/GOO |
| $F_3Sn^-$ | | | | | | |
| $SnF_3^-$ | | | | | | |
| | >1.2 | | | EIAP | From $SnF_4$ | 77PAB/PER |
| -632 | >1.2 | | | EIAP | From $SnF_4$ | 75BEN/WAN |
| -887 | 2.6 | | | EIAP | From $SnF_4$ | 74FRA/WAN |
| $F_3V^-$ | | | | | | |
| $VF_3^-$ | | | | | | |
| -1033±48 | 1.6±0.4 | | | EIAP | From $VOF_3$ | 75FLE/SVE |
| $F_4Cr^-$ | | | | | | |
| $CrF_3 \cdot\cdot F^-$ | | | | | | |
| -1467±15 | | | | TDEq | | 83IGO |
| | | | | | $FeF_3^- + CrF_4^- \rightleftharpoons FeF_4^- + CrF_3^-$, $\Delta_{rxn}H$ = 9 kJ | |
| $F_4Fe^-$ | | | | | | |
| $FeF_3 \cdot\cdot F^-$ | | | | | | |
| -1423±18 [c] | | *451±10* | | TDEq | $F^-A$: 92.5 kJ > $FeF_2$ | 86SID/BOR |
| -1490 [c] | | *456±14* | | TDEq | $F^-A$: 37 kJ < $AlF_3$ | 84CHI/KOR |
| -1412±14 [c] | 5.45±0.20 [i] | *439±14* | | TDEq | $F^-A$: 62 kJ < $AlF_3$ | 81SOR/SID |
| $F_4Ge_2^-$ | | | | | | |
| $Ge_2F_4^-$ | | | | | | |
| <-121 | | | | IMRB | | 72HAR/CRA |
| $F_4La^-$ | | | | | | |
| $LaF_3 \cdot\cdot F^-$ | | | | | | |
| -2004±33 | | | | TDEq | | 79GUS/GOR |
| $F_4Mn^-$ | | | | | | |
| $MnF_3 \cdot\cdot F^-$ | | | | | | |
| -1463±60 [c] | | *421±13* | | TDEq | $F^-A$: 72±3 kJ < $AlF_3$ | 84CHI/KOR |
| -1466±60 | 5.23±0.03 [i] | | | TDEq | $F^-A$: 79 kJ < $AlF_3$ | 84KOR/CHI |
| $F_4OP^-$ | | | | | | |
| $F_3PO \cdot\cdot F^-$ | | | | | | |
| • -1660±13 [c] | | *200±8* [g] | *168±8* | IMRE | | 85LAR/MCM |
| -1594±46 [c] | | *134±42* | | IMRB | $F^-A$: $SF_4$ > $F_3PO$ > $SF_5$ | 71RHY/DIL |
| $F_4OU^-$ | | | | | | |
| $UOF_3 \cdot\cdot F^-$ | | | | | | |
| | 3.80±0.43 | | | TDEq | | 84GOR/PYA |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $F_4P^-$ | | | | | | | |
| $PF_3\cdot\cdot F^-$ | | | | | | | |
| • | −1336±13[c] | | *168±8*[g] | *136±8* | IMRE | | 83LAR/MCM |
| | | | *209±21* | | IMRB | $F^-$A: < $OPF_3$, > F, $SF_4$, $Me_3SiF$, HCN, $SO_2$ | 78SUL/BEA |
| $F_4PS^-$ | | | | | | | |
| $F_3PS\cdot\cdot F^-$ | | | | | | | |
| | −1374±106[c] | | *134±42* | | IMRB | $F^-$A: between $SF_4$, $SF_5$ | 71RHY/DIL |
| $F_4Pt^-$ | | | | | | | |
| $PtF_4^-$ | | | | | | *$\Delta_f H(A)$= −524±25* | *83KOR/BON* |
| | | 5.20±0.16 | | | TDEq | EA: 2.5 kJ > $MnF_4$ | 84KOR/CHI |
| $F_4Rh^-$ | | | | | | | |
| $RhF_4^-$ | | | | | | | |
| | | 5.00±0.20[i] | *401±14* | | TDEq | $F^-$A: 22 kJ < $MnF_3$ | 84CHI/KOR |
| $F_4S^-$ | | | | | | | |
| $SF_4^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −763±21* | *85JANAF* |
| • | −990±31[b] | 2.4±0.1 | | | IMRB | EA: between $NO_2^-$, $HS^-$ | 81BAB/STR2 |
| | | 0.8±0.2 | | | NBIP | | 78COM/REI |
| | | 1.3±0.1 | | | ES | | 74DON/HAR |
| $F_4Sc^-$ | | | | | | | |
| $ScF_3\cdot\cdot F^-$ | | | | | | | |
| | −2013±13[c] | | *495±10* | | TDEq | $F^-$A: 10 kJ < $AlF_3$ | 81SKO/NIK |
| | −2009±13[c] | | *487±10* | | TDEq | $F^-$A: 17 kJ < $AlF_3$ | 81NIK/SID |
| | | | *470±10* | | TDEq | Reanalyzed data, 18 kJ < $AlF_3$ | 86NIK/IGO |
| $F_4Se^-$ | | | | | | | |
| $SeF_4^{-\cdot}$ | | | | | | | |
| | | 1.7±0.1 | | | EIAP | From $SeF_6$ | 73HAR/THY |
| | −795±42 | | | | EIAP | From $SeF_6$ | 69BRI |
| $F_4Te^-$ | | | | | | | |
| $TeF_4^{-\cdot}$ | | | | | | | |
| | | 2.2±0.1 | | | EIAP | From $TeF_6$ | 73HAR/THY |
| | −895±42 | | | | EIAP | | 69BRI |
| $F_4Ti^-$ | | | | | | | |
| $TiF_4^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −1552±2* | *82TN270* |
| | | >0.0 | | | EIAP | | 74BEN/PAB |
| $F_4U^-$ | | | | | | | |
| $UF_4^-$ | | | | | | *$\Delta_f H(A)$= −1599±2* | *82TN270* |
| • | −1725±30 | 1.24±0.36[i] | *415±42*[k] | | TDEq | Critical review | 84PYA/GUS |
| | | <1.8 | | | IMRB | | 80SID/SKO |
| $F_4W^-$ | | | | | | | |
| $WF_4^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −1029* | *81WOO* |
| | −1280[b] | 2.6 | | | EIAP | From $WF_6$ | 77DEW/NEU |
| | | >2.3±0.1 | | | EIAP | From $WF_6$ | 73THY/HAR2 |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_4W^-$ | | | | | | |
| $WF_4^{-\cdot}$ | | | | | *$\Delta_f H(A)$= -1029* | *81WOO* |
| | >1.0 | | | EIAP | From $WF_6$ | 77HIL |
| $F_5Cr^-$ | | | | | | |
| $CrF_4\cdot\cdot F^-$ | | | | | | |
| -1753±15 | | | | TDEq | | 83IGO |
| | | | $FeF_3^- + CrF_5^- \rightleftharpoons FeF_4^- + CrF_4^-$, $\Delta_{rxn}H$ = -48 kJ | | | |
| $F_5Fe_2^-$ | | | | | | |
| $FeF_2\cdot\cdot FeF_3^-$ | | | | | | |
| * -1740±43 [c] | 3.80±0.40 [i] | *202±37* | | TDEq | | 86SID/BOR |
| -1769±17 [c] | | *201±4* | | TDAs | $\Delta_f H(A^-)$ at 0K | 81SOR/SID |
| $F_5Ge^-$ | | | | | | |
| $GeF_4\cdot\cdot F^-$ | | | | | | |
| -1856±26 | | *418±29* [k] | | Latt | | 84MAL/ROS |
| <-2038 [c] | | *>405* | | IMRB | | 72HAR/CRA |
| $F_5Hf^-$ | | | | | | |
| $HfF_5^-$ | | | | | | |
| -2386±17 [c] | | *429±17* | | TDEq | Reanalyzed literature data, 59 kJ < $AlF_3$ | 86NIK/IGO |
| | | *405±9* | | TDEq | $F^-A$: 84 kJ < $AlF_3$ | 80NIK/SOR |
| $F_5Mn^-$ | | | | | | |
| $MnF_5^-$ | | | | | | |
| -1565±84 | | *348±84* | | TDEq | $F^-A$: 73 kJ < $MnF_3$ | 84KOR/CHI |
| $F_5Mo^-$ | | | | | | |
| $MoF_5^-$ | | | | | *$\Delta_f H(A)$= -1241* | *85JANAF* |
| | >3.5 | | | NBAP | From $MoF_6$ | 78COM/REI |
| | >3.3±0.4 | | | NBAP | From $MoF_6$ | 77MAT/ROT |
| $F_5Pt^-$ | | | | | | |
| $PtF_5^-$ | | | | | | |
| | 6.50 | | | TDEq | | 79SID/NIK |
| $F_5S^-$ | | | | | | |
| $SF_5^-$ | | | | | | |
| * -1195±31 [c] | 3.01±0.29 [i] | *183±8* [g] | *151±8* | IMRE | | 83LAR/MCM |
| <-1263±33 | >3.7±0.3 [i] | | | IMRB | $F^-A$: $SF_4$ > $SF_5$ | 81BAB/STR2 |
| -1251±25 | | | | NBAP | From $SF_6$ | 74LEF/TAN |
| -1269±33 [b] | 3.7±0.2 | | | Est | Literature average | 82JANAF |
| | 2.7±0.2 | | | NBAP | From $SF_6$ | 78COM/REI |
| | >2.9±0.1 | | | NBAP | From $SF_6$ | 75HUB/LOS |
| | >2.8±0.1 | | | EnCT | | 73LIF/TIE |
| | >2.8±0.2 | | | NBAP | From $SF_6$ | 73COM/COO |
| | 3.2±0.2 | | | EIAP | From $SF_6$, new EA($F^-$) | 61CUR2 |
| | 3.66±0.04 | | | SI | | 64KAY/PAG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_5Se^-$ | | | | | | |
| $SeF_5^-$ | | | | | *$\Delta_f H(A)$= −476±42* | *69BRI* |
| −1385±40 | >5.1 [i] | | | NBAP | From $SeF_6$ | 78COM/REI |
