

# Evaluated Gas Phase Basicities and Proton Affinities of Molecules: An Update

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Received August 11, 1997; revised manuscript received 23 March 1998

The available data on gas-phase basicities and proton affinities of approximately 1700 molecular, radical and atomic neutral species are evaluated and compiled. Tables of the data are sorted (1) according to empirical formula and (2) according to evaluated gas basicity. This publication constitutes an update of a similar evaluation published in 1984.

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[S0047-2689(98)00203-7]

Key words: enthalpy; entropy; gas basicity; Gibbs energy; ion-molecule reactions; proton affinity; protonation entropy; proton transfer.

## Contents

1. Introduction. . . . .	413	3.8. Ethene: CH <sub>2</sub> CH <sub>2</sub> . . . . .	420
1.1. Dedication to Professor Robert W. Taft. . . . .	413	3.9. Carbon Monoxide: CO. . . . .	420
1.2. Background. . . . .	414	3.10. Carbon Dioxide: CO <sub>2</sub> . . . . .	421
1.3. Definitions. . . . .	414	4. Evaluation of Thermodynamic Ladders. . . . .	421
2. Sources of Proton Affinity/Gas Basicity Data. . . . .	414	5. Generation of the Scale of Absolute Proton Affinities from the Scale of Relative Gas Basicities. . . . .	422
2.1. Absolute Proton Affinity Values. . . . .	414	5.1. Evaluation of Entropy Change Data. . . . .	422
2.1.1. Ionization Threshold Measurements. . . . .	414	5.2. Procedures Followed in Evaluating Absolute Proton Affinities from the Scale of Relative Gas Basicities. . . . .	423
2.1.2. Absolute Values of Proton Affinities from Quantum Chemical Calculations. . . . .	415	5.3. Sample Evaluations. . . . .	424
2.2. Relative Gas Basicity/Proton Affinity Values. . . . .	415	5.4. Uncertainty of the Proton Affinity Scale. . . . .	425
2.2.1. Gas Phase Equilibrium Constant Data. . . . .	415	5.5. Problems Remaining. . . . .	425
2.2.2. Relative Gas Basicities from Bracketing Experiments. . . . .	416	6. Description of the Tables. . . . .	425
2.2.3. Relative Proton Affinity Data from the "Kinetic Method". . . . .	416	7. References. . . . .	427
2.2.4. Relative Gas Basicity/Proton Affinity Data from the "Thermokinetic Method". . . . .	416		
2.2.5. Other Sources of Relative Proton Affinity Data. . . . .	417		
2.3. Remarks Concerning Temperature Dependence of Proton Affinities and Protonation Entropies. . . . .	417		
3. Evaluation of Absolute Proton Affinities from Ionization Threshold Measurements. . . . .	418		
3.1. Ketene: CH <sub>2</sub> CO. . . . .	418		
3.2. Isobutene: (CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> . . . . .	418		
3.3. Acetaldehyde: CH <sub>3</sub> CHO. . . . .	419		
3.4. Propene: CH <sub>3</sub> CHCH <sub>2</sub> . . . . .	419		
3.5. Formaldehyde: CH <sub>2</sub> O. . . . .	419		
3.6. Hydrogen sulfide: H <sub>2</sub> S. . . . .	420		
3.7. Water: H <sub>2</sub> O. . . . .	420		

## List of Tables

1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases. . . . .	429
2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M. . . . .	458
3. Annotated References to Tables 1 and 2. . . . .	639

## 1. Introduction

### 1.1. Dedication to Professor Robert W. Taft

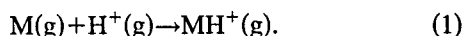
This evaluation of gas basicity and proton affinity data is dedicated to the late Professor Robert W. Taft, whose research led to the early determination of an extensive scale of gas-phase basicity data. The existence of this comprehensive body of internally consistent, interlocking experimental measurements in a very real sense made it possible to tie together and evaluate data from a wide variety of sources generated by various experimental techniques. We are indebted to Professor Taft for pioneering this type of research, and for demonstrating its scientific interest and importance.

## 1.2. Background

This publication is an update and revision of the evaluation of the scale of gas phase basicity/proton affinity data carried out in this laboratory, and published in 1984.<sup>1</sup> Prior to its appearance, there had been a number of reviews of the field<sup>2-8</sup> and two unevaluated compilations,<sup>9,10</sup> but no single reference had presented a comprehensive collection of data on gas phase proton affinities evaluated for internal consistency. The 1984 evaluation has been proven to be sufficiently useful that it is still widely cited, and current publications often compare new data to data in the proton affinity scale as presented there (the so-called "NBS (National Bureau of Standards) Scale"). However, in the intervening years, a large amount of new data has appeared in the literature, so the so-called "NBS Scale" is seriously out-of-date, missing data for about 900 compounds. In addition, recent studies include several seminal publications, both experimental and theoretical, which present information indicating that portions of the scale as presented in the 1984 publication are incorrect, and therefore in need of re-evaluation.

## 1.3. Definitions

The gas basicity and proton affinity of a species (molecule, radical, or atom), M, are defined in terms of the hypothetical gas-phase reaction:



The gas basicity of M at temperature T, GB(M, T), is the negative of the Gibbs free energy change for this reaction:

$$GB(M, T) \equiv -\Delta G_{Rn1}^0(T) \quad (2)$$

Thermochemical quantities having a subscript Rn followed by an integer means that the quantity is associated with the reaction or process indicated by the integer. The proton affinity, PA(M, T), is the negative of the corresponding enthalpy change:

$$\begin{aligned} PA(M, T) &\equiv -\Delta H_{Rn1}^0(T) \\ &= \Delta_f H^0(M, T) + \Delta_f H^0(H^+, T) - \Delta_f H^0(MH^+, T). \end{aligned} \quad (3)$$

The corresponding entropy change can be expressed in terms of absolute entropies of the species involved:

$$\Delta S_{Rn1}^0(T) = S^0(MH^+, T) - S^0(M, T) - S^0(H^+, T) \quad (4)$$

$$= \Delta S_p(M, T) - S^0(H^+, T), \quad (5)$$

where  $\Delta S_p(M, T)$  is defined as the entropy of protonation of M:

$$\Delta S_p(M, T) \equiv S^0(MH^+, T) - S^0(M, T). \quad (6)$$

Since the defining process is understood to always involve gaseous species, the phase designations for the species indicated in reaction (1) are dropped when indicating those species in thermochemical quantities. The relationship between gas basicity, proton affinity and entropy of protonation is obtained by combining Eqs. (2), (3) and (5) to give

$$GB(M, T) = PA(M, T) + T[\Delta S_p(M, T) - S^0(H^+, T)]. \quad (7)$$

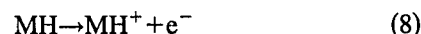
## 2. Sources of Proton Affinity/Gas Basicity Data

Most of the published data on gas phase basicities/proton affinities of molecules are derived from measurements which lead to *relative* scales of basicities/proton affinities, but do not provide *absolute* values for these quantities. Absolute values are assigned to the entire relative thermochemical scales using data for molecules whose position in the relative scale has been established, and for which absolute values of enthalpies of formation of both M and MH<sup>+</sup> are known from other measurements. Thus the evaluation of the basicity/proton affinity scales has three components: (1) an evaluation of the thermochemical data leading to the scale of *relative* gas basicities; (2) an evaluation of measured entropy changes for proton transfer reactions, or an estimation of entropy changes for species for which experimental data are not available, followed by the generation of the scale of *relative* proton affinities, and (3) the evaluation of data leading to the assignment of absolute values to the scales. Before describing the evaluation of these scales, we first describe briefly the methods by which absolute values of proton affinity and relative values of gas basicity are obtained.

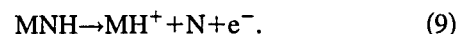
### 2.1. Absolute Proton Affinity Values

#### 2.1.1. Ionization Threshold Measurements

Experiments in which the enthalpy of formation of MH<sup>+</sup> is determined lead directly to values for the proton affinity when combined with the value for the enthalpy of formation of the corresponding neutral molecule, M. If MH is a sufficiently stable species that it can be introduced into a mass spectrometer or be generated *in situ*, or if MH<sup>+</sup> is formed as a product ion from the fragmentation of some larger molecular species, absolute values for the enthalpy of formation can be obtained, either by determining the ionization energy of MH:



or the appearance energy of MH<sup>+</sup> from a larger molecule, MNH:



Since the thermochemical scales provide data on *relative* proton affinities, it is necessary to assign absolute proton affinity values to the entire scale. This is only possible if an absolute proton affinity can be reliably assigned to one or more molecules in the scale. Absolute values for proton affinities can be derived from Eq. (3) by simply inserting available values for enthalpies of formation of M(g), MH<sup>+</sup>(g), and H<sup>+</sup>(g) when these are all known. Unfortunately, there are relatively few species for which this is possible.

Enthalpies of formation of all relevant species are known for the lower members of the homologous series when M is

an olefin and  $MH^+$  an alkyl ion. For this reason, the proton affinities of ethylene, propene, and isobutene have often been used as the basis for assigning absolute values to the proton affinity scale,<sup>1</sup> and were considered to be reliable anchors. However, as will be discussed below, new results indicate some changes are necessary; for example, the accepted value for the enthalpy of formation of the tert-butyl cation has changed based on new measurements, and the positions of ethylene and propene in the basicity scale are not necessarily as well established as previously thought.

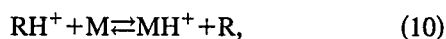
### 2.1.2. Absolute Values of Proton Affinities from Theoretical Calculations

It has been shown that standard *ab initio* molecular orbital calculations at the G2 level of theory<sup>11</sup> consistently yield values of proton affinities within 10 kJ mol<sup>-1</sup> of experimental values, which is usually within error limits of the latter. In a recent paper, Smith and Radom<sup>12</sup> reported computed proton affinity values for 31 molecules over an energy range of about 500 kJ mol<sup>-1</sup>, that is, values that effectively spanned most of the experimental scale reported from equilibrium constant determinations. Further work by East, Smith and Radom<sup>13</sup> provides a set of theoretically predicted values of entropy changes associated with protonation of these molecules. In view of the difficulties in pinning down values to be assigned to species in an experimentally derived thermochemical scale (which may display "shifts" over time, for various reasons discussed elsewhere in this paper), the data from these papers provided an invaluable guide to the evaluation of the proton affinity data presented here.

## 2.2. Relative Gas Basicity/Proton Affinity Values

### 2.2.1. Gas Phase Equilibrium Constant Data

Most of the data presented here are based on measurements of the equilibrium constants of gas phase proton transfer reactions between M and a reference species, R, at a single temperature:



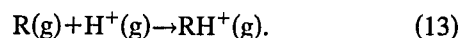
where:

$$-R_g T \ln K_{Rn10} = \Delta G_{Rn10}^0 = \Delta H_{Rn10}^0 - T \Delta S_{Rn10}^0 \quad (11)$$

and  $R_g$  is the universal gas constant. The equilibrium constant for reaction (10) is obtained from a mass spectrometric observation of the relative abundances of the ions,  $RH^+$  and  $MH^+$ , in a mixture of compounds R and M of known composition:

$$K_{Rn10} = \{[MH^+]/[RH^+]\} \cdot \{[R]/[M]\}. \quad (12)$$

When the ratio of ions is observed under conditions such that thermodynamic equilibrium has been attained, the resulting value for the equilibrium constant of reaction (10) directly provides a value for the Gibbs free energy change of reaction at temperature  $T$ . We note that reaction (10) can be resolved into reaction (1) and an analogous process in which M is replaced by R, namely:



The gas basicity, proton affinity and protonation entropy of R in reaction (13) are similarly defined as for M in Eqs. (2)–(7) in which M is replaced by R. Then, the Gibbs free energy change of reaction (10) is equal to the relative gas phase basicities of compounds R and M,  $\Delta GB(M,R,T)$ , at the temperature  $T$ , i.e.,

$$-\Delta G_{Rn10}^0(T) = GB(M,T) - GB(R,T) \equiv \Delta GB(M,R,T). \quad (14)$$

Scales of relative gas phase basicities derived from equilibrium constant determinations can lead to a quantitative scale of relative proton affinities,  $\Delta PA(M,R)$ , only if the entropy change of reaction (10), or the relative protonation entropy,  $\Delta \Delta S_p(M,R)$ , is known or can be reliably estimated.

$$-\Delta H_{Rn10}^0 = PA(M,T) - PA(R,T) \equiv \Delta PA(M,R), \quad (15)$$

$$\Delta S_{Rn10}^0 = \Delta S_p(M,T) - \Delta S_p(R,T) \equiv \Delta \Delta S_p(M,R). \quad (16)$$

The reader should note that the definitions of relative proton affinities and relative protonation entropies do not show an explicit temperature dependence, even though the quantities involved in their definitions do show such explicit dependence. Unlike relative gas basicity, relative proton affinities and relative protonation entropies are quite temperature independent; more about this feature is explained in Section 2.3.

Some of the data available and presented here are based on measurements of  $K_{Rn10}$  over a range of temperatures. When such data are treated in a van't Hoff manner, i.e., when  $\ln K_{Rn10}$  is plotted against  $T^{-1}$ , then values of  $\Delta H_{Rn10}^0$  and  $\Delta S_{Rn10}^0$  can, in principle, be derived directly from the slope and intercept of the fitted line, respectively,

$$\ln K_{Rn10} = -\Delta H_{Rn10}^0/R_g T + \Delta S_{Rn10}^0/R_g. \quad (17)$$

In the van't Hoff treatment, the values of  $\Delta H_{Rn10}^0$  and  $\Delta S_{Rn10}^0$  are considered to be constants over the temperature range for which  $K_{Rn10}$  is measured (see Sec. 2.3.).

In the 1984 evaluation,<sup>1</sup> proton affinity values were derived from the scale of gas basicities using calculated entropy changes derived from standard statistical mechanics treatments. In most cases, the estimates were based on the simplifying assumption that the protonation entropy of M in reaction (1) can be approximated adequately by the temperature independent expression:

$$\Delta S_p(M) = R_g \ln[\sigma(M)/\sigma(MH^+)], \quad (18)$$

where  $\sigma(M)$  and  $\sigma(MH^+)$  are the rotational symmetry numbers of M and  $MH^+$ .

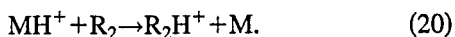
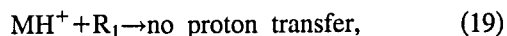
For the present evaluation, extensive thermochemical ladders from two laboratories<sup>14-16</sup> were available which included determinations of equilibrium constants over a range of temperatures, i.e., which included entropy change determinations. However, as discussed below in the description of the evaluation procedures, there was poor agreement between the entropy change measurements from different labo-

ratories; this was taken as an indication that inherent experimental problems make such determinations unreliable. Therefore, instead of using the (inconsistent) experimental data directly, or resorting to the use of Eq. (18), a procedure was adopted which incorporates an analysis of the data for the entire thermochemical ladder at different temperatures, and the imposition of a requirement that the entropy changes be reasonable and internally consistent.

Most measurements of proton transfer equilibrium constants have been carried out using one of three types of mass spectrometers which operate in very different pressure regimes: an ion cyclotron resonance spectrometer<sup>17(a)</sup> (ICR,  $\sim 10^{-4}$  Pa, 1 Torr = 133.3224 Pa), a high pressure mass spectrometer<sup>17(b)</sup> (HPMS, 100–1000 Pa), or a flowing afterglow<sup>17(c)</sup> apparatus (FA, 100–1000 Pa). Questions have been raised about whether thermodynamic equilibrium is in fact attained at the low pressures of an ICR experiment (in spite of the long reaction times employed); the generally good agreement between thermochemical scales determined through ICR experiments and those from higher pressure HPMS and FA measurements argues in favor of the validity of the ICR scales.

### 2.2.2. Relative Gas Basicities from Bracketing Experiments

In some cases, measurements of proton transfer equilibrium constants are difficult or impossible. This happens when M is an unstable molecule, or in systems where  $MH^+$  undergoes fast reactions with M, or a reaction other than proton transfer with R, see reaction (10). In these cases, upper and lower bounds of the basicity can usually be estimated through the technique known as "bracketing." The ion  $MH^+$  is reacted with a series of molecules,  $R_1$  and  $R_2$  in reactions (19) and (20), and the occurrence or nonoccurrence of proton transfer is noted:



Under the assumption that proton transfer will be observed only if the reaction is associated with a negative value of the Gibbs free energy change, the basicity of M is taken to be between the basicities of  $R_1$  and  $R_2$ . Note that since it is the Gibbs free energy change that determines whether proton transfer occurs, the quantity that is bracketed is the gas basicity and not necessarily the proton affinity.

Results obtained from bracketing experiments are generally less reliable than those obtained from other types of experiments because of numerous possible complications. For example, exothermic proton transfer reactions sometimes do not occur if there is an energetically favorable alternate channel open to the reactants. If there are several isomeric structures of the species involved in reactions (19) or (20), the observed proton transfer reaction may be accompanied by a rearrangement of those species in the reaction complex to more stable structures; in this case, the observed "bracketing" does not reflect the thermochemistry of the expected proton transfer reaction.

### 2.2.3. Relative Proton Affinity Data from the "Kinetic Method"

Another often-used approach is based on the observation of the collision-induced dissociation of proton-bound dimer ions, here written as  $M \cdot H^+ \cdot R$ , formed in association reactions:



A semi-quantitative relationship<sup>18,19</sup> between the ratios of the two product ions and the relative proton affinities has been developed, and can be used to derive relative proton affinity values of M and R provided the entropy changes associated with processes (21) and (22) are similar. Clearly, the ratio of rate coefficients for reactions (21) and (22) is equal to the ratio of the product ions,  $[MH^+]/[RH^+]$ . Applying an Arrhenius-type relationship to each of the unimolecular decompositions yields

$$\ln\{[MH^+]/[RH^+]\} = \ln\{k_{Rn21}/k_{Rn22}\} \\ = (E_{Rn22} - E_{Rn21})/R_g T, \quad (23)$$

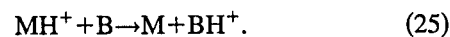
where the  $E$ 's are the activation energies of the reactions, and the familiar frequency factors or  $A$  factors cancel out if the entropy changes for reactions (21) and (22) are similar. If it is assumed that the reverse of reactions of (21) and (22) occur with no activation barriers, then  $E_{Rn22} - E_{Rn21} = \Delta PA(M,R)$ , which can be substituted into Eq. (23), yielding

$$\ln\{[MH^+]/[RH^+]\} = \Delta PA(M,R)/R_g T. \quad (24)$$

Measuring and plotting the ratio in Eq. (24) against the proton affinities of a series of reference molecules, R, results in a straight line if the temperature is effectively constant. The proton affinity of M is determined from where the line intercepts the PA axis. The value of  $PA(M)$  determined by this method depends on the PA values used for each of the reference bases, R, which are being re-evaluated. For this reason, data obtained by this method are tabulated in this compilation as if they were "bracketed" by the PA values of the nearest bases below and above where the plotted line crosses zero.

### 2.2.4. Relative Gas Basicity/Proton Affinity Data from the "Thermokinetic Method"

Still another approach developed recently to determine gas basicity or proton affinity information uses a correlation observed between the measured reaction efficiency (RE) of a process like reaction (25) and the corresponding Gibbs free energy change<sup>20</sup>



The observed correlation is expressed as

$$RE = k_{Rn25}/k_{coll} = [1 + \exp(\Delta G_{Rn25}^0 + \Delta G_a^0)/R_g T]^{-1}, \quad (26)$$

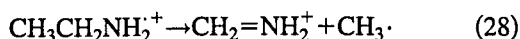
where  $k_{Rn25}$  and  $k_{coll}$  are the experimental and collision<sup>21</sup> rate coefficients, respectively, for reaction (25),  $\Delta G_{Rn25}^0$  is the

standard free energy change and  $\Delta G_a^0$  is an "apparent" energy barrier for reaction (25). Substituting  $GB(M,T) - GB(B,T)$  for  $\Delta G_{Rn25}^0$  into Eq. (26) yields:

$$RE = (1 + \exp\{[GB(M,T) - GB(B,T) + \Delta G_a^0]/R_g T\})^{-1}. \quad (27)$$

By measuring and plotting the reaction efficiency of  $MH^+$  with a series of bases, B, of known gas basicity, the gas basicity of M,  $GB(M,T)$ , can be evaluated.

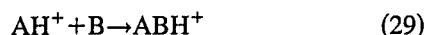
This method appears to be well suited to the study of unstable or labile molecules, M, but whose protonated ions,  $MH^+$ , can be generated from a suitable precursor and whose reactivity with a series of bases can be measured. An example is the recent measurement<sup>22</sup> of the proton affinity of the imine  $CH_2=NH$ . This molecule is not stable enough to permit an equilibrium type measurement but its protonated ion,  $CH_2=NH_2^+$ , could be generated in the gas phase by  $\alpha$ -cleavage of amine radical cations according to:



Clearly, values for  $GB(M,T)$  obtained by this correlation depend upon values used for the gas basicities of the series of reference bases, which are being re-evaluated here. As the values for the reference bases change,  $GB(M,T)$  must be re-determined from a plot of Eq. (27). For this reason, data obtained by this method are tabulated in this compilation as if they were bracketed by the GB values of the nearest bases below and above that of M.

### 2.2.5. Other Sources of Relative Proton Affinity Data

Quantitative information about relative proton affinities has also been obtained through the determination of the energy barrier associated with endothermic proton transfer reactions through an Arrhenius treatment of the temperature dependence of the rate coefficients. Also, determinations of the equilibrium constants of association reactions:



can give values for enthalpies of formation of the product ion,  $ABH^+$ , provided the enthalpies of formation of  $AH^+$  and B are known; if the enthalpy of formation of AB is also known, its proton affinity can be derived.

### 2.3. Remarks Concerning Temperature Dependence of Proton Affinities and Protonation Entropies

The experimental determinations of proton affinities and protonation entropies that are derived from equilibrium proton transfer measurements were performed at various temperatures mostly at or above 298 K and below 700 K. A valid question may be how do *absolute* proton affinities and protonation entropies vary with temperature. Differentiating Eq. (3) with respect to temperature gives

$$\begin{aligned} \partial PA(M)/\partial T &= -\partial \Delta H_{Rn1}^0/\partial T \\ &= C_p(H^+) + C_p(M) - C_p(MH^+), \quad (30) \end{aligned}$$

where the  $C_p$ 's are the molar heat capacities at constant pressure of the parenthetically indicated species. At room temperature and above,  $C_p(H^+)$  is assumed to have the classical value of  $(5/2)R_g$ , while  $C_p(MH^+)$  will be close to but greater than  $C_p(M)$ . Thus, the difference in absolute proton affinity of M at 298 and 600 K will be less than  $6.2 \text{ kJ mol}^{-1}$  but still a nontrivial temperature dependence.

The *relative* proton affinities,  $\Delta PA(M,R)$ , of a pair of molecules M and R in reaction (10), or the enthalpy change of reaction (10), is essentially temperature independent, i.e.,

$$\begin{aligned} -\Delta H_{Rn10}^0(T_1) &= PA(M, T_1) - PA(R, T_1) \\ &\approx -\Delta H_{Rn10}^0(T_2) \\ &= PA(M, T_2) - PA(R, T_2). \quad (31) \end{aligned}$$

This follows from what was found above about the temperature dependence of an individual molecule, but can be shown more formally by differentiating Eq. (15) with respect to temperature

$$\begin{aligned} \partial \Delta PA(M,R)/\partial T &= -\partial \Delta H_{Rn10}^0/\partial T \\ &= C_p(RH^+) + C_p(M) - C_p(MH^+) - C_p(R) \quad (32) \end{aligned}$$

and noting that because of the structural similarities of reactants and products the heat capacity terms of Eq. (32) will essentially cancel to zero. When a relative proton affinity is derived from a van't Hoff analysis of a proton transfer equilibrium over a suitable temperature range, it is safe to assume that  $\Delta H_{Rn10}^0$  is independent of temperature over that range. The above discussion suggests that the temperature independence of  $\Delta H_{Rn10}^0$  can be safely assumed throughout the range  $298 \text{ K} \leq T \leq 600 \text{ K}$ . This feature is actually a generally observed phenomenon for reactions in which the number of reactants and products is the same, as is the case for proton transfer reactions. Similar considerations also apply to relative protonation entropies, i.e.,

$$\begin{aligned} \Delta S_{Rn10}(T_1) &= \Delta S_p(M, T_1) - \Delta S_p(R, T_1) \\ &\approx \Delta S_{Rn10}(T_2) \\ &= \Delta S_p(M, T_2) - \Delta S_p(R, T_2). \quad (33) \end{aligned}$$

This is the reason that the relative proton affinities  $[\Delta PA(M,R)]$  and relative protonation entropies  $[\Delta \Delta S_p(M,R)]$ , defined by Eqs. (15) and (16), are not written as being explicitly temperature dependent. Thus, in those instances where this evaluation relies on relative proton affinity data that are derived from a van't Hoff analysis [Eq. (17)] over a temperature range that may be far removed from 298 K, within the uncertainty of such measurements, it is considered appropriate to apply the derived relative proton affinity to the 298 K PA value of molecule R to deduce a 298 K PA value of molecule M according to Eq. (15). Likewise for the relative entropy of protonation. In this evaluation, the proton affinity scale uses as its primary anchor point the 298 K proton affinity value for  $NH_3$ . In Table 1, which lists the

TABLE A. Bases whose proton affinities were determined absolutely or derived from the procedure described in Sec. 5

Base	Reg. No.	GB(298) <sup>a</sup>	PA(298) <sup>a</sup>	$\Delta S_p(298)^b$
(CH <sub>3</sub> ) <sub>3</sub> N	75-50-3	918.1	948.9	5.6
pyridine	110-86-1	898.1	930.0	2.0
(CH <sub>3</sub> ) <sub>2</sub> NH	124-40-3	896.5	929.5	-2.0
C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	75-04-7	878.0	912.0	-5.1
CH <sub>3</sub> NH <sub>2</sub>	74-89-5	864.5	899.0	-7
NH <sub>3</sub>	7664-41-7	819.0	853.6	-6.4
CH <sub>2</sub> CO	463-51-4	793.6	825.3	2.4
(CH <sub>3</sub> ) <sub>2</sub> CO	67-64-1	782.1	812.0	8.7
(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub>	115-11-7	775.6	802.1	20.0
(CH <sub>3</sub> ) <sub>2</sub> O	115-10-6	764.5	792.0	16.5
C <sub>2</sub> H <sub>5</sub> CN	107-12-0	763.0	794.1	4.7
C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	108-88-3	756.3	784.0	16
CH <sub>2</sub> CHCN	107-13-1	753.7	784.7	4.9
HCOOCH <sub>3</sub>	107-31-3	751.5	782.5	5.0
CH <sub>3</sub> CN	75-05-8	748.0	779.2	4.3
CH <sub>3</sub> CHO	75-07-0	736.5	768.5	1.5
CH <sub>3</sub> OH	67-56-1	724.5	754.3	9
CH <sub>3</sub> CHCH <sub>2</sub>	115-07-1	722.7	751.6	12
CH <sub>2</sub> O	50-00-0	683.3	712.9	9.5
H <sub>2</sub> S	7783-06-4	673.8	705	4.3
H <sub>2</sub> O	7732-18-5	660.0	691.0	5.0
CS <sub>2</sub>	75-15-0	657.7	681.9	28
CH <sub>2</sub> CH <sub>2</sub>	74-85-1	651.5	680.5	11.5
CO	630-08-0	562.8	594.0	4.2
CO <sub>2</sub>	124-38-9	515.8	540.5	26

<sup>a</sup>In units of kJ mol<sup>-1</sup>.<sup>b</sup>In units of J (mol K)<sup>-1</sup>.

evaluated gas basicity, proton affinity and protonation entropy of each molecule considered, all these quantities are therefore referred to a temperature of 298 K. If, however, the present evaluation is used to compute a value of  $\Delta H_f(\text{MH}^+, T)$  using Eq. (3) at a temperature different than 298 K, the above mentioned temperature dependence of the proton affinity of M will have to be considered.

### 3. Evaluation of Absolute Proton Affinities from Ionization Threshold Measurements

The proton affinity of a species, M, can be determined *absolutely* if all of the enthalpies of formation indicated in Eq. (3) are known. Values of  $\Delta H_f(\text{M}, 298 \text{ K})$  are reliably known for a number of species, M, as well as the proton's enthalpy of formation [ $\Delta H_f(\text{H}^+, 298 \text{ K}) = 1530 \text{ kJ mol}^{-1}$ ]. Values for  $\Delta H_f(\text{MH}^+, 298 \text{ K})$  are known for a much smaller set of  $\text{MH}^+$ ; they are mainly derived from ionization threshold measurements according to reactions (8) or (9). Here in Sec. 3 is a description of experiments that lead to values of  $\Delta H_f(\text{MH}^+, 298 \text{ K})$  and thus to absolute values of PA(M, 298 K) for ten molecules that are independent of equilibrium thermochemical scales and depend only on auxiliary thermochemical data for precursor and product molecules, i.e., for the MNH and N species in reaction (9), respectively. In all cases in this section, the most recent and reliable values of the auxiliary data are used, which may differ from that used in the original papers. The absolute proton affinity values for

these 10 compounds, along with their gas basicities and entropies of protonation, are summarized in Table A. Table A also contains the same data for 15 other molecules whose values have been evaluated by the procedure described in Sec. 5.

#### 3.1. Ketene: CH<sub>2</sub>CO

The PA(CH<sub>2</sub>CO) is defined by the enthalpy change of the reaction:

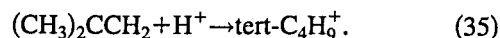


Traeger *et al.*,<sup>23</sup> have measured appearance energies for the acetyl cation, CH<sub>3</sub>CO<sup>+</sup>, formed by photoionization of a series of methyl ketones and have determined an enthalpy of formation for the acetyl cation as  $\Delta_f H^0(\text{CH}_3\text{CO}^+, 298 \text{ K}) = (657.0 \pm 1.5) \text{ kJ mol}^{-1}$ . Taking  $\Delta_f H^0(\text{CH}_2\text{CO}, 298 \text{ K})^{24} = (-47.7 \pm 2.5) \text{ kJ mol}^{-1}$  yields PA(CH<sub>2</sub>CO, 298 K) = (825.3 ± 3) kJ mol<sup>-1</sup> and is the selected value for this evaluation.