| | 3.3±0.1 | | | EIAP | From $SeF_6$ | 73HAR/THY |
| <−1197 | | | | EIAP | From $SeF_6$ | 69BRI |
| $F_5Si^-$ | | | | | | |
| $SiF_4\cdot\cdot F^-$ | | | | | | |
| • −2115±19 [c] | | *251±17* [g] | *226±17* | IMRE | | 85LAR/MCM |
| | | *285±21* | | IMRB | $F^-A$: < $BF_3$, > $iPr_2BF$ | 77MUR/BEA3 |
| <−2318 | | | | IMRB | | 70MAC/THY |
| $F_5Te^-$ | | | | | | |
| $TeF_5^-$ | | | | | *$\Delta_f H(A)$= −586±42* | *69BRI* |
| | 4.5 | | | NBAP | From $TeF_6$ | 78COM/REI |
| | 4.2±0.1 | | | EIAP | From $TeF_6$ | 73HAR/THY |
| <−1397 | | | | EIAP | From $TeF_6$ | 69BRI |
| $F_5Th^-$ | | | | | | |
| $ThF_4\cdot\cdot F^-$ | | | | | | |
| −2432±13 | | *436±15* [k] | | TDEq | $F^-A$: 88 kJ < $AlF_3$, 15 kJ < $ZrF_4$ | 83SID/ZHU |
| $F_5U^-$ | | | | | | |
| $UF_5^-$ | | | | | | |
| −2275±19 [c] | 2.99±0.20 [i] | *427±15* | | TDEq | Reanalyzed literature data, 61 kJ < $AlF_3$ | 86NIK/IGO |
| • −2322±15 | 3.47±0.26 [i] | *424* [k] | | TDEq | Critical review, other literature data corrected | 84PYA/GUS |
| −2256±4 [c] | 3.30±0.16 [i] | *410±1* | | TDEq | $F^-A$: 93 kJ < $AlF_3$ | 80SID/SKO |
| −2297±33 | 3.78±0.40 [i] | *448±36* [k] | | TDEq | | 80PYA/GUS |
| −2297±33 | | | | TDEq | | 79GUS/GOR |
| −2297±33 | >1.9±0.4 [i] | | | NBAP | From $UF_6$ | 77MAT/ROT |
| −2265±14 | 4.0±0.4 [i] | | | NBAP | From $UF_6$ | 77COM |
| $F_5W^-$ | | | | | | |
| $WF_5^-$ | | | | | *$\Delta_f H(A)$= −1397* | *81WOO* |
| >−1631 | <3.5 | | | IMRB | EA: $WF_5$ < $WF_6$ | 79GEO/BEA |
| | >1.8±0.3 | | | NBAP | From $WF_6$ | 78COM/REI |
| <−1338±25 | >0.4±0.2 | | | EIAP | From $WF_6$ | 77HIL |
| | 1.2±0.3 | | | NBAP | From $WF_6$ | 77DIS/LAC |
| | 1.3±0.2 | | | EIAP | From $WF_6$ | 77DEW/NEU |
| −1409±29 | 0.8±0.2 | *270* [k] | | EIAP | From $WF_6$ | 73THY/HAR2 |
| $F_5Zr^-$ | | | | | | |
| $ZrF_4\cdot\cdot F^-$ | | | | | | |
| −2338±31 [c] | | *415±8* | | TDEq | $F^-A$: 92±3 kJ < $AlF_3$ | 82SKO/SOR |
| −2343±17 [c] | | *403±4* | | TDEq | $F^-A$: 97 kJ < $AlF_3$ | 81SKO/NIK |
| $F_6Fe_2^-$ | | | | | | |
| $Fe_2F_6^-$ | | | | | | |
| −2071±38 | 4.45±0.24 [i] | | | TDEq | | 86SID/BOR |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $F_6Ge_2^-$ | | | | | | |
| $Ge_2F_6^-$ | | | | | | |
| <−117 | | | | IMRB | | 72HAR/CRA |
| $F_6Ir^-$ | | | | | | |
| $IrF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −544±21* | *82TN270* |
| | >5.1±0.5 | | | NBIP | | 78COM/REI |
| $F_6Mo^-$ | | | | | | |
| $MoF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1558±1* | *85JANAF* |
| | >5.1±0.5 | | | NBIP | | 78COM/REI |
| | >4.5±0.4 | | | NBIP | | 77MAT/ROT |
| $F_6P^-$ | | | | | | |
| $PF_5\cdot\cdot F^-$ | | | | | | |
| • −2200±46 [c] | | *356±42* [g] | *308±42* | IMRE | | 85LAR/MCM |
| | | *423±33* | | latt | | 84MAL/ROS |
| $F_6Pt^-$ | | | | | | |
| $PtF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −676±28* | *86KOR/NIK* |
| • −1448±57 [b] | 8.00±0.30 | | | TDEq | EA: 272 kJ > $PtF_4$ | 81NIK/SID2 |
| | >5.1±0.5 | | | NBIP | | 78COM/REI |
| $F_6Re^-$ | | | | | | |
| $ReF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1349* | *84BAR/YEH* |
| | >5.1±0.5 | | | NBIP | | 78COM/REI |
| $F_6S^-$ | | | | | | |
| $SF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1221±1* | *85JANAF* |
| • −1322±10 [b] | 1.05±0.10 | *159±15* [k] | | TDEq | | 85GRI/CHO |
| | 0.542 | | | LPD | | 82DRZ/BRA |
| | 0.8 | | | Kine | | 83LIF |
| | | | Review: literature consistent with $\Delta S^{\ddagger}$ for detachment = −59 J/mol−K | | | |
| | 0.5±0.2 | | | NBIP | | 78COM/REI |
| | 1.4±0.1 | | | Kine | | 83HEN/BEN |
| | >0.7 | | | ECD | | 83CHE/WEN |
| | 1.2±0.3 | | | Est | Literature average | 82JANAF |
| <−1310 | | | | CIDT | | 78REF/FRA |
| | 0.3±0.1 | | | NBIP | | 75HUB/LOS |
| | 0.8±0.1 | | | NBIP | | 74LEF/TAN |
| | >0.6±0.1 | | | EnCT | | 73LIF/TIE |
| | 0.5±0.1 | | | NBIP | | 73COM/COO2 |
| | 0.5±0.2 | | | NBIP | | 73COM/COO |
| | 0.9±0.5 | | | IMRB | | 71FEH |
| | 0.4 | | | IMRB | | 70LIF/HUG |
| | >0.7 | | | ECD | | 68CHE/GEO |
| | 1.1 | | | ES | | 66COM/CHR |
| | 1.5±0.2 | | | SI | | 64KAY/PAG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$F_6Sb^-$** | | | | | | |
| $SbF_5\cdot\cdot F^-$ | | | | | | |
| | >6.0 | | | NBAP | From $Sb_2F_{10}$ | 80COM/REI |
| **$F_6Se^-$** | | | | | | |
| $Se\dot{F}_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1117±21* | *82TN270* |
| −1397±40 [b] | 2.9±0.2 | | | NBIP | | 78COM/REI |
| **$F_6Te^-$** | | | | | | |
| $TeF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1318±21* | *82TN270* |
| • −1636±31 [b] | 3.3±0.1 | | | NBIP | | 78COM/REI |
| | 3.3±0.2 | | | NBIP | | 73COM/COO2 |
| | 3.3±0.2 | | | NBIP | | 73COM/COO |
| **$F_6U^-$** | | | | | | |
| $UF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −2147±2* | *82TN270* |
| • −2680±25 | 5.58±0.31 [i] | | | TDEq | Critical review | 84PYA/GUS |
| −2649±30 | 5.20±0.34 [i] | | | TDEq | $F^-A$: 55±8 kJ > $UF_4$ | 83SKO/SOR |
| −2628±24 [c] | 4.89±0.25 [i] | *424±17* | | TDEq | $F^-A$:(1100K) 14±1 kJ > $UF_4$. $\Delta_f H(A^-)$:298K | 80SID/SKO |
| | 6.33±0.50 | | | TDEq | | 80PYA/GUS |
| −2724±42 | 5.8±0.3 [i] | | | Latt | | 84MAL/ROS |
| | >3.6 | | | IMRB | | 80STR/NEW |
| | >5.5 | | | IMRB | | 80ANN/STO |
| | >4.3±0.4 | | | NBIP | | 77MAT/ROT |
| | >5.1 | | | NBIP | | 77COM |
| | 4.9±0.5 | | | IMRB | Endo $F^-$ transfer to $BF_3$ at 1.5 eV observed | 76BEA |
| | 2.9 | | | SI | | 69PAG/GOO |
| **$F_6W^-$** | | | | | | |
| $WF_6^{-\cdot}$ | | | | | *$\Delta_f H(A)$= −1722±8* | *82TN270* |
| −2046±28 [b] | 3.4±0.2 | | | IMRB | | 85VIG/PAU |
| −2061±25 | 3.5±0.1 | | | IMRB | EA: > $F^-$, < $Cl^-$ | 79GEO/BEA |
| | >5.1±0.5 | | | NBIP | | 78COM/REI |
| | >4.9±0.4 | | | NBIP | | 77MAT/ROT |
| | 3.7±0.2 | | | NBIP | | 77DIS/LAC |
| | 2.7 | | | SI | | 69PAG/GOO |
| **$F_7Fe_2^-$** | | | | | | |
| $FeF_3\cdot\cdot FeF_4^-$ | | | | | | |
| −2379±37 [c] | 4.5±0.2 [i] | *189±24* | | TDAs | | 86SID/BOR |
| −2280±18 | | *204±4* | | TDAs | $\Delta_f H(A^-)$ at 0K | 81SOR/SID |