For comparison, Smith and Radom<sup>12</sup> have calculated a 298 K PA value for ketene as 825.0 kJ mol<sup>-1</sup>, indistinguishable from the photoionization value. The selected value for the entropy of protonation comes from East *et al.*,<sup>13</sup> who calculate  $\Delta S_p(\text{CH}_2\text{CO}, 298 \text{ K}) = 2.4 \text{ J (mol K)}^{-1}$ . The selected value for GB(CH<sub>2</sub>CO, 298 K) = (793.6 ± 3) kJ mol<sup>-1</sup>.

#### 3.2. Isobutene: (CH<sub>3</sub>)<sub>2</sub>CCH<sub>2</sub>

The proton affinity of isobutene is defined by the enthalpy change associated with the reaction:



It was recognized in the 1984 scale of gas basicities/proton affinities<sup>1</sup> that the enthalpy of formation of tert-C<sub>4</sub>H<sub>9</sub><sup>+</sup> was not as well established as that for ethyl or sec-propyl cations, and so the PA of isobutene was in need of additional corroborating evidence. The value cited for the enthalpy of formation of tert-C<sub>4</sub>H<sub>9</sub><sup>+</sup> in the earlier publication<sup>1</sup> was 694 kJ mol<sup>-1</sup>, based on several apparently consistent pieces of data (appearance energy measurements, an ionization energy for the tert-butyl radical, and a chloride ion transfer equilibrium constant). However, in each instance, there is some uncertainty, usually in the supporting thermochemical data. Indeed, one of the reasons for updating this gas basicity/proton affinity scale is due to the recognition that the proton affinity span between isobutene and NH<sub>3</sub> was not as indicated in the 1984 scale. This discrepancy was first noted by Meot-Ner(Mautner) and Sieck<sup>14</sup> and confirmed by Szulejko and McMahon.<sup>15</sup>

The first indication that it was the proton affinity of isobutene that was in need of significant revision came from the calculations of Smith and Radom,<sup>12</sup> whose *ab initio* results put PA[(CH<sub>3</sub>)<sub>2</sub>CCH<sub>2</sub>, 298 K] = 802.1 kJ mol<sup>-1</sup>. The first experimental verification that the proton affinity of isobutene needed revision came from the extensive thermochemical ladder of Szulejko and McMahon,<sup>15</sup> in which the proton affinity of CO was used as the anchor point. Since then two

more recent determinations of  $\Delta_f H^0(\text{tert-C}_4\text{H}_9^+, 298 \text{ K})$  have appeared that are consistent with each other and with the present thermochemical scale. Keister *et al.*<sup>25</sup> measured  $\Delta_f H^0(\text{tert-C}_4\text{H}_9^+, 298 \text{ K}) = (711 \pm 3.6) \text{ kJ mol}^{-1}$  by dissociative ionization of a supersonically cooled beam of tert-butyl iodide using the photoelectron photoion coincidence technique. Most of the uncertainty in their result comes from the uncertainty in  $\Delta_f H^0(\text{tert-C}_4\text{H}_9\text{I}, 298 \text{ K})^{26} = (-72.0 \pm 3.3) \text{ kJ mol}^{-1}$ . Traeger<sup>27</sup> used threshold photoionization mass spectrometry and measured  $\Delta_f H^0(\text{tert-C}_4\text{H}_9^+, 298 \text{ K}) = (711.4 \pm 1.1) \text{ kJ mol}^{-1}$  from the appearance energies of tert-C<sub>4</sub>H<sub>9</sub><sup>+</sup> from isobutane, neopentane and tert-butyl iodide, in excellent agreement with the Keister *et al.* results. Using the average of these experimental estimates for  $\Delta_f H^0(\text{tert-C}_4\text{H}_9^+, 298 \text{ K})$  and using  $\Delta_f H^0[(\text{CH}_3)_2\text{CCH}_2, 298 \text{ K}]^{26} = (-16.9 \pm 0.9) \text{ kJ mol}^{-1}$  yields  $\text{PA}[(\text{CH}_3)_2\text{CCH}_2, 298 \text{ K}] = (802.1 \pm 1.4) \text{ kJ mol}^{-1}$ , which is in excellent agreement with the calculations of Smith and Radom<sup>12</sup> and is the selected value in this compilation. For  $\Delta S_p[(\text{CH}_3)_2\text{CCH}_2, 298 \text{ K}]$ , an average of various experimental determinations and a value calculated by East *et al.*<sup>13</sup> is used and assigned  $20 \text{ J (mol K)}^{-1}$ , which sets  $\text{GB}[(\text{CH}_3)_2\text{CCH}_2, 298 \text{ K}] = (775.6 \pm 1.2) \text{ kJ mol}^{-1}$ .

As indicated by Traeger,<sup>27</sup> accepting these new values of  $\text{PA}[(\text{CH}_3)_2\text{CCH}_2, 298 \text{ K}]$  and  $\Delta_f H^0(\text{tert-C}_4\text{H}_9^+, 298 \text{ K})$  requires some changes in the accepted enthalpy of formation of the tert-butyl radical or of its ionization energy. More recent estimates of  $\Delta_f H^0(\text{tert-C}_4\text{H}_9, 298 \text{ K})$  put that value at  $(46.0 \pm 2.5)^{28} \text{ kJ mol}^{-1}$  and at  $(51.3 \pm 1.8)^{29} \text{ kJ mol}^{-1}$ . At the time of the 1984 evaluation,<sup>1</sup> this value was considered to vary from 35 to 44  $\text{kJ mol}^{-1}$ .

### 3.3. Acetaldehyde: CH<sub>3</sub>CHO

The proton affinity of acetaldehyde is defined as the enthalpy change associated with the reaction:

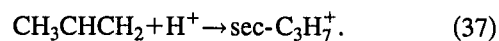


Ruscic and Berkowitz<sup>30</sup> have determined the 0 K appearance energy of  $\text{CH}_3\text{CHOH}^+$  from  $\text{C}_2\text{H}_5\text{OH}$  as  $(10.801 \pm 0.005) \text{ eV}$  using photoionization mass spectrometry. Assuming that the thermal  $(\text{H}_{298}^0 - \text{H}_0^0)$  correction needed for  $\text{CH}_3\text{CHOH}^+$  is intermediate between that for  $\text{CH}_3\text{CHO}$  and  $\text{C}_2\text{H}_5\text{OH}$ , they derive a value of  $\Delta_f H^0(\text{CH}_3\text{CHOH}^+, 298 \text{ K}) \leq (595.4 \pm 0.4) \text{ kJ mol}^{-1}$   $[(142.3 \pm 0.1) \text{ kcal mol}^{-1}]$ . These authors<sup>30</sup> comment further on the inequalities by saying "Although this is rigorously a lower limit, it is very likely close to the true value, since it is based on an appearance potential of a first fragment resulting from a simple bond cleavage." Bogan *et al.*<sup>31</sup> also determined the appearance energy of  $\text{CH}_3\text{CHOH}^+$  from  $\text{C}_2\text{H}_5\text{OH}$  as 10.81 eV using a discharge flow photoionization mass spectrometer, in close agreement with Ruscic and Berkowitz.<sup>30</sup> Accepting  $\Delta_f H^0(\text{CH}_3\text{CHO}, 298 \text{ K})^{26} = (-166.1 \pm 0.5) \text{ kJ mol}^{-1}$  gives  $\text{PA}(\text{CH}_3\text{CHO}, 298 \text{ K}) = (768.5 \pm 1.6) \text{ kJ mol}^{-1}$  and is taken as the selected value for this evaluation.

Smith and Radom<sup>12</sup> have calculated a 298 K proton affinity value for  $\text{CH}_3\text{CHO}$  of  $770.2 \text{ kJ mol}^{-1}$ , in good agreement with the experimental values above. East *et al.*<sup>13</sup> calculate a  $\Delta S_p(\text{CH}_3\text{CHO}, 298 \text{ K}) = 1.5 \text{ J (mol K)}^{-1}$ . Using as selected values the experimental results for proton affinity<sup>30,31</sup> and the theoretical value<sup>13</sup> for the entropy of protonation of  $\text{CH}_3\text{CHO}$  puts  $\text{GB}(\text{CH}_3\text{CHO}, 298 \text{ K}) = (736.5 \pm 1.6) \text{ kJ mol}^{-1}$ .

### 3.4. Propene: CH<sub>3</sub>CHCH<sub>2</sub>

The proton affinity of  $\text{CH}_3\text{CH}=\text{CH}_2$  is defined as the enthalpy change for the reaction:



Rosenstock *et al.*<sup>32</sup> determined appearance energies for  $\text{sec-C}_3\text{H}_7^+$  from  $2\text{-C}_3\text{H}_7\text{Br}$  and  $2\text{-C}_3\text{H}_7\text{I}$  as  $(10.42 \pm 0.01) \text{ eV}$  and  $(9.77 \pm 0.02) \text{ eV}$ , respectively, using the photoelectron photoion coincidence technique. Using  $\Delta_f H^0(2\text{-C}_3\text{H}_7\text{Br}, 298 \text{ K})^{26} = (-98.3 \pm 0.9) \text{ kJ mol}^{-1}$  and  $\Delta_f H^0(2\text{-C}_3\text{H}_7\text{I}, 298 \text{ K})^{26} = (41.6 \pm 1.7) \text{ kJ mol}^{-1}$  and related thermal corrections<sup>26</sup> yielded the values  $(799.6 \pm 2) \text{ kJ mol}^{-1}$  and  $(798.7 \pm 3) \text{ kJ mol}^{-1}$ , respectively, for the enthalpy of formation of  $\text{sec-C}_3\text{H}_7^+$  at 298 K formed from  $2\text{-C}_3\text{H}_7\text{Br}$  and  $2\text{-C}_3\text{H}_7\text{I}$ . Baer<sup>33</sup> similarly reported  $\Delta_f H^0(\text{sec-C}_3\text{H}_7^+, 298 \text{ K}) = (798.3 \pm 4) \text{ kJ mol}^{-1}$ . Using  $\Delta_f H^0(\text{CH}_3\text{CHCH}_2, 298 \text{ K})^{26} = (20.1 \pm 0.8) \text{ kJ mol}^{-1}$  and an average of the above experimental values for  $\Delta_f H^0(\text{sec-C}_3\text{H}_7^+, 298 \text{ K})$ , yields  $\text{PA}(\text{CH}_3\text{CHCH}_2, 298 \text{ K}) = (751.6 \pm 3) \text{ kJ mol}^{-1}$  and is the selected value. For comparison, Smith and Radom<sup>12</sup> calculated a 298 K proton affinity for propene of  $744.3 \text{ kJ mol}^{-1}$ .

For the entropy of protonation, the selected value,  $\Delta S_p(\text{CH}_3\text{CHCH}_2, 298 \text{ K}) = 12 \text{ J (mol K)}^{-1}$  comes from East *et al.*<sup>23</sup> Based on these values, the selected gas basicity value is  $\text{GB}(\text{CH}_3\text{CHCH}_2, 298 \text{ K}) = (722.7 \pm 3) \text{ kJ mol}^{-1}$ .

### 3.5. Formaldehyde: CH<sub>2</sub>O

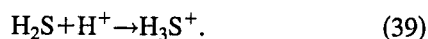
The proton affinity of formaldehyde is defined by the enthalpy change accompanying the process:



Traeger and Holmes<sup>34</sup> measured an appearance energy of  $(11.578 \pm 0.007) \text{ eV}$  for  $\text{CH}_2\text{OH}^+$  from  $\text{CH}_3\text{OH}$ , resulting in a  $\Delta_f H^0(\text{CH}_2\text{OH}^+, 298 \text{ K}) = (708.5 \pm 0.8) \text{ kJ mol}^{-1}$ . Using  $\Delta_f H^0(\text{CH}_2\text{O}, 298 \text{ K})^{26} = (-108.8 \pm 0.8) \text{ kJ mol}^{-1}$  sets  $\text{PA}(\text{CH}_2\text{O}, 298 \text{ K}) = (712.9 \pm 1.1) \text{ kJ mol}^{-1}$ . For comparison, Smith and Radom<sup>12</sup> calculated a 298 K proton affinity for formaldehyde of  $711.8 \text{ kJ mol}^{-1}$ . East *et al.*<sup>13</sup> computed  $\Delta S_p(\text{CH}_2\text{O}, 298 \text{ K}) = 9.5 \text{ J (mol K)}^{-1}$ . The selected values for this evaluation uses the experimental PA value derived from the appearance energy measurement<sup>34</sup> and the theoretical entropy of protonation<sup>13</sup> which combined gives  $\text{GB}(\text{CH}_2\text{O}, 298 \text{ K}) = (683.3 \pm 1.1) \text{ kJ mol}^{-1}$ .

### 3.6. Hydrogen sulfide: H<sub>2</sub>S

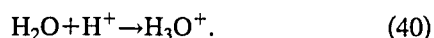
The proton affinity of H<sub>2</sub>S is defined by the enthalpy change for the reaction:



Prest *et al.*<sup>35</sup> and Walters and Blais<sup>36</sup> have determined appearance energies for H<sub>3</sub>S<sup>+</sup> from the van der Waals dimer (H<sub>2</sub>S)<sub>2</sub> as (10.249 ± 0.012) eV and (10.263 ± 0.010) eV, respectively. Using  $\Delta_f H^0(\text{H}_2\text{S}, 298 \text{ K})^{37} = (-20.6 \pm 0.8) \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{HS}, 298 \text{ K})^{37} = (139.3 \pm 5) \text{ kJ mol}^{-1}$ , the thermal corrections<sup>37</sup> for H<sub>2</sub>S and HS, taking the dimerization energy in (H<sub>2</sub>S)<sub>2</sub> as 6 kJ mol<sup>-1</sup>, and assuming the thermal correction for H<sub>3</sub>S<sup>+</sup> is equal to that for the isoelectronic PH<sub>3</sub>, results in estimates for  $\Delta_f H^0(\text{H}_3\text{S}^+, 298 \text{ K})$  of (803.8 ± 5.2) kJ mol<sup>-1</sup> and (805.1 ± 5.2) kJ mol<sup>-1</sup>. Taking the average of these two estimates results in a PA(H<sub>2</sub>S, 298 K) = (705.0 ± 5.3) kJ mol<sup>-1</sup>, and is the selected value. For comparison, Smith and Radom<sup>12</sup> computed a value of 707.7 kJ mol<sup>-1</sup> for this quantity. The selected value for  $\Delta S_p(\text{H}_2\text{S}, 298 \text{ K}) = 4.3 \text{ J (mol K)}^{-1}$  based on the difference in absolute entropies<sup>37</sup> of PH<sub>3</sub> and H<sub>2</sub>S. These correspond to  $GB(\text{H}_2\text{S}, 298 \text{ K}) = (673.8 \pm 5.3) \text{ kJ mol}^{-1}$ .

### 3.7. Water: H<sub>2</sub>O

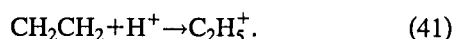
The proton affinity of H<sub>2</sub>O is defined by the reaction:



Ng *et al.*<sup>38</sup> measured an appearance energy of (11.73 ± 0.03) eV for H<sub>3</sub>O<sup>+</sup> from the van der Waals dimer (H<sub>2</sub>O)<sub>2</sub>. Using  $\Delta_f H^0(\text{H}_2\text{O}, 298 \text{ K})^{37} = (-241.8 \pm 0.04) \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{OH}, 298 \text{ K})^{37} = (39.0 \pm 1.2) \text{ kJ mol}^{-1}$ , thermal corrections for H<sub>2</sub>O and OH, a dimerization<sup>39</sup> binding energy of 16 kJ mol<sup>-1</sup> for (H<sub>2</sub>O)<sub>2</sub>, and approximating the thermal correction for H<sub>3</sub>O<sup>+</sup> to be that of NH<sub>3</sub>, yields  $\Delta_f H^0(\text{H}_3\text{O}^+, 298 \text{ K}) = (592.6 \pm 5) \text{ kJ mol}^{-1}$ . This leads to a proton affinity value of (695.6 ± 5) kJ mol<sup>-1</sup>. For comparison, Smith and Radom<sup>12</sup> and Pople and Curtiss<sup>39</sup> calculate values of 688.4 and 691.6 kJ mol<sup>-1</sup>. Because of the rather large and uncertain binding energy of the van der Waals dimer, the selected value for PA(H<sub>2</sub>O, 298 K) = (691 ± 3) kJ mol<sup>-1</sup> is based on the theoretical estimations<sup>12,39</sup> and also on a proton transfer equilibrium measurement.<sup>40</sup> A value of  $\Delta S_p(\text{H}_2\text{O}, 298 \text{ K}) = 5 \text{ J (mol K)}^{-1}$  is selected from East *et al.*,<sup>13</sup> corresponding to a selected  $GB(\text{H}_2\text{O}, 298 \text{ K}) = (660.0 \pm 3) \text{ kJ mol}^{-1}$ .

### 3.8. Ethene: CH<sub>2</sub>CH<sub>2</sub>

The proton affinity of ethene is defined according to the enthalpy change:



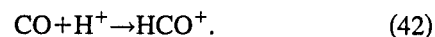
Ruscic *et al.*<sup>41</sup> determined an adiabatic ionization energy of (8.117 ± 0.008) eV for the ethyl radical. Using a value of  $\Delta_f H^0(\text{C}_2\text{H}_5, 298 \text{ K})^{42} = (118.6 \pm 1.7) \text{ kJ mol}^{-1}$  and reported

vibrational frequencies for the ethyl radical<sup>43</sup> and the ethyl cation<sup>44</sup> for the necessary thermal corrections yields  $\Delta_f H^0(\text{C}_2\text{H}_5^+, 298 \text{ K}) = (902 \pm 1.9) \text{ kJ mol}^{-1}$ . Rosenstock *et al.*<sup>32</sup> using the photoelectron photoion coincidence technique, measured an appearance energy of (10.52 ± 0.01) eV for C<sub>2</sub>H<sub>5</sub><sup>+</sup> from C<sub>2</sub>H<sub>5</sub>I. Using a value of  $\Delta_f H^0(\text{C}_2\text{H}_5\text{I}, 298 \text{ K}) = -7.7 \text{ kJ mol}^{-1}$  and thermal corrections for I and C<sub>2</sub>H<sub>5</sub>I given by Wagman *et al.*<sup>45</sup> and estimating the thermal correction for ethyl cation as indicated above, results in  $\Delta_f H^0(\text{C}_2\text{H}_5^+, 298 \text{ K}) = (903.1 \pm 2) \text{ kJ mol}^{-1}$ . Baer,<sup>33</sup> using the same technique and the same system as Rosenstock *et al.*,<sup>32</sup> obtained an appearance energy of 10.49 eV, resulting in the slightly lower value of  $\Delta_f H^0(\text{C}_2\text{H}_5^+, 298 \text{ K}) = 900.2 \text{ kJ mol}^{-1}$ . Using the average of these three values yields  $\Delta_f H^0(\text{C}_2\text{H}_5^+, 298 \text{ K}) = (901.8 \pm 1.5) \text{ kJ mol}^{-1}$ . Accepting the value  $\Delta_f H^0(\text{C}_2\text{H}_4, 298 \text{ K})^{26} = (52.3 \pm 0.8) \text{ kJ mol}^{-1}$  yields PA(C<sub>2</sub>H<sub>4</sub>, 298 K) = (680.5 ± 1.7) and is the selected value.

Smith and Radom<sup>12</sup> calculate a 298 K PA value 681.9 kJ mol<sup>-1</sup>, in good agreement with the experimental values. A value of  $\Delta S_p(\text{C}_2\text{H}_4, 298 \text{ K}) = 11.5 \text{ J (mol K)}^{-1}$  is selected as an average of various experimental determinations and a theoretical value,<sup>13</sup> and  $GB(\text{C}_2\text{H}_4, 298 \text{ K}) = (651.5 \pm 1.7) \text{ kJ mol}^{-1}$ .

### 3.9. Carbon Monoxide: CO

The proton affinity of CO is specified by the enthalpy change associated with the reaction:



The gas phase protonation thermochemistry of CO is rather unique in that experimental spectroscopic and thermochemical information exists for both CO and the formyl cation (HCO<sup>+</sup>). Armed with such data, the PA, GB and  $\Delta S_p$  of CO can be specified entirely from experimental studies subject only to the uncertainties associated with appearance energy measurements and the thermochemical quantities of relevant precursors. The proton affinity, gas basicity and protonation entropy of CO is an excellent choice to anchor a proton affinity ladder as in fact it was by one of the principal data sets used in this evaluation.<sup>15</sup> Unfortunately, the position of CO in the PA scale is rather near the bottom, separated by a scarcity of molecules for confidently linking it to the upper part of the scale.

Traeger<sup>46</sup> reported an appearance energy of HCO<sup>+</sup> from HCOOH as 12.76 eV from which a value of  $\Delta_f H^0(\text{HCO}^+, 298 \text{ K}) = (825.6 \pm 2.7) \text{ kJ mol}^{-1}$  is derived. Using  $\Delta_f H^0(\text{CO}, 298 \text{ K})^{47} = (-110.5 \pm 0.2) \text{ kJ mol}^{-1}$  results in PA(CO, 298 K) = (594 ± 3) kJ mol<sup>-1</sup>, and is the selected value for this quantity.

Protonated CO has been completely spectroscopically characterized in the microwave and infrared regions. In a microwave measurement, Woods *et al.*<sup>48</sup> observed the  $J=0 \rightarrow 1$  rotational transition at 89,188 MHz. Both Gudeman *et al.*<sup>49</sup> and Amano<sup>50</sup> have reported  $\nu_1 = 3088.7 \text{ cm}^{-1}$ . Kawaguchi *et al.*<sup>51</sup> have measured the doubly degenerate

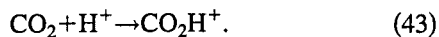


bending mode at  $\nu_2=828.2\text{ cm}^{-1}$ . Foster *et al.*<sup>52</sup> have reported a value for  $\nu_3=2183.9\text{ cm}^{-1}$ . Each of the vibrational studies have revealed P and R branch structures which prove that  $\text{HCO}^+$  is linear and have rotational line separations consistent with each other and with the microwave measurements. From these spectroscopic data for  $\text{HCO}^+$  the absolute entropy of  $\text{HCO}^+$  can be calculated, yielding the protonation entropy of CO at any temperature. They yield  $\Delta S_p(\text{CO}, 298\text{ K})=4.2\text{ J}(\text{mol K})^{-1}$ , which is the selected value for this quantity.

Kormornicki and Dixon<sup>53</sup> report a calculated 298 K proton affinity of CO as  $593.1\text{ kJ mol}^{-1}$ , while Smith and Radom<sup>12</sup> report a value  $593.0\text{ kJ mol}^{-1}$ , both of which agree well with values derived from the above appearance measurement. East *et al.*<sup>13</sup> report  $\Delta S_p(\text{CO}, 298\text{ K})=3.8\text{ J}(\text{mol K})^{-1}$ , close to value determined using spectroscopic data.

### 3.10. Carbon Dioxide: $\text{CO}_2$

The proton affinity of  $\text{CO}_2$  is the enthalpy change associated with the process:



In a photoelectron photoion coincidence measurement, Ruscic *et al.*<sup>54</sup> determined an appearance energy of  $(12.30 \pm 0.02)\text{ eV}$  for  $\text{CO}_2\text{H}^+$  from formic acid ( $\text{HCO}_2\text{H}$ ). Using a  $\Delta_f H^0(\text{HCO}_2\text{H}, 298\text{ K})=(-378.7 \pm 0.4)\text{ kJ mol}^{-1}$ ,<sup>45</sup> and the thermal correction for  $\text{HCO}_2\text{H}$  and estimating the thermal correction for  $\text{CO}_2\text{H}^+$  using theoretical vibrational frequencies<sup>44,55</sup> yields an estimate of  $\Delta_f H^0(\text{CO}_2\text{H}^+, 298\text{ K})=(596 \pm 2)\text{ kJ mol}^{-1}$ . This corresponds to  $\text{PA}(\text{CO}_2, 298\text{ K})=(540.5 \pm 2)\text{ kJ mol}^{-1}$  based on  $\Delta_f H^0(\text{CO}_2, 298\text{ K})^{47}=(-393.5 \pm 0.1)\text{ kJ mol}^{-1}$ . Traeger and Kompe<sup>56</sup> used photoionization mass spectrometry to measure appearance energies of  $\text{CO}_2\text{H}^+$  from a series of carboxylic acid precursors. As a mean value from their measurements, they arrive at  $\Delta_f H^0(\text{CO}_2\text{H}^+, 298\text{ K})=(600 \pm 3)\text{ kJ mol}^{-1}$ ; specifically, however, the appearance energy of  $\text{CO}_2\text{H}^+$  from  $\text{HCO}_2\text{H}$  was  $12.31\text{ eV}$ , in close agreement with the Ruscic value.

For comparison, Kormornicki and Dixon<sup>53</sup> calculate a PA value of  $541.0\text{ kJ mol}^{-1}$  while Smith and Radom<sup>12</sup> calculate  $539.3\text{ kJ mol}^{-1}$ , both at 298 K and both close to the experimental value. The selected value of  $\text{PA}(\text{CO}_2, 298\text{ K})$  is  $(540.5 \pm 2)\text{ kJ mol}^{-1}$ , based on the above appearance observations. For  $\Delta S_p(\text{CO}_2, 298\text{ K})$  the value from East *et al.*<sup>13</sup> is chosen,  $26\text{ J}(\text{mol K})^{-1}$ , which puts  $\text{GB}(\text{CO}_2, 298\text{ K})=(515.8 \pm 2)\text{ kJ mol}^{-1}$ .

## 4. Evaluation of Thermodynamic Ladders

The proton affinity and gas basicity scales presented here result primarily from an evaluation of a large body of inter-related data comprising a long thermochemical ladder. Since such a thermochemical scale imposes the requirements of internal consistency in three parameters,  $\Delta G^0$  (at different temperatures),  $\Delta H^0$ , and  $\Delta S^0$ , the evaluation of such data

necessarily requires that the complete scale be evaluated as a whole. That is, a compound-by-compound evaluation of the data for individual compounds is not possible, but at the same time, final values for the proton affinities and entropy changes for individual compounds must be consistent with what is known about enthalpies of formation of the relevant ion,  $\text{MH}^+$ , and molecule, M, as well as with entropy changes for the protonation reaction that would be predicted from statistical mechanics and values (when available) of absolute entropies of the relevant species. In addition, trends in homologous series or compounds of a particular structural type must make sense.

The evaluation of such a body of data, therefore, presents a particular challenge. The strategy followed here, to summarize the discussion briefly, is: (a) to compare directly the data from four extensive gas basicity scales obtained over a long period of time in four different laboratories; (b) to find that nearly all disagreements among the scales consist of relative "contractions" or "expansions" of the scales (which are known to be attributed to problems in temperature measurements in the earlier studies), and to proceed to "standardize" the various scales (i.e., to make appropriate corrections for temperature); (c) to use the recently published theoretical values for proton affinities<sup>12</sup> and entropy changes<sup>13</sup> as a guide to assigning absolute proton affinity values and evaluating entropy changes; and (d) to examine the resulting gas basicity and proton affinity scales compound-by-compound to verify internal consistency and "reasonableness" of all the proton affinity and entropy change values.

The evaluation of gas basicity/proton affinity scales presented here takes as its starting point an evaluation of several extensive thermochemical ladders generated in different laboratories over a wide time range. These are:

(1) **The data of Kebarle–Lau:** The early high pressure mass spectrometric proton transfer equilibrium constant determinations carried out in the laboratory of Kebarle<sup>57–62</sup> and summarized in the 1979 thesis of Lau<sup>63</sup> include only a few entropy change determinations. Comparison of this scale with more recent work (see items 3 and 4, below) indicates that the scale is slightly constricted; if one takes the operating temperature as 650 K rather than 600 K, the scale is expanded [Eq. (11)], bringing it into good agreement with the recent results.

(2) **The data of Taft *et al.*:** The large body of work emanating from the ICR laboratory of Taft and collaborators was published in dozens of research papers and summarized by Taft in reviews.<sup>4,8</sup> An updated comprehensive list of these determinations was made available to the present authors by Taft.<sup>64</sup> For the original measurements of gas basicities, the temperature of the ICR cell was not measured, but assumed to be 300 K. Subsequently, it has been determined that in many cases ICR cells thought to operate at "room temperature" were actually operating at higher temperatures. At the time of the 1984 evaluation,<sup>1</sup> Taft had estimated the operating temperature of the ICR cell to be 320 K, so the scale reported there was corrected to that temperature. A recent

paper from that laboratory<sup>65</sup> cites a temperature of 373 K for the operating temperature of the cell. Although the extensive scale of ICR data originated from experiments in which, as we now know, the exact temperature is ill-defined, the great value of this large body of data for multiply interconnected thermochemical steps mitigates in favor of making an attempt to reconstruct the probable temperature. One aspect of the current evaluation involved identifying the probable operating temperature at which the bulk of the earlier data from the Taft laboratory were taken. Therefore, multiple comparisons were made between the data in question and data from equilibrium constant determinations in numerous other laboratories where temperature measurements were carried out at the time of the experiments (including ICR, flowing afterglow, and high pressure mass spectrometry determinations); in general, current analysis indicates that had the operating temperature for the Taft laboratory measurements been  $(350 \pm 5)$  K for that part of the scale above water, the Gibbs free energy changes measured would match well. Accordingly, in the present evaluation, Gibbs free energy values reported in these early studies<sup>64</sup> (which covered the scale above water) have been corrected [Eq. (11)] by multiplying originally reported Gibbs free energy values by 350/300. The lower portion of the basicity scale was better matched by assuming an operating temperature of 320 K; these conclusions were confirmed by one of the authors of the series of papers from that laboratory.<sup>66</sup>

(3) **The data of Meot-Ner (Mautner)–Sieck:** In 1991, Meot-Ner (Mautner) and Sieck<sup>14</sup> determined a scale of temperature-dependent proton transfer equilibrium constants using high pressure mass spectrometry. This study reported that the span between the proton affinities of isobutene and ammonia was  $50.6 \text{ kJ mol}^{-1}$ ; since this span had been evaluated<sup>1</sup> in 1984 to be  $33.5 \text{ kJ mol}^{-1}$ , based on the earlier (constricted) scales reported in the literature, the Meot-Ner (Mautner)–Sieck paper gave a strong indication that a re-evaluation of the entire scale was needed. After the appearance of the results by Szulejko and McMahon<sup>15(b)</sup> (see item 4, below), Sieck carefully re-measured certain sections of the scale where there were discrepancies between the two sets of results, getting slightly different results for some equilibrium constants; those revised results<sup>16</sup> have been made available for this evaluation. In particular, the authors found that their thermochemical ladder as originally reported was somewhat expanded in the region of the scale between acetaldehyde and methyl acetate; an adjustment by a factor of 0.87, is recommended by Sieck, and has been adopted in this evaluation.