| **$F_7MnPt^-$** | | | | | | |
| $MnF_3\cdot\cdot PtF_4^-$ | | | | | | |
| −2054±105 | | | | TDEq | | 84KOR/CHI |
| **$F_7Mn_2^-$** | | | | | | |
| $MnF_3\cdot\cdot MnF_4^-$ | | | | | | |
| −2517±84 | | | | TDAs | | 84KOR/CHI |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $F_7Sc_2^-$ | | | | | | | |
| $ScF_3\cdot\cdot ScF_4^-$ | | | | | | | |
| | | | *228±1* | *199±1* | TDAs | | 81NIK/SID |
| $F_7U^-$ | | | | | | | |
| $UF_6\cdot\cdot F^-$ | | | | | | | |
| | −2630±30 | | *237±30* [k] | | TDEq | Critical review | 84PYA/GUS |
| | −2588±46 [c] | | *192±42* | | IMRB | | 76BEA |
| $F_7W^-$ | | | | | | | |
| $WF_6\cdot\cdot F^-$ | | | | | | | |
| | −2266±24 | <6.5 | *289±21* [k] | | IMRB | $F^-$A: $SiF_4 < WF_6 < BF_3$ | 79GEO/BEA |
| $F_8Ge_2^-$ | | | | | | | |
| $Ge_2F_8^-$ | | | | | | | |
| | <−151 | | | | IMRB | | 72HAR/CRA |
| $F_8KSc_2^-$ | | | | | | | |
| $KScF_4\cdot\cdot ScF_4^-$ | | | | | | | |
| | | | *144±3* | *120±4* | TDAs | | 81NIK/SID |
| $F_8U_2^-$ | | | | | | | |
| $U_2F_8^-$ | | | | | | | |
| | >−3598±100 | 2.30 [i] | | | TDEq | | 84PYA/GOR |
| $F_9U_2^-$ | | | | | | | |
| $U_2F_9^-$ | | | | | | | |
| | −4130±30 | 4.30±0.52 | *500±50* [k] | | TDEq | | 84PYA/GOR |
| | −4138±33 | | | | TDEq | | 80PYA/GUS |
| $F_9Zr_2^-$ | | | | | | | |
| $ZrF_4\cdot\cdot ZrF_5^-$ | | | | | | | |
| | −4228±15 [c] | | *214±4* | | TDAs | | 82SKO/SOR |
| $F_{10}U_2^-$ | | | | | | | |
| $U_2F_{10}^-$ | | | | | | | |
| | −4490±30 | 4.50±0.40 [i] | *520±50* [k] | | TDEq | | 84PYA/GOR |
| $F_{11}U_2^-$ | | | | | | | |
| $U_2F_{11}^-$ | | | | | | | |
| | −4850±40 | 6.10±0.70 [i] | *540±50* [k] | | TDEq | | 84PYA/GOR |
| $F_{12}U_2^-$ | | | | | | | |
| $U_2F_{12}^-$ | | | | | | | |
| | >−5200±79 | 7.90±0.80 [i] | | | TDEq | | 84PYA/GOR |
| $Fe^-$ | | | | | | *$\Delta_f H(AH)=$ 471±29* | *79DEN/VAN* |
| $Fe^-$ | | | | | | *BDE(A–H)= 163±29* | *79DEN/VAN* |
| * | 402±1 [b] | 0.151±0.003 | 1461±30 [e] | | LPES | | 86LEO/LIN |
| * | | | 1420±13 [g] | 1389±13 | IMRB | | 85SAL/LAN |
| | | 0.163±0.035 | | | LPES | | 85HOT/LIN |
| | >361±42 [a] | <0.3±0.2 | 1420±13 [e] | | EIAP | From $Fe(CO)_5$ | 76COM/STO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$FeH^-$** | | | | | | |
| $FeH^-$ | | | | | | |
| • | 0.934±0.010 | | | LPES | | 83STE/FEI |
| **$FeH_2^-$** | | | | | | |
| $FeH_2^-$ | | | | | | |
| • | 1.049±0.014 | | | LPES | | 86MIL/FEI |
| **$FeD_2^-$** | | | | | | |
| $FeD_2^-$ | | | | | | |
| • | 1.038±0.013 | | | LPES | | 86MIL/FEI |
| **$FeO^-$** | | | | | *$\Delta_f H(AH)$= 133±17* | *80MUR* |
| $FeO^-$ | | | | - | *BDE(A-H)= 336±38* | *85JANAF* |
| • 107±56 [a] | 1.492±0.020 | 1504±40 [c] | | LPES | | 77ENG/LIN |
| **$Fe_2^-$** | | | | | | |
| $Fe_2^-$ | | | | | | |
| • | 0.902±0.008 | | | LPES | | 86LEO/LIN |
| **$Ga^-$** | | | | *DH* | *$\Delta_f H(AH)$= 220±13* | |
| $Ga^-$ | | | | | *BDE(A-H)= 262±8* | *81KAN/MOO* |
| 236±36 [a] | 0.3±0.1 | 1546±23 [c] | | PD | | 85HOT/LIN |
| **$Ge^-$** | | | | | | |
| $Ge^-$ | | | | | *$\Delta_f H(A)$= 377±2* | *82TN270* |
| • 258±2 [b] | 1.233±0.003 | | | LPES | | 86MIL/MIL |
| **$GeH_3^-$** | | | | | *$\Delta_f H(AH)$= 91±2* | *82TN270* |
| $GeH_3^-$ | | | | | *BDE(A-H)= 345±10* | *83NOB/WAL* |
| • 50±17 [a] | 1.739±0.043 | 1490±15 [c] | 1455±15 [h] | LPD | | 74REE/BRA |
| **$H^-$** | | | | | | |
| $H^-$ | | | | | *BDE(A-H)= 436* | *85JANAF* |
| • 145 [a] | 0.8 | 1675 [c] | 1649 [h] | Calc | Given: 0.754209(3) eV | 85HOT/LIN |
| | 0.78±0.02 | | | PD | | 70FEL |
| **$HIS^-$** | | | | | | |
| $ISH^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 105* | *76REF* |
| −48 | 1.1 | | | Endo | $I^- + H_2S \rightarrow$ | 76REF |
| **$HI_2^-$** | | | | | | |
| $HI\cdot\cdot I^-$ | | | | | | |
| • −233±9 [c] | | *71±8* | *41±11* | TDAs | | 85CAL/KEB |
| **$HK_2O^-$** | | | | | | |
| $K_2OH^-$ | | | | | | |
| −345±12 | | | | TDEq | | 84BUR/KUD |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $HMg^-$ | | | | | | | |
| $MgH^-$ | | | | | | | |
| • | | 1.05±0.06 | | | PD | | 77RAC/FEL |
| $HMn^-$ | | | | | | | |
| $MnH^-$ | | | | | | *$\Delta_f H(A)$= 256* | *79HUB/HER* |
| • | 172 [b] | 0.869±0.010 | | | LPES | | 83STE/FEI |
| $HMoO_4^-$ | | | | | | *$\Delta_f H(AH)$= -887±21* | *82TN270* |
| $HMoO_4^-$ | | | | | | | |
| | −1055±61 [a] | | 1362±40 | | TDEq | $e^- + H_2MoO_4 = HMoO_4^- + H$ | 79MIL |
| $HN^-$ | | | | | | *$\Delta_f H(AH)$= 189±1* | *85GIB/GRE* |
| $NH^{-\cdot}$ | | | | | | *BDE(A−H)= 406±18* | *85JANAF* |
| • | 340±21 [a] | 0.381±0.014 | 1682±20 [c] | 1653±21 [h] | LPES | See also 85NEU/LYK | 76ENG/LIN |
| | | 0.380±0.030 | | | LPES | | 74CEL/BEN |
| $HNO^-$ | | | | | | | |
| $HNO^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 100±4* | *82BAU/COX* |
| • | 68±6 [b] | 0.338±0.015 | | | LPES | | 83ELL/ELL |
| | | | | >1498 | IMRB | | 77SUL |
| $DNO^-$ | | | | | | | |
| $DNO^{-\cdot}$ | | | | | | | |
| • | | 0.330±0.015 | | | LPES | | 83ELL/ELL |
| $HNO_3^-$ | | | | | | | |
| $HNO_3^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= -135* | *82TN270* |
| | −190±15 [b] | 0.6±0.1 | | | NBIP | | 76MAT/ROT2 |
| | | 0.6±0.2 | | | EnCT | | 82PAU/DAL |
| $HN_2O^-$ | | | | | | | |
| $HN=NO^-$ | | | | | | | |
| | <247 | | | | IMRB | $RONO + NH_2^- \rightarrow$ | 81KIN/MAR |
| | <130±21 | | | | IMRB | $CH_2=N^- + N_2O \rightarrow$ | 85KAS/DEP |
| $HN_2O_4^-$ | | | | | | | |
| $HONO\cdot\cdot NO_2^-$ | | | | | | | |
| • | −405±22 [c] | | *136±4* | | TDAs | | 80LEE/KEE |
| $HN_2O_6^-$ | | | | | | | |
| $HNO_3\cdot\cdot NO_3^-$ | | | | | | | |
| • | −545±10 [c] | | *103±8* | *87±7* | TDEq | | 77DAV/FEH |
| $HNi^-$ | | | | | | | |
| $NiH^-$ | | | | | | | |
| • | | 0.481±0.007 | | | LPES | | 87MIL/FEI |
| $HO^-$ | | | | | | *$\Delta_f H(AH)$= -242* | *82TN270* |
| $HO^-$ | | | | | | *BDE(A−H)= 499* | *85JANAF* |
| • | −137 [a] | 1.828 | 1635 [e] | 1607±1 [h] | LPD | Given: 1.827670(21) eV | 82SCH/MEA |
| | | 1.825±0.002 | | | LPD | | 74HOT/PAT |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$HO^-$** | | | | | *$\Delta_f H(AH)$= -242* | *82TN270* |