(4) **The data of Szulejko–McMahon:** Szulejko and McMahon published similar proton affinity scales determining temperature-dependent equilibrium constants in a high pressure mass spectrometer in 1991<sup>15(a)</sup> and 1993.<sup>15(b)</sup> These results confirmed the expansion of the gas basicity/proton affinity scales as reported by Meot-Ner (Mautner) and Sieck.<sup>14</sup>

(5) **The data of Smith–Radom:** Smith and Radom<sup>12</sup> produced a scale of proton affinity values generated by *ab initio* computations. That scale included proton affinity values for

31 molecules over an energy range of about  $500 \text{ kJ mol}^{-1}$ , that is, values that effectively spanned most of the experimental scale reported from equilibrium constant determinations. The same group<sup>13</sup> has also published a set of theoretically predicted values of entropy changes associated with protonation of these molecules. These data based on theory were used extensively as a tool for the evaluation of the experimental data.

Except for small details, the experimental gas basicity scales at 600 K from the three high pressure mass spectrometry laboratories are in generally good agreement (after making the temperature corrections described above). The scale from the ion cyclotron resonance experiments is in good agreement with the other three sets of results when the temperature difference is taken into account.

However, the proton affinity scales derived from the van't Hoff plots of the three high pressure mass spectrometry data sets<sup>14–16,57–63</sup> are in poor agreement. For this reason, the starting point for the evaluation was *not* the reported proton affinity scales,<sup>14–16,57–63</sup> but rather the 600 and 350 K gas basicity scales which appear to be well established from the good agreement and internal consistency among data generated by Kebarle *et al.*,<sup>57–63</sup> Meot-Ner (Mautner) and Sieck,<sup>14,16</sup> Szulejko and McMahon,<sup>15</sup> and Taft *et al.*<sup>64,65</sup>

Data on relative gas basicities from other laboratories were related to particular molecules included in these extensive scales, then treated the same as these data to generate proton affinity values. Details of the procedure are described in Sec. 5.

## 5. Generation of the Scale of Absolute Proton Affinities from the Scale of Relative Gas Basicities

### 5.1. Evaluation of Entropy Change Data

The current evaluation of proton affinity data relies heavily on data from recent high pressure mass spectrometric studies<sup>14–16</sup> in which entropy changes for individual proton transfer reactions were determined experimentally by measuring the equilibrium constants as a function of temperature. In principle, these studies produce a scale of experimentally derived entropy changes, and hence an experimental scale of proton affinity values. However, from the disagreements between the data sets from Refs. 14 and 16 compared to data from Ref. 15, it was obvious that at least one set of data suffered from undefined experimental problems. Several options were explored by the two sets of researchers to explain the differences; a suggestion, for example, that the Meot-Ner (Mautner)–Sieck data were taken under conditions where the ions underwent too few collisions to be thermally equilibrated was tested, and found not to be the explanation for the discrepancies.

A telling result appears to be the fact that the two laboratories do reproduce one another's scales of Gibbs free energy changes at 600 K. A value for a Gibbs free energy change (relative gas basicity) of a proton transfer reaction is ob-

tained *directly* from the measured equilibrium constant [Eq. (11)], unlike the entropy and enthalpy changes of reaction which require multiple measurements over a wide temperature range [Eq. (17)]. High pressure mass spectrometric van't Hoff plot determinations are performed typically at temperatures between 450 and 650 K. Clustering reactions of protonated molecules with polar neutral molecules frequently occur at the lower end of this temperature range, while pyrolysis and isomerization reactions of molecules and ions may ensue at the upper end. These types of processes, which are difficult to detect and evaluate, may well conspire to perturb the equilibrium constant measurement and yield inaccurate van't Hoff plots, that otherwise appear precise and internally consistent. The Gibbs free energy changes measured at temperatures close to 600 K seem to suffer least from the combined effects of clustering, isomerization, and pyrolysis, judging from the good agreement between the different data sets. ICR experiments, generally carried out at a temperature of about 350 K and at much lower pressures, are apparently not as susceptible to errors resulting from clustering and pyrolysis.

For the above reasons, the entropy changes determined in the high pressure mass spectrometric studies<sup>14-16</sup> were not accepted as the "best" values for relevant entropy changes, although in some cases (where clustering and pyrolysis would be expected to be minimal, and sufficient information to carry out an estimate was missing), the data were used, or consulted in making the final decision.

Entropy changes were instead derived through a combination of (a) estimating the entropy change from Gibbs free energy change determinations and the corresponding calculated enthalpy changes;<sup>12</sup> (b) comparing Gibbs free energy changes measured in a high pressure mass spectrometer with values taken at a lower temperature in an ICR; (c) comparing values derived from the procedures described in (a) and (b) with theoretically-calculated entropy changes<sup>13,67</sup> and with "expected" values from statistical mechanics or from considerations of isoelectronic species. A requirement of "reasonableness" and internal consistency was imposed on all entropy change data adopted in the evaluation. Details are given in Sections 5.2 and 5.3.

## 5.2. Procedures Followed in Evaluating Absolute Proton Affinities from the Scale of Relative Gas Basicities

The following steps were followed in producing an evaluated proton affinity scale from the composite gas basicity scale. This amounts in large part to carrying out an evaluation of entropy changes for the proton transfer reactions.

(1) The relative gas basicity scales at 600 and 350 K were related to the basicity of ammonia.



$$\Delta\text{GB}(\text{B}, \text{NH}_3, T) = -\Delta G_{\text{Rn44}}^0(T). \quad (45)$$

Ammonia was chosen as the primary anchor for the scale because it was considered that quantum chemical calcula-

tions lead to a reliable value for the proton affinity of this molecule. Smith and Radom report computational values of 853.6 kJ mol<sup>-1</sup> at 298 K and 858.8 kJ mol<sup>-1</sup> at 600 K (in good agreement with earlier *ab initio* results,<sup>68,69</sup> and also incidentally, with the value of 853.3 kJ mol<sup>-1</sup> recommended in the previous evaluation<sup>1</sup>).

Furthermore, the entropy change associated with protonation of ammonia can be calculated reliably, since both NH<sub>3</sub> and NH<sub>4</sub><sup>+</sup> have well-known structures and are devoid of complications associated with internal rotors, nonclassical structures, internal solvation, and so on. Therefore, the absolute gas basicity of ammonia at any given temperature can be assigned with high reliability. The entropy change for the half reaction associated with protonation of ammonia is taken as -6.4 J (mol K)<sup>-1</sup> and -4.5 J (mol K)<sup>-1</sup> at 298 and 600 K, respectively.

(2) The first set of standards comprising the primary evaluated scale were taken to be the molecules included in the *ab initio* calculations published by Smith and Radom.<sup>12</sup> This scale made up a "ladder" to which all other results could be linked.

- (a) Taking results from that publication<sup>12</sup> for the absolute enthalpy changes of reaction (44) for the 31 molecules, and using that "theoretical" proton affinity scale with the corresponding Gibbs free energy changes taken from the experimental scale of relative basicities at 600 K, values for  $\Delta S_{\text{Rn44}}^0$  were calculated. Since the entropy change for the half reaction associated with protonation of ammonia is known, this leads to a value for the entropy change for protonation of molecule B. This value for the entropy change was then evaluated to see if it was reasonable. The requirement of "reasonableness" included not only comparing the derived value of  $\Delta S_{\text{p}}^0(\text{B})$  with values predicted from statistical mechanics, or from comparisons with entropy changes derived from absolute entropies of isoelectronic species, but also a comparison, when possible, with entropy changes derived from theoretical calculations.<sup>13,67</sup>
- (b) The value of  $\Delta G_{\text{Rn44}}^0(600 \text{ K})$  and the value derived for  $\Delta S_{\text{Rn44}}^0$  were used to estimate  $\Delta G_{\text{Rn44}}^0(350 \text{ K})$ , assuming that  $\Delta S_{\text{Rn44}}^0$  is independent of temperature. When this value was found to be in agreement with the temperature-corrected experimental values reported by Taft *et al.*<sup>64</sup> to within 4 kJ mol<sup>-1</sup>, then the proton affinity, gas basicity, and entropy change for protonation of B were considered to be established.

Note that this procedure amounts to using the "reasonableness" of the value for the entropy change, as well as the internal consistency among the different data sets, as a criterion for the correctness of the evaluation. The required overall internal consistency also provides a secondary check on the absolute values adopted for the proton affinities; primary checks are agreements with values derived from absolute enthalpies of formation [Eq. (3)] where possible. This procedure yielded a framework proton affinity/gas basicity ladder including data for 25 molecules, and covering the proton

affinity range from about 540 to 950 kJ mol<sup>-1</sup>. The gas basicities, entropy changes, and proton affinities used for these compounds are listed in Table A.

(3) Data for other molecules were then referenced to one or more of these primary standards, or to other molecules with well-established gas basicities from the initial reference scales. The extensive gas basicity scales,<sup>14-16,57-65</sup> as well as measurements carried out to elucidate proton affinities of molecules not included in those scales, could all be related to the primary scale. There remained the problem of deriving values for entropy changes for proton transfer to molecules not included in the primary scale of 25 molecules (Table A).

- (a) For the compounds in the composite 600 K gas basicity scale<sup>14-16,57-63</sup> which also appear in the 350 K gas basicity scale<sup>64</sup> from the ICR experiments, a value for the entropy change was also derived from the difference in these two points. This derived value was then evaluated for reasonableness and internal consistency with entropy changes assigned to other related molecules in the scale.
- (b) When a calculated entropy change was available,<sup>13,67</sup> the derived value was also compared to the calculated value; in most cases there was very good agreement between the values of  $\Delta S_p^0(B)$  derived from the experimental basicity scales, but when there was a discrepancy, if the "reasonableness" of the entropy change obtained in step (a) was questionable, the theoretical value was chosen.

It should be noted that the evaluation procedure is, in fact, an evaluation of the entire scale of gas basicities/proton affinities (rather than a compound-by-compound evaluation of data for individual compounds), and imposes the requirement of internal consistency not only between scales measured at different temperatures, but also between values for the entropy changes for protonation of the different compounds included in the scales. That is, it is expected that entropy changes for protonation of all structurally similar amines, alcohols, ketones, or aldehydes, for example, should be similar. As mentioned before, most of the discrepancies between the data sets reported by Meot-Ner (Mautner) and Sieck<sup>14,16</sup> and by Szulejko and McMahon<sup>15</sup> disappear when one ignores the reported proton affinity scales (e.g., the entropy change values), and takes as a starting point for the evaluation the gas basicity scales at 600 K.

### 5.3. Sample Evaluations

(1) The evaluation of the gas basicity/proton affinity of methyl amine, B=CH<sub>3</sub>NH<sub>2</sub>: The 600 K gas basicity ladders reported by Meot-Ner (Mautner) and Sieck<sup>14</sup> and Szulejko and McMahon<sup>15</sup> give  $\Delta G_{Rn44}^0$  values of -45 and -46 kJ mol<sup>-1</sup>, respectively, for reaction (44). The difference between the proton affinity values for methyl amine and for ammonia calculated by Smith and Radom<sup>12</sup> is -47 kJ mol<sup>-1</sup>. Averaging the two 600 K relative basicity values, these data lead to a value of  $\Delta S_{Rn44}^0$

= -2.5 J (mol K)<sup>-1</sup> for the entropy change of the proton transfer between ammonia and methyl amine. Taking a value of -6.4 J (mol K)<sup>-1</sup> for the entropy change of the half reaction associated with the protonation of ammonia, the entropy change for the half reaction of protonation of methyl amine derived from these results is -9 J (mol K)<sup>-1</sup>. To check if this value is reasonable, first take the difference in the absolute symmetry number corrected entropies of C<sub>2</sub>H<sub>6</sub> (the isoelectronic analog of CH<sub>3</sub>NH<sub>3</sub><sup>+</sup>) and CH<sub>3</sub>NH<sub>2</sub> at 600 K; this difference is -7.3 J (mol K)<sup>-1</sup>. Taking the derived value of the entropy change of reaction, one predicts a Gibbs free energy change at 350 K for the proton transfer from NH<sub>4</sub><sup>+</sup> to CH<sub>3</sub>NH<sub>2</sub> of -46 kJ mol<sup>-1</sup>. The experimental value from the expanded Taft scale<sup>64</sup> is -44.8 kJ mol<sup>-1</sup>. Since there is excellent internal agreement among the various gas basicity scales, and the derived value of the entropy change for protonation of methyl amine is reasonable, the data are accepted for the evaluation. Absolute values for the proton affinity and gas basicity are assigned relative to the absolute values selected for ammonia.

(2) The evaluation of the gas basicity/proton affinity of isobutene, B=(CH<sub>3</sub>)<sub>2</sub>CCH<sub>2</sub>: Smith and Radom<sup>12</sup> compute a value for the 298 K proton affinity of 802.1 kJ mol<sup>-1</sup>, leading to an enthalpy change associated with proton transfer from NH<sub>4</sub><sup>+</sup> of  $\Delta H_{Rn44}^0 = 51.5$  kJ mol<sup>-1</sup>. Meot-Ner (Mautner) and Sieck<sup>14</sup> report a 600 K Gibbs free energy change of 38.5 kJ mol<sup>-1</sup> for this reaction, but this is in the region of the scale for which Sieck recommends a slightly greater value is 38.8 kJ mol<sup>-1</sup>. Szulejko and McMahon<sup>15</sup> report a value of 32 kJ mol<sup>-1</sup> for this quantity. Averaging these two values and calculating a value for  $\Delta S_{Rn44}^0$  taking the enthalpy change of reaction from the theoretical data, one obtains a value of 26 J (mol K)<sup>-1</sup> for the protonation entropy of isobutene. Taking the difference in absolute entropies at 298 K of isobutene and B(CH<sub>3</sub>)<sub>3</sub>,<sup>45</sup> the isoelectronic analog of the tert-butyl ion, one estimates that the entropy change for the half reaction should be about 22 J (mol K)<sup>-1</sup>, in reasonably good agreement with the value derived from the data analysis. Using these data, one predicts a value for the 350 K Gibbs free energy change of the proton transfer reaction from ammonia to isobutene of 42.2 kJ mol<sup>-1</sup>, in close agreement with the value taken from the expanded Taft scale,<sup>64</sup> 42.1 kJ mol<sup>-1</sup>.

(3) The evaluation of the gas basicity/proton affinity of dimethyl ether, B=(CH<sub>3</sub>)<sub>2</sub>O: Smith and Radom<sup>12</sup> compute a 298 K proton affinity of 792 kJ mol<sup>-1</sup> for dimethyl ether, which yields a calculated enthalpy change for proton transfer from NH<sub>4</sub><sup>+</sup> of  $\Delta H_{Rn44}^0 = 61.6$  kJ mol<sup>-1</sup>. The corresponding Gibbs free energy change, averaging the results from Szulejko and McMahon<sup>15</sup> and the adjusted results from Meot-Ner (Mautner) and Sieck,<sup>14</sup> is 45.6 kJ mol<sup>-1</sup>. Using these values as the enthalpy and Gibbs free energy for reaction (44), a value of  $\Delta S_{Rn44}^0 = 26.7$  J (mol K)<sup>-1</sup> and  $\Delta S_{pl}[(CH_3)_2O] = 20.3$  J (mol K)<sup>-1</sup> is obtained. Combining this  $\Delta S_{Rn44}^0$  value with the averaged 600 K Gibbs free energy change, one gets a 350 K Gibbs free energy value of

52.3 kJ mol<sup>-1</sup>, in good agreement with 53.5 kJ mol<sup>-1</sup> obtained from the expanded Taft scale.<sup>64</sup>

But how reasonable is this value for  $\Delta S_p[(\text{CH}_3)_2\text{O}] = 20.3 \text{ J (mol K)}^{-1}$ ? The difference in absolute entropies at 298 K between  $(\text{CH}_3)_2\text{NH}$  [the isoelectronic neutral analog of  $(\text{CH}_3)_2\text{OH}^+$ ] and  $(\text{CH}_3)_2\text{O}$  is about  $7 \text{ J (mol K)}^{-1}$ . For the present evaluation, this is not considered "reasonable" agreement. However, a theoretically predicted value obtained by East *et al.*,<sup>13</sup> gives  $\Delta S_p[(\text{CH}_3)_2\text{O}] = 16.5 \text{ J (mol K)}^{-1}$ . For this evaluation, the theoretically predicted value and the value derived from the present procedure is deemed in good agreement. This may indicate something unusual about the protonation of ethers whose entropy of protonation may not be reliably estimated using an isoelectronic neutral analog, e.g., a much lower inversion barrier is expected in the oxonium ion than in the amine.

#### 5.4. Uncertainty of the Proton Affinity Scale

In Sec. 3, the standard uncertainty assigned to the absolute proton affinity of the molecules indicated is the usual root-sum-of-squares combination of individual uncertainties associated with relevant enthalpies of formation and the uncertainty of some key measurement, such as an ionization or an appearance energy. The uncertainty assigned to all of the other molecules in this evaluation is based on our best judgment using all the relevant information and a general knowledge and experience with inter-locking thermochemical scales and is considered to be about  $8 \text{ kJ mol}^{-1}$ .

#### 5.5. Problems Remaining

As discussed recently by Koppel, Anvia and Taft,<sup>65</sup> the scale of gas basicities is not yet well established in the low basicity region, that is, in the region of the scale below the basicities of compounds such as water and hydrogen sulfide. As pointed out by those authors, measurements made in ion cyclotron resonance spectrometers are internally consistent, but are inconsistent with data taken in high pressure mass spectrometers (which data are themselves internally inconsistent).

Without access to more information, it is not possible at this time to resolve these discrepancies. Therefore, for that part of the scale below propene, many of the suggested gas basicity and proton affinity values are broad averages of rather disparate contributing values or are based somewhat indiscriminately on the most recent measurements.

### 6. Description of the Tables

Table 1 presents a summary of the evaluated proton affinity and gas basicity data sorted by molecular formula according to the Hill sort scheme.<sup>70</sup> The format is: molecular formula in the Hill format; Chemical Abstracts Registry Number; compound name or semiempirical formula; GB: evaluated value of gas basicity in kJ mol<sup>-1</sup>; PA: evaluated value of proton affinity in kJ mol<sup>-1</sup>;  $\Delta S_p$ : evaluated entropy

change for the half reaction:  $\text{M} \rightarrow \text{MH}^+$ . The last column gives an indication of the reason for the  $\Delta S_p$  value assigned to each compound. All of the thermochemical quantities are referred to 298 K. Aside from indicating the reasons for  $\Delta S_p$  values, references are not given in this table, since cited values may be derived from numerous references; the latter are given in Table 2.

Some of the entries in the second column consist of a Registry Number followed by a colon and a lower-case letter. This indicates that the corresponding molecule has estimates of proton affinity related to different sites of protonation. An example is carbon monoxide (CO) which has two entries as "630-08-0:a" (referring to protonation at C) and "630-0808:b" (referring to protonation at O). Other entries in this column begin with the "#" character followed by a number. These refer to molecules for which a Registry Number could not be found. The number following the "#" character has meaning only as an internal indexing pointer for this compilation.

The bold entries in the GB column indicate values that are derived from bracketing measurements (see Section 2.2.2.). The values so tabulated are the average GB values of the bracketing partners. It is necessary to refer to Table 2 to identify the bracketing partners and to get an indication of what may be the range of values associated with this average. Most reports of bracketing measurements do not indicate the temperature at which the observations are made. Even in cases where temperature is indicated, the tabulated values are averages of GB values referred to 298 K; no temperature corrections are included in such averages.

Some of the entries in the PA and  $\Delta S_p$  columns contain "NE." This means that the protonation entropy is expected to have a large negative value but which cannot be reliably estimated. Most of the molecules having this entry are large, flexible, polyfunctional molecules, such as polypeptides, for which cyclization of the protonated molecule is expected and for which only a gas basicity value has been reported. It is necessary for such molecules to refer to Table 2 to determine the temperature for which the tabulated GB value refers.

Since the site of protonation and the protonation entropy of functionally similar molecules are expected to be nearly equal, many  $\Delta S_p$  values are assigned to molecules based on their type. Thus, all tertiary amines have the same  $\Delta S_p$  values as  $(\text{CH}_3)_3\text{N}$ , all symmetrical secondary amines have the same  $\Delta S_p$  values as  $(\text{CH}_3)_2\text{NH}$  and all unsymmetrical secondary amines have the same  $\Delta S_p$  values as  $(\text{CH}_3)_2\text{NH}$  adjusted for the difference in rotational symmetry. Similarly, all symmetrical ketones have the same  $\Delta S_p$  values as acetone; unsymmetrical ketones have the value of symmetrical ketones modified for the symmetry difference. Molecules which protonate at an alkene function and give rise to a free internal rotor are assigned the  $\Delta S_p$  value of propene. As such, many of the entries under " $\Delta S_p$  Reasons" simply give the functional type to which the molecule belongs. Many other molecules do not fall neatly into such categories and their  $\Delta S_p$  values are assigned based on their rotational symmetry. For these molecules, the entry under " $\Delta S_p$  Reasons"

is of the form of Eq. (18). Other molecules give a reason in the form of a reference "squib," which is described in the next section. For these molecules, the cited reference is either the primary source of the assigned value of  $\Delta S_p$  or contains what is believed to be a reasonable explanation of the value.

For many atomic species in Table 1, column six starts with "rot. est.," followed by a number in parenthesis. This means that the protonation entropy of that atom was approximated as being equal to the rotational entropy, where the diatomic species consist of that atom and hydrogen and has a bond length in nanometers as indicated in parenthesis. The bond length was estimated from the sum of the valence radii of the atom and hydrogen. The vibrational contribution to  $\Delta S_p$  of these atoms is small and is ignored.

Table 2 presents a complete summary of the gas basicity data from the literature, along with the evaluated values for gas basicities at 298 K, entropy changes and proton affinities; these evaluations are summarized in Table 1 in a format sorted according to molecular formula. The data in Table 2 are presented in order of descending gas basicity. To find detailed experimental data for any particular molecule in Table 2, it is most convenient to first locate the molecule of interest in Table 1, then cross reference to the evaluated gas basicity value to locate the species in Table 2.

The structure of Table 2 can be best explained by actually referring to the table. Each page of Table 2 shows the column headings for the table and tabulated information for a few molecules. To begin with, it should be noted that the headings for the first three columns, along with the seventh, tenth and thirteenth columns, consist of two lines. The upper line of these column headings is in bold-face type while the lower line is in regular type. Meanwhile, the tabulated information is grouped for each individual molecule such that the first (header) row of a group is in bold-face type followed by one or more rows in regular type. The bold-faced column headings [namely, "[Formula]," "Reg No(M)," "Base(M)," "GB(M)," "PA(M)" and " $\Delta S_p(M)$ "] are meant to describe only the bold-faced data on the header row of each group of tabulated data. Similarly, the regular type headings on the lower line of the column headings describe the data contained on rows below the header row.

The header row for each grouping contains information about the base of interest, indicated by M in parenthesis and corresponding to the M indicated in reaction (10) and in Eqs. (12), (14), (15), and (16). The first column contains the molecular formula expressed in the Hill format, as indicated from the bold-faced column heading. In the second column is the Chemical Abstracts Registry Number for that base. The third column has either a line formula that is suggestive of the base's structure or a name for the base if its structure is too complicated or would be ambiguous to write as such a formula. The seventh and tenth columns contain, respectively, the *evaluated* gas basicity [GB(M)] and proton affinity [PA(M)] in  $\text{kJ mol}^{-1}$ ; the thirteenth column contains the evaluated entropy of protonation [ $\Delta S_p(M)$ ] in  $\text{J (mol K)}^{-1}$ . These three quantities are all referred to 298 K.

The regular type rows below each header row contain summaries of measurements, calculations or other kinds of data that pertain to the base specified in the header row. The structure of information on these rows is intended to accommodate the fact that the vast majority of data comprising this compilation is derived from proton transfer equilibrium measurements. The data for these types of measurements are given in considerable detail, with reference bases, thermochemical quantities and temperatures specifically noted.

The first column gives identifiers for literature references and are presented in a so-called "squib":

00ABC/DEF,

where 00 gives the year of publication (assumed to be in the twentieth century), ABC are the first three letters of the last name of the first author, and DEF are the first three letters of the last name of the second author. As an example, the publication

Koppel, I. A., Anvia, F., and Taft, R. W., *J. Phys. Org. Chem.* 7, 717 (1994).

would be represented in a squib as 94KOP/ANV. The complete citations of all references are given in the References section; references are sorted alphabetically according to the alphabetical part of the squib and then chronologically by year. Each entry is annotated, with experimental information such as type of instrument used, and where relevant, additional information about the study. In the case of bracketing experiments, the annotation will include the identities of bracketing compounds.

The second and third columns [labeled "Reg No(R)" and "Base(R)"] of regular-face rows gives the Chemical Abstracts Registry Number and identity, respectively, of the reference base used in proton transfer equilibrium measurements. The letter R in parenthesis corresponds to the R in reaction (10) and in Eqs. (12), (14), (15), and (16). In cases where the data come from bracketing experiments, the Registry Numbers and identities of both bracketing partners, corresponding to  $R_1$  and  $R_2$  of reactions (19) and (20), are given in these columns, separated by a semicolon. Some indication is given in the third column when the data comes from some other source or type of measurement; more information about these can be found in the references.

The fourth column [ $T(K)$ ] gives the absolute temperature of those measurements done at a single temperature or the maximum temperature of variable temperature experiments. The fifth column [GB(R)] is the evaluated 298 K gas basicity of the reference base employed. The sixth column [ $\Delta\text{GB}(M,R,T)$ ] gives the change in gas basicity *at the temperature, T, indicated in the fourth column*; it is the actual value reported. The algebraic sign of this quantity is made clear by referring to Eqs. (6) and (9) and noting that R refers to the reference base and M refers to the base of interest. The seventh column [regular-face type GB(M)] gives the 298 K gas basicity value for the particular measurement based on the entry in the previous column adjusted to 298 K and the

GB value of the reference. Note that the seventh column is not simply the sum of the previous two columns, but rather is given by the equation:

$$\text{GB}(M) = \text{GB}(R) + \Delta\text{GB}(M, R, T) - \Delta\Delta S_p(M, R)(T - 298 \text{ K}), \quad (46)$$

where  $\Delta\Delta S_p(M, R)$  is given by Eq. (16). Equation (46) is derived from Eqs. (14) and (16), and the familiar equation from thermodynamics:

$$(\partial\Delta G/\partial T)_p = -\Delta S, \quad (47)$$

where the subscript means that the partial differentiation is at constant pressure and where  $S$  is considered sufficiently independent of temperature as to be treated as a constant in the integration.

Some of the entries in column 7 show a range of values. These values are the GB values (to the nearest integer) of the bracketing partners indicated in the third column.

In most cases, the derivation of the evaluated gas basicity value given in the first line of an entry will be obvious from an examination of the experimental data listed below the header.

The eighth column [PA(R)] is the evaluated 298 K proton affinity of the reference base employed. The ninth column [ $\Delta\text{PA}(M, R)$ ] gives the measured change in proton affinity, and is considered to be independent of temperature and *not* necessarily referred to the temperature given in column 4. The tenth column [regular-face type PA(M)] is the proton affinity of M deduced from the particular measurement; it is the sum of the previous two columns. In the eleventh column [ $\Delta S_p(R)$ ] is the evaluated 298 K entropy of protonation of the reference base. The twelfth column [ $\Delta\Delta S_p(M, R)$ ] shows the measured entropy change. Like the change in proton affinity, this quantity is treated as independent of temperature and not referred to any particular temperature. The last column [ $\Delta S_p(M)$ ] is the sum of the two columns to its left and is the value inferred from this particular measurement.