| $HO^-$ | | | | | *BDE(A-H)= 499* | *85JANAF* |
| | 1.829±0.010 | | | LPES | | 74CEL/BEN |
| | 1.83±0.04 | | | PD | | 66BRA |
| | 1.8±0.2 | | | EIAP | From MeOH, EtOH, nPrOH | 64TSU/HAM |
| • | 1.9±0.1 | | | SI | | 69PAG/GOO |
| **$DO^-$** | | | | | *$\Delta_f H(AH)$= -249* | *82TN270* |
| $DO^-$ | | | | | *BDE(A-H)= 504±1* | *82TN270* |
| -139±1 [a] | 1.826 | 1640±1 [c] | 1615±1 [h] | LPD | Given: 1.822549(37) eV | 82SCH/MEA |
| | 1.823±0.002 | | | LPD | | 74HOT/PAT |
| **$HO_2^-$** | | | | | *$\Delta_f H(AH)$= -136±1* | *82TN270* |
| $HOO^-$ | | | | | *BDE(A-H)= 365±3* | *82TN270* |
| • -94±10 [a] | 1.08±0.12 [d] | 1573±9 [g] | 1542±8 | IMRE | | 81BIE/SCH |
| • | 1.078±0.017 | | | LPES | | 85OAK/HAR |
| | 1.9±0.1 | | | Ther | From a solution phase thermodynamic cycle | 80BEN/NAN |
| | 1.19±0.01 | | 1536±12 | IMRE[o] | | 81BIE/SCH |
| **$DO_2^-$** | | | | | | |
| $DOO^-$ | | | | | | |
| • | 1.089±0.017 | | | LPES | | 85OAK/HAR |
| **$HO_2S^-$** | | | | | | |
| $HSO_2^-$ | | | | | | |
| -415 [c] | | *264±67* [g] | *238±67* | IMRB | | 85LAH/HAY |
| **$HO_3S^-$** | | | | | | |
| $SO_2\cdot\cdot OH^-$ | | | | | | |
| < -802 [c] | | > *368* | | IMRB | $CO_2\cdot\cdot HO^- + SO_2 \rightarrow$ | 84HIE/PAU |
| **$HO_4S^-$** | | | | | *$\Delta_f H(AH)$= -735±8* | *85JANAF* |
| $HSO_4^-$ | | | | | | |
| < -953±17 [a] | | < 1312±8 | < 1281±10 [h] | EIAP | From $H_2SO_4$ (Appearance Potential = 0eV) | 86ADA/SMI |
| | 4.5 [d] | < 1320 [g] | < 1289 | IMRB | $I^- + H_2SO_4 \rightarrow$ | 80VIG/PER |
| **$HO_4W^-$** | | | | | *$\Delta_f H(AH)$= -906±4* | *85JANAF* |
| $HWO_4^-$ | | | | | | |
| -1084±46 [a] | | 1352±41 | 1322±48 [h] | TDEq | $H_2WO_4 + e^- = HWO_4^- + H$ measured | 70JEN/MIL |
| **$HP^-$** | | | | | *$\Delta_f H(AH)$= 139±3* | *86BER/CUR* |
| $PH^{-}\cdot$ | | | | | *BDE(A-H)= 315±11* | *86BER/CUR* |
| • 137±12 [a] | 1.028±0.010 | 1528±9 [c] | | LPES | | 76ZIT/LIN |
| | 1.00±0.06 | | | PD | | 77RAC/FEL |
| 218±18 | > 0.5±0.2 | | | EIAP | From $PH_3$ | 69HAL/PLA |
| | < 1.1 | | | IMRB | | 64EBI/KRA |
| **$HS^-$** | | | | | *$\Delta_f H(AH)$= -21±1* | *82TN270* |
| $HS^-$ | | | | | *BDE(A-H)= 381±1* | *82TN270* |
| • -81±10 [a] | 2.32±0.10 [d] | 1469±9 [g] | 1443±8 | IMRE | | 79BAR/SCO |
| • | 2.310±0.010 | 1470±2 [c] | 1443±3 [h] | LPD | | 80JAN/REE |
| | | 1473±9 [g] | 1446±8 | IMRE | | 78CUM/KEB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$HS^-$** | | | | | | *$\Delta_f H(AH)$= -21±1* | *82TN270* |
| $HS^-$ | | | | | | *BDE(A–H)= 381±1* | *82TN270* |
| | | 2.302±0.001 | | | LPD | | 74EYL/ATK |
| | | 2.32±0.01 | | | PD | | 68STE |
| | –69 | 2.2 [i] | | | Endo | | 76REF |
| | | 2.30±0.04 | | | SI | | 69PAG/GOO |
| | | | | 1453±8 | IMRE[o] | | 79BAR/SCO |
| **$HSe^-$** | | | | | | *$\Delta_f H(AH)$= 30±8* | *82TN270* |
| $HSe^-$ | | | | | | *BDE(A–H)= 368±19* | *72DON/LIT* |
| • | –34±28 [a] | 2.213 | 1466±19 [c] | 1440±19 [h] | LPD | | 86STO/LAR |
| | | 2.21±0.03 | | | PD | | 72SMY/BRA3 |
| | | | 1434±38 [g] | 1407±38 | IMRB | Between $H_2S$, HCl | 72DIX/HOL |
| **$HSi^-$** | | | | | | *$\Delta_f H(AH)$= 237±16* | *81DON/WAL* |
| $SiH^{-\cdot}$ | | | | | | *BDE(A–H)= 353±8* | *81DON/WAL* |
| • | 249±3 [b] | 1.277±0.009 | | | LPES | | 75KAS/HER |
| **$HTe^-$** | | | | | | *$\Delta_f H(AH)$= 100±2* | *82TN270* |
| $TeH^-$ | | | | | | | |
| • | | 2.102±0.015 | | | LPES | | 86FRE/SNO |
| **$HZn^-$** | | | | | | | |
| $ZnH^-$ | | | | | | | |
| | | <0.9 | | | PD | | 77RAC/FEL |
| **$H_2IO^-$** | | | | | | | |
| $HOH\cdot\cdot I^-$ | | | | | | | |
| • | –472 [c] | | *42±4* | *23±9* | TDAs | | 84CAL/KEB |
| | | | *46* | *22±1* | TDAs | | 80KEE/CAS2 |
| | | | *43±8* | *23±8* | TDAs | | 70ARS/YAM |
| **$H_2Mn^-$** | | | | | | | |
| $MnH_2^-$ | | | | | | | |
| • | | 0.444±0.016 | | | LPES | | 86MIL/FEI |
| **$D_2Mn^-$** | | | | | | | |
| $MnD_2^-$ | | | | | | | |
| • | | 0.465±0.014 | | | LPES | | 86MIL/FEI |
| **$H_2N^-$** | | | | | | *$\Delta_f H(AH)$= -46* | *82TN270* |
| $NH_2^-$ | | | | | | *BDE(A–H)= 449±3* | *82TN270* |
| • | 113±4 [a] | 0.75±0.06 [d] | 1689±3 [g] | 1657±3 | IMRE | | 76MAC/HEM |
| • | | 0.776±0.037 | | | LPES | | 74CEL/BEN |
| | | 0.744±0.022 | | | LPD | | 72SMY/BRA2 |
| | | 0.740±0.030 | | | LPD | | 71SMY/MCI |
| | | 0.76±0.04 | | | PD | | 71FEL |
| | 49±19 | | | | EIAP | From $NH_3$ | 68COL/HUB |
| | | 1.1 | | | SI | | 69PAG/GOO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $H_2NO_3^-$ | | | | | | |
| $HOH\cdot\cdot NO_2^-$ | | | | | | |
| • −494 [c] | | *64* | *34±1* | TDAs | | 80LEE/KEE |
| | | *60±8* | *33±8* | TDAs | | 71PAY/YAM |
| | | | *34±24* | Endo | | 82PAU/DAL |
| • −431 [c] | 2.850 | | | LPD | | 79SMI/LEE2 |
| $H_2NO_4^-$ | | | | | | |
| $HOH\cdot\cdot NO_3^-$ | | | | | | |
| • −610 [c] | | *61±1* | *30±1* | TDAs | | 80LEE/KEE |
| | | *52±8* | *28±8* | TDAs | | 71PAY/YAM |
| $H_2NO_4^-$ | | | | | | |
| $HOOH\cdot\cdot NO_2^-$ | | | | | | |
| −410±15 [c] | | *85±4* | *60±4* | TDEq | Relative to $HOH\cdot\cdot NO_2^-$, 80KEE/LEE | 84BOH/FAH |
| $H_2NO_5^-$ | | | | | | |
| $HOOH\cdot\cdot NO_3^-$ | | | | | | |
| • −524±6 [c] | | *80±4* | *54±4* | TDEq | Relative to $HOH\cdot\cdot NO_3^-$, 80KEE/LEE | 84BOH/FAH |
| $H_2NS^-$ | | | | | | |
| $H_2NS^-$ | | | | | | |
| | | 1493±16 [g] | 1467±13 | IMRB | | 81DEP/BIE |
| | | | Between $CF_3CH_2OH$ and $H_2S$, comparable to MeSH | | | |
| | | | 1480±13 | IMRB | $NH_2^-$ + COS → | 84BIE/GRA |
| | | | 1476±13 | IMRB[o] | | 81DEP/BIE |
| $H_2Ni^-$ | | | | | | |
| $NiH_2^-$ | | | | | | |
| • | 1.934±0.008 | | | LPES | | 86MIL/FEI |
| $D_2Ni^-$ | | | | | | |
| $NiD_2^-$ | | | | | | |
| • | 1.926±0.007 | | | LPES | | 86MIL/FEI |
| $H_2O^-$ | | | | | | |
| $HO\cdot\cdot H^-$ | | | | | | |
| −34±17 | | *287* [k] | | IMRB | | 84DEK/NIB |
| $H_2O_3^-$ | | | | | | |
| $HOH\cdot\cdot O_2^-$ | | | | | | |
| • −361 [c] | | *77±8* | *52±8* | TDAs | | 70ARS/KEB |
| | | | *49±8* | IMRE | | 71PAR |
| $H_2P^-$ | | | | | *$\Delta_f H(AH)$= 5±2* | *61GUN/GRE* |