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TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[Ar]	7440-37-1	Ar	346.3	369.2	32	$S(\text{HCl})-S(\text{Ar})$
[AsF <sub>3</sub> ]	7784-35-2	AsF <sub>3</sub>	<b>604.2</b>	636.7	0	Rln(3/3)
[AsH <sub>3</sub> ]	7784-42-1	AsH <sub>3</sub>	712.0	747.9	-11.5	Rln(3/12)
[BHO <sub>2</sub> ]	13460-50-9	HO-B=O	<b>730.5</b>	763.0	0	Rln(1/1)
[BH <sub>3</sub> O <sub>3</sub> ]	10043-35-3	B(OH) <sub>3</sub>	698.4	728.1	9.1	Rln(3/1)
[B <sub>2</sub> H <sub>6</sub> ]	19287-45-7	B <sub>2</sub> H <sub>6</sub>	586.0	615	11.5	Rln(4/1)
[B <sub>3</sub> H <sub>3</sub> N <sub>3</sub> ]	61110-11-0	B-Borazynyl radical	<b>770.6</b>	803.0	0	Rln(1/1)
[B <sub>3</sub> H <sub>6</sub> N <sub>3</sub> ]	6569-51-3	Borazine	772.8	802.5	9.1	Rln(6/2)
[B <sub>4</sub> H <sub>8</sub> ]	12007-71-5	B <sub>4</sub> H <sub>8</sub>	<b>752.4</b>	784.9	0	?
[B <sub>4</sub> H <sub>10</sub> ]	18283-93-7	B <sub>4</sub> H <sub>10</sub>	572.5	605	0	?
[B <sub>5</sub> H <sub>8</sub> ]	65930-58-7	B <sub>5</sub> H <sub>8</sub>	<b>731.0</b>	763.4	0	Rln(4/4)
[B <sub>5</sub> H <sub>9</sub> ]	19624-22-7	B <sub>5</sub> H <sub>9</sub>	<b>666.9</b>	699.4	0	?
[BaO]	1304-28-5	BaO	1187.6	1215.4	15.5	89GUR/VEY
[Br]	10097-32-2	Br	531.2	554.4	31	rot est (0.114)
[BrH]	10035-10-6	HBr	557.7	584.2	20	97EAS/SMI
[BrLi]	7550-35-8	LiBr	792.5	819	20	linear-to-bent est.
[CB <sub>3</sub> F <sub>3</sub> ]	75-63-8	CF <sub>3</sub> Br	550.3	580.0	9.1	Rln(3/1)
[CB <sub>3</sub> N]	506-68-3	BrCN	719.2	749.8	6	nitriles
[CClF]	1691-88-9	CFCl	<b>740.0</b>	772.4	0	Rln(1/1)
[CClF <sub>3</sub> ]	75-72-9	CF <sub>3</sub> Cl	541.5	571.3	9.1	Rln(3/1)
[CCIN]	506-77-4	ClCN	691.5	722.1	6	nitriles
[CCl <sub>2</sub> ]	1605-72-7	CCl <sub>2</sub>	828.5	861	0	Rln(2/2)
[CCl <sub>2</sub> S]	463-71-8	Cl <sub>2</sub> CS	721.8	752.5	5.8	Rln(2/1)
[CFN]	1495-50-7	FCN	601.3	632	6	nitriles
[CF <sub>2</sub> ]	2154-59-8	CF <sub>2</sub>	732.5	765	0	Rln(2/2)
[CF <sub>2</sub> O]	353-50-4	F <sub>2</sub> CO	637.0	666.7	9	sym ketones
[CF <sub>3</sub> I]	2314-97-8	CF <sub>3</sub> I	598.2	628.0	9.1	Rln(3/1)
[CF <sub>3</sub> NO]	334-99-6	CF <sub>3</sub> NO	<b>670.8</b>	703.3	0	Rln(1/1)
[CF <sub>4</sub> ]	75-73-0	CF <sub>4</sub>	503.7	529.3	23.3	average
[CHCl]	2108-20-5	CHCl	<b>839.9</b>	874.1	-5.8	Rln(1/2)
[CHF]	13453-52-6	CFH	<b>763.8</b>	797.9	-5.8	Rln(1/2)
[CHF <sub>3</sub> ]	75-46-7	CHF <sub>3</sub>	<b>589.7</b>	619.5	9.1	Rln(3/1)
[CHF <sub>3</sub> O <sub>3</sub> S]	1493-13-6	CF <sub>3</sub> SO <sub>3</sub> H	<b>666.9</b>	699.4	0	Rln(1/1)
[CHN]	6914-07-4	HNC	739.8	772.3	0	97EAS/SMI
[CHN]	74-90-8	HCN	681.6	712.9	4	97EAS/SMI
[CHNO]	75-13-8	HNCO	718.8	753	-5.8	Rln(1/2)
[CHNO]	506-85-4	HCNO	725.5	758	0	Rln(1/1)
[CHO]	2597-44-6	HCO	601.8	636	-5.8	Rln(1/2)
[CHO <sub>2</sub> ]	2564-86-5	•COOH	590.9	623.4	0	89HOL/LOS
[CHP]	6829-52-3	HCP	666.5	699	0	Rln(1/1)
[CH <sub>2</sub> Co]	116492-58-1	CoCH <sub>2</sub>	<b>905.2</b>	937.7	0	Rln(2/?)
[CH <sub>2</sub> F <sub>2</sub> ]	75-10-5	CH <sub>2</sub> F <sub>2</sub>	<b>589.7</b>	620.5	5.8	Rln(2/1)
[CH <sub>2</sub> F <sub>2</sub> Si]	51675-50-4	F <sub>2</sub> Si=CH <sub>2</sub>	<b>713.4</b>	742.3	12	propene
[CH <sub>2</sub> Fe]	95250-85-4	FeCH <sub>2</sub>	<b>905.2</b>	937.7	0	Rln(2/?)
[CH <sub>2</sub> N <sub>2</sub> ]	420-04-2	NH <sub>2</sub> -CN	774.9	805.6	6	nitriles
[CH <sub>2</sub> N <sub>2</sub> ]	334-88-3	CH <sub>2</sub> NN	<b>826.7</b>	858.9	1	$S(\text{CH}_3\text{CN})-S(\text{CH}_2\text{NN})$
[CH <sub>2</sub> O]	50-00-0	H <sub>2</sub> C=O	683.3	712.9	9.5	97EAS/SMI
[CH <sub>2</sub> O]	19710-56-6	HCOH (hydroxymethylene)	<b>933.4</b>	965.9	0	Rln(1/1)
[CH <sub>2</sub> OS]	40100-16-1	CH <sub>2</sub> =S=O	<b>766.4</b>	798.9	0	Rln(1/1)
[CH <sub>2</sub> O <sub>2</sub> ]	64-18-6	HCOOH	710.3	742.0	2.7	97EAS/SMI
[CH <sub>2</sub> S]	865-36-1	H <sub>2</sub> C=S	<b>730.5</b>	759.7	11	97EAS/SMI
[CH <sub>2</sub> Se]	6596-50-5	H <sub>2</sub> C=Se	<b>734.9</b>	764.0	11	H <sub>2</sub> CS
[CH <sub>2</sub> Te]	43309-26-8	H <sub>2</sub> C=Te	766.8	796	11	H <sub>2</sub> CS
[CH <sub>3</sub> BO <sub>2</sub> ]	#1524	CH <sub>3</sub> O-B=O	<b>730.5</b>	763.0	0	Rln(1/1)
[CH <sub>3</sub> Br]	74-83-9	CH <sub>3</sub> Br	638.0	664.2	21	isoel analog
[CH <sub>3</sub> Cl]	74-87-3	CH <sub>3</sub> Cl	621.1	647.3	21	$S(\text{CH}_3\text{SH})-S(\text{CH}_3\text{Cl})$
[CH <sub>3</sub> F]	593-53-3	CH <sub>3</sub> F	571.5	598.9	17	$S(\text{CH}_3\text{OH})-S(\text{CH}_3\text{F})$
[CH <sub>3</sub> I]	74-88-4	CH <sub>3</sub> I	665.5	691.7	21	isoel analog
[CH <sub>3</sub> N]	2053-29-4	CH <sub>2</sub> =NH	<b>818.7</b>	852.9	-5.8	Rln(1/2)
[CH <sub>3</sub> NO]	75-12-7	HCONH <sub>2</sub>	791.2	822.2	5	amides
[CH <sub>3</sub> NO <sub>2</sub> ]	4312-87-2	HCOONH <sub>2</sub>	802.2	834.7	0	Rln(1/1)
[CH <sub>3</sub> NO <sub>2</sub> ]	75-52-5	CH <sub>3</sub> NO <sub>2</sub>	721.6	754.6	-1.6	$S(\text{CH}_3\text{COOH})-S(\text{CH}_3\text{NO}_2)$
[CH <sub>3</sub> NO <sub>2</sub> ]	624-91-9	CH <sub>3</sub> ONO	<b>766.4</b>	798.9	0	Rln(1/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[CH <sub>3</sub> NO <sub>3</sub> ]	598-58-3	CH <sub>3</sub> ONO <sub>2</sub>	<b>714.8</b>	733.6	46	94CAC/ATT
[CH <sub>3</sub> N <sub>3</sub> ]	624-90-8	CH <sub>3</sub> NNN	800.5	833	0	Rln(1/1)
[CH <sub>3</sub> O]	2597-43-5	•CH <sub>2</sub> OH	662.5	695	0	?
[CH <sub>3</sub> S]	17032-46-1	•CH <sub>2</sub> SH	<b>701.5</b>	733.9	0	Rln(1/1)
[CH <sub>4</sub> ]	74-82-8	CH <sub>4</sub>	520.6	543.5	32	73HEM/RUN
[CH <sub>4</sub> N]	10507-29-6	•CH <sub>2</sub> NH <sub>2</sub>	<b>801.6</b>	832.8	4	S(CH <sub>3</sub> NH <sub>2</sub> )-S(•CH <sub>2</sub> NH <sub>2</sub> )
[CH <sub>4</sub> N <sub>2</sub> ]	26981-93-1:a	CH <sub>3</sub> N=NH at terminal N	812.5	845	0	Rln(1/1)
[CH <sub>4</sub> N <sub>2</sub> ]	26981-93-1:b	CH <sub>3</sub> N=NH at interior N	808.5	841	0	Rln(1/1)
[CH <sub>4</sub> N <sub>2</sub> S]	62-56-6	SC(NH <sub>2</sub> ) <sub>2</sub>	863.9	893.7	9	sym ketones
[CH <sub>4</sub> O]	67-56-1	CH <sub>3</sub> OH	724.5	754.3	9	97EAS/SMI
[CH <sub>4</sub> O <sub>3</sub> S]	75-75-2	CH <sub>3</sub> SO <sub>3</sub> H	<b>728.9</b>	761.3	0	?
[CH <sub>4</sub> S]	74-93-1	CH <sub>3</sub> SH	742	773.4	3.5	97EAS/SMI
[CH <sub>3</sub> N]	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	864.5	899.0	-7	97EAS/SMI
[CH <sub>3</sub> NO]	67-62-9	CH <sub>3</sub> ONH <sub>2</sub>	812.3	844.8	0	Rln(1/1)
[CH <sub>3</sub> N <sub>3</sub> ]	113-00-8	(NH <sub>2</sub> ) <sub>2</sub> C=NH	949.4	986.3	-14.9	Rln(1/6)
[CH <sub>3</sub> P]	593-54-4	CH <sub>3</sub> PH <sub>2</sub>	817.6	851.5	-5	S(CH <sub>3</sub> SiH <sub>3</sub> )-S(CH <sub>3</sub> PH <sub>2</sub> )
[CH <sub>6</sub> N <sub>2</sub> ]	60-34-4	CH <sub>3</sub> NHNH <sub>2</sub>	866.4	898.8	0	Rln(1/1)
[CN]	2074-87-5	CN at N	>564	>595	4.2	CO
[CNS]	15941-77-2	NCS	718.5	751	0	Rln(1/1)
[CO]	630-08-0:a	CO at C	562.8	594	4.2	exp. spectra
[CO]	630-08-0:b	CO at O	402.2	426.3	28	85DEF/MCL
[COS]	463-58-1	OCS at S	602.6	628.5	22	avg[CO <sub>2</sub> ,CS <sub>2</sub> ]-Rln(2/1)
[COSe]	1603-84-5	OCS <sub>e</sub> at Se	644.1	670	22	OCS
[COTe]	#1602	OCTe at Te	692.1	718	22	OCS
[CO <sub>2</sub> ]	124-38-9	CO <sub>2</sub>	515.8	540.5	26	97EAS/SMI
[CS]	2944-05-0	CS	760	791.5	3.3	97EAS/SMI
[CS <sub>2</sub> ]	75-15-0	CS <sub>2</sub>	657.7	681.9	28	88MCI/ADA
[CSe]	16674-18-3	CSe at C	800.2	831.8	3	CS
[CSe <sub>2</sub> ]	506-80-9	CSe <sub>2</sub>	700.9	725	28	CS <sub>2</sub>
[CTe]	12012-15-6	CTe at C	860.4	892	3	CS
[CTe <sub>2</sub> ]	12192-34-6	CTe <sub>2</sub>	747.8	771	31	CS <sub>2</sub> -like
[C <sub>2</sub> ClF <sub>3</sub> O]	354-32-5	CF <sub>3</sub> COCl	649.8	681.6	2	aldehydes
[C <sub>2</sub> Cl <sub>3</sub> N]	545-06-2	CCl <sub>3</sub> CN	692.6	723.2	6	nitriles
[C <sub>2</sub> D <sub>6</sub> O]	17222-37-6	(CD <sub>3</sub> ) <sub>2</sub> O	753.0	780.4	17	sym ethers
[C <sub>2</sub> F <sub>3</sub> N]	353-85-5	CF <sub>3</sub> CN	657.7	688.4	6	nitriles
[C <sub>2</sub> F <sub>4</sub> O]	354-34-7	CF <sub>3</sub> CFO	636.7	668.6	2	aldehydes
[C <sub>2</sub> H]	2122-48-7	HCC•	720.8	753	0	Rln(1/1)
[C <sub>2</sub> HCl <sub>3</sub> O]	75-87-6	CCl <sub>3</sub> CHO	690.5	722.3	2	CH <sub>3</sub> CHO
[C <sub>2</sub> HCl <sub>3</sub> O <sub>2</sub> ]	76-03-9	CCl <sub>3</sub> COOH	739.1	770.0	5	acids
[C <sub>2</sub> HF]	2713-09-9	HCCF	661.3	686	26	HCCF
[C <sub>2</sub> HF <sub>3</sub> ]	359-11-5	C <sub>2</sub> F <sub>3</sub> H	<b>666.9</b>	699.4	0	Rln(1/1)
[C <sub>2</sub> HF <sub>3</sub> O]	75-90-1	CF <sub>3</sub> CHO	653.6	685.5	2	aldehydes
[C <sub>2</sub> HF <sub>3</sub> O <sub>2</sub> ]	76-05-1	CF <sub>3</sub> COOH	680.7	711.7	5	acids
[C <sub>2</sub> H <sub>2</sub> ]	74-86-2	C <sub>2</sub> H <sub>2</sub>	616.7	641.4	26	AUE
[C <sub>2</sub> H <sub>2</sub> CIN]	107-14-2	CClH <sub>2</sub> CN	715.1	745.7	6	nitriles
[C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ]	1630-78-0	(E)-CHFCHF	<b>657.9</b>	688.6	5.8	Rln(2/1)
[C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ]	75-38-7	CH <sub>2</sub> =CF <sub>2</sub>	705.1	734	12	propene
[C <sub>2</sub> H <sub>2</sub> O]	463-51-4	CH <sub>2</sub> =C=O	793.6	825.3	2.4	97EAS/SMI
[C <sub>2</sub> H <sub>2</sub> S]	18282-77-4	CH <sub>2</sub> =C=S	<b>795.4</b>	826.2	5.8	Rln(2/1)
[C <sub>2</sub> H <sub>3</sub> ]	2669-89-8	C <sub>2</sub> H <sub>3</sub>	<b>719.8</b>	755.2	-10	S(C <sub>2</sub> H <sub>4</sub> )-S(C <sub>2</sub> H <sub>3</sub> )+Rln(2) (spin corr)
[C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub> ]	79-11-8	CH <sub>2</sub> ClCOOH	734.5	765.4	5	acids
[C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O]	115-20-8	CCl <sub>3</sub> CH <sub>2</sub> OH	698.9	729.3	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>3</sub> F]	75-02-5	CH <sub>2</sub> =CHF	700.1	729	12	propene
[C <sub>2</sub> H <sub>3</sub> FO <sub>2</sub> ]	144-49-0	CH <sub>2</sub> FCOOH	734.5	765.4	5	acids
[C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O]	75-89-8	CF <sub>3</sub> CH <sub>2</sub> OH	669.9	700.2	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O]	421-14-7	CF <sub>3</sub> OCH <sub>3</sub>	690.0	719.2	11	unsym ethers
[C <sub>2</sub> H <sub>3</sub> N]	75-05-8	CH <sub>3</sub> CN	748	779.2	4.3	S(CH <sub>3</sub> CCH)-S(CH <sub>3</sub> CN)
[C <sub>2</sub> H <sub>3</sub> N]	593-75-9	CH <sub>3</sub> NC	806.6	839.1	0.1	HNC
[C <sub>2</sub> H <sub>3</sub> NO]	624-83-9	CH <sub>3</sub> NCO	<b>732.0</b>	764.4	0	Rln(1/1)
[C <sub>2</sub> H <sub>3</sub> NS]	556-64-9	CH <sub>3</sub> SCN	<b>766.1</b>	796.7	6	nitriles
[C <sub>2</sub> H <sub>3</sub> NS]	556-61-6	CH <sub>3</sub> NCS	766.7	799.2	0	Rln(1/1)
[C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> ]	288-88-0	1,2,4-Triazole	855.9	886.0	8	pyridines+Rln(2/1)
[C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> ]	288-36-8	1,2,3-triazole	847.4	879.3	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>2</sub> H <sub>3</sub> O]	4400-01-5	•CH <sub>2</sub> CHO	741.5	774	0	89HOL/LOS
[C <sub>2</sub> H <sub>3</sub> O]	3170-69-2	CH <sub>3</sub> CO•	620.5	653	0	89HOL/LOS
[C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ]	#1498	•CH <sub>2</sub> COOH	737.5	770	0	89HOL/LOS
[C <sub>2</sub> H <sub>4</sub> ]	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	651.5	680.5	11.5	AUE; 97EAS/SMI
[C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> O]	359-13-7	CF <sub>2</sub> HCH <sub>2</sub> OH	697.0	727.4	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>4</sub> F <sub>3</sub> N]	753-90-2	CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	812.9	846.8	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> ]	540-61-4	NCCH <sub>2</sub> NH <sub>2</sub>	791.0	824.9	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>2</sub> H <sub>4</sub> O]	75-21-8	c-C <sub>2</sub> H <sub>4</sub> O	745.3	774.2	12	AUE
[C <sub>2</sub> H <sub>4</sub> O]	75-07-0	CH <sub>3</sub> CHO	736.5	768.5	1.5	97EAS/SMI
[C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ]	64-19-7	CH <sub>3</sub> COOH	752.8	783.7	5	acids
[C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ]	107-31-3	HCOOCH <sub>3</sub>	751.5	782.5	5	97EAS/SMI
[C <sub>2</sub> H <sub>4</sub> S]	420-12-2	c-C <sub>2</sub> H <sub>4</sub> S(Thiirane)	777.6	807.4	9	sym sulfides
[C <sub>2</sub> H <sub>5</sub> ]	2025-56-1	C <sub>2</sub> H <sub>5</sub> •	583.5	616	0	?
[C <sub>2</sub> H <sub>5</sub> Br]	74-96-4	C <sub>2</sub> H <sub>5</sub> Br	669.7	696.2	20	C <sub>2</sub> H <sub>5</sub> Cl
[C <sub>2</sub> H <sub>5</sub> BrO]	540-51-2	BrCH <sub>2</sub> CH <sub>2</sub> OH	735.7	766.1	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>5</sub> Cl]	75-00-3	C <sub>2</sub> H <sub>5</sub> Cl	666.9	693.4	20	S(C <sub>2</sub> H <sub>5</sub> SH)-S(C <sub>2</sub> H <sub>5</sub> Cl)
[C <sub>2</sub> H <sub>5</sub> ClO]	107-07-3	ClCH <sub>2</sub> CH <sub>2</sub> OH	735.7	766.1	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>5</sub> F]	353-36-6	C <sub>2</sub> H <sub>5</sub> F	655.8	683.4	16	S(C <sub>2</sub> H <sub>5</sub> OH)-S(C <sub>2</sub> H <sub>5</sub> F)
[C <sub>2</sub> H <sub>5</sub> FO]	371-62-0	FCH <sub>2</sub> CH <sub>2</sub> OH	685.2	715.6	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>5</sub> FSi]	125413-85-6	F(CH <sub>3</sub> )Si=CH <sub>2</sub>	742.2	771.1	12	propene
[C <sub>2</sub> H <sub>5</sub> F <sub>2</sub> N]	430-67-1	CF <sub>2</sub> HCH <sub>2</sub> NH <sub>2</sub>	836.6	870.5	-5.1	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>2</sub> H <sub>5</sub> I]	75-03-6	C <sub>2</sub> H <sub>5</sub> I	698.3	724.8	20	ethyl halides
[C <sub>2</sub> H <sub>5</sub> N]	593-67-9	CH <sub>2</sub> =CHNH <sub>2</sub>	866.5	898.9	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> N]	151-56-4	Azirdine	872.5	905.5	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>2</sub> H <sub>5</sub> N]	20729-41-3	CH <sub>3</sub> CH=NH	852.6	885.1	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> N]	1761-67-7	CH <sub>2</sub> =NCH <sub>3</sub>	852.1	884.6	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> NO]	123-39-7	HCONHCH <sub>3</sub>	820.3	851.3	5	amides
[C <sub>2</sub> H <sub>5</sub> NO]	60-35-5	CH <sub>3</sub> CONH <sub>2</sub>	832.6	863.6	5	amides
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ]	79-24-3	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	733.2	765.7	0	?
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ]	56-40-6	glycine	852.2	886.5	-6	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ]	546-88-3	Acetamide,N-hydroxy	823.0	854.0	5	amides
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ]	109-95-5	C <sub>2</sub> H <sub>5</sub> ONO	786.4	818.9	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> NS]	62-55-5	CH <sub>3</sub> CSNH <sub>2</sub>	852.8	884.6	2	unsym ketones
[C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> ]	871-31-8	CH <sub>3</sub> CH <sub>2</sub> NNN	845.5	878	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> O]	4422-54-2	•CH <sub>2</sub> CH <sub>2</sub> OH	712.5	745	0	89HOL/LOS
[C <sub>2</sub> H <sub>5</sub> O]	16520-04-0	•CH <sub>2</sub> OCH <sub>3</sub>	723.6	756.1	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> O]	2348-46-1	CH <sub>3</sub> CH(•)OH	687.7	720.1	0	Rln(1/1)
[C <sub>2</sub> H <sub>5</sub> P]	6569-82-0	c-C <sub>2</sub> H <sub>4</sub> PH	768.3	802.5	-5.8	Rln(1/2)
[C <sub>2</sub> H <sub>6</sub> ]	74-84-0	C <sub>2</sub> H <sub>6</sub>	569.9	596.3	20	94CAR/SCH
[C <sub>2</sub> H <sub>6</sub> B <sub>4</sub> ]	20693-67-8	1,6-C <sub>2</sub> B <sub>4</sub> H <sub>6</sub>	834.8	863.8	11.5	Rln(4/1)
[C <sub>2</sub> H <sub>6</sub> FN]	406-34-8	CH <sub>2</sub> FCH <sub>2</sub> NH <sub>2</sub>	858.0	892.0	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>2</sub> H <sub>6</sub> Hg]	593-74-8	(CH <sub>3</sub> ) <sub>2</sub> Hg	740.8	771.6	5.8	Rln(2/1)
[C <sub>2</sub> H <sub>6</sub> N]	#804	•CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	854.5	887	0	89HOL/LOS
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> ]	143-37-3	CH <sub>3</sub> C(=NH)NH <sub>2</sub>	938.2	970.7	0	Rln(1/1)
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> ]	4143-41-3	(E)-CH <sub>3</sub> N=NCH <sub>3</sub>	834.4	865.1	5.8	Rln(2/1)
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O]	598-41-4	H <sub>2</sub> NCH <sub>2</sub> CONH <sub>2</sub> (glycinamide)	882.3	NE	NE	not estimated
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ]	4164-28-7	(CH <sub>3</sub> ) <sub>2</sub> NNO <sub>2</sub>	795.8	828.3	0	?
[C <sub>2</sub> H <sub>6</sub> O]	64-17-5	C <sub>2</sub> H <sub>5</sub> OH	746	776.4	7	CH <sub>3</sub> OH
[C <sub>2</sub> H <sub>6</sub> O]	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	764.5	792	16.5	97EAS/SMI
[C <sub>2</sub> H <sub>6</sub> OS]	67-68-5	(CH <sub>3</sub> ) <sub>2</sub> SO	853.7	884.4	5.8	Rln(2/1)
[C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ]	107-21-1	HOCH <sub>2</sub> CH <sub>2</sub> OH	773.6	815.9	-33	95CHE/STO
[C <sub>2</sub> H <sub>6</sub> S]	75-18-3	(CH <sub>3</sub> ) <sub>2</sub> S	801.2	830.9	9.1	97EAS/SMI
[C <sub>2</sub> H <sub>6</sub> S]	75-08-1	C <sub>2</sub> H <sub>5</sub> SH	758.4	789.6	4	CH <sub>3</sub> SH
[C <sub>2</sub> H <sub>6</sub> S <sub>2</sub> ]	624-92-0	CH <sub>3</sub> SSCH <sub>3</sub>	782.8	815.3	0	Rln(1/1)
[C <sub>2</sub> H <sub>7</sub> B <sub>5</sub> ]	20693-69-0	2,4-C <sub>2</sub> B <sub>5</sub> H <sub>7</sub>	665.0	697.4	0	Rln(1/1)
[C <sub>2</sub> H <sub>7</sub> N]	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	878	912.0	-5.1	97EAS/SMI
[C <sub>2</sub> H <sub>7</sub> N]	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	896.5	929.5	-2	97EAS/SMI
[C <sub>2</sub> H <sub>7</sub> NO]	141-43-5	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> OH	896.8	930.3	-3.3	80MAU/HAM
[C <sub>2</sub> H <sub>7</sub> O <sub>3</sub> P]	868-85-9	(CH <sub>3</sub> O) <sub>2</sub> PHO	862.4	894.8	0	Rln(1/1)
[C <sub>2</sub> H <sub>7</sub> P]	676-59-5	(CH <sub>3</sub> ) <sub>2</sub> PH	877.9	912.0	-5.8	Rln(1/2)
[C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ]	57-14-7	(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub>	894.7	927.1	0	Rln(1/1)
[C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ]	107-15-3	1,2-Diaminoethane	912.5	951.6	-22.1	80MAU/HAM
[C <sub>2</sub> N <sub>2</sub> ]	460-19-5	NC-CN	645.8	674.7	11.8	nitriles+Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>2</sub> O]	12071-23-7	CCO	747.0	774.7	16	93MAC/SUD
[C <sub>2</sub> S]	12602-41-4	C <sub>2</sub> S	840.7	869.6	12	92MAC/SUD
[C <sub>3</sub> ]	12075-35-3	C <sub>3</sub>	736.3	767.0	5.8	Rln(2/1)
[C <sub>3</sub> F <sub>5</sub> N]	422-04-8	C <sub>2</sub> F <sub>5</sub> CN	661.3	692.0	6	nitriles
[C <sub>3</sub> F <sub>6</sub> O]	684-16-2	(CF <sub>3</sub> ) <sub>2</sub> CO	639.7	670.4	5.8	Rln(2/1)
[C <sub>3</sub> HN]	1070-71-9	HCC-CN	720.5	751.2	6	nitriles
[C <sub>3</sub> HNO]	145798-71-6	HNCCCO	828.5	861	0	?
[C <sub>3</sub> HNO]	4452-08-8	NCCHCO	751.5	784	0	Rln(1/1)
[C <sub>3</sub> HN <sub>3</sub> ]	290-87-9	1,3,5-Triazine	819.6	848.8	11	pyridines+Rln(6/2)
[C <sub>3</sub> H <sub>2</sub> ]	16165-40-5	cyclopropenylidene	915.9	951.1	-9.1	Rln(2/6)
[C <sub>3</sub> H <sub>2</sub> F <sub>4</sub> O]	360-52-1	CF <sub>2</sub> HCOCF <sub>2</sub> H	669.0	698.8	9	sym ketones
[C <sub>3</sub> H <sub>2</sub> F <sub>6</sub> O]	920-66-1	(CF <sub>3</sub> ) <sub>2</sub> CHOH	656.2	686.6	7	CH <sub>3</sub> OH
[C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> ]	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	694.1	723.0	12	nitriles+Rln(2/1)
[C <sub>3</sub> H <sub>2</sub> N <sub>4</sub> O <sub>4</sub> ]	38858-89-8	3,5-dinitroimidazole	727.5	759.4	2	pyridines
[C <sub>3</sub> H <sub>3</sub> ]	2932-78-7	HCCCCH <sub>2</sub> •	708.5	741	0	89HOL/LOS
[C <sub>3</sub> H <sub>3</sub> ]	28933-84-8	c-C <sub>3</sub> H <sub>3</sub> •	701.8	734.3	0	Rln(2/2)
[C <sub>3</sub> H <sub>3</sub> CIN <sub>2</sub> ]	15965-31-8	4-Cl-pyrazole	834.9	868.5	-3.8	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub> O]	918-00-3	CCl <sub>3</sub> COCH <sub>3</sub>	736.3	768.3	1.5	CH <sub>3</sub> CHO
[C <sub>3</sub> H <sub>3</sub> FN <sub>2</sub> ]	35277-02-2	4-fluoropyrazole	829.4	863.0	-4	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O]	421-50-1	CF <sub>3</sub> COCH <sub>3</sub>	692.0	723.9	2	unsym ketones
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> OS]	41879-94-1	CF <sub>3</sub> COSCH <sub>3</sub>	734.3	765.2	5	esters
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub> ]	431-47-0	CF <sub>3</sub> COOCH <sub>3</sub>	709.6	740.5	5	acids
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub> ]	32042-38-9	HCOOCH <sub>2</sub> CF <sub>3</sub>	714.6	745.5	5	acids
[C <sub>3</sub> H <sub>3</sub> N]	107-13-1	CH <sub>2</sub> =CHCN	753.7	784.7	4.9	97EAS/SMI
[C <sub>3</sub> H <sub>3</sub> NO]	631-57-2	CH <sub>2</sub> COCN	716.2	746.9	6	nitriles
[C <sub>3</sub> H <sub>3</sub> NO]	288-42-6	oxazole	844.5	876.4	2	pyridines
[C <sub>3</sub> H <sub>3</sub> NO]	288-14-2	Isooxazole	816.8	848.6	2	pyridines
[C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> ]	17640-15-2	CH <sub>2</sub> COOCN	714.7	745.7	5	esters
[C <sub>3</sub> H <sub>3</sub> NS]	288-47-1	thiazole	872.1	904	2	pyridines
[C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O]	2075-46-9	4-NO <sub>2</sub> -pyrazole	788.7	822.2	-3.8	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub> ]	26621-44-3	3(5)-nitroimidazole	789.0	820.8	2	pyridines
[C <sub>3</sub> H <sub>4</sub> ]	463-49-0	H <sub>2</sub> C=C=CH <sub>2</sub>	745.8	775.3	10	AUE
[C <sub>3</sub> H <sub>4</sub> ]	2781-85-3	Cyclopropene	787.8	818.5	5.8	Rln(2/1)
[C <sub>3</sub> H <sub>4</sub> ]	74-99-7	CH <sub>3</sub> CCH	723.0	748	25	AUE
[C <sub>3</sub> H <sub>4</sub> CIN]	542-76-7	Cl(CH <sub>2</sub> ) <sub>2</sub> CN	742.4	773.1	6	nitriles
[C <sub>3</sub> H <sub>4</sub> F <sub>2</sub> O]	453-14-5	CFH <sub>2</sub> COCFH <sub>2</sub>	733.0	762.8	9	(CH <sub>3</sub> ) <sub>2</sub> CO
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ]	288-32-4	Imidazole	909.2	942.8	-3.8	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ]	288-13-1	Pyrazole	860.5	894.1	-3.8	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S]	96-50-4	2-Aminothiazole	898.7	930.6	2	pyridines
[C <sub>3</sub> H <sub>4</sub> O]	6004-44-0	CH <sub>3</sub> CH=CO	803.4	834.1	6	ketene+Rln(3/2)
[C <sub>3</sub> H <sub>4</sub> O]	107-02-8	CH <sub>2</sub> =CHCHO	765.1	797.0	2	CH <sub>3</sub> CHO
[C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> ]	96-49-1	1,3-Dioxolane-2-one	784.4	814.2	9	sym ketones
[C <sub>3</sub> H <sub>5</sub> ]	2417-82-5	c-C <sub>3</sub> H <sub>5</sub> •	702.0	738.9	-14.9	Rln(1/6)
[C <sub>3</sub> H <sub>5</sub> ]	1981-80-2	CH <sub>2</sub> =CHCH <sub>2</sub> •	707.4	736	13	S(C <sub>3</sub> H <sub>6</sub> )+Rln(2/1)-S(C <sub>3</sub> H <sub>5</sub> •)
[C <sub>3</sub> H <sub>5</sub> ClO <sub>2</sub> ]	541-41-3	ClCOOC <sub>2</sub> H <sub>5</sub>	733.8	764.8	5	esters
[C <sub>3</sub> H <sub>5</sub> FO]	430-51-3	CH <sub>3</sub> COCH <sub>2</sub> F	763.5	795.4	2	unsym ketones
[C <sub>3</sub> H <sub>5</sub> FO <sub>2</sub> ]	461-64-3	FCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	726.0	757.0	5	esters
[C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> O]	460-43-5	CF <sub>3</sub> CH <sub>2</sub> OCH <sub>3</sub>	718.4	747.6	11	unsym ethers
[C <sub>3</sub> H <sub>5</sub> N]	107-12-0	C <sub>2</sub> H <sub>5</sub> CN	763.0	794.1	4.7	S(C <sub>2</sub> H <sub>5</sub> CCH)-S(C <sub>2</sub> H <sub>5</sub> CN)
[C <sub>3</sub> H <sub>5</sub> N]	18295-52-8	vinylimine	879.7	912.1	0	Rln(1/1)
[C <sub>3</sub> H <sub>5</sub> N]	19540-05-7	1-Azabicyclo[1.1.0]butane	856.1	886.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>3</sub> H <sub>5</sub> N]	2450-71-7	HCCCCH <sub>2</sub> NH <sub>2</sub>	853.5	887.4	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>5</sub> N]	624-79-3	C <sub>2</sub> H <sub>5</sub> NC	818.9	851.3	0	HNC
[C <sub>3</sub> H <sub>5</sub> NO]	930-21-2	2-Azetidinone	821.7	852.6	5	amides
[C <sub>3</sub> H <sub>5</sub> NO]	1738-36-9	CH <sub>3</sub> OCH <sub>2</sub> CN	727.4	758.1	6	nitriles
[C <sub>3</sub> H <sub>5</sub> NO]	79-06-1	2-propenamidine	839.8	870.7	5	amides
[C <sub>3</sub> H <sub>5</sub> NS]	35120-10-6	CH <sub>3</sub> SCH <sub>2</sub> CN	754.1	784.8	6	nitriles
[C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> ]	1820-80-0	3(5)-aminopyrazole	889.6	921.5	2	pyridines
[C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> ]	28466-26-4	4-NH <sub>2</sub> -pyrazole	874.0	907.6	-3.8	pyridines+Rln(1/2)
[C <sub>3</sub> H <sub>5</sub> O]	3122-07-4	•CH <sub>2</sub> COCH <sub>3</sub>	787.5	820	0	89HOL/LOS
[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ]	#1324	•CH <sub>2</sub> COOCH <sub>3</sub>	783.5	816	0	89HOL/LOS
[C <sub>3</sub> H <sub>5</sub> O <sub>3</sub> P]	279-53-8	2,6,7-Trioxa-1-phosphabicyclo[2.2.1]heptane	770.6	803.1	0	Rln(1/1)
[C <sub>3</sub> H <sub>6</sub> ]	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>	722.7	751.6	12	97EAS/SMI