| $PH_2^-$ | | | | | *BDE(A−H)= 354±5* | *86BER/CUR* |
| • 27±10 [a] | 1.19±0.14 [d] | 1552±8 [g] | 1520±8 | IMRE | | 79BAR/SCO |
| • | 1.271±0.010 | 1544±6 [c] | | LPES | | 76ZIT/LIN |
| | 1.25±0.03 | | | PD | | 72SMY/BRA |
| | 1.300±0.030 | | | LPD | | 71SMY/MCI |
| | | 1524±19 | | EIAP | | 69HAL/PLA |
| < 9±21 [a] | < 1.4±0.3 [d] | < 1534±19 | | EIAP | | 64EBI/KRA |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $H_2P^-$ | | | | | | | |
| $PH_2^-$ | | | | | | *$\Delta_f H(AH)$= 5±2* | *61GUN/GRE* |
| | | | | | | *BDE(A–H)= 354±5* | *86BER/CUR* |
| | | 1.6 | | | SI | | 69PAG/GOO |
| | | | | 1519±8 | IMRE° | | 79BAR/SCO |
| $H_2Si^-$ | | | | | | | |
| $SiH_2^{-\cdot}$ | | | | | | *$\Delta_f H(AH)$= 203±6* | *87BOO/ARM* |
| | | | | | | *BDE(A–H)= 304±15* | *87BOO/ARM* |
| * | 181±10 [b] | 1.123±0.022 | 1508±17 [c] | | LPES | | 75KAS/HER |
| $H_3O^-$ | | | | | | | |
| $HOH\cdot\cdot H^-$ | | | | | | | |
| | −169±17 | | *72±21* [k] | | Endo | $HOH\cdot\cdot HO^- + H_2 \rightarrow$ | 84PAU/HEN |
| | −199±49 | | | | IMRB | $H^- + HCO_2H \rightarrow$ | 83KLE/NIB |
| $H_3OSi^-$ | | | | | | | |
| $H_3SiO^-$ | | | | | | | |
| | <−107 | | | | IMRB | $HO^- + SiH_4 \rightarrow$ | 76PAY/TAN |
| $H_3O_2^-$ | | | | | | | |
| $HOH\cdot\cdot OH^-$ | | | | | | | |
| * | −479 [c] | | *100±8* | *78±8* | TDAs | | 71PAY/YAM |
| * | | 2.9±0.2 | | | PD | | 68GOL/STE |
| | | | *112±4* | *84±7* | TDEq | | 86MEO/SIE2 |
| | | | *94±8* | *71±8* | TDAs | | 70ARS/KEB |
| | | | *149±29* | | CIDT | | 70DEP/GIA |
| $D_3O_2^-$ | | | | | | | |
| $DOD\cdot\cdot OD^-$ | | | | | | | |
| | −491 [c] | | *112±3* | *84±5* | TDAs | | 86MEO/SIE |
| $H_3O_5S^-$ | | | | | | | |
| $HOH\cdot\cdot HSO_4^-$ | | | | | | | |
| | | | *50±4* | *25±4* | TDAs | | 84BOH/FAH |
| $H_3O_6S^-$ | | | | | | | |
| $HOOH\cdot\cdot HSO_4^-$ | | | | | | | |
| | −1156±22 [c] | | *67±4* | *45±4* | TDEq | Relative to $HOH\cdot\cdot HSO_4^-$, 84BOH/FAH | 84BOH/FAH |
| $H_3P_2^-$ | | | | | | | |
| $P_2H_3^-$ | | | | | | | |
| | <66 | | | | IMRB | $PH_2^- + PH_3 \rightarrow$ | 72SMY/BRA |
| $H_3Si^-$ | | | | | | | |
| $SiH_3^-$ | | | | | | *$\Delta_f H(AH)$= 35±2* | *81BEL/PER* |
| | | | | | | *BDE(A–H)= 386±8* | *87BOO/ARM* |
| * | 63±10 [a] | 1.45±0.17 [d] | 1558±8 [g] | 1522±8 | IMRE | | 79BAR/SCO |
| * | | 1.406±0.014 | 1562±10 [c] | | LPES | | 86NIM/ELL2 |
| | | <1.440±0.030 | | | LPD | | 74REE/BRA |
| | 486±10 | | | | EIAP | | 64EBI/KRA |
| | | | | 1519±8 | IMRE° | | 79BAR/SCO |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $D_3Si^-$ | | | | | | |
| $SiD_3^-$ | | | | | | |
| | 1.386±0.022 | | | LPES | | 86NIM/ELL2 |
| $H_4N^{-\cdot}$ | | | | | | |
| $NH_3\cdot\cdot H^-$ | | | | | | |
| | 1.110±0.019 | | | LPES | | 87SNO/COE3 |
| | 1.110±0.019 | | | LPES | | 85COE/SNO |
| $H_5N_2^-$ | | | | | | |
| $NH_3\cdot\cdot NH_2^-$ | | | | | | |
| 16 [c] | | *50* | | PDis | | 87SNO/COE2 |
| $H_5Si^-$ | | | | | | |
| $SiH_4\cdot\cdot H^-$ | | | | | | |
| 86 [c] | | *94±19* | | IMRE | | 86HAJ/SQU |
| $H_7N_2^-$ | | | | | | |
| $(NH_3)_2\cdot\cdot H^-$ | | | | | | |
| −114 [c] | 1.460±0.019 | | | LPES | | 87SNO/COE3 |
| $H_8N_3^-$ | | | | | | |
| $(NH_3)_2\cdot\cdot NH_2^-$ | | | | | | |
| | 1.780±0.019 | | | LPES | | 87SNO/COE2 |
| $I^-$ | | | | | | |
| $I^-$ | | | | | *$\Delta_f H(A)=$ 107* | *82BAU/COX* |
| • −188±1 [a] | 3.059 | 1315 [e] | 1294±1 [h] | LOG | | 83WEB/MCD |
| $IK_2^-$ | | | | | | |
| $K_2I^-$ | | | | | | |
| −244±11 | | | | TDEq | | 84BUR/KUD |
| $ILi^-$ | | | | | | |
| $LiI^{-\cdot}$ | | | | | *$\Delta_f H(A)=$ −91±8* | *85JANAF* |
| <−199 [b] | >1.1 | | | EIAP | From $(LiI)_2$ | 64EBI |
| $IN^-$ | | | | | | |
| $IN^{-\cdot}$ | | | | | *$\Delta_f H(A)=$ 215* | *76REF2* |
| 96±21 | 1.3±0.2 | | | Endo | $I^- + NO_2 \rightarrow$ | 76REF2 |
| $IO^-$ | | | | | | |
| $IO^-$ | | | | | | |
| <−66 | >2.5 [i] | | | Endo | $I^- + CO \rightarrow$ | 77VOG/MIS |
| −42±35 | >2.1±0.3 [i] | | | Endo | $I^- + O_2 \rightarrow$ | 77VOG/DRE |
| −79±21 | 2.6 [i] | | | Endo | $I^- + O_2 \rightarrow$ | 76REF/FRA2 |
| −48 | 2.3 [i] | | | Endo | $I^- + SO_2 \rightarrow$ | 76REF/FRA |
| <−147 | >3.3 [i] | | | IMRB | $O^- + I_2 \rightarrow$ | 59HEN/MUC |

## Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}$(AH) $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}$(AH) $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$IOS^-$** | | | | | | |
| $ISO^-$ | | | | | | |
| −67 | | | | Endo | $I^- + SO_2 \rightarrow$ | 76REF/FRA |
| **$IO_2S^-$** | | | | | | |
| $SO_2\cdot\cdot I^-$ | | | | | | |
| • −545±10 [c] | | *60±8* | *38±11* | TDAs | | 85CAL/KEB |
| −539±2 [c] | | *54* | *37±1* | TDAs | | 80KEE/LEE |
| **$IS^-$** | | | | | | |
| $IS^-$ | | | | | *$\Delta_f H(A)$= 310* | *76REF/FRA* |
| 47±29 | 2.7±0.3 [i] | | | Endo | $I^-$ + $H_2S$ and $CS_2 \rightarrow$ | 76REF |
| **$I_2^-$** | | | | | | |
| $I_2^{-\cdot}$ | | | | | *$\Delta_f H(A)$= 62* | *82BAU/COX* |
| • −181 [b] | 2.5±0.1 | | | NBIP | | 73BAE/AUE |
| | 1.72±0.05 | | | NBIP | Vertical EA | 76HUB/KLE |
| | 2.3 | | | ECD | Vertical EA: 1.7 eV | 81AYA/WEN |
| | 2.4±0.2 | | | EnCT | | 73HUG/LIF |
| | 2.4±0.1 | | | NBIP | | 71MOU/ATE |
| | 2.6±0.1 | | | EIAP | From $CHI_3$ | 71DEC/FRA |
| | 2.6±0.1 | | | EnCT | | 71CHU/BER |
| **$I_2K^-$** | | | | | | |
| $KI\cdot\cdot I^-$ | | | | | | |
| −483±8 | | | | TDEq | | 84BUR/KUD |
| **$I_2Sn^-$** | | | | | | |
| $SnI_2^{-\cdot}$ | | | | | | |
| | 1.7 | | | EIAP | From $SnI_4$ | 77PAB/PER |
| **$I_3^-$** | | | | | | |
| $I_3^-$ | | | | | | |
| −482 | | *356* [k] | | Latt | | 77FIN/GAT |
| <−207 | | | | IMRB | | 28HOG/HAR |
| | | | | | $I_2^-$ + $I_2 \rightarrow$; First negative ion/molecule reaction reported. | |
| **$I_3K_2^-$** | | | | | | |
| $K_2I_3^-$ | | | | | | |
| −760±15 | | | | TDEq | | 84BUR/KUD |
| **$I_3Sn^-$** | | | | | | |
| $SnI_3^-$ | | | | | | |
| | 3.21±0.01 | | | EIAP | From $SnI_4$ | 78PAB/MAR |
| | 3.2 | | | EIAP | From $SnI_4$ | 77PAB/PER |
| **$I_3Ti^-$** | | | | | | |
| $TiI_3^-$ | | | | | *$\Delta_f H(A)$= −150±33* | *85JANAF* |
| <−240±18 | >0.9 | | | EIAP | From $TiI_4$ | 74BEN/PAB |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ <br> $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) <br> eV | $\Delta H_{acid}(AH)$ <br> $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ <br> $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$In^-$** | | | | | | | |
| $In^-$ | | | | | | *$\Delta_f H(A)$= 244* | *82TN270* |
| • | 215±36 [a] | 0.3±0.2 | 1508±28 [c] | | PD | | 85HOT/LIN |
| | | 0.8±0.2 | | | EIAP | From InBr | 80BRU/COT |
| **$Ir^-$** | | | | | | | |
| $Ir^-$ | | | | | | *$\Delta_f H(A)$= 665±2* | *82TN270* |
| • | 514±3 [b] | 1.565±0.008 | | | LPES | | 85HOT/LIN |
| **$K^-$** | | | | | | | |
| $K^-$ | | | | | | *$\Delta_f H(A)$= 89* | *82TN270* |
| • | 41 [b] | 0.501 | 1448±15 [c] | 1428±17 [h] | LPD | | 85HOT/LIN |
| **$KO_4S^-$** | | | | | | | |
| $KSO_4^-$ | | | | | | | |
| | −992±11 | | | | TDEq | | 85RUD/SID2 |
| **$Li^-$** | | | | | | | |
| $Li^-$ | | | | | | *$\Delta_f H(A)$= 161* | *82TN270* |
| • | 101 [a] | 0.618±0.001 | 1492 [c] | 1470±1 [h] | LPD | | 85HOT/LIN |
| **$Mo^-$** | | | | | | | |
| $Mo^-$ | | | | | | *$\Delta_f H(A)$= 658±2* | *82TN270* |
| • | 586±3 [b] | 0.746±0.010 | | | LPES | | 85HOT/LIN |
| | | | | 1402±13 | IMRB | | 85SAL/LAN |
| **$MoO_3^-$** | | | | | | | |
| $MoO_3^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −362* | *81WOO* |
| | −655±40 | 2.58±0.41 [i] | | | TDEq | $H + HMoO_4^- = H_2O + MoO_3^-$ | 79MIL |
| **$NO^-$** | | | | | | | |
| $NO^-$ | | | | | | *$\Delta_f H(A)$= 91* | *82BAU/COX* |
| • | 89±18 [a] | 2.4±0.010 | 1519±9 [c] | 1492±10 [h] | LPES | | 72SIE/CEL |
| | | 0.1±0.1 | | | ECD | | 83CHE/WEN |
| | | 2.0±0.1 | | | CIDT | | 78TIE/WU |
| | | 0.0±0.1 | | | NBIP | | 77DUR/PAR |
| | | 0.7±0.2 | | | Endo | | 76REF2 |
| | | 2.500±0.007 | | | ETS | | 74BUR |
| | | >0.1±0.1 | | | NBIP | | 73NAL/COM |
| | | 1.5±0.1 | | | EnCT | | 73HUG/LIF |
| | | 2.60±0.02 | | | Kine | | 72PAR/SUG |
| | | >6.0±0.1 | | | EnCT | | 71CHA |
| | | >9.0 | | | EnCT | | 71BER/CHU |
| | | 0.0±0.2 | | | NBIP | | 70LAC/HER |
| | | >0.7±0.1 | | | EIAP | From $NO_2$ | 69STO/COM |
| | | 0.8±0.1 | | | EIAP | From EtONO, nBuONO | 68WIL/HAM |
| | | 0.8 | | | SI | | 69PAG/GOO |
| | | 0.9 | | | SI | | 64FAR/PAG |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $NOS^-$ | | | | | | |
| $NSO^-$ | | | | | | |
| <−142 | | | 1414±21 | IMRB | $NH_2^- + SO_2 \rightarrow$ | 84BIE/GRA |
| $NO_2^-$ | | | | | *$\Delta_fH(AH)$= −80±8* | *82BAU/COX* |
| $NO_2^-$ | | | | | *BDE(A−H)= 331±9* | *82BAU/COX* |
| • −189±10 [b] | 2.30±0.10 | 1421±18 [e] | 1389±18 [h] | TDEq | | 87KEB/CHO |
| | 2.359±0.100 | | | LPES | | 74HER/PAT |
| | 2.31±0.11 | | | IMRE | | 85GRI/CAL |
| | 2.1±0.2 | | | ECD | | 83CHE/WEN |
| | 2.350±0.100 | | | LPD | | 79SMI/LEE2 |
| | 2.800±0.050 | | | LPD | | 74RIC/STE |
| | <2.6 | | | IMRB | | 72FER/DUN |
| | 2.4±0.1 | | | CIDT | | 78TIE/WU |
| | 2.1 | | | EnCT | | 76REF2 |
| | >2.5±0.1 | | | NBIP | | 73NAL/COM |
| | 2.50±0.05 | | | NBIP | | 73LEF/JAC |
| | 2.3±0.1 | | | IMRB | | 73HUG/LIF |
| | 2.38±0.06 | | | IMRB | | 72DUN/FEH |
| | 2.5±0.1 | | | NBIP | | 72BAE |
| | 1.8±0.2 | | | NBIP | | 77DUR/PAR |
| | <3.9 | | | PD | | 71MIL/JAC |
| | 2.0 | | | EnCT | | 71BER/CHU |
| | 2.3±0.1 | | | EnCT | | 70LIF/HUG |
| | 2.1±0.2 | | | IMRB | | 69VOG |
| 9±29 | | | | IMRE | $CO_3^- + NO \rightarrow$ [isomer?] | 70ADA/BOH |
| | 3.10±0.05 | | | PD | | 69WAR |
| | 3.9±0.2 | | | EIAP | From $MeNO_2$, $EtNO_2$ | 64TSU/HAM |
| | >3.8 | | | IMRB | | 62CUR |
| | 1.800±0.050 | | | LPD | | 74RIC/STE |
| | 4.0 | | | SI | | 64FAR/PAG |
| $NO_3^-$ | | | | | *$\Delta_fH(AH)$= −135* | *82BAU/COX* |
| $NO_3^-$ | | | | | *BDE(A−H)= 424±21* | *77DAV/FEH* |
| • −307±1 [a] | 3.92±0.24 [i] | 1358±1 | 1330±1 | TDEq | | 77DAV/FEH |
| | | | | | Relative to HBr, reevaluated with current HBr acidity | |
| | | 1358±2 | | TDEq | | 72FER/DUN |
| | | 1371±24 | | Endo | $I^- + HNO_3 \rightarrow$ | 76REF/FRA3 |
| | | 1380±20 | | NBAP | From $HNO_3$ | 76MAT/ROT2 |
| | 3.70±0.20 | | | IMRE | $NO_3^- + NO = NO_2^- + NO_2$ | 72MCF/DUN |
| | | 1491 | | Endo | | 71BER/CHU |
| <−10 | | | | IMRB | $O_4^- + NO \rightarrow NO_3^- + O_2$; isomer? | 70ADA/BOH |
| −135±21 [c] | | *276±21* | | PDis | | 78SMI/LEE |
| | | *<193* | | PDis | isomer: $O_4^- + NO \rightarrow$ | 79SMI/LEE2 |
| $NO_4S^-$ | | | | | | |
| $SO_2\cdot\cdot NO_2^-$ | | | | | | |
| • −594±12 [c] | | *108±1* | *62±1* | TDAs | | 80KEE/LEE |
| | | *102±4* | *62±4* | TDEq | Relative to $HOH\cdot\cdot NO_2^-$, 80KEE/LEE | 84BOH/FAH |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $NO_5S^-$ | | | | | | | |
| $SO_2\cdot\cdot NO_3^-$ | | | | | | | |
| • | −676±11 [c] | | *72±8* | *40±8* | TDEq | Relative to $HOH\cdot\cdot NO_3^-$, 80KEE/LEE | 84BOH/FAH |
| | | | *76±5* | *37±4* | TDAs | | 83WLO/LUC |
| $NS^-$ | | | | | | | |
| $NS^{-\cdot}$ | | | | | | | |
| • | | 1.194±0.011 | | | LPES | | 82BUR/FEI |
| $N_2O^-$ | | | | | | | |
| $N_2O^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 82* | *82BAU/COX* |
| | 61±10 [b] | 0.2±0.1 | *47±12 [k]* | | CIDT | | 78TIE/WU |
| | 67±12 [c] | 0.2±0.1 [i] | *41±10* | | CIDT | Vertical detachment: −2.23±0.20 eV | 76HOP/WAH |
| | | | | | | | 73NAL/COM |
| | | 0.3±0.2 | | | ECD | | 71WEN/CHE |
| | | 0.760±0.100 | | | LPES | Vertical detachment | 86COE/SNO |
| $N_2O_2^-$ | | | | | | | |
| $N_2\cdot\cdot O_2^-$ | | | | | | | |
| | >−99 [c] | | *<57* | | IMRB | $N_2\cdot\cdot O_2^- + O_2 \rightarrow O_4^-$ | 70ADA/BOH |
| $N_2O_3^-$ | | | | | | | |
| $N_2O\cdot\cdot O_2^-$ | | | | | | | |
| | >−17 [c] | | *<57* | | IMRB | $N_2O\cdot\cdot O_2^- + O_2 \rightarrow O_4^- + N_2O$ | 70ADA/BOH |
| $N_3^-$ | | | | | | *$\Delta_f H(AH)$= 294±2* | *82TN270* |
| $N_3^-$ | | | | | *D-EA* | *BDE(A−H)= 387±21* | |
| • | | 2.762±0.043 | | | LPD | | 85ILL/COM |
| • | 203±15 [a] | 2.7±0.1 | 1439±13 [g] | 1414±12 | IMRB | Acidity near $HCO_2H$ | 81PEL/JAC |