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>3</sub> H <sub>6</sub> ]	75-19-4	c-C <sub>3</sub> H <sub>6</sub>	722.2	750.3	14.9	Rln(6/1)
[C <sub>3</sub> H <sub>6</sub> CINO]	96-30-0	CICON(CH <sub>3</sub> ) <sub>2</sub>	814.8	845.8	5	amides
[C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N]	460-39-9	CF <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	853.2	887.2	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N]	2730-67-8	CF <sub>3</sub> CH <sub>2</sub> NHCH <sub>3</sub>	848.0	881.1	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N]	677-41-8	CF <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	772.2	803.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ]	1467-79-4	(CH <sub>3</sub> ) <sub>2</sub> NCN	821.4	852.1	6	nitriles
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ]	151-18-8	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN	832.5	866.4	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ]	5616-32-0	CH <sub>3</sub> NHCH <sub>2</sub> CN	830.7	863.8	-2	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S]	96-45-7	2-imidazolinethione	891.2	921.9	5.8	Rln(2/1)
[C <sub>3</sub> H <sub>6</sub> O]	107-25-5	CH <sub>2</sub> =CH-OCH <sub>3</sub>	830.3	859.2	12	propene
[C <sub>3</sub> H <sub>6</sub> O]	75-56-9	2-Methylloxirane	772.7	803.3	6	oxirane-Rln(2/1)
[C <sub>3</sub> H <sub>6</sub> O]	503-30-0	c-C <sub>3</sub> H <sub>6</sub> O(Oxetane)	773.9	801.3	17	sym ethers
[C <sub>3</sub> H <sub>6</sub> O]	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	754.0	786.0	1.5	CH <sub>3</sub> CHO
[C <sub>3</sub> H <sub>6</sub> O]	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	782.1	812	8.7	97EAS/SMI
[C <sub>3</sub> H <sub>6</sub> OS]	21119-13-1	CH <sub>3</sub> C(=S)OCH <sub>3</sub>	816.5	846.0	10	CH <sub>2</sub> S
[C <sub>3</sub> H <sub>6</sub> OS]	1534-08-3	CH <sub>3</sub> C(=O)SCH <sub>3</sub>	798.0	829.0	5	esters
[C <sub>3</sub> H <sub>6</sub> OS <sub>2</sub> ]	19708-81-7	CH <sub>3</sub> OC(S)SCH <sub>3</sub>	830.8	862.6	2	unsym ketones
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ]	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	768.4	799.4	5	esters
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ]	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	790.7	821.6	5	esters
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ]	79-09-4	C <sub>2</sub> H <sub>5</sub> COOH	766.2	797.2	5	esters
[C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> ]	616-38-6	(CH <sub>3</sub> O) <sub>2</sub> CO	799.2	830.2	5	acids
[C <sub>3</sub> H <sub>6</sub> S]	1822-74-8	CH <sub>2</sub> =CH-SCH <sub>3</sub>	829.3	858.2	12	propene
[C <sub>3</sub> H <sub>6</sub> S]	287-27-4	Thietane	805.0	834.8	9	sym sulfides
[C <sub>3</sub> H <sub>6</sub> S]	1072-43-1	2-Methylthiirane	801.5	833.3	2	thiirane-Rln(2/1)
[C <sub>3</sub> H <sub>6</sub> S <sub>2</sub> ]	2168-84-5	CH <sub>3</sub> C(=S)SCH <sub>3</sub>	831.5	860.7	11	CH <sub>2</sub> S
[C <sub>3</sub> H <sub>6</sub> Se]	76573-19-8	CH <sub>2</sub> =CH-SeCH <sub>3</sub>	822.0	850.9	12	propene
[C <sub>3</sub> H <sub>7</sub> ]	2025-55-0	i-C <sub>3</sub> H <sub>7</sub> •	638.9	671.4	0	?
[C <sub>3</sub> H <sub>7</sub> N]	765-30-0	c-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	869.9	904.7	-7.9	S(C <sub>3</sub> H <sub>5</sub> CH <sub>3</sub> )-S(C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> )
[C <sub>3</sub> H <sub>7</sub> N]	503-29-7	Azetidine	908.6	943.4	-7.8	(CH <sub>3</sub> ) <sub>2</sub> NH+Rln(1/2)
[C <sub>3</sub> H <sub>7</sub> N]	1072-44-2	N-Methylaziridine	904.1	934.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>3</sub> H <sub>7</sub> N]	75-55-8	2-Methylaziridine	892.1	925.1	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>3</sub> H <sub>7</sub> N]	107-11-9	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	875.5	909.5	-5.1	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>7</sub> N]	38697-07-3	(CH <sub>3</sub> ) <sub>2</sub> C=NH	<b>898.2</b>	932.3	-5.8	Rln(1/2)
[C <sub>3</sub> H <sub>7</sub> N]	4427-28-5	CH <sub>2</sub> =C(CH <sub>3</sub> )NH <sub>2</sub>	909.3	941.8	0	Rln(1/1)
[C <sub>3</sub> H <sub>7</sub> NO]	68-12-2	(CH <sub>3</sub> ) <sub>2</sub> NCHO	856.6	887.5	5	amides
[C <sub>3</sub> H <sub>7</sub> NO]	79-05-0	C <sub>2</sub> H <sub>5</sub> CONH <sub>2</sub>	845.3	876.2	5	amides
[C <sub>3</sub> H <sub>7</sub> NO]	79-16-3	Acetamide, N-methyl	857.6	888.5	5	amides
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	56-41-7	L-alanine	867.7	901.6	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	5806-90-6	Acetamide, N-methoxy	848.0	879.0	5	amides
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	541-42-4	i-C <sub>3</sub> H <sub>7</sub> ONO	<b>813.0</b>	845.5	0	Rln(1/1)
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	107-97-1	Sarcosine	888.7	921.2	0	Rln(1/1)
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	13115-24-7	Acetamide, N-hydroxy-N-methyl	845.3	876.2	5	amides
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S]	52-90-4	L-Cysteine	869.3	903.2	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> ]	56-45-1	L-Serine	880.7	914.6	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>7</sub> NS]	758-16-7	(CH <sub>3</sub> ) <sub>2</sub> NC(=S)H	875.5	906.4	5	amides
[C <sub>3</sub> H <sub>7</sub> O]	31594-81-7	•CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH	703.5	736	0	89HOL/LOS
[C <sub>3</sub> H <sub>7</sub> O <sub>3</sub> P]	3741-36-4	2-Methoxy-1,3,2-dioxaphospholane	862.7	895.1	0	Rln(1/1)
[C <sub>3</sub> H <sub>8</sub> ]	74-98-6	C <sub>3</sub> H <sub>8</sub>	607.8	625.7	49	75HIR/KEB
[C <sub>3</sub> H <sub>8</sub> FN]	462-41-9	FCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	886.9	920.9	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>8</sub> Ge]	82064-99-1	(CH <sub>3</sub> ) <sub>2</sub> Ge=CH <sub>2</sub>	822.2	851.1	12	propene
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O]	96-31-1	OC(NHCH <sub>3</sub> ) <sub>2</sub>	873.5	903.3	9	sym ketones
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S]	534-13-4	SC(NHCH <sub>3</sub> ) <sub>2</sub>	895.1	926.0	5	amides
[C <sub>3</sub> H <sub>8</sub> O]	67-63-0	i-C <sub>3</sub> H <sub>7</sub> OH	762.6	793.0	7	CH <sub>3</sub> OH
[C <sub>3</sub> H <sub>8</sub> O]	71-23-8	n-C <sub>3</sub> H <sub>7</sub> OH	756.1	786.5	7	CH <sub>3</sub> OH
[C <sub>3</sub> H <sub>8</sub> O]	540-67-0	CH <sub>3</sub> OC <sub>2</sub> H <sub>5</sub>	781.2	808.6	17	unsym ethers
[C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ]	109-86-4	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OH	729.8	768.8	-22	1,2-diaminoethane
[C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ]	504-63-2	HO(CH <sub>2</sub> ) <sub>3</sub> OH	825.9	876.2	-60	95CHE/STO
[C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> ]	56-81-5	HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> OH	820	874.8	-75	80MAU/HAM
[C <sub>3</sub> H <sub>8</sub> Pb]	82065-01-8	(CH <sub>3</sub> ) <sub>2</sub> Pb=CH <sub>2</sub>	911.5	938.0	20	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>
[C <sub>3</sub> H <sub>8</sub> S]	75-33-2	i-C <sub>3</sub> H <sub>7</sub> SH	772.3	803.6	4	CH <sub>3</sub> SH
[C <sub>3</sub> H <sub>8</sub> S]	107-03-9	n-C <sub>3</sub> H <sub>7</sub> SH	763.6	794.9	4	CH <sub>3</sub> SH
[C <sub>3</sub> H <sub>8</sub> S]	624-89-5	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub>	815.3	846.5	4	unsym sulfides
[C <sub>3</sub> H <sub>8</sub> Si]	4112-23-6	(CH <sub>3</sub> ) <sub>2</sub> Si=CH <sub>2</sub>	921.0	947.5	20	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>3</sub> H <sub>8</sub> Sn]	82065-00-7	(CH <sub>3</sub> ) <sub>2</sub> Sn=CH <sub>2</sub>	867.1	893.6	20	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>
[C <sub>3</sub> H <sub>9</sub> As]	593-88-4	(CH <sub>3</sub> ) <sub>3</sub> As	864.9	897.3	0	Rln(3/3)
[C <sub>3</sub> H <sub>9</sub> B <sub>3</sub> O]	121-43-7	B(OCH <sub>3</sub> ) <sub>3</sub>	<b>783.4</b>	815.8	0	Rln(1/1)
[C <sub>3</sub> H <sub>9</sub> N]	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	918.1	948.9	5.6	97EAS/SMI
[C <sub>3</sub> H <sub>9</sub> N]	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	883.9	917.8	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>9</sub> N]	624-78-2	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NH	909.2	942.2	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>3</sub> H <sub>9</sub> N]	75-31-0	i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	889.0	923.8	-8	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>9</sub> NO]	156-87-6	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> OH	917.3	962.5	-43	80MAU/HAM
[C <sub>3</sub> H <sub>9</sub> NO]	109-85-3	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	894.6	928.6	-5.1	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>3</sub> H <sub>9</sub> NO]	1184-78-7	(CH <sub>3</sub> ) <sub>3</sub> NO	953.5	983.2	9.1	Rln(3/1)
[C <sub>3</sub> H <sub>9</sub> OP]	676-96-0	OP(CH <sub>3</sub> ) <sub>3</sub>	880.0	909.7	9.1	Rln(3/1)
[C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> P]	121-45-9	P(OCH <sub>3</sub> ) <sub>3</sub>	899.9	929.7	9.1	Rln(3/1)
[C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> PS]	152-18-1	SP(OCH <sub>3</sub> ) <sub>3</sub>	853.9	883.6	9.1	Rln(3/1)
[C <sub>3</sub> H <sub>9</sub> O <sub>4</sub> P]	512-56-1	OP(OCH <sub>3</sub> ) <sub>3</sub>	860.8	890.6	9.1	Rln(3/1)
[C <sub>3</sub> H <sub>9</sub> P]	594-09-2	(CH <sub>3</sub> ) <sub>3</sub> P	926.3	958.8	0	Rln(3/3)
[C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ]	109-76-2	1,3-Diaminopropane	940.0	987.0	-49	80MAU/HAM
[C <sub>3</sub> H <sub>10</sub> OSi]	1066-40-6	Silanol, trimethyl	<b>781.5</b>	814.0	0	Rln(1/1)
[C <sub>3</sub> O]	11127-17-6	CCCO	847.7	880.2	0	Rln(1/1)
[C <sub>3</sub> S]	109545-35-9	C <sub>3</sub> S	900.5	933	0	Rln(1/1)
[C <sub>4</sub> F <sub>7</sub> N]	375-00-8	C <sub>3</sub> F <sub>7</sub> CN	662.6	693.2	6	nitriles
[C <sub>4</sub> HF <sub>9</sub> O]	2378-02-1	(CF <sub>3</sub> ) <sub>3</sub> COH	646.7	676.8	8	CH <sub>3</sub> OH
[C <sub>4</sub> H <sub>2</sub> ]	460-12-8	HCC-CCH	712.8	737.2	27	AUE
[C <sub>4</sub> H <sub>2</sub> F <sub>9</sub> N]	2809-92-9	(CF <sub>3</sub> ) <sub>3</sub> CNH <sub>2</sub>	752.9	783.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>3</sub> NO]	145355-49-3	CH <sub>3</sub> NCCCO	887.5	920	0	?
[C <sub>4</sub> H <sub>3</sub> NO]	57681-10-4	NCC(CH <sub>3</sub> )CO	765.5	798	0	Rln(1/1)
[C <sub>4</sub> H <sub>4</sub> F <sub>4</sub> O <sub>2</sub> ]	1683-88-1	CF <sub>3</sub> COOCH <sub>2</sub> CH <sub>2</sub> F	704.7	735.7	5	acids
[C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> O]	333-36-8	(CF <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> O	674.9	702.3	17	sym ethers
[C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> O]	1515-14-6	(CF <sub>3</sub> ) <sub>2</sub> C(CH <sub>3</sub> )OH	660.9	691.2	7	CH <sub>3</sub> OH
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ]	290-37-9	Pyrazine	847.0	877.1	7.8	pyridines+Rln(4/2)
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ]	289-80-5	Pyridazine	877.1	907.2	7.8	pyridines+Rln(2/1)
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ]	289-95-2	Pyrimidine	855.7	885.8	7.8	pyridines+Rln(2/1)
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O]	557-01-7	2(1H)-Pyrimidinone	<b>841.7</b>	872.7	5	amides
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	66-22-8	Uracil	<b>841.7</b>	872.7	5	amides
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub> ]	2001-93-6	Dithiouracil	<b>880.5</b>	911.4	5	amides
[C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub> ]	32683-48-0	1-methyl-3,5-dinitroimidazole	757.0	788.8	2	pyridines
[C <sub>4</sub> H <sub>4</sub> O]	110-00-9	Furan	770.9	803.4	0	Rln(1/1)
[C <sub>4</sub> H <sub>4</sub> S]	110-02-1	Thiophene	784.3	815.0	5.8	Rln(2/1)
[C <sub>4</sub> H <sub>4</sub> Cl <sub>3</sub> O <sub>2</sub> ]	515-84-4	CCl <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	759.4	790.4	5	esters
[C <sub>4</sub> H <sub>4</sub> F <sub>3</sub> O <sub>2</sub> ]	383-63-1	CF <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	727.9	758.8	5	esters
[C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> N]	407-01-2	(CF <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> NH	805.1	838.1	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>5</sub> N]	5500-21-0	c-C <sub>3</sub> H <sub>5</sub> CN	777.5	808.2	6	nitriles
[C <sub>4</sub> H <sub>5</sub> N]	109-97-7	pyrrole	843.8	875.4	2.8	97EAS/SMI
[C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> ]	623-49-4	NCCOOC <sub>2</sub> H <sub>5</sub>	714.7	745.7	5	acids
[C <sub>4</sub> H <sub>5</sub> NS]	3581-87-1	2-Methylthiazole	898.7	930.6	2	pyridines
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O]	71-30-7	Cytosine	918	949.9	2	pyridines
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ]	54210-33-2	1-methyl-5-nitroimidazole	818.4	850.3	2	pyridines
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ]	54210-32-1	1-methyl-3-nitroimidazole	815.7	847.6	2	pyridines
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ]	3034-42-2	1-Methyl-5-nitroimidazole	863.5	895.3	2	pyridines
[C <sub>4</sub> H <sub>6</sub> ]	590-19-2	CH <sub>2</sub> =C=CHCH <sub>3</sub>	<b>749.8</b>	778.9	11	AUE
[C <sub>4</sub> H <sub>6</sub> ]	822-35-5	Cyclobutene	753.6	784.4	5.8	Rln(2/1)
[C <sub>4</sub> H <sub>6</sub> ]	3100-04-7	1-Methylcyclopropene	826.9	856.0	11	?
[C <sub>4</sub> H <sub>6</sub> ]	503-17-3	CH <sub>3</sub> -CC-CH <sub>3</sub>	745.1	775.8	5.8	Rln(2/1)
[C <sub>4</sub> H <sub>6</sub> ]	106-99-0	CH <sub>2</sub> =CHCH=CH <sub>2</sub>	757.6	783.4	22	propene+Rln(2/1)
[C <sub>4</sub> H <sub>6</sub> F <sub>3</sub> NO]	1547-87-1	CF <sub>3</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	818.0	849.0	5	amides
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	7554-65-6	4-methylpyrazole	873.4	906.8	-3	pyridines+Rln(1/2)
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	822-36-6	4-Methylimidazole	920.9	952.8	2	pyridines
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	693-98-1	2-Methylimidazole	929.6	963.4	-4	pyridines+Rln(1/2)
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	616-47-7	1-methylimidazole	927.7	959.6	2	pyridines
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	930-36-9	1-methylpyrazole	880.1	912.0	2	pyridines
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	1453-58-3	3(5)-methylpyrazole	874.2	906.0	2	pyridines
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O]	16703-51-8	(CH <sub>3</sub> ) <sub>2</sub> NCOCN	797.1	829.0	2	unsym ketones
[C <sub>4</sub> H <sub>6</sub> O]	78-85-3	CH <sub>2</sub> =C(CH <sub>3</sub> )CHO	776.8	808.7	2	CH <sub>3</sub> CHO
[C <sub>4</sub> H <sub>6</sub> O]	4170-30-3	CH <sub>3</sub> CH=CHCHO	799.0	830.8	2	CH <sub>3</sub> CHO

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>4</sub> H <sub>8</sub> O]	1708-29-8	2,5-Dihydrofuran	796	823.4	17	sym ethers
[C <sub>4</sub> H <sub>6</sub> O]	78-94-4	CH <sub>2</sub> =CHCOCH <sub>3</sub>	802.8	834.7	2	unsym ketones
[C <sub>4</sub> H <sub>6</sub> O]	1191-95-3	cyclobutanone	772.7	802.5	9	sym ketones
[C <sub>4</sub> H <sub>8</sub> O]	1191-99-7	2,3-Dihydrofuran	834.4	866.9	0	Rln(1/1)
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	79-41-4	CH <sub>3</sub> C(=CH <sub>2</sub> )COOH	785.7	816.7	5	acids
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	431-03-8	CH <sub>3</sub> COCOCH <sub>3</sub>	770.1	801.9	2	unsym ketones
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	96-48-0	$\gamma$ -Butyrolactone	808.1	840.0	2	unsym ketones
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	108-05-4	CH <sub>3</sub> COOCH=CH <sub>2</sub>	782.9	813.9	5	esters
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	96-33-3	CH <sub>2</sub> =CHCOOCH <sub>3</sub>	794.8	825.8	5	esters
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	543-75-9	Dihydro-1,4-dioxin	792.8	823.5	5.8	Rln(2/1)
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	1759-53-1	Cyclopropane carboxylic acid	790.4	821.4	5	acids
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	107-93-7	(E)-CH <sub>3</sub> CH=CHCOOH	793	824.0	5	acids
[C <sub>4</sub> H <sub>7</sub> ]	15157-95-6	CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> •	747.3	778	6	S(i-C <sub>4</sub> H <sub>8</sub> ) + spin-S(C <sub>4</sub> H <sub>7</sub> •)
[C <sub>4</sub> H <sub>7</sub> ]	#1452	CH <sub>3</sub> CH=CHCH <sub>2</sub> •	754.4	785.1	6	S(2-C <sub>4</sub> H <sub>8</sub> ) + spin-S(C <sub>4</sub> H <sub>7</sub> •)
[C <sub>4</sub> H <sub>7</sub> F <sub>2</sub> NO]	667-50-5	CF <sub>2</sub> HCON(CH <sub>3</sub> ) <sub>2</sub>	833.1	864.1	5	amides
[C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> O]	461-24-5	C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CF <sub>3</sub>	735.0	762.4	17	(CH <sub>3</sub> ) <sub>2</sub> O
[C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> S]	5187-62-2	CF <sub>3</sub> CH <sub>2</sub> SC <sub>2</sub> H <sub>5</sub>	766.4	797.6	4	unsym sulfides
[C <sub>4</sub> H <sub>7</sub> N]	109-74-0	n-C <sub>3</sub> H <sub>7</sub> CN	767.7	798.4	6	nitriles
[C <sub>4</sub> H <sub>7</sub> N]	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	772.8	803.6	5.7	S(i-PrCCH)-S(i-PrCN)
[C <sub>4</sub> H <sub>7</sub> N]	627-36-1	i-C <sub>3</sub> H <sub>7</sub> NC	824.3	856.8	0	HNC
[C <sub>4</sub> H <sub>7</sub> NO]	79-39-0	2-propenamide, 2-methyl-	849.4	880.4	5	amides
[C <sub>4</sub> H <sub>7</sub> NO]	23350-58-5	2-butenamide	856.1	887.1	5	amides
[C <sub>4</sub> H <sub>7</sub> NO]	2679-13-2	N-methyl-2-azetidinone	851.3	882.2	5	amides
[C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub> ]	56-84-8	L-aspartic acid	875	908.9	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> ]	1192-21-8	1-methyl-5-aminopyrazole	917.6	949.5	2	pyridines
[C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> ]	1904-31-0	1-methyl-3-aminopyrazole	905.5	937.4	2	pyridines
[C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> ]	39687-97-3	N'-cyano-N,N-dimethyl formamidine	857.3	889.7	0	Rln(1/1)
[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ]	4598-47-4	1,4-Dioxyl radical	770.7	803.2	0	Rln(1/1)
[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> P]	61580-09-4	4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.1]heptane	791.5	823.9	0	?
[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> P]	280-45-5	2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane	836.4	868.8	0	Rln(3/3)
[C <sub>4</sub> H <sub>8</sub> ]	624-64-6	E-CH <sub>3</sub> CH=CHCH <sub>3</sub>	719.9	747	18	propene + Rln(2/1)
[C <sub>4</sub> H <sub>8</sub> ]	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	775.6	802.1	20	97EAS/SMI
[C <sub>4</sub> H <sub>8</sub> Cl <sub>3</sub> N]	36726-94-0	CCl <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	882.0	912.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>8</sub> F <sub>3</sub> N]	819-46-5	CF <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	869.6	903.5	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>8</sub> F <sub>3</sub> N]	819-06-7	CF <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	871.9	902.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> ]	926-64-7	NCCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	853.7	884.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> ]	1606-49-1	1,4,5,6-tetrahydropyrimidine	967.8	1002.0	-5.8	Rln(1/2)
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> ]	70-47-3	L-Asparagine	891.5	929	-17	80MAU/HAM
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> ]	556-50-3	diglycine	882	NE	NE	not estimated
[C <sub>4</sub> H <sub>8</sub> O]	109-92-2	C <sub>2</sub> H <sub>5</sub> OCH=CH <sub>2</sub>	840.4	870.1	9.5	91MAU/SIE
[C <sub>4</sub> H <sub>8</sub> O]	109-99-9	Tetrahydrofuran	794.7	822.1	17	sym ethers
[C <sub>4</sub> H <sub>8</sub> O]	78-84-2	i-C <sub>3</sub> H <sub>7</sub> CHO	765.5	797.3	2	CH <sub>3</sub> CHO
[C <sub>4</sub> H <sub>8</sub> O]	78-93-3	CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>	795.5	827.3	2	unsym ketones
[C <sub>4</sub> H <sub>8</sub> O]	116-11-0	CH <sub>2</sub> =C(CH <sub>3</sub> )OCH <sub>3</sub>	866.1	894.9	12	propene
[C <sub>4</sub> H <sub>8</sub> O]	123-72-8	n-C <sub>3</sub> H <sub>7</sub> CHO	760.8	792.7	2	CH <sub>3</sub> CHO
[C <sub>4</sub> H <sub>8</sub> OS]	926-67-0	CH <sub>3</sub> C(S)OC <sub>2</sub> H <sub>5</sub>	831.8	863.6	2	unsym ketones
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	625-55-8	HCOOCH(CH <sub>3</sub> ) <sub>2</sub>	780.3	811.3	5	esters
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	123-91-1	1,4-Dioxane	770.0	797.4	17	sym ethers
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	505-22-6	1,3-Dioxane	796.2	825.4	11	unsym ethers
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	804.7	835.7	5	esters
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	110-74-7	HCO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )	773.9	804.9	5	esters
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	554-12-1	C <sub>2</sub> H <sub>5</sub> COOCH <sub>3</sub>	799.2	830.2	5	esters
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ]	922-69-0	CH <sub>2</sub> =C(OCH <sub>3</sub> ) <sub>2</sub>	928.1	957.0	12	propene
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S]	38103-96-7	C <sub>2</sub> H <sub>5</sub> S(OCH <sub>3</sub> )CO	802.9	833.9	5	esters
[C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> ]	623-53-0	C <sub>2</sub> H <sub>5</sub> OCOOCCH <sub>3</sub>	810.8	842.7	2	unsym ketones
[C <sub>4</sub> H <sub>8</sub> S]	110-01-0	c-C <sub>4</sub> H <sub>8</sub> S	819.3	849.1	9	sym sulfides
[C <sub>4</sub> H <sub>8</sub> S]	7594-44-7	CH <sub>2</sub> =C(CH <sub>3</sub> )-SCH <sub>3</sub>	859.7	888.6	12	propene
[C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> ]	51102-74-0	CH <sub>2</sub> =C(SCH <sub>3</sub> ) <sub>2</sub>	902.2	931.1	12	propene
[C <sub>4</sub> H <sub>8</sub> Se]	114659-08-4	CH <sub>2</sub> =C(CH <sub>3</sub> )-SeCH <sub>3</sub>	850.5	879.4	12	propene
[C <sub>4</sub> H <sub>8</sub> Se <sub>2</sub> ]	99030-02-1	CH <sub>2</sub> =C(SeCH <sub>3</sub> ) <sub>2</sub>	892.6	921.5	12	propene
[C <sub>4</sub> H <sub>9</sub> N]	1190-79-0	CH <sub>3</sub> CH=NC <sub>2</sub> H <sub>5</sub>	909.4	941.9	0	Rln(1/1)
[C <sub>4</sub> H <sub>9</sub> N]	123-75-1	Pyrrolidine	915.3	948.3	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>9</sub> N]	5763-87-1	(CH <sub>3</sub> ) <sub>2</sub> NCH=CH <sub>2</sub>	924.4	956.8	0	Rln(1/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>4</sub> H <sub>9</sub> N]	2878-14-0	CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> NH <sub>2</sub>	883.5	917.5	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>9</sub> N]	4923-79-9	Azetidine, N-methyl-	851.7	882.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>9</sub> NO]	110-91-8	Morpholine	891.2	924.3	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>9</sub> NO]	1187-58-2	C <sub>2</sub> H <sub>5</sub> CONHCH <sub>3</sub>	889.4	920.4	5	amides
[C <sub>4</sub> H <sub>9</sub> NO]	563-83-7	i-C <sub>3</sub> H <sub>7</sub> CONH <sub>2</sub>	846.7	878.6	2	amides
[C <sub>4</sub> H <sub>9</sub> NO]	625-50-3	Acetamide, N-ethyl-	867.0	898.0	5	amides
[C <sub>4</sub> H <sub>9</sub> NO]	127-19-5	Dimethylacetamide	877.0	908.0	5	amides
[C <sub>4</sub> H <sub>9</sub> NO]	6281-94-3	n-C <sub>3</sub> H <sub>7</sub> NHCHO	847.4	878.4	5	amides
[C <sub>4</sub> H <sub>9</sub> NOS]	16703-45-0	CH <sub>3</sub> OC(S)N(CH <sub>3</sub> ) <sub>2</sub>	869.0	900.0	5	amides
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	105-40-8	CH <sub>3</sub> NHCOOC <sub>2</sub> H <sub>5</sub>	857.8	888.8	5	esters
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	7541-16-4	(CH <sub>3</sub> ) <sub>2</sub> NCOOCH <sub>3</sub>	847.3	878.3	5	esters
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	540-80-7	t-C <sub>4</sub> H <sub>9</sub> ONO	<b>831.4</b>	863.9	0	CH <sub>3</sub> ONO
[C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> ]	72-19-5	L-threonine	888.5	922.5	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>9</sub> NS]	631-67-4	CH <sub>3</sub> C(S)N(CH <sub>3</sub> ) <sub>2</sub>	894.4	925.3	5	amides
[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> P]	31121-06-9	2-Methoxy-1,3,2-dioxaphosphorinane	892.8	925.3	0	Rln(1/1)
[C <sub>4</sub> H <sub>10</sub> ]	75-28-5	iso-C <sub>4</sub> H <sub>10</sub>	671.3	677.8	87	76HIR/KEB
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	110-85-0	Piperazine	914.7	943.7	11.5	Rln(4/1)
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	1609-01-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>3</sub>	970.0	1002.5	0	Rln(1/1)
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	4901-75-1	c-C(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NHNH	871.3	903.8	0	Rln(1/1)
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	110-70-3	CH <sub>3</sub> NHCH <sub>2</sub> CH <sub>2</sub> NHCH <sub>3</sub>	946.9	989.2	-33	80MAU/HAM
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O]	139033-03-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-OCH <sub>3</sub>	915.8	948.3	0	Rln(1/1)
[C <sub>4</sub> H <sub>10</sub> O]	78-92-2	CH <sub>3</sub> CH <sub>2</sub> CH(OH)CH <sub>3</sub>	784.6	815	7	CH <sub>3</sub> OH
[C <sub>4</sub> H <sub>10</sub> O]	71-36-3	n-C <sub>4</sub> H <sub>9</sub> OH	758.9	789.2	7	CH <sub>3</sub> OH
[C <sub>4</sub> H <sub>10</sub> O]	78-83-1	i-C <sub>4</sub> H <sub>9</sub> OH	762.2	793.7	3	S(i-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> )-S(i-
[C <sub>4</sub> H <sub>10</sub> O]	75-65-0	t-C <sub>4</sub> H <sub>9</sub> OH	772.2	802.6	7	CH <sub>3</sub> OH
[C <sub>4</sub> H <sub>10</sub> O]	598-53-8	(CH <sub>3</sub> ) <sub>2</sub> CHOCH <sub>3</sub>	797.1	826.3	11	unsym ethers
[C <sub>4</sub> H <sub>10</sub> O]	557-17-5	n-C <sub>3</sub> H <sub>7</sub> OCH <sub>3</sub>	785.7	814.9	11	unsym ethers
[C <sub>4</sub> H <sub>10</sub> O]	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	801	828.4	17	sym ethers
[C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ]	110-71-4	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OCH <sub>3</sub>	820.2	858.0	-18	84SHA/BLA; 83MAU
[C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ]	110-63-4	HO(CH <sub>2</sub> ) <sub>4</sub> OH	854.9	915.6	-95	80MAU/HAM
[C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> ]	3068-00-6	HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> CH <sub>2</sub> OH	841	905.9	-109	86SUN/KUL
[C <sub>4</sub> H <sub>10</sub> S]	513-53-1	CH <sub>3</sub> CH <sub>2</sub> CH(SH)CH <sub>3</sub>	781.7	813	4	unsym sulfides
[C <sub>4</sub> H <sub>10</sub> S]	109-79-5	n-C <sub>4</sub> H <sub>9</sub> SH	770.5	801.7	4	CH <sub>3</sub> SH
[C <sub>4</sub> H <sub>10</sub> S]	352-93-2	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S	827.0	856.7	9	sym sulfides
[C <sub>4</sub> H <sub>10</sub> S]	75-66-1	t-C <sub>4</sub> H <sub>9</sub> SH	785.1	816.4	4	CH <sub>3</sub> SH
[C <sub>4</sub> H <sub>10</sub> S]	513-44-0	i-C <sub>4</sub> H <sub>9</sub> SH	771.4	802.6	4	CH <sub>3</sub> SH
[C <sub>4</sub> H <sub>11</sub> N]	4747-21-1	CH <sub>3</sub> NH(i-C <sub>3</sub> H <sub>7</sub> )	919.4	952.4	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>11</sub> N]	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	886.6	921.5	-8	S(C <sub>5</sub> H <sub>12</sub> )-S(n-BuNH <sub>2</sub> )+Rln2
[C <sub>4</sub> H <sub>11</sub> N]	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	899.9	934.1	-6	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>11</sub> N]	13952-84-6	sec-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	895.7	929.7	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>11</sub> N]	598-56-1	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	929.1	960.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>4</sub> H <sub>11</sub> N]	78-81-9	i-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	890.8	924.8	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>4</sub> H <sub>11</sub> N]	109-89-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	919.4	952.4	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>11</sub> NO]	13325-10-5	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>4</sub> OH	932.1	984.5	-67	80MAU/HAM
[C <sub>4</sub> H <sub>11</sub> NO]	3710-84-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NOH	882.2	914.7	0	Rln(1/1)
[C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub> ]	111-42-2	(HOCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NH	920	953	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>4</sub> H <sub>12</sub> NOP]	50663-05-3	OP(N(CH <sub>3</sub> ) <sub>2</sub> )(CH <sub>3</sub> ) <sub>2</sub>	903.0	935.5	0	Rln(1/1)
[C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ]	6415-12-9	(CH <sub>3</sub> ) <sub>2</sub> NN(CH <sub>3</sub> ) <sub>2</sub>	917.9	948.7	5.8	Rln(2/1)
[C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ]	110-60-1	1,4-butanediamine	954.3	1005.6	-63	93CHE/WU; 80MAU/HAM
[C <sub>4</sub> H <sub>12</sub> OSi]	1825-61-2	(CH <sub>3</sub> ) <sub>3</sub> SiOCH <sub>3</sub>	<b>814.6</b>	847.0	0	Rln(1/1)
[C <sub>4</sub> H <sub>12</sub> Sn]	594-27-4	(CH <sub>3</sub> ) <sub>4</sub> Sn	<b>797.4</b>	823.7	20.6	Rln(12/1)
[C <sub>4</sub> H <sub>14</sub> N <sub>3</sub> OP]	3732-86-3	OP(NH <sub>2</sub> )(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>	915.0	947.5	0	Rln(1/1)
[C <sub>4</sub> H <sub>14</sub> OSi <sub>2</sub> ]	3277-26-7	((CH <sub>3</sub> ) <sub>2</sub> SiH) <sub>2</sub> O	<b>814.6</b>	845.3	5.8	Rln(2/1)
[C <sub>4</sub> NiO <sub>4</sub> ]	13463-39-3	(CO) <sub>4</sub> Ni	716.0	742.3	20.6	Rln(12/1)
[C <sub>5</sub> F <sub>5</sub> N]	700-16-3	Pentafluoropyridine	733.0	764.9	2	pyridines
[C <sub>5</sub> FeO <sub>5</sub> ]	13463-40-6	(CO) <sub>5</sub> Fe	798.5	833.0	-7	91ALL/CRA
[C <sub>5</sub> HMnO <sub>5</sub> ]	16972-33-1	(CO) <sub>5</sub> MnH	803.0	835.5	0	?
[C <sub>5</sub> H <sub>3</sub> ClN <sub>4</sub> ]	87-42-3	6-Chloropurine	<b>841.7</b>	873.6	2	pyridines
[C <sub>5</sub> H <sub>4</sub> BrN]	626-55-1	3-Br-pyridine	878.2	910.0	2	pyridines
[C <sub>5</sub> H <sub>4</sub> BrN]	109-04-6	2-Br-pyridine	873.0	904.8	2	pyridines
[C <sub>5</sub> H <sub>4</sub> BrN]	1120-87-2	4-Br-pyridine	886.0	917.8	2	pyridines
[C <sub>5</sub> H <sub>4</sub> ClN]	109-09-1	2-Cl-pyridine	869	900.9	2	pyridines
[C <sub>5</sub> H <sub>4</sub> ClN]	626-61-9	4-Cl-pyridine	884.2	916.1	2	pyridines



TABLE I. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>5</sub> H <sub>4</sub> ClN]	626-60-8	3-Cl-pyridine	871.5	903.4	2	pyridines
[C <sub>5</sub> H <sub>4</sub> ClNO]	1851-22-5	3-chloro-pyridine-1-oxide	869.7	902.2	0	Rln(1/1)
[C <sub>5</sub> H <sub>4</sub> FN]	372-47-4	3-F-pyridine	870.1	902.0	2	pyridines
[C <sub>5</sub> H <sub>4</sub> FN]	372-48-5	2-F-pyridine	852.7	884.6	2	pyridines
[C <sub>5</sub> H <sub>4</sub> FN]	694-52-0	4-F-pyridine	881.2	913.1	2	pyridines
[C <sub>5</sub> H <sub>4</sub> FNO]	695-37-4	3-fluoro-pyridine-1-oxide	867.6	900.1	0	Rln(1/1)
[C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> ]	1124-33-0	4-(NO <sub>2</sub> )-pyridine-1-oxide	837.3	868.0	5.8	Rln(2/1)
[C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> ]	120-73-0	Purine	888.2	920.1	2	pyridines
[C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O]	68-94-0	Hypoxanthine	880.5	912.3	2	pyridines
[C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	1122-61-8	4-(NO <sub>2</sub> )-pyridine	842.5	874.3	2	pyridines
[C <sub>5</sub> H <sub>5</sub> ]	2143-53-5	c-C <sub>5</sub> H <sub>5</sub> radical	799.1	831.5	0	Rln(2/2)
[C <sub>5</sub> H <sub>5</sub> As]	289-31-6	Arsabenzene	752.4	784.8	0	Rln(2/2)
[C <sub>5</sub> H <sub>5</sub> N]	110-86-1	pyridine	898.1	930	2	pyridines
[C <sub>5</sub> H <sub>5</sub> NNiO]	12071-73-7	(C <sub>5</sub> H <sub>5</sub> )NiNO	798.6	827.0	13.4	Rln(5/1)
[C <sub>5</sub> H <sub>5</sub> NO]	694-59-7	pyridine-1-oxide	892.9	923.6	5.8	Rln(2/1)
[C <sub>5</sub> H <sub>5</sub> NO]	109-00-2	3-(OH)-pyridine	897.7	929.5	2	pyridines
[C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> ]	73-24-5	Adenine	912.5	942.8	7	79MAU
[C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O]	73-40-5	Guanine	927.6	959.5	2	pyridines
[C <sub>5</sub> H <sub>5</sub> P]	289-68-9	Phosphabenzene	785.3	817.7	0	Rln(2/2)
[C <sub>5</sub> H <sub>6</sub> ]	542-92-7	1,3-c-C <sub>5</sub> H <sub>6</sub>	798.4	821.6	31	AUE
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ]	504-29-0	2-Pyridinamine	915.3	947.2	2	pyridines
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ]	462-08-8	3-Pyridinamine	922.6	954.4	2	pyridines
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ]	504-24-5	4-Pyridinamine	947.8	979.7	2	pyridines
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ]	65-71-4	Thymine	850.0	880.9	5	amides
[C <sub>5</sub> H <sub>6</sub> O]	534-22-5	2-methylfuran	833.5	865.9	0	Rln(1/1)
[C <sub>5</sub> H <sub>6</sub> O]	930-27-8	3-methylfuran	821.5	854.0	0	Rln(1/1)
[C <sub>5</sub> H <sub>6</sub> S]	554-14-3	2-Methylthiophene	826.5	859.0	0	Rln(1/1)
[C <sub>5</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ]	352-23-8	CF <sub>3</sub> CH <sub>2</sub> COOC <sub>2</sub> H <sub>5</sub>	766.3	797.3	5	esters
[C <sub>5</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ]	383-66-4	CF <sub>3</sub> CO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )	732.9	763.9	5	esters
[C <sub>5</sub> H <sub>7</sub> O]	#1169	•CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CO	806.2	838.6	0	?
[C <sub>5</sub> H <sub>8</sub> ]	598-23-2	(CH <sub>3</sub> ) <sub>2</sub> CHCCH	787.8	814.9	18	AUE
[C <sub>5</sub> H <sub>8</sub> ]	627-21-4	C <sub>2</sub> H <sub>5</sub> CCCH <sub>3</sub>	778.0	810.2	1	2-butyne
[C <sub>5</sub> H <sub>8</sub> ]	693-86-7	c-C <sub>3</sub> H <sub>5</sub> CH=CH <sub>2</sub>	787.5	816.3	12	propene
[C <sub>5</sub> H <sub>8</sub> ]	3907-06-0	3,3-Dimethylcyclopropene	817.1	847.8	5.8	?
[C <sub>5</sub> H <sub>8</sub> ]	2004-70-8	(E)CH <sub>3</sub> CH=CHCH=CH <sub>2</sub>	804.4	834.1	9.1	AUE
[C <sub>5</sub> H <sub>8</sub> ]	1489-60-7	1-Methylcyclobutene	807.3	841.5	-5.8	Rln(1/2)
[C <sub>5</sub> H <sub>8</sub> ]	142-29-0	c-C <sub>5</sub> H <sub>8</sub>	733.8	766.3	0	Rln(2/2)
[C <sub>5</sub> H <sub>8</sub> ]	78-79-5	CH <sub>2</sub> =CHC(CH <sub>3</sub> )=CH <sub>2</sub>	797.6	826.4	12	propene
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	694-31-5	1,5-Dimethylpyrazole	902.8	934.3	3	pyrazole(pyrrrole)
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	35520-41-3	trans-dimethylamino acrylonitrile	864.3	896.8	0	Rln(1/1)
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	6338-45-0	1,4-Dimethylimidazole	944.9	976.7	2	pyridines
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	1739-84-0	1,2-Dimethylimidazole	952.6	984.7	2	pyridines
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	694-48-4	1,3-Dimethylpyrazole	902.3	933.9	3	pyrazole(pyrrrole)
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	10447-93-5	1,5-Dimethylimidazole	945.8	977.6	2	pyridines
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	1072-68-0	1,4-Dimethylpyrazole	896.8	928.4	3	pyrazole
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	67-51-6	3,5-dimethylpyrazole	900.1	933.5	-3	pyrazole-Rln2
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ]	2820-37-3	3(5),4-dimethylpyrazole	895.4	927.3	2	pyridines
[C <sub>5</sub> H <sub>8</sub> O]	107-86-8	3-methyl-2-butenal	825.0	856.9	2	unsym ketones
[C <sub>5</sub> H <sub>8</sub> O]	814-78-8	CH <sub>3</sub> C(=O)C(=CH <sub>2</sub> )CH <sub>3</sub>	811.3	843.1	2	unsym ketones
[C <sub>5</sub> H <sub>8</sub> O]	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	823	854.9	2	unsym ketones
[C <sub>5</sub> H <sub>8</sub> O]	110-87-2	2H-Pyran, 3, 4-dihydro-	833.4	865.8	0	Rln(1/1)
[C <sub>5</sub> H <sub>8</sub> O]	120-92-3	Cyclopentanone	794.0	823.7	9	sym ketones
[C <sub>5</sub> H <sub>8</sub> O]	625-33-2	CH <sub>3</sub> CH=CHC(=O)CH <sub>3</sub>	832.5	864.3	2	unsym ketones
[C <sub>5</sub> H <sub>8</sub> O]	6038-09-1	2-methyl-2-butenal(Z)	812.1	843.9	2	unsym ketones
[C <sub>5</sub> H <sub>8</sub> O]	34314-83-5	4-Methyl-2,3-dihydrofuran	836.2	868.6	0	?
[C <sub>5</sub> H <sub>8</sub> O]	1576-87-0	2-pentenal(E)	807.2	839.0	2	aldehydes
[C <sub>5</sub> H <sub>8</sub> O]	1487-15-6	5-Methyl-2,3-dihydrofuran	877.9	910.3	0	Rln(1/1)
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	565-63-9	(Z)CH <sub>3</sub> CH=C(CH <sub>3</sub> )COOH	791.5	822.5	5	acids
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	623-43-8	CH <sub>3</sub> CH=CHCOOCH <sub>3</sub>	820.4	851.3	5	esters
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	836.8	873.5	-14	83MAU
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	13991-37-2	(E)CH <sub>3</sub> CH <sub>2</sub> CH=CHCOOH	792.6	823.6	5	acids
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	3721-95-7	Cyclobutane carboxylic acid	786.4	817.4	5	acids
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	80-62-6	CH <sub>2</sub> =C(CH <sub>3</sub> )COOCH <sub>3</sub>	800.5	831.4	5	esters
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	811.2	842.1	5	esters

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ]	541-47-9	(CH <sub>3</sub> ) <sub>2</sub> C=CHCOOH	791.9	822.9	5	acids
[C <sub>5</sub> H <sub>9</sub> F <sub>3</sub> N]	134166-59-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> CF <sub>3</sub>	933.8	966.2	0	Rln(1/1)
[C <sub>5</sub> H <sub>9</sub> N]	110-59-8	n-C <sub>4</sub> H <sub>9</sub> CN	771.7	802.4	6	nitriles
[C <sub>5</sub> H <sub>9</sub> N]	7223-38-3	HCCCCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	909.5	940.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>9</sub> N]	630-18-2	t-C <sub>4</sub> H <sub>9</sub> CN	780.2	810.9	6	nitriles
[C <sub>5</sub> H <sub>9</sub> N]	7188-38-7	t-C <sub>4</sub> H <sub>9</sub> NC	838.3	870.7	0.1	HNC
[C <sub>5</sub> H <sub>9</sub> NO]	5264-35-7	c-C <sub>4</sub> H <sub>8</sub> N(2-OCH <sub>3</sub> )	925.5	957.9	0	Rln(1/1)
[C <sub>5</sub> H <sub>9</sub> NO]	872-50-4	1-Methyl-2-pyrrolidinone	891.6	923.5	2	unsym ketones
[C <sub>5</sub> H <sub>9</sub> NO]	2141-62-0	C <sub>2</sub> H <sub>5</sub> CH(OC <sub>2</sub> H <sub>5</sub> )CH <sub>2</sub> CN	776.5	807.2	6	nitriles
[C <sub>5</sub> H <sub>9</sub> NO]	2680-03-7	2-propenamamide, N,N-dimethyl	873.4	904.3	5	amides
[C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> ]	147-85-3	L-proline	886.0	920.5	-7	93L/HAR
[C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> ]	1117-77-7	CH <sub>3</sub> CONHCH <sub>2</sub> COOCH <sub>3</sub>	861	892.0	5	amides
[C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub> ]	56-86-0	L-GlutamicAcid	879.1	913.0	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> ]	134166-58-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> CN	915.5	948.0	0	Rln(1/1)
[C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> ]	51-45-6	Histamine	961.9	999.8	-18	histidine
[C <sub>5</sub> H <sub>9</sub> O <sub>3</sub> P]	1449-91-8	4-Methyl-2,6,7-trioxa-1-phosphabicyclo[2.2.2]octane	850.3	882.8	0	Rln(3/3)
[C <sub>5</sub> H <sub>10</sub> ]	513-35-9	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub>	779.9	808.8	12	propene
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> ]	2305-59-1	4,4-dimethyl-2-imidazoline	955.7	988.1	0	Rln(1/1)
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O]	80-73-9	1,3-Dimethyl-2-imidazolidinone	886.0	918.4	0	?
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ]	56-85-9	L-Glutamine	900	937.8	-18	Asparagine
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> ]	7361-43-5	ser-gly	886.4	NE	NE	not estimated
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> ]	687-63-8	gly-ser	880.9	NE	NE	not estimated
[C <sub>5</sub> H <sub>10</sub> O]	96-47-9	c-C <sub>4</sub> H <sub>7</sub> O(2-CH <sub>3</sub> )	811.6	840.8	11	unsym ethers
[C <sub>5</sub> H <sub>10</sub> O]	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	807	836.8	9	sym ketones
[C <sub>5</sub> H <sub>10</sub> O]	142-68-7	c-C <sub>5</sub> H <sub>10</sub> O	795.4	822.8	17	sym ethers
[C <sub>5</sub> H <sub>10</sub> O]	107-87-9	n-C <sub>3</sub> H <sub>7</sub> COCH <sub>3</sub>	800.9	832.7	2	unsym ketone
[C <sub>5</sub> H <sub>10</sub> O]	110-62-3	n-C <sub>4</sub> H <sub>9</sub> CHO	764.8	796.6	2	CH <sub>3</sub> CHO
[C <sub>5</sub> H <sub>10</sub> O]	4696-26-8	trans-CH <sub>3</sub> CH=CH-OC <sub>2</sub> H <sub>5</sub>	848.0	876.9	12	propene
[C <sub>5</sub> H <sub>10</sub> O]	563-80-4	(i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub>	804.4	836.3	2	unsym ketones
[C <sub>5</sub> H <sub>10</sub> O]	928-55-2	C <sub>2</sub> H <sub>5</sub> OCH=CHCH <sub>3</sub>	847.7	876.6	12	propene
[C <sub>5</sub> H <sub>10</sub> O]	557-31-3	C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CH=CH <sub>2</sub>	804.5	833.7	11	unsym ethers
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	5057-98-7	cis-1,2-cyclopentanediol	853.1	885.6	0	Rln(1/1)
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	623-42-7	C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub>	805.4	836.4	5	esters
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	592-84-7	HCO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )	775	806.0	5	esters
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	108-21-4	isopropyl acetate	805.6	836.6	5	esters
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	547-63-7	i-C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub>	805.7	836.6	5	esters
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	109-60-4	CH <sub>3</sub> COOC <sub>3</sub> H <sub>7</sub>	805.6	836.6	5	esters
[C <sub>5</sub> H <sub>10</sub> S]	1613-51-0	Tetrahydrothiopyran	826.0	855.8	9	sym sulfides
[C <sub>5</sub> H <sub>11</sub> N]	6163-56-0	CH <sub>3</sub> CH=CHN(CH <sub>3</sub> ) <sub>2</sub>	934.5	967.0	0	Rln(1/1)
[C <sub>5</sub> H <sub>11</sub> N]	1743-55-1	(CH <sub>3</sub> ) <sub>2</sub> C=NC <sub>2</sub> H <sub>5</sub>	943.5	976.0	0	Rln(1/1)
[C <sub>5</sub> H <sub>11</sub> N]	2155-94-4	CH <sub>2</sub> =CHCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	926.8	957.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>11</sub> N]	120-94-5	N-Methylpyrrolidine	934.8	965.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>11</sub> N]	110-89-4	Piperidine	921	954.0	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>5</sub> H <sub>11</sub> NO]	754-10-9	t-C <sub>4</sub> H <sub>9</sub> CONH <sub>2</sub>	857.2	889.0	2	amides
[C <sub>5</sub> H <sub>11</sub> NOS]	#638	C <sub>2</sub> H <sub>5</sub> OC(S)N(CH <sub>3</sub> ) <sub>2</sub>	880.0	911.0	5	amides
[C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> ]	72-18-4	L-valine	876.7	910.6	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> ]	687-48-9	(CH <sub>3</sub> ) <sub>2</sub> NCOOC <sub>2</sub> H <sub>5</sub>	865.6	896.6	5	esters
[C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> S]	63-68-3	L-Methionine	901.5	935.4	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> ]	28504-67-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NCH <sub>3</sub>	990.8	1023.2	0	Rln(1/1)
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> ]	38704-89-1	Pyrazolidine, 1,2-dimethyl	928.6	959.3	5.8	Rln(2/1)
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> ]	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	976.3	1008.7	0	Rln(1/1)
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O]	632-22-4	[(CH <sub>3</sub> ) <sub>2</sub> N] <sub>2</sub> C=O	899.6	930.6	5	amides
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S]	2782-91-4	SC[N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub>	916.6	947.6	5	amides
[C <sub>5</sub> H <sub>12</sub> O]	625-54-7	C <sub>2</sub> H <sub>5</sub> O(i-C <sub>3</sub> H <sub>7</sub> )	813.5	842.7	11	unsym ethers
[C <sub>5</sub> H <sub>12</sub> O]	1634-04-4	t-C <sub>4</sub> H <sub>9</sub> OCH <sub>3</sub>	812.4	841.6	11	unsym ethers
[C <sub>5</sub> H <sub>12</sub> O]	75-84-3	neo-C <sub>3</sub> H <sub>7</sub> OH	765.2	795.5	7	CH <sub>3</sub> OH
[C <sub>5</sub> H <sub>12</sub> O]	628-28-4	n-C <sub>4</sub> H <sub>9</sub> OCH <sub>3</sub>	791.2	820.3	11	unsym ethers
[C <sub>5</sub> H <sub>12</sub> O <sub>2</sub> ]	17081-21-9	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>3</sub> OCH <sub>3</sub>	858.6	897.2	-20.6	83MAU
[C <sub>5</sub> H <sub>12</sub> S]	1679-08-9	neo-C <sub>3</sub> H <sub>7</sub> SH	778.2	809.5	4	CH <sub>3</sub> SH
[C <sub>5</sub> H <sub>12</sub> Si]	754-05-2	(CH <sub>3</sub> ) <sub>3</sub> SiCH=CH <sub>2</sub>	804.1	833	12	propene
[C <sub>5</sub> H <sub>13</sub> N]	5813-64-9	neo-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	894.0	928.3	-6	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>5</sub> H <sub>13</sub> N]	594-39-8	t-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	903.6	937.8	-6	CH <sub>3</sub> NH <sub>2</sub>