| | | >2.540 | | | LPES | | 76ENG/LIN |
| | 199±29 | 3.1±0.3 [i] | 1418±21 [f] | | EIAP | From $MeN_3$ and $HN_3$ | 58FRA/DIB |
| $N_3O_2^-$ | | | | | | | |
| $N_2O\cdot\cdot NO^-$ | | | | | | | |
| | 151±18 [b] | 0.258±0.009 | *19 [k]* | | LPES | | 87COE/SNO |
| $N_4O_2^-$ | | | | | | | |
| $(N_2O)_2^-$ | | | | | | | |
| | | 0.950±0.100 | | | LPES | | 86COE/SNO |
| $N_5O_3^-$ | | | | | | | |
| $(N_2O)_2\cdot\cdot NO^-$ | | | | | | | |
| | 213±18 [c] | 0.513±0.022 | *19 [k]* | | LPES | | 87COE/SNO |
| $Na^-$ | | | | | | *$\Delta_f H(AH)$= 130* | *82TN270* |
| $Na^-$ | | | | | | *BDE(A−H)= 195±1* | *85JANAF* |
| • | 54±1 [b] | 0.548 | 1455±1 [c] | 1434±3 [h] | LPD | | 85HOT/LIN |
| $Nb^-$ | | | | | | | |
| $Nb^-$ | | | | | | *$\Delta_f H(A)$= 733±8* | *85JANAF* |
| • | 647±11 [b] | 0.893±0.025 | | | LPES | | 85HOT/LIN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| **$Ni^-$** | | | | | | |
| $Ni^-$ | | | | | $\Delta_f H(A)=$ 430±2 | 82TN270 |
| • 318±3 [b] | 1.156±0.010 | | | LPES | | 85HOT/LIN |
| **$O^-$** | | | | | $\Delta_f H(AH)=$ 39±1 | 85JANAF |
| $O^-$ | | | | | $BDE(A-H)=$ 428±1 | 85JANAF |
| • 108±2 [a] | 1.461 | 1599±1 [e] | 1574±2 [h] | LPD | Given: 1.461122(3) eV | 85NEU/LYK |
| | 1.462 | | | LPD | | 85HOT/LIN |
| **$OP^-$** | | | | | | |
| $OP^-$ | | | | | $\Delta_f H(A)=$ −33±13 | 83PED/MAR |
| • −139±14 [b] | 1.092±0.010 | | | LPES | | 76ZIT/LIN |
| **$OS^-$** | | | | | | |
| $SO^{-\cdot}$ | | | | | $\Delta_f H(A)=$ 5±1 | 85JANAF |
| • −100±6 [b] | 1.09±0.05 | | | PD | | 70FEL |
| −111 | 1.12±0.01 [i] | | | Endo | $I^- + SO_2 \rightarrow$ | 76REF/FRA |
| | 1.1 | | | EIAP | From $SO_2$ | 73HAR/FRA |
| | >1.2±0.1 | | | EIAP | From $SO_2$ | 72THY |
| | <1.1 | | | IMRB | | 61KRA/MUL |
| | <1.1 | | | IMRB | EA: < $SO_2$ | 59HEN/MUC |
| −100 | 1.2 | | | EIAP | From $SO_2$ | 58REE/DIB |
| **$OS_2^-$** | | | | | | |
| $S_2O^-$ | | | | | $\Delta_f H(A)=$ −53 | 86NIM/ELL |
| • −234±1 [b] | 1.877±0.008 | | | LPES | | 86NIM/ELL |
| **$OSe^-$** | | | | | | |
| $SeO^-$ | | | | | $\Delta_f H(A)=$ 53 | 82TN270 |
| • −87±2 [b] | 1.456±0.020 | | | LPES | | 86COE/SNO2 |
| **$OTe^-$** | | | | | | |
| $TeO^-$ | | | | | $\Delta_f H(A)=$ 69±21 | 83PED/MAR |
| • −95±23 [b] | 1.697±0.022 | | | LPES | | 86FRE/COE |
| **$O_2^-$** | | | | | $\Delta_f H(AH)=$ 10±8 | 82TN270 |
| $O_2^{-\cdot}$ | | | | | $BDE(A-H)=$ 206±8 | 82TN270 |
| • −42±1 [b] | 0.440±0.008 | 1476±9 [e] | 1449±9 [h] | LPES | | 72CEL/BEN |
| | 0.430±0.030 | | | LPES | | 71CEL/BEN |
| | 0.45±0.05 | | | ECD | | 83CHE/WEN |
| | 0.4±0.1 | | | CIDT | From $O_2^-$ | 78TIE/WU |
| | 0.4±0.1 | | | NBIP | | 77DUR/PAR |
| | 0.45±0.02 | | | ETS | | 74BUR |
| | 0.5±0.1 | | | NBIP | | 72BAE |
| | >0.5±0.1 | | | EnCT | | 71TIE/HUG |
| | 0.46±0.05 | | | NBIP | | 71NAL/COM |
| | >0.6±0.1 | | | EnCT | | 71CHA |
| | >0.5 | | | EnCT | | 71BER/CHU |
| | 1.12±0.07 | | | IMRB | | 70VOG/HAU |
| | 0.5±0.2 | | | NBIP | | 70LAC/HER |
| | >1.3±0.2 | | | EnCT | | 70BAI/MAH |
| | >1.1±0.1 | | | EIAP | From $NO_2$ | 69STO/COM |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ *$\Delta H_{aff}(X\cdot\cdot Y^-)$* | $\Delta G_{acid}(AH)$ *$\Delta G_{aff}(X\cdot\cdot Y^-)$* | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $O_2^-$ | | | | | | | |
| $O_2^{-\cdot}$ | | | | | | *$\Delta_f H(AH)$= 10±8* | *82TN270* |
| | | | | | | *BDE(A–H)= 206±8* | *82TN270* |
| | | 0.43±0.02 | | | Kine | | 66PAC/PHE |
| | | 0.15±0.05 | | | PD | | 58BUR/SMI |
| $O_2P^-$ | | | | | | | |
| $PO_2^-$ | | | | | | *$\Delta_f H(A)$= −280±2* | *85JANAF* |
| | −645±18 | 3.80±0.22 [i] | | | TDEq | | 86RUD/VOV |
| | −569 [b] | 3.00 | | | IMRE | | 79WOR/KOB |
| $O_2S^-$ | | | | | | | |
| $SO_2^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −297±1* | *85JANAF* |
| • | −403±2 [b] | 1.107±0.008 | | | LPES | | 86NIM/ELL |
| | | 1.097±0.036 | | | LPES | | 74CEL/BEN |
| | | 1.00±0.05 | | | PD | | 70FEL |
| | | 1.1 | | | EnCT | | 76REF/FRA |
| | | 1.1±0.2 | | | NBIP | | 75ROT/TAN |
| | | 1.0±0.1 | | | EnCT | | 73HUG/LIF |
| | | 1.1±0.1 | | | IMRB | Between $NH_2^-$, $C^-$ | 61KRA/MUL |
| $O_2Se^-$ | | | | | | | |
| $SeO_2^-$ | | | | | | | |
| • | | 1.823±0.040 | | | LPES | | 87SNO/COE |
| $O_2Te^-$ | | | | | | | |
| $TeO_2^-$ | | | | | | | |
| | | >2.200 | | | LPES | | 87SNO/COE |
| $O_3^-$ | | | | | | | |
| $O_3^-$ | | | | | | *$\Delta_f H(A)$= 143±2* | *82TN270* |
| • | −60±2 [b] | 2.103±0.003 | | | LPES | | 79NOV/ENG |
| | | 1.9±0.1 | | | PD | | 71WON/VOR |
| | −66 [c] | 2.2±0.4 [i] | *174±19* | | PDis | | 78SMI/LEE |
| | −66 [c] | | *174±5* | | CIDT | | 78LIF/WU |
| | >−99 [c] | 2.06±0.06 [i] | *<207* | | PDis | | 78COS/MOS |
| | −66 [c] | 2.2 [i] | *174±10* | | CIDT | Excited state: 81 kJ up | 77WU/TIE |
| | | >1.8 | | | IMRB | | 77DOT/DAV |
| | | 2.1±0.2 | | | NBIP | | 75ROT/TAN |
| | | >2.0 | | | EnCT | $I^- + O_3 \rightarrow$ | 71BER/CHU |
| $O_3P^-$ | | | | | | *$\Delta_f H(AH)$= −565±63* | *85HEN/VIG* |
| $PO_3^-$ | | | | | | *BDE(A–H)= 456±167* | *85HEN/VIG* |
| | −943±16 | 4.49±0.53 [i] | | | TDEq | | 86RUD/VOV |
| | −993±23 | | | | TDEq | | 83SID/RUD |
| | <−772±78 [a] | >4.6 [d] | <1323±15 [g] | <1293±13 | IMRB | | 85HEN/VIG |
| | −795 | 3.5 | | | IMRB | | 79WOR/KOB |
| $O_3Re^-$ | | | | | | | |
| $ReO_3^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= −284±21* | *75GOU/MIL* |
| | −574±40 | 3.01±0.43 [i] | | | TDEq | | 75GOU/MIL |
| | | >2.5 | | | IMRB | | 72CEN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_fH(A^-)$ $\Delta_fH(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $O_3S^-$ | | | | | | |
| $SO_3^{-\cdot}$ | | | | | *$\Delta_fH(A)$= −396±1* | *82TN270* |
| −560±15 [b] | 1.7±0.2 | | | NBIP | | 75ROT/TAN |
| −601±8 | | | | TDEq | | 85RUD/SID2 |
| $O_3W^-$ | | | | | | |
| $WO_3^{-\cdot}$ | | | | | *$\Delta_fH(A)$= −293* | *81WOO* |
| −698±40 | 3.64±0.41 [i] | | | TDEq | $HWO_4^- + H = WO_3^- + H_2O$ | 70JEN/MIL |
| | >2.5 | | | IMRB | | 72CEN |
| $O_4^-$ | | | | | | |
| $O_2\cdot\cdot O_2^-$ | | | | | | |