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>5</sub> H <sub>13</sub> N]	996-35-0	(CH <sub>3</sub> ) <sub>2</sub> (i-C <sub>3</sub> H <sub>7</sub> )N	939.6	970.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>13</sub> N]	926-63-6	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	931.9	962.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>13</sub> N]	616-39-7	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N	940.0	971.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>13</sub> N]	110-58-7	n-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	889.5	923.5	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>5</sub> H <sub>13</sub> N]	19961-27-4	(C <sub>2</sub> H <sub>5</sub> )(i-C <sub>3</sub> H <sub>7</sub> )NH	926.7	960.0	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>5</sub> H <sub>13</sub> N <sub>2</sub> OP]	16606-18-1	c-P(O)CH <sub>3</sub> N(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> )	915.0	947.5	0	Rln(1/1)
[C <sub>5</sub> H <sub>13</sub> N <sub>3</sub> ]	80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	997.4	1031.6	-5.8	Rln(1/2)
[C <sub>5</sub> H <sub>13</sub> N <sub>3</sub> ]	32150-27-9	CH <sub>3</sub> C(N(CH <sub>3</sub> ) <sub>2</sub> )=NN(CH <sub>3</sub> ) <sub>2</sub>	963.4	995.8	0	Rln(1/1)
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ]	462-94-2	1,5-Diaminopentane	946.2	999.6	-70	80MAU/HAM
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ]	51-80-9	(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	919.8	952.2	0	(CH <sub>3</sub> ) <sub>3</sub> N-Rln2
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ]	109-55-7	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	975.3	1025.0	-58	80MAU/HAM
[C <sub>5</sub> H <sub>15</sub> NSi]	18135-05-2	(CH <sub>3</sub> ) <sub>3</sub> SiN(CH <sub>3</sub> ) <sub>2</sub>	936	966.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>5</sub> H <sub>15</sub> N <sub>2</sub> OP]	2511-17-3	OP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub> (CH <sub>3</sub> )	918.9	951.3	0	Rln(1/1)
[C <sub>6</sub> CrO <sub>6</sub> ]	13007-92-6	(CO) <sub>6</sub> Cr	714.6	739.2	26.4	Rln(24/1)
[C <sub>6</sub> F <sub>6</sub> ]	392-56-3	C <sub>6</sub> F <sub>6</sub>	624.4	648.0	30	aromatics
[C <sub>6</sub> HF <sub>5</sub> ]	363-72-4	C <sub>6</sub> HF <sub>5</sub>	662.7	690.4	16	aromatics
[C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> ]	551-62-2	1,2,3,4-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	672.7	700.4	16	aromatics
[C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> ]	2367-82-0	1,2,3,5-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	719.6	747.3	16	aromatics
[C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> ]	327-54-8	1,2,4,5-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>	718.8	746.5	16	aromatics
[C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> ]	1489-53-8	1,2,3-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	696.6	724.3	16	aromatics
[C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> ]	367-23-7	1,2,4-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	699.4	729.5	8	93SZU/MCM
[C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> ]	372-38-3	1,3,5-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	715.4	741.9	20	93SZU/MCM
[C <sub>6</sub> H <sub>3</sub> MnO <sub>5</sub> ]	13601-24-6	(CO) <sub>5</sub> MnCH <sub>3</sub>	735.4	764.4	11.5	Rln(4/1)
[C <sub>6</sub> H <sub>3</sub> O <sub>5</sub> Re]	14524-92-6	(CO) <sub>5</sub> ReCH <sub>3</sub>	745.9	774.9	11.5	Rln(4/1)
[C <sub>6</sub> H <sub>4</sub> ]	462-80-6	ortho-benzyne	808.5	841	0	Rln(2/2)
[C <sub>6</sub> H <sub>4</sub> FO]	2145-21-3	4-F-phenoxy	822	854.5	0	?
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	367-11-3	1,2-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	703.5	731.2	16	average
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	540-36-3	1,4-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	692.8	718.7	22	aromatics
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	372-18-9	1,3-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	722	749.7	16	average
[C <sub>6</sub> H <sub>4</sub> F <sub>3</sub> N]	368-48-9	2-(CF <sub>3</sub> )-pyridine	855.2	887.1	2	pyridines
[C <sub>6</sub> H <sub>4</sub> F <sub>3</sub> N]	3796-23-4	3-(CF <sub>3</sub> )-pyridine	860.7	892.5	2	pyridines
[C <sub>6</sub> H <sub>4</sub> F <sub>3</sub> N]	3796-24-5	4-(CF <sub>3</sub> )-pyridine	862.0	893.9	2	pyridines
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ]	100-70-9	2-Pyridinecarbonitrile	841	872.9	2	pyridines
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ]	100-48-1	4-Pyridinecarbonitrile	848.8	880.6	2	pyridines
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ]	100-54-9	3-Pyridinecarbonitrile	845.1	877.0	2	pyridines
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O]	14906-59-3	4-cyano-pyridine-1-oxide	842.7	873.4	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O]	14906-64-0	3-cyano-pyridine-1-oxide	847.1	879.6	0	Rln(1/1)
[C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> ]	106-51-4	p-benzoquinone	769.3	799.1	9	96IRI/MAU
[C <sub>6</sub> H <sub>6</sub> ]	116139-00-5	HCCCH <sub>2</sub> CH(•)CCH	716.4	748.9	0	?
[C <sub>6</sub> H <sub>5</sub> ]	2396-01-2	phenyl radical	851.5	884	0	Rln(1/1)
[C <sub>6</sub> H <sub>5</sub> ]	116138-99-9	CH <sub>3</sub> -CC-CC-CH <sub>2</sub> •	786.6	819.1	0	?
[C <sub>6</sub> H <sub>5</sub> Br]	108-86-1	C <sub>6</sub> H <sub>5</sub> Br	725.8	754.1	14	C <sub>6</sub> H <sub>5</sub> Cl
[C <sub>6</sub> H <sub>5</sub> Cl]	108-90-7	C <sub>6</sub> H <sub>5</sub> Cl	724.6	753.1	13.5	average
[C <sub>6</sub> H <sub>5</sub> F]	462-06-6	C <sub>6</sub> H <sub>5</sub> F	726.6	755.9	10.5	average
[C <sub>6</sub> H <sub>5</sub> NO]	586-96-9	Nitrosobenzene	823.6	854.3	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>5</sub> NO]	872-85-5	4-Pyridinecarboxaldehyde	872.8	904.6	2	pyridines
[C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> ]	98-95-3	C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>	769.5	800.3	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> ]	622-37-7	phenyl azide	787.5	820	0	Rln(1/1)
[C <sub>6</sub> H <sub>5</sub> O]	2122-46-5	C <sub>6</sub> H <sub>5</sub> O radical	827	857.7	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>6</sub> ]	71-43-2	C <sub>6</sub> H <sub>6</sub>	725.4	750.4	25	97EAS/SMI
[C <sub>6</sub> H <sub>6</sub> BrN]	591-19-5	3-BrC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	841.4	873.2	2	anilines
[C <sub>6</sub> H <sub>6</sub> CIN]	18368-63-3	2-Cl-6-(CH <sub>3</sub> )-pyridine	876.2	908.0	2	pyridines
[C <sub>6</sub> H <sub>6</sub> CIN]	3678-62-4	2-Cl-4-(CH <sub>3</sub> )-pyridine	889.4	921.2	2	pyridines
[C <sub>6</sub> H <sub>6</sub> CIN]	106-47-8	4-ClC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	842.0	873.8	2	anilines
[C <sub>6</sub> H <sub>6</sub> CIN]	108-42-9	3-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	836.3	868.1	2	anilines
[C <sub>6</sub> H <sub>6</sub> CINO]	17228-63-6	6-Chloro-1-methyl-2(1H)pyridinone	885.5	918.5	-1.9	
[C <sub>6</sub> H <sub>6</sub> CINO]	17228-64-7	2-Cl-6-(CH <sub>3</sub> O)-pyridine	878.0	909.9	2	pyridines
[C <sub>6</sub> H <sub>6</sub> FN]	371-40-4	4-F-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	839.7	871.5	2	anilines
[C <sub>6</sub> H <sub>6</sub> FN]	372-19-0	3-F-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	835.5	867.3	2	anilines
[C <sub>6</sub> H <sub>6</sub> IN]	626-01-7	3-I-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	846.8	878.7	2	anilines
[C <sub>6</sub> H <sub>6</sub> N]	2348-49-4	C <sub>6</sub> H <sub>5</sub> NH radical	917.4	949.8	0	?
[C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O]	98-92-0	nicotinamide	886.4	918.3	2	pyridines
[C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ]	100-01-6	4-Nitroaniline	834.2	866.0	2	anilines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> ]	2004-03-7	6-Methylpurine	<b>907.3</b>	939.2	2	pyridines
[C <sub>6</sub> H <sub>6</sub> O]	6921-27-3	(HCCCH <sub>2</sub> ) <sub>2</sub> O	756.5	783.9	17	sym ethers
[C <sub>6</sub> H <sub>6</sub> O]	108-95-2	C <sub>6</sub> H <sub>5</sub> OH	786.3	817.3	5	S(C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> )-S(C <sub>6</sub> H <sub>5</sub> OH)
[C <sub>6</sub> H <sub>7</sub> N]	6921-28-4	(HCCCH <sub>2</sub> ) <sub>2</sub> NH	876.9	910.0	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>7</sub> N]	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	850.6	882.5	2	S(C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> )-S(C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> )
[C <sub>6</sub> H <sub>7</sub> N]	109-06-8	2-(CH <sub>3</sub> )-pyridine	917.3	949.1	2	pyridines
[C <sub>6</sub> H <sub>7</sub> N]	108-99-6	3-(CH <sub>3</sub> )-pyridine	911.6	943.4	2	pyridines
[C <sub>6</sub> H <sub>7</sub> N]	108-89-4	4-(CH <sub>3</sub> )-pyridine	915.3	947.2	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NO]	95-55-6	2-(OH)C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	866.9	898.8	2	anilines
[C <sub>6</sub> H <sub>7</sub> NO]	620-08-6	4-(CH <sub>3</sub> O)-pyridine	929.8	961.7	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NO]	591-27-5	3-(OH)C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	866.9	898.8	2	anilines
[C <sub>6</sub> H <sub>7</sub> NO]	1628-89-3	2-(CH <sub>3</sub> O)-pyridine	902.8	934.7	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NO]	7295-76-3	3-(CH <sub>3</sub> O)-pyridine	910.9	942.7	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NO]	694-85-9	1-Methyl-2-pyridinone	894.8	925.8	5	amides
[C <sub>6</sub> H <sub>7</sub> NO]	1003-73-2	3-methyl-pyridine-1-oxide	902.8	935.2	0	Rln(1/1)
[C <sub>6</sub> H <sub>7</sub> NS]	18794-33-7	3-(CH <sub>3</sub> S)-pyridine	904.7	936.5	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NS]	18438-38-5	2-(CH <sub>3</sub> S)-pyridine	906.0	937.8	2	pyridines
[C <sub>6</sub> H <sub>7</sub> NS]	22581-72-2	4-(CH <sub>3</sub> S)-pyridine	923.3	955.2	2	pyridines
[C <sub>6</sub> H <sub>8</sub> ]	592-57-4	1,3-c-C <sub>6</sub> H <sub>8</sub>	804.5	837	0	Rln(2/2)
[C <sub>6</sub> H <sub>8</sub> ]	628-41-1	1,4-c-C <sub>6</sub> H <sub>8</sub>	808.0	837	11.5	Rln(4/1)
[C <sub>6</sub> H <sub>8</sub> ]	15082-13-0	1-Methyl-3-methylene-cyclobutene	856.9	891.0	-5.8	Rln(1/2)
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ]	95-54-5	1,2-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	865.8	896.5	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ]	108-45-2	1,3-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	899.2	929.9	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ]	106-50-3	1,4-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>	874.0	905.9	2	anilines
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O]	1656-48-0	O(CH <sub>2</sub> CH <sub>2</sub> CN) <sub>2</sub>	<b>786.4</b>	813.8	17	sym ethers
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> ]	37622-90-5	4-(C <sub>2</sub> H <sub>5</sub> COO)-pyrazole	846.5	880.7	-5.8	Rln(1/2)
[C <sub>6</sub> H <sub>8</sub> O]	625-86-5	2,5-dimethylfuran	835.2	865.9	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>8</sub> O]	20843-07-6	3,4-dimethylfuran	838.3	869.0	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>8</sub> O]	3710-43-8	2,4-dimethylfuran	862.3	894.7	0	Rln(1/1)
[C <sub>6</sub> H <sub>8</sub> O]	6705-50-6	Bicyclo[2.2.1]hept-2-ene,7-oxa-	804.7	837.1	0	Rln(1/1)
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ]	504-02-9	c-hexane-1,3-dione	849.4	881.2	2	unsym ketones
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ]	765-87-7	c-hexane-1,2-dione	818.9	849.6	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ]	637-88-7	c-hexane-1,4-dione	782.7	812.5	9	sym ketones
[C <sub>6</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> ]	367-64-6	CF <sub>3</sub> CO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )	733.8	764.8	5	esters
[C <sub>6</sub> H <sub>9</sub> N]	625-84-3	2,5-Dimethylpyrrole	887.1	918.7	3	pyrrole
[C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> ]	71-00-1	L-histidine	950.2	988	-18	94WU/FEN
[C <sub>6</sub> H <sub>9</sub> O <sub>3</sub> P]	281-33-4	2,8,9-Trioxa-1-phosphadamantane	866.8	899.3	0	Rln(3/3)
[C <sub>6</sub> H <sub>10</sub> ]	1528-30-9	c-C <sub>3</sub> H <sub>8</sub> =CH <sub>2</sub>	803.5	832.4	12	propene
[C <sub>6</sub> H <sub>10</sub> ]	1501-58-2	1,2-Dimethylcyclobutene	807.3	838.0	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>10</sub> ]	1118-58-7	CH <sub>3</sub> CH=CHC(CH <sub>3</sub> )=CH <sub>2</sub>	836	864.9	12	propene
[C <sub>6</sub> H <sub>10</sub> ]	764-35-2	2-hexyne	781.1	806.1	25	CH <sub>3</sub> CCH
[C <sub>6</sub> H <sub>10</sub> ]	693-02-7	1-hexyne	774.8	799.8	25	CH <sub>3</sub> CCH
[C <sub>6</sub> H <sub>10</sub> ]	513-81-5	CH <sub>2</sub> =C(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub>	807.8	835.0	17.8	propene+Rln(2/1)
[C <sub>6</sub> H <sub>10</sub> ]	693-89-0	1-Methylcyclopentene	787.1	816.5	10	?
[C <sub>6</sub> H <sub>10</sub> ]	4663-22-3	c-C <sub>3</sub> H <sub>5</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	842.7	871.6	12	propene
[C <sub>6</sub> H <sub>10</sub> ]	4549-74-0	CH <sub>3</sub> CH=C(CH <sub>3</sub> )CH=CH <sub>2</sub>	823.4	852.3	12	propene
[C <sub>6</sub> H <sub>10</sub> ]	16906-27-7	1-ethenyl-1-methylcyclopropane	826.9	855.7	12	propene
[C <sub>6</sub> H <sub>10</sub> ]	3664-56-0	1,3,3-Trimethylcyclopropene	865.9	895.4	10	AUE
[C <sub>6</sub> H <sub>10</sub> ]	110-83-8	c-C <sub>6</sub> H <sub>10</sub>	752.0	784.5	0	Rln(2/2)
[C <sub>6</sub> H <sub>10</sub> F <sub>3</sub> N]	657-36-3	4-Trifluoromethylpiperidine	892.0	925.1	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>10</sub> F <sub>3</sub> NO]	400-59-9	CF <sub>3</sub> CONH(n-C <sub>4</sub> H <sub>9</sub> )	819.4	850.3	5	amides
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ]	1530-87-6	Piperidine, 1-carbonitrile-	846.1	876.7	6	nitriles
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ]	5519-42-6	3,4,5-Trimethylpyrazole	916.0	949.3	-3	pyridines-Rln2
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ]	1072-91-9	1,3,5-Trimethylpyrazole	917.4	949.3	2	pyridines
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ]	4395-98-6	4-Cyanopiperidine	879.2	912.3	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ]	121508-72-3	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-propynyl)	960.7	993.1	0	Rln(1/1)
[C <sub>6</sub> H <sub>10</sub> O]	557-40-4	(CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>2</sub> O	800.0	827.4	17	sym ethers
[C <sub>6</sub> H <sub>10</sub> O]	286-20-4	Cyclohexene oxide	<b>815.6</b>	848.1	0	Rln(1/1)
[C <sub>6</sub> H <sub>10</sub> O]	1567-72-2	3-methyl-3-penten-2-one(Z)	834.5	866.4	2	unsym ketones
[C <sub>6</sub> H <sub>10</sub> O]	108-94-1	cyclohexanone	811.2	841.0	9	sym ketones
[C <sub>6</sub> H <sub>10</sub> O]	141-79-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH(C=O)CH <sub>3</sub>	846.9	878.7	2	unsym ketones
[C <sub>6</sub> H <sub>10</sub> O]	279-49-2	Bicyclo[2.2.1]heptane,7-oxa	816.8	844.2	17	sym ethers
[C <sub>6</sub> H <sub>10</sub> O]	4376-23-2	3-hexen-2-one(E)	833.8	865.6	2	unsym ketones

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> ]	3400-45-1	cyclopentane carboxylic acid	786.4	817.4	5	acids
[C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> ]	110-13-4	CH <sub>3</sub> COCH <sub>2</sub> CH <sub>2</sub> COCH <sub>3</sub>	851.8	892.0	-26	83MAU
[C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> ]	22157-30-8	CH <sub>3</sub> C(OCH <sub>3</sub> )=CHCOOCH <sub>3</sub>	885.8	916.8	5	esters
[C <sub>6</sub> H <sub>11</sub> N]	124-02-7	(CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>2</sub> NH	916.3	949.3	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>11</sub> NO]	931-20-4	c-C <sub>5</sub> H <sub>9</sub> N(2-O)1-CH <sub>3</sub>	892.6	924.4	2	unsym ketones
[C <sub>6</sub> H <sub>11</sub> NO]	6976-91-6	2-propenamide, N,N,2-trimethyl-	880.6	911.5	5	amides
[C <sub>6</sub> H <sub>11</sub> NO]	23135-18-4	2-propenamide, N,N-dimethyl-	899.4	930.3	5	amides
[C <sub>6</sub> H <sub>11</sub> NO]	4030-18-6	Acetylpyrrolidine	894.4	925.4	5	amides
[C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> ]	26629-33-4	CH <sub>3</sub> CONHCH(CH <sub>3</sub> )COOCH <sub>3</sub>	888.0	938.6	-61	83MAU
[C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> ]	134166-60-2	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> CH <sub>2</sub> CN	948.3	980.8	0	Rln(1/1)
[C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> ]	556-33-2	triglycine	916.8	966.8	-59	93CHE/WU
[C <sub>6</sub> H <sub>12</sub> ]	625-27-4	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>2</sub> CH <sub>3</sub>	783.1	812	12	propene
[C <sub>6</sub> H <sub>12</sub> ]	563-79-1	(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub>	785.9	813.9	15	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>
[C <sub>6</sub> H <sub>12</sub> ]	592-41-6	1-hexene	776.3	805.2	12	propene
[C <sub>6</sub> H <sub>12</sub> ]	110-82-7	c-C <sub>6</sub> H <sub>12</sub>	666.9	686.9	42	C <sub>2</sub> H <sub>6</sub> ; c-C <sub>3</sub> H <sub>6</sub>
[C <sub>6</sub> H <sub>12</sub> ]	922-61-2	CH <sub>3</sub> CH=C(CH <sub>3</sub> )C <sub>2</sub> H <sub>5</sub>	784.0	812.9	12	propene
[C <sub>6</sub> H <sub>12</sub> N]	60598-49-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-propenyl)	972.3	1004.8	0	Rln(1/1)
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ]	5397-67-1	1H,5H-pyrazolo[1,2-a]pyrazole, tetrahydro	947.3	978.0	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ]	280-57-9	1,4-Diazabicyclo[2.2.2]octane	934.6	963.4	12	(CH <sub>3</sub> ) <sub>3</sub> N+Rln(6/3)
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ]	133835-16-2	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(c-propyl)	973.8	1006.2	0	Rln(1/1)
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ]	1948-31-8	di-L-alanine	905.6	NE	NE	not estimated
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> ]	6620-95-7	ser-ser	886.4	NE	NE	not estimated
[C <sub>6</sub> H <sub>12</sub> O]	592-90-5	c-C <sub>6</sub> H <sub>12</sub> O(Oxepane)	806.8	834.2	17	sym ethers
[C <sub>6</sub> H <sub>12</sub> O]	75-97-8	t-C <sub>4</sub> H <sub>9</sub> COCH <sub>3</sub>	808.2	840.1	2	unsym ketones
[C <sub>6</sub> H <sub>12</sub> O]	1003-17-4	2,2-Dimethyltetrahydrofuran	818.5	847.7	11	unsym ethers
[C <sub>6</sub> H <sub>12</sub> O]	589-38-8	3-hexanone	811.3	843.2	2	unsym ketones
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ]	823-18-7	cis-1,3-cyclohexandiol	849.7	882.2	0	?
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ]	598-98-1	t-C <sub>4</sub> H <sub>9</sub> -COOCH <sub>3</sub>	814.2	845.2	5	esters
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ]	5515-64-0	trans-1,3-cyclohexanol	797.9	828.6	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ]	123-42-2	(CH <sub>3</sub> ) <sub>2</sub> C(OH)CH <sub>2</sub> (C=O)CH <sub>3</sub>	791.1	822.9	2	unsym ketones
[C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ]	26655-34-5	alpha-D-glucose	778.9	NE	NE	not estimated
[C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ]	28905-12-6	beta-D-glucose	778.9	NE	NE	not estimated
[C <sub>6</sub> H <sub>13</sub> N]	111-49-9	Hexahydroazepine	923.5	956.7	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>13</sub> N]	626-67-5	1-Methylpiperidine	940.1	971.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>13</sub> N]	1611-12-7	n-C <sub>3</sub> H <sub>7</sub> CH=NC <sub>2</sub> H <sub>5</sub>	923.0	955.5	0	Rln(1/1)
[C <sub>6</sub> H <sub>13</sub> N]	78733-72-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=CHCH <sub>3</sub>	972.9	1005.4	0	Rln(1/1)
[C <sub>6</sub> H <sub>13</sub> N]	108-91-8	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	899.6	934.4	-8	S(C <sub>6</sub> H <sub>11</sub> CH <sub>3</sub> )-
[C <sub>6</sub> H <sub>13</sub> N]	6906-32-7	(CH <sub>3</sub> ) <sub>2</sub> C=CHN(CH <sub>3</sub> ) <sub>2</sub>	934.5	967.0	0	Rln(1/1)
[C <sub>6</sub> H <sub>13</sub> NO]	760-79-2	n-C <sub>3</sub> H <sub>7</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	890.8	921.7	5	amides
[C <sub>6</sub> H <sub>13</sub> NO]	685-91-6	CH <sub>3</sub> CON(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	894.4	925.4	5	amides
[C <sub>6</sub> H <sub>13</sub> NO]	21678-37-5	i-C <sub>3</sub> H <sub>7</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	891.8	923.7	2	amides
[C <sub>6</sub> H <sub>13</sub> NO]	53687-79-9	c-C <sub>3</sub> H <sub>10</sub> N(2-OCH <sub>3</sub> )	936.7	969.9	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> ]	61-90-5	L-leucine	880.6	914.6	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> ]	73-32-5	L-isoleucine	883.5	917.4	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>6</sub> H <sub>13</sub> O <sub>3</sub> P]	7735-82-2	cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane	919.1	951.6	0	Rln(1/1)
[C <sub>6</sub> H <sub>13</sub> O <sub>3</sub> P]	41821-91-4	trans-2-Methoxy-cis,cis-4,6-dimethyl-1,3,2-dioxaphosphorinane	914.1	946.6	0	Rln(1/1)
[C <sub>6</sub> H <sub>13</sub> P]	39763-50-3	(CH <sub>2</sub> ) <sub>3</sub> PCH <sub>3</sub>	936.7	969.4	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ]	32150-25-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-propyl)	979.2	1011.7	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ]	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	981.0	1013.5	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ]	151328-40-4	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NC <sub>2</sub> H <sub>5</sub>	996.7	1029.1	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ]	26163-37-1	Pyridazine, hexahydro-1,2-dimethyl	935.4	966.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O]	134166-62-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methoxyethyl)	986.4	1018.9	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ]	56-87-1	L-lysine	951.0	996	-42	93CHE/WU
[C <sub>6</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> ]	74-79-3	L-Arginine	1006.6	1051.0	-40	80MAU/HAM
[C <sub>6</sub> H <sub>14</sub> O]	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	828.1	855.5	17	sym ethers
[C <sub>6</sub> H <sub>14</sub> O]	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	810.5	837.9	17	sym ethers
[C <sub>6</sub> H <sub>14</sub> O]	637-92-3	C <sub>2</sub> H <sub>5</sub> O(t-C <sub>4</sub> H <sub>9</sub> )	826.9	856.0	11	unsym ethers
[C <sub>6</sub> H <sub>14</sub> O]	1118-00-9	neo-C <sub>5</sub> H <sub>11</sub> OCH <sub>3</sub>	796.7	825.8	11	unsym ethers
[C <sub>6</sub> H <sub>14</sub> OSi]	1833-53-0	CH <sub>2</sub> =(CH <sub>3</sub> )OSi(CH <sub>3</sub> ) <sub>3</sub>	898.2	930.6	0	Rln(1/1)
[C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> ]	13179-96-9	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>4</sub> OCH <sub>3</sub>	880.6	931.5	-62	84SHA/BLA
[C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> ]	111-96-6	CH <sub>3</sub> (OCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> OCH <sub>3</sub>	870.9	918.8	-52	84SHA/BLA; 83MAU

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>6</sub> H <sub>14</sub> S]	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	834.9	864.7	9	sym sulfides
[C <sub>6</sub> H <sub>14</sub> S]	625-80-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	846.6	876.4	9	sym sulfides
[C <sub>6</sub> H <sub>15</sub> N]	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	951	981.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>15</sub> N]	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	929.3	962.3	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>15</sub> N]	111-26-2	n-C <sub>6</sub> H <sub>13</sub> NH <sub>2</sub>	893.5	927.5	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>6</sub> H <sub>15</sub> N]	927-62-8	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )N	938.2	969.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>15</sub> N]	921-04-0	(sec-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> ) <sub>2</sub> N	945.1	975.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>15</sub> N]	7239-24-9	(CH <sub>3</sub> ) <sub>2</sub> (i-C <sub>4</sub> H <sub>9</sub> )N	937.8	968.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>15</sub> N]	108-18-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	938.6	971.9	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>6</sub> H <sub>15</sub> N]	918-02-5	(CH <sub>3</sub> ) <sub>2</sub> (t-C <sub>4</sub> H <sub>9</sub> )N	948.6	979.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>15</sub> NO]	4048-33-3	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>6</sub> OH	915.7	969.0	-70	80MAU
[C <sub>6</sub> H <sub>15</sub> N <sub>3</sub> ]	13439-84-4	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NCH <sub>3</sub>	1015.2	1047.7	0	Rln(1/1)
[C <sub>6</sub> H <sub>15</sub> OP]	597-50-2	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> PO	906.8	936.6	9.1	Rln(3/1)
[C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P]	78-40-0	OP(OC <sub>2</sub> H <sub>5</sub> ) <sub>3</sub>	879.6	909.3	9.1	Rln(3/1)
[C <sub>6</sub> H <sub>15</sub> P]	554-70-1	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> P	952.0	984.5	0	Rln(3/3)
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	60678-65-1	(n-C <sub>3</sub> H <sub>7</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub>	934.3	966.8	0	Rln(1/1)
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	23337-93-1	Hydrazine, 1,2-diethyl-1,2-dimethyl	933.0	963.7	5.8	Rln(2/1)
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	110-18-9	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	970.6	1012.8	-33	80MAU/HAM
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	124-09-4	1,6-Diaminohexane	946.2	999.5	-70	80MAU/HAM
[C <sub>6</sub> H <sub>16</sub> N <sub>3</sub> OP]	7778-06-5	c-OP{N(CH <sub>3</sub> ) <sub>2</sub> }N(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> )	929.3	961.7	0	Rln(1/1)
[C <sub>6</sub> H <sub>16</sub> OSi]	597-52-4	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> SiOH	794.8	822.1	17	88LI/STO
[C <sub>6</sub> H <sub>17</sub> NSi]	18182-40-6	(CH <sub>3</sub> ) <sub>3</sub> SiCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	943.8	974.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> OP]	680-31-9	OP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	928.7	958.6	9.1	Rln(3/1)
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> P]	1608-26-0	P(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	897.7	930.1	0	Rln(1/1)
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> PS]	3732-82-9	SP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	912.2	942.0	9.1	Rln(3/1)
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> PSe]	7422-73-3	SeP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	904.3	934.1	9.1	Rln(3/1)
[C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub> ]	107-46-0	(CH <sub>3</sub> ) <sub>3</sub> SiOSi(CH <sub>3</sub> ) <sub>3</sub>	816.2	846.4	7.8	87LI/STO
[C <sub>6</sub> MoO <sub>6</sub> ]	13939-06-5	(CO) <sub>6</sub> Mo	738.1	762.6	26.4	Rln(24/1)
[C <sub>6</sub> O <sub>6</sub> V]	20644-87-5	(CO) <sub>6</sub> V	775.3	799.9	26.4	Rln(24/1)
[C <sub>6</sub> O <sub>6</sub> W]	14040-11-0	(CO) <sub>6</sub> W	733.4	758.0	26.4	Rln(24/1)
[C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	619-72-7	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CN	745.1	775.7	6	nitriles
[C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	619-24-9	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CN	750.7	781.4	6	nitriles
[C <sub>7</sub> H <sub>5</sub> ClO]	587-04-2	3-ClC <sub>6</sub> H <sub>4</sub> CHO	781.1	813.0	2	CH <sub>3</sub> CHO
[C <sub>7</sub> H <sub>5</sub> ClO]	104-88-1	4-ClC <sub>6</sub> H <sub>4</sub> CHO	799.4	831.3	2	CH <sub>3</sub> CHO
[C <sub>7</sub> H <sub>5</sub> CrNO <sub>3</sub> ]	36312-04-6	(C <sub>5</sub> H <sub>5</sub> )Cr(CO) <sub>2</sub> NO	786.7	819.1	0	Rln(1/1)
[C <sub>7</sub> H <sub>5</sub> D <sub>3</sub> ]	1124-18-1	C <sub>6</sub> H <sub>5</sub> CD <sub>3</sub>	762	789.7	16	toluene
[C <sub>7</sub> H <sub>5</sub> FO]	456-48-4	3-FC <sub>6</sub> H <sub>4</sub> CHO	782.5	814.3	2	aldehydes
[C <sub>7</sub> H <sub>5</sub> FO]	459-57-4	4-FC <sub>6</sub> H <sub>4</sub> CHO	795.3	827.1	2	aldehydes
[C <sub>7</sub> H <sub>5</sub> N]	100-47-0	C <sub>6</sub> H <sub>5</sub> CN	780.9	811.5	6	nitriles
[C <sub>7</sub> H <sub>5</sub> N]	931-54-4	C <sub>6</sub> H <sub>5</sub> NC	<b>836.0</b>	868.4	0	Rln(1/1)
[C <sub>7</sub> H <sub>5</sub> N]	2510-22-7	4-ethynyl-pyridine	898.2	930.1	2	pyridines
[C <sub>7</sub> H <sub>5</sub> NO]	273-53-0	benzoxazole	859.8	891.6	2	pyridines
[C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> ]	555-16-8	4-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> CHO	763.2	795.1	2	aldehydes
[C <sub>7</sub> H <sub>5</sub> O <sub>2</sub> Rh]	12192-97-1	(C <sub>5</sub> H <sub>5</sub> )Rh(CO) <sub>2</sub>	851.8	882.5	5.8	Rln(2/1)
[C <sub>7</sub> H <sub>6</sub> ClNO]	618-48-4	3-Cl-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>846.3</b>	877.2	5	amides
[C <sub>7</sub> H <sub>6</sub> ClNO]	619-56-7	4-Cl-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>846.3</b>	877.2	5	amides
[C <sub>7</sub> H <sub>6</sub> F]	2599-73-7	3-FC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> radical	<b>804</b>	836.5	0	?
[C <sub>7</sub> H <sub>6</sub> FNO]	455-37-8	3-F-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>846.3</b>	877.2	5	amides
[C <sub>7</sub> H <sub>6</sub> FNO]	824-75-9	4-F-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>846.3</b>	877.2	5	amides
[C <sub>7</sub> H <sub>6</sub> F <sub>3</sub> N]	98-16-8	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	825.1	856.9	2	anilines
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	274-76-0	Imidazo(1,2-a)pyridine	940.3	972.1	2	pyridines
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	271-44-3	1H-Indazole	868.9	900.8	2	pyridines
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	271-63-6	7-Azaindole	908.3	940.2	2	pyridines
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	51-17-2	Benzimidazole	920.5	953.8	-3	pyridine-Rln2
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	2237-30-1	3-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CN	810.4	842.3	2	anilines
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> ]	619-80-7	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>814.4</b>	845.3	5	amides
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> ]	645-09-0	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>823.2</b>	854.2	5	amides
[C <sub>7</sub> H <sub>6</sub> O]	539-80-0	2,4,6-Cycloheptatriene-1-one	<b>891.0</b>	920.8	9	sym ketones
[C <sub>7</sub> H <sub>6</sub> O]	502-87-4	4-Methylene-2,5-cyclohexadiene-1-one	894.0	923.8	9	sym ketones
[C <sub>7</sub> H <sub>6</sub> O]	100-52-7	C <sub>6</sub> H <sub>5</sub> CHO	802.1	834.0	2	CH <sub>3</sub> CHO
[C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> ]	65-85-0	C <sub>6</sub> H <sub>5</sub> COOH	790.1	821.1	5	acids
[C <sub>7</sub> H <sub>7</sub> ]	2154-56-5	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub>	800.7	831.4	6	isoel analog
[C <sub>7</sub> H <sub>7</sub> ]	3551-27-7	c-C <sub>7</sub> H <sub>7</sub> radical	<b>800.0</b>	832.4	0	?