| −194 [c] | 2.0±0.2 [i] | *151±19* | | PDis | | 78SMI/LEE |
| | 1.9±0.2 | | | PD | | 72BUR2 |
| −99 [c] | | *57±1* | *17±1* | TDAs | | 68CON/NES |
| | | | *17±2* | IMRE | | 71PAR |
| | | *< 77±8* | | IMRB | | 70ADA/BOH |
| | | | $O_4^- + H_2O \rightarrow O_2^-\cdot\cdot H_2O + O_2$, anchored on 70ARS/KEB | | | |
| $O_4Re^-$ | | | | | *$\Delta_fH(AH)$= −665±42* | *82TN270* |
| $ReO_4^-$ | | | | | | |
| −976±30 | | | | TDEq | | 83SID/RUD |
| −867±82 [a] | 4.46±0.52 [i] | 1328±40 | | TDEq | | 75GOU/MIL |
| | >2.5 | | | IMRB | | 72CEN |
| $O_4S^-$ | | | | | | |
| $SO_4^{-\cdot}$ | | | | | | |
| −744±10 | | | | TDEq | | 85RUD/SID2 |
| $O_4S_2^-$ | | | | | | |
| $SO_2\cdot\cdot SO_2^-$ | | | | | | |
| −801±4 [c] | | *100±1* | *58±2* | TDAs | | 80KEE/LEE |
| $O_5S_2^-$ | | | | | | |
| $SO_2\cdot\cdot SO_3^-$ | | | | | | |
| −912±17 [c] | | *56* | *32±1* | TDAs | | 80KEE/LEE |
| $P^-$ | | | | | *$\Delta_fH(AH)$= 236±8* | *86BER/CUR* |
| $P^-$ | | | | | *BDE(A−H)= 298±10* | *85JANAF* |
| • 244±1 [b] | 0.747 | 1538±10 [e] | 1514±10 [h] | LPD | | 85HOT/LIN |
| | 0.77±0.05 | | | EIAP | From $P_4$ | 74BEN/MAR |
| $P_2^-$ | | | | | | |
| $P_2^-$ | | | | | *$\Delta_fH(A)$= 144±2* | *85JANAF* |
| • 88±5 [b] | 0.589±0.025 | | | LPES | | 85SNO/COE |
| | <0.7 | | | PD | | 77FEL/RAC |
| 156±20 | 0.2±0.2 | | | EIAP | From $P_4$ | 74BEN/MAR |
| $P_3^-$ | | | | | | |
| $P_3^-$ | | | | | *$\Delta_fH(A)$= 249±17* | *74BEN/MAR* |
| 160±19 | 0.9±0.4 | | | EIAP | From $P_4$ | 74BEN/MAR |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| **$Pb^-$** | | | | | | | |
| $Pb^-$ | | | | | | *$\Delta_f H(A)$= 195±2* | *82TN270* |
| • | 160±3 [b] | 0.364±0.008 | | | LPES | | 85HOT/LIN |
| **$Pd^-$** | | | | | | | |
| $Pd^-$ | | | | | | *$\Delta_f H(A)$= 378±2* | *82TN270* |
| • | 325±3 [b] | 0.557±0.008 | | | LPES | | 85HOT/LIN |
| **$Pt^-$** | | | | | | | |
| $Pt^-$ | | | | | | *$\Delta_f H(A)$= 565±2* | *82TN270* |
| • | 360±2 [b] | 2.128±0.002 | | | LPD | | 85HOT/LIN |
| **$Rb^-$** | | | | | | | |
| $Rb^-$ | | | | | | *$\Delta_f H(A)$= 81* | *82TN270* |
| • | 34 [b] | 0.486 | | | LPD | | 85HOT/LIN |
| **$Re_2^-$** | | | | | | | |
| $Re_2^-$ | | | | | | | |
| • | | 1.571±0.008 | | | LPES | | 86LEO/MIL2 |
| **$Rh^-$** | | | | | | | |
| $Rh^-$ | | | | | | *$\Delta_f H(A)$= 557±2* | *82TN270* |
| • | 447±3 [b] | 1.137±0.008 | | | LPES | | 85HOT/LIN |
| **$S^-$** | | | | | | *$\Delta_f H(AH)$= 139±5* | *85JANAF* |
| $S^-$ | | | | | | *BDE(A–H)= 356±5* | *85JANAF* |
| • | 77 [b] | 2.077 | 1467±5 [c] | 1444±6 [h] | LPD | | 85HOT/LIN |
| **$S_2^-$** | | | | | | | |
| $S_2^{-\cdot}$ | | | | | | *$\Delta_f H(A)$= 129±1* | *85JANAF* |
| • | −32±5 [b] | 1.663±0.040 | | | LPES | | 74CEL/BEN |
| | <46±10 | >0.8±0.1 [i] | | | IMRB | | 68DIL/FRA |
| | | | | | | $S^- + COS \rightarrow S_2^- + CO$. Also $S_2^- + COS \rightarrow S_3^- + CO$, etc. to n=6 | |
| | | >2.5±0.8 | | | EIAP | From $CS_2$ | 72THY |
| **$S_3^-$** | | | | | | | |
| $S_3^-$ | | | | | | *$\Delta_f H(A)$= 142±8* | *85JANAF* |
| • | −60±11 [b] | 2.093±0.025 | | | LPES | | 86NIM/ELL |
| | | 2.0±0.1 | | | PD | | 77FEL/RAC |
| **$Sb^-$** | | | | | | | |
| $Sb^-$ | | | | | | *$\Delta_f H(A)$= 262±2* | *82TN270* |
| • | 159±7 [b] | 1.07±0.05 | | | PD | | 85HOT/LIN |
| **$Sc^-$** | | | | | | | |
| $Sc^-$ | | | | | | *$\Delta_f H(A)$= 378±4* | *82TN270* |
| • | 360±6 [b] | 0.188±0.020 | | | LPES | | 85HOT/LIN |
| **$Se^-$** | | | | | | | |
| $Se^-$ | | | | | | *$\Delta_f H(A)$= 227* | *82TN270* |
| • | 32 [b] | 2.021 | | | LPD | | 85HOT/LIN |

Table 2. Negative Ion Table - Continued

| Ion $\Delta_f H(A^-)$ $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|
| $Se_2^-$ | | | | | | |
| $Se_2^-$ | | | | | *$\Delta_f H(A)$= 146±8* | *82TN270* |
| * −41±15 [b] | 1.940±0.070 | | | LPES | | 87SNO/COE |
| $Se_3^-$ | | | | | | |
| $Se_3^-$ | | | | | | |
| | >2.200 | | | LPES | | 87SNO/COE |
| $Si^-$ | | | | | *$\Delta_f H(AH)$= 377±8* | *85JANAF* |
| $Si^-$ | | | | | *BDE(A−H)= 297±10* | *82TN270* |
| * 322±3 [b] | 1.385±0.005 | 1475±11 [e] | 1453±12 [h] | LPES | | 75KAS/HER |
| $Sn^-$ | | | | | | |
| $Sn^-$ | | | | | *$\Delta_f H(A)$= 302±2* | *82TN270* |
| * 195±4 [b] | 1.113±0.020 | | | LPES | | 86MIL/MIL |
| | 1.1±0.1 | | | PD | | 85HOT/LIN |
| $Ta^-$ | | | | | | |
| $Ta^-$ | | | | | *$\Delta_f H(A)$= 782* | *82TN270* |
| * 751±1 [b] | 0.322±0.012 | | | LPES | | 85HOT/LIN |
| $Te^-$ | | | | | *$\Delta_f H(AH)$= 143* | *79HUB/HER* |
| $Te^-$ | | | | | | |
| * 6 [b] | 1.971 | | | LPD | | 85HOT/LIN |
| $Te_2^-$ | | | | | | |
| $Te_2^-$ | | | | | *$\Delta_f H(A)$= 168±8* | *82TN270* |
| * −17±15 [b] | 1.920±0.070 | | | LPES | | 87SNO/COE |
| $Te_3^-$ | | | | | | |
| $Te_3^-$ | | | | | | |
| | <2.700 | | | LPES | | 87SNO/COE |
| $Ti^-$ | | | | | *$\Delta_f H(AH)$= 532* | *79HUB/HER* |
| $Ti^-$ | | | | | | |
| * 462±3 [b] | 7.9±0.014 | 1460 [f] | | LPES | | 85HOT/LIN |
| $Tl^-$ | | | | | | |
| $Tl^-$ | | | | | *$\Delta_f H(A)$= 182±1* | *82TN270* |
| * 163±20 [b] | 0.2±0.2 | | | PD | | 85HOT/LIN |
| | 1.1±0.2 | | | EIAP | From TlBr | 80BRU/COT |
| $V^-$ | | | | | | |
| $V^-$ | | | | | *$\Delta_f H(A)$= 515±8* | *85JANAF* |
| * 464±10 [b] | 0.525±0.012 | | | LPES | | 85HOT/LIN |
| | | | 1389±13 | IMRB | | 85SAL/LAN |
| $W^-$ | | | | | | |
| $W^-$ | | | | | *$\Delta_f H(A)$= 851±6* | *85JANAF* |
| * 772±7 [b] | 0.815±0.008 | | | LPES | | 85HOT/LIN |

Table 2. Negative Ion Table - Continued

| Ion | $\Delta_f H(A^-)$ / $\Delta_f H(X\cdot\cdot Y^-)$ | EA(A) eV | $\Delta H_{acid}(AH)$ / $\Delta H_{aff}(X\cdot\cdot Y^-)$ | $\Delta G_{acid}(AH)$ / $\Delta G_{aff}(X\cdot\cdot Y^-)$ | Method | Comment | Reference |
|---|---|---|---|---|---|---|---|
| $Y^-$ | | | | | | | |
| $Y^-$ | | | | | | *$\Delta_f H(A)$= 421±2* | *82TN270* |
| • | 392±3 [b] | 0.307±0.012 | | | LPES | | 85HOT/LIN |
| $Zr^-$ | | | | | | | |
| $Zr^-$ | | | | | | *$\Delta_f H(A)$= 610±8* | *85JANAF* |
| • | 569±10 [b] | 0.426±0.014 | | | LPES | | 85HOT/LIN |

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