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>7</sub> H <sub>7</sub> Br]	106-38-7	4-Br-toluene	745.8	775.3	10	aromatics
[C <sub>7</sub> H <sub>7</sub> Br]	95-46-5	2-Br-toluene	745.8	775.3	10	aromatics
[C <sub>7</sub> H <sub>7</sub> Br]	591-17-3	3-Br-toluene	752.5	782.0	10	aromatics
[C <sub>7</sub> H <sub>7</sub> Cl]	95-49-8	2-Cl-toluene	761.1	790.5	10	aromatics
[C <sub>7</sub> H <sub>7</sub> Cl]	106-43-4	4-Cl-toluene	735.2	762.9	16	aromatics
[C <sub>7</sub> H <sub>7</sub> Cl]	108-41-8	3-Cl-toluene	754.5	783.9	10	aromatics
[C <sub>7</sub> H <sub>7</sub> F]	95-52-3	2-F-toluene	743.8	773.3	10	aromatics
[C <sub>7</sub> H <sub>7</sub> F]	352-70-5	3-F-toluene	756.0	785.4	10	aromatics
[C <sub>7</sub> H <sub>7</sub> F]	352-32-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> F	736.1	763.8	16	aromatics
[C <sub>7</sub> H <sub>7</sub> I]	615-37-2	2-I-toluene	750.8	780.3	10	aromatics
[C <sub>7</sub> H <sub>7</sub> N]	16118-22-2	C <sub>6</sub> H <sub>5</sub> CH=NH	<b>879.4</b>	911.9	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> N]	56911-25-2	2,3-Cyclobutenopyridine	922.0	953.9	2	pyridines
[C <sub>7</sub> H <sub>7</sub> N]	56911-27-4	3,4-Cyclobutenopyridine	925.6	957.5	2	pyridines
[C <sub>7</sub> H <sub>7</sub> N]	100-43-6	4-Vinylpyridine	912.3	944.1	2	pyridines
[C <sub>7</sub> H <sub>7</sub> NO]	350-03-8	3-(CH <sub>3</sub> CO)-pyridine	884.3	916.2	2	pyridines
[C <sub>7</sub> H <sub>7</sub> NO]	1122-54-9	1-(4-Pyridinyl)-ethanone	882.9	914.7	2	pyridines
[C <sub>7</sub> H <sub>7</sub> NO]	55-21-0	C <sub>6</sub> H <sub>5</sub> CONH <sub>2</sub>	<b>861.2</b>	892.1	5	amides
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	118-92-3	2-NH <sub>2</sub> -benzoic acid	<b>869.0</b>	901.5	0	?
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	150-13-0	4-NH <sub>2</sub> -benzoic acid	<b>832.3</b>	864.7	0	?
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	99-05-8	3-NH <sub>2</sub> -benzoic acid	<b>832.3</b>	864.7	0	?
[C <sub>7</sub> H <sub>7</sub> NO]	556-18-3	4-NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CHO	878.6	910.4	2	anilines
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	93-60-7	methylnicotinate	893.8	925.6	2	pyridines
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	14188-94-4	1-(3-pyridinyl-1-oxide)ethanone	880.6	913.1	0	?
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	99-99-0	4-Nitrotoluene	782.7	815.2	0	?
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	2459-09-8	Pyridine-4-carboxylic acid, methyl ester	894.7	926.6	2	pyridines
[C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub> ]	619-73-8	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> OH	778.0	810.5	0	86SUN/KUL
[C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> ]	13351-73-0	1-methylbenzotriazole	898.7	931.2	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> ]	16584-00-2	2-methyl-2H-benzotriazole	855.9	890.1	-5.8	Rln(1/2)
[C <sub>7</sub> H <sub>7</sub> O]	155174-22-4	3-OH-benzyl	853	885.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> O]	3174-48-9	4-Me-phenoxy	852	884.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> O]	88170-17-6	4-OH-benzyl	864	896.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> O]	155174-21-3	2-OH-benzyl	846	878.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> O]	3174-49-0	2-Me-phenoxy	842	874.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>7</sub> O]	41115-75-7	3-Me-phenoxy	845	877.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>8</sub> ]	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	756.3	784.0	16	toluene
[C <sub>7</sub> H <sub>8</sub> ]	121-46-0	Bicyclo[2.2.1]hepta-2,5-diene	820.3	849.3	11.5	Rln(4/1)
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O]	3544-24-9	3-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>869.9</b>	900.9	5	amides
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O]	2835-68-9	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	<b>896.9</b>	927.9	5	amides
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> ]	100-15-2	N-Methyl-4-nitroaniline	865.1	891.6	20	anilines
[C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> ]	27258-04-4	Di(1-pyrazolyl)methane	893.9	924.7	5.8	Rln(2/1)
[C <sub>7</sub> H <sub>8</sub> O]	694-71-3	Bicyclo[2.2.1]hept-2-ene-7-one	798.3	830.2	2	unsym ketones
[C <sub>7</sub> H <sub>8</sub> O]	100-51-6	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH	748.0	778.3	7	CH <sub>3</sub> OH
[C <sub>7</sub> H <sub>8</sub> O]	100-66-3	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub>	807.2	839.6	0	?
[C <sub>7</sub> H <sub>8</sub> O]	694-98-4	Bicyclo[2.2.1]hept-2-ene-5-one	813.4	845.3	2	unsym ketones
[C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> ]	1004-36-0	2,6-Dimethyl-4-pyrone	907.3	941.5	-5.8	Rln(1/2)
[C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> S]	3112-85-4	C <sub>6</sub> H <sub>5</sub> SO <sub>2</sub> CH <sub>3</sub>	780.3	812.7	0	Rln(1/1)
[C <sub>7</sub> H <sub>8</sub> S]	100-68-5	C <sub>6</sub> H <sub>5</sub> SCH <sub>3</sub>	843.7	872.6	12	
[C <sub>7</sub> H <sub>9</sub> N]	95-53-4	2-methylaniline	859.1	890.9	2	anilines
[C <sub>7</sub> H <sub>9</sub> N]	536-75-4	4-(C <sub>2</sub> H <sub>5</sub> )-pyridine	919.2	951.1	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	931.1	963.0	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	108-44-1	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	864.0	895.8	2	anilines
[C <sub>7</sub> H <sub>9</sub> N]	100-46-9	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub>	879.4	913.3	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>7</sub> H <sub>9</sub> N]	100-71-0	2-(C <sub>2</sub> H <sub>5</sub> )-pyridine	920.6	952.4	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	589-93-5	2,5-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	926.9	958.8	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	108-47-4	2,4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	930.8	962.9	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	583-61-9	2,3-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	927.0	958.9	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	100-61-8	C <sub>6</sub> H <sub>5</sub> NHCH <sub>3</sub>	890.1	916.6	20	anilines
[C <sub>7</sub> H <sub>9</sub> N]	591-22-0	3,5-(CH <sub>3</sub> ) <sub>3</sub> -pyridine	923.5	955.4	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	106-49-0	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	864.8	896.7	2	anilines
[C <sub>7</sub> H <sub>9</sub> N]	583-58-4	3,4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	925.5	957.3	2	pyridines
[C <sub>7</sub> H <sub>9</sub> N]	536-78-7	3-(C <sub>2</sub> H <sub>5</sub> )-pyridine	915.5	947.4	2	pyridines
[C <sub>7</sub> H <sub>9</sub> NO]	536-90-3	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	881.1	913.0	2	anilines
[C <sub>7</sub> H <sub>9</sub> NO]	90-04-0	2-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	873.3	905.2	2	anilines
[C <sub>7</sub> H <sub>9</sub> NO]	23579-92-2	2-(CH <sub>3</sub> OCH <sub>2</sub> )-pyridine	926.4	958.3	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>7</sub> H <sub>9</sub> NO]	104-94-9	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	868.5	900.3	2	anilines
[C <sub>7</sub> H <sub>9</sub> NS]	1783-81-9	3-CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	870.3	902.1	2	anilines
[C <sub>7</sub> H <sub>10</sub> ]	498-66-8	Bicyclo[2.2.1]hept-2-ene	804.0	836.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>10</sub> CIN]	#449	3-Chloro-1-azabicyclo[2.2.2]oct-2-ene	916.7	947.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ]	18437-57-5	N,N-Dimethyl-3-pyridinamine	943.1	969.6	20	anilines
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ]	1122-58-3	N,N-Dimethyl-4-pyridinamine	971.1	997.6	20	anilines
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ]	5683-33-0	N,N-Dimethyl-2-pyridinamine	941.6	968.2	20	anilines
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ]	4027-57-0	3(5)-methyl-5(3)-ethoxycarbonylpyrazole	870.8	902.6	2	pyridines
[C <sub>7</sub> H <sub>10</sub> O]	10218-02-7	Bicyclo[2.2.1]heptan-7-one	802.4	832.1	9	sym ketones
[C <sub>7</sub> H <sub>10</sub> O]	497-38-1	Bicyclo[2.2.1]heptan-2-one	815.5	847.4	2	unsym ketones
[C <sub>7</sub> H <sub>10</sub> O]	1121-37-5	(c-C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CO	850.6	880.4	9	sym ketones
[C <sub>7</sub> H <sub>10</sub> S]	38381-24-7	(c-C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CS	874.5	904.3	9	sym ketones
[C <sub>7</sub> H <sub>11</sub> F <sub>2</sub> N]	#524	3,3-Difluoro-1-azabicyclo[2.2.2]octane	904.8	935.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>11</sub> N]	766-05-2	c-C <sub>8</sub> H <sub>11</sub> CN	784.4	815.0	6	nitriles
[C <sub>7</sub> H <sub>11</sub> N]	87-62-7	2,6-dimethylaniline	869.8	901.7	2	anilines
[C <sub>7</sub> H <sub>11</sub> N]	13929-94-7	1-Azabicyclo[2.2.2]oct-2-ene	938.6	969.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>11</sub> NO]	3731-38-2	1-Azabicyclo[2.2.2]octan-3-one	905.2	936.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> ]	765-47-9	c-C <sub>5</sub> H <sub>6</sub> -1,2-(CH <sub>3</sub> ) <sub>2</sub>	791.9	822.6	5.8	Rln(2/1)
[C <sub>7</sub> H <sub>12</sub> ]	1000-86-8	(CH <sub>3</sub> ) <sub>2</sub> C=CHC(CH <sub>3</sub> )=CH <sub>2</sub>	857.6	886.5	12	propene
[C <sub>7</sub> H <sub>12</sub> ]	591-49-1	1-Methylcyclohexene	792.6	825.1	0	?
[C <sub>7</sub> H <sub>12</sub> BrN]	#364	3-Bromo-1-azabicyclo[2.2.2]octane	931.8	962.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> CIN]	42332-45-6	3-Chloro-1-azabicyclo[2.2.2]octane	923.5	954.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> CIN]	5960-95-2	1-azabicyclo[2.2.2]-octane, 4-chloro	918.6	949.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> CIN]	96943-88-3	1-azabicyclo[2.2.2]-octane, 2-chloro	920.0	950.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> FN]	#321	3-Fluoro-1-azabicyclo[3.2.1]octane	936.7	967.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ]	3001-72-7	1,5-diazabicyclo[4.3.0]non-5-ene	1005.9	1038.3	0	Rln(1/1)
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ]	45676-04-8	1-t-Butylimidazole	954.9	987.0	2	pyridines
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ]	15802-80-9	3(5)-t-butylpyrazole	891.0	922.8	2	pyridines
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ]	52096-24-9	n-Butylpyrazole	897.3	928.8	3	pyrazole
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ]	704-15-4	gly-pro	905.6	NE	NE	not estimated
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ]	2578-57-6	pro-gly	925.1	NE	NE	not estimated
[C <sub>7</sub> H <sub>12</sub> O]	589-92-4	4-methylcyclohexanone	813.0	844.9	2	unsym ketones
[C <sub>7</sub> H <sub>12</sub> O]	502-42-1	cycloheptanone	815.9	845.6	9	sym ketones
[C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> ]	98-89-5	Cyclohexane carboxylic acid	792.8	823.8	5	acids
[C <sub>7</sub> H <sub>13</sub> N]	100-76-5	1-azabicyclo[2.2.2]-octane	952.5	983.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>13</sub> N]	7242-92-4	Bicyclo[2.2.1]heptan-2-amine,exo	901.3	935.3	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>7</sub> H <sub>13</sub> N]	31002-73-0	Bicyclo[2.2.1]heptan-2-amine,endo	901.3	935.3	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> ]	673-46-1	N <sub>α</sub> ,N <sub>α</sub> -dimethylhistamine	990.1	1022.0	2	pyridines
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> ]	5807-14-7	1,5,7-triazabicyclo[4.4.0]dec-5-ene	1022.1	1054.6	0	Rln(1/1)
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	3146-40-5	ala-gly-gly	917.8	NE	NE	not estimated
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	19729-30-7	gly-gly-ala	914.8	NE	NE	not estimated
[C <sub>7</sub> H <sub>14</sub> ]	625-65-0	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH(CH <sub>3</sub> ) <sub>2</sub>	783.1	812	12	propene
[C <sub>7</sub> H <sub>14</sub> CIN]	49665-74-9	c-C <sub>5</sub> H <sub>9</sub> N,2-CH <sub>2</sub> Cl,1-CH <sub>3</sub>	934.2	965.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ]	6238-14-8	3-Amino-1-azabicyclo[2.2.2]octane	954.7	985.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ]	6523-29-1	2-Methyl-1,2-diazabicyclo[2.2.2]-octane	938.1	968.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ]	14287-89-9	2,3-diazabicyclo[2.2.1]heptane, 2,3-dimethyl	945.6	978.0	0	Rln(1/1)
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ]	151328-39-1	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(c-C <sub>3</sub> H <sub>5</sub> )	991.7	1024.1	0	Rln(1/1)
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> ]	1963-21-9	gly-val	874.1	NE	NE	not estimated
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> ]	686-43-1	val-gly	874.1	NE	NE	not estimated
[C <sub>7</sub> H <sub>14</sub> O]	100-49-2	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> OH	771.7	802.1	7	CH <sub>3</sub> OH
[C <sub>7</sub> H <sub>14</sub> O]	931-56-6	c-C <sub>6</sub> H <sub>11</sub> OCH <sub>3</sub>	811.3	840.5	11	unsym ethers
[C <sub>7</sub> H <sub>14</sub> O]	123-19-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	815.3	845.0	9	sym ketones
[C <sub>7</sub> H <sub>14</sub> O]	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	820.5	850.3	9	sym ketones
[C <sub>7</sub> H <sub>14</sub> S]	2550-37-0	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> SH	782.4	813.6	4	CH <sub>3</sub> SH
[C <sub>7</sub> H <sub>14</sub> S]	6572-99-2	Heptamethylenesulfide	830.7	860.5	9	sym sulfides
[C <sub>7</sub> H <sub>14</sub> S]	7133-37-1	c-C <sub>6</sub> H <sub>11</sub> SCH <sub>3</sub>	833.3	864.5	4	unsym sulfides
[C <sub>7</sub> H <sub>15</sub> N]	78733-73-0	(CH <sub>3</sub> ) <sub>2</sub> NC(C <sub>2</sub> H <sub>5</sub> )=CHCH <sub>3</sub>	961	991.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>15</sub> N]	3218-02-8	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> NH <sub>2</sub>	895.8	926.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>15</sub> NO]	24331-71-3	t-C <sub>4</sub> H <sub>9</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	895.2	927.1	2	amides
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	94793-20-1	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>3</sub> H <sub>7</sub> )	997.9	1030.3	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	49840-68-8	1H-1,2-diazepine, hexahydro-1,2-dimethyl	936.1	966.8	5.8	Rln(2/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	85599-92-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylpropyl)	985.7	1018.1	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	94793-19-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(i-C <sub>3</sub> H <sub>7</sub> )	999.2	1031.6	0	Rln(1/1)



TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	3717-82-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-butyl)	980.5	1013.0	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	67161-18-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methylpropyl)	982.0	1014.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	23314-06-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(t-C <sub>4</sub> H <sub>9</sub> )	988.3	1020.8	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O]	151328-41-5	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(CH <sub>2</sub> ) <sub>2</sub> OCH <sub>3</sub>	1003.8	1036.2	0	Rln(1/1)
[C <sub>7</sub> H <sub>16</sub> O]	17348-59-3	(i-C <sub>3</sub> H <sub>7</sub> )O(t-C <sub>4</sub> H <sub>9</sub> )	841.5	870.7	11	unsym ethers
[C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> ]	111-89-7	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>5</sub> OCH <sub>3</sub>	879.5	931.3	-65	84SHA/BLA
[C <sub>7</sub> H <sub>17</sub> N]	57757-60-5	(t-C <sub>5</sub> H <sub>11</sub> )(CH <sub>3</sub> ) <sub>2</sub> N	951.5	982.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>17</sub> N]	10076-31-0	(CH <sub>3</sub> ) <sub>2</sub> (neo-C <sub>5</sub> H <sub>11</sub> )N	939.5	970.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>17</sub> N]	4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	947.9	978.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>17</sub> N]	6006-15-1	(i-C <sub>3</sub> H <sub>7</sub> )N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	965.6	996.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>7</sub> H <sub>17</sub> N]	111-68-2	n-C <sub>7</sub> H <sub>15</sub> NH <sub>2</sub>	889.3	923.2	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>7</sub> H <sub>17</sub> N <sub>3</sub> ]	13439-88-8	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NC <sub>2</sub> H <sub>5</sub>	1019.0	1051.4	0	Rln(1/1)
[C <sub>7</sub> H <sub>17</sub> N <sub>3</sub> ]	101398-58-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	996.4	1028.8	0	Rln(1/1)
[C <sub>7</sub> H <sub>17</sub> P]	3405-42-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> (CH <sub>3</sub> )P	950.9	983.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ]	60678-73-1	(t-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub>	936.4	968.8	0	Rln(1/1)
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ]	110-95-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	985.4	1035.2	-58	80MAU/HAM
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ]	52598-10-4	(n-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub>	938.1	970.5	0	Rln(1/1)
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ]	646-19-5	1,7-Diaminoheptane	944.9	998.5	-71	80MAU/HAM
[C <sub>7</sub> H <sub>19</sub> NSi]	23138-94-5	(CH <sub>3</sub> ) <sub>3</sub> Si(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	949.4	980.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> N]	368-77-4	3-(CF <sub>3</sub> )-C <sub>6</sub> H <sub>4</sub> -CN	760.8	791.4	6	nitriles
[C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> N]	455-18-5	4-(CF <sub>3</sub> )-C <sub>6</sub> H <sub>4</sub> -CN	758.3	787.2	11.8	nitriles+Rln(2/1)
[C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> ]	626-17-5	1,3-(CN) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	750.4	779.3	11.8	nitriles+Rln(2/1)
[C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> ]	623-26-7	1,4-(CN) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	751.8	779.0	17.5	nitriles+Rln(4/1)
[C <sub>8</sub> H <sub>5</sub> Cl]	873-73-4	4-Cl-C <sub>6</sub> H <sub>4</sub> -CCH	801.7	832.4	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>5</sub> Cl]	766-83-6	3-Cl-C <sub>6</sub> H <sub>4</sub> -CCH	779.8	812.3	0	Rln(1/1)
[C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O]	2902-69-4	C <sub>6</sub> H <sub>5</sub> COCCl <sub>3</sub>	787.0	818.9	2	unsym ketones
[C <sub>8</sub> H <sub>5</sub> F]	2561-17-3	3-FC <sub>6</sub> H <sub>4</sub> -CCH	776.3	808.7	0	Rln(1/1)
[C <sub>8</sub> H <sub>5</sub> F]	766-98-3	4-FC <sub>6</sub> H <sub>4</sub> -CCH	796.7	827.4	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> O]	455-19-6	p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO	773.8	805.6	2	CH <sub>3</sub> CHO
[C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> O]	434-45-7	C <sub>6</sub> H <sub>5</sub> COCF <sub>3</sub>	767.4	799.2	2	unsym ketones
[C <sub>8</sub> H <sub>6</sub> NO]	105-07-7	4-CNC <sub>6</sub> H <sub>4</sub> CHO	766.3	796.9	6	nitriles
[C <sub>8</sub> H <sub>6</sub> ]	536-74-3	C <sub>6</sub> H <sub>5</sub> -CCH	801.3	832.0	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>6</sub> CIN]	64407-07-4	3-(CH <sub>2</sub> Cl)-C <sub>6</sub> H <sub>4</sub> -CN	780.6	811.2	6	nitriles
[C <sub>8</sub> H <sub>6</sub> CIN]	874-86-2	4-(CH <sub>2</sub> Cl)-C <sub>6</sub> H <sub>4</sub> -CN	782.1	812.8	6	nitriles
[C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> NO]	1801-10-1	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	836.0	866.9	5	amides
[C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> NO]	1891-90-3	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	831.8	862.8	5	amides
[C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> ]	253-66-7	Cinnoline	904.4	936.3	2	pyridines
[C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> ]	91-19-0	Quinoxaline	873.7	903.8	8	pyridines+Rln(2/1)
[C <sub>8</sub> H <sub>7</sub> Br]	2039-82-9	4-BrC <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>	809.8	838.7	12	propene
[C <sub>8</sub> H <sub>7</sub> Br]	2039-86-3	3-BrC <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>	793.5	822.4	12	propene
[C <sub>8</sub> H <sub>7</sub> Cl]	2039-85-2	3-ClC <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>	812.6	841.5	12	propene
[C <sub>8</sub> H <sub>7</sub> ClO]	99-02-5	3-Cl-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	815.1	846.9	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> ClO]	99-91-2	4-Cl-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	824.8	856.6	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub> ]	2905-65-9	3-Cl-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	804.4	835.4	5	esters
[C <sub>8</sub> H <sub>7</sub> ClO <sub>2</sub> ]	1126-46-1	4-Cl-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	811.1	842.1	5	esters
[C <sub>8</sub> H <sub>7</sub> FO]	403-42-9	4-F-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	826.8	858.6	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> FO]	455-36-7	3-F-C <sub>6</sub> H <sub>4</sub> COCH <sub>3</sub>	813.8	845.7	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> FO <sub>2</sub> ]	455-68-5	3-F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	801.9	832.9	5	esters
[C <sub>8</sub> H <sub>7</sub> FO <sub>2</sub> ]	403-33-8	4-F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	810.3	841.3	5	esters
[C <sub>8</sub> H <sub>7</sub> FO <sub>4</sub> S]	124397-38-2	4-SO <sub>2</sub> F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	771.6	802.6	5	esters
[C <sub>8</sub> H <sub>7</sub> FO <sub>4</sub> S]	124397-36-0	3-SO <sub>2</sub> F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	775.1	806.1	5	esters
[C <sub>8</sub> H <sub>7</sub> N]	14235-81-5	4-H <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -CCH	882.0	912.7	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>7</sub> N]	140-29-4	Benzyl cyanide	774.8	805.5	6	nitriles
[C <sub>8</sub> H <sub>7</sub> N]	120-72-9	Indole	901.9	933.4	3	pyrrole
[C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub> S]	22821-76-7	4-(CH <sub>3</sub> SO <sub>2</sub> )-C <sub>6</sub> H <sub>4</sub> -CN	768.0	798.7	6	nitriles
[C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub> S]	22821-75-6	3-(CH <sub>3</sub> SO <sub>2</sub> )-C <sub>6</sub> H <sub>4</sub> -CN	768.8	799.5	6	nitriles
[C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> ]	121-89-1	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	794.1	826.0	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> ]	100-19-6	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	792.5	824.3	2	unsym ketones
[C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub> ]	619-50-1	4-O <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	782.3	813.2	5	esters
[C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub> ]	618-95-1	3-O <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	784.7	815.7	5	esters
[C <sub>8</sub> H <sub>8</sub> ]	277-10-1	Cubane	833.6	859.9	20.6	Rln(24/2)
[C <sub>8</sub> H <sub>8</sub> ]	100-42-5	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	809.2	839.5	7.4	AUE
[C <sub>8</sub> H <sub>8</sub> ]	32796-95-5	1,2-C <sub>6</sub> H <sub>4</sub> (=CH <sub>2</sub> ) <sub>2</sub>	871.7	898.8	18	propene+Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>8</sub> H <sub>8</sub> ]	502-86-3	1,4-C <sub>6</sub> H <sub>4</sub> (=CH <sub>2</sub> ) <sub>2</sub>	873.5	900.6	18	propene+Rln(4/2)
[C <sub>8</sub> H <sub>8</sub> FeO]	12080-06-7	(C <sub>5</sub> H <sub>5</sub> )Fe(CO) <sub>2</sub> CH <sub>3</sub>	759.5	792.0	0	Rln(1/1)
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	934-37-2	2-Methylimidazo(1,2-a)pyridine	959.0	990.9	2	pyridines
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	933-69-7	5-Methylimidazo(1,2-a)pyridine	955.4	987.4	2	pyridines
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	1632-83-3	1-methylbenzimidazole	935.2	967.0	2	pyridines
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	4838-00-0	2-Methyl-2H-indazole	909.6	941.4	2	pyridines
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	874-39-5	7-Methylimidazo(1,2-a)pyridine	962.7	994.6	2	pyridines
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	13436-48-1	1-methylindazole	890.5	922.4	2	pyridines
[C <sub>8</sub> H <sub>8</sub> O]	104-87-0	4-(CH <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> CHO	820.0	851.8	2	CH <sub>3</sub> CHO
[C <sub>8</sub> H <sub>8</sub> O]	620-23-5	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO	808.1	840.0	2	CH <sub>3</sub> CHO
[C <sub>8</sub> H <sub>8</sub> O]	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	829.3	861.1	2	unsym ketones
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	99-04-7	Benzoic acid, 3-methyl	798.8	829.8	5	acids
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	123-11-5	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CHO	849.3	881.1	2	aldehydes
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	99-93-4	4-HO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	851.9	883.7	2	unsym ketones
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	819.5	850.5	5	esters
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	118-90-1	Benzoic acid, 2-methyl	807.8	838.8	5	acids
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	591-31-1	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CHO	812.2	844.1	2	aldehydes
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	121-71-1	3-HO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	831.8	863.6	2	unsym ketones
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	99-94-5	Benzoic acid, 4-methyl	805.7	836.7	5	acids
[C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> ]	19438-10-9	3-HO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	819.1	850.0	5	esters
[C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> ]	99-76-3	4-HO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	832.5	863.4	5	esters
[C <sub>8</sub> H <sub>9</sub> ]	2348-51-8	C <sub>6</sub> H <sub>5</sub> CHCH <sub>3</sub> radical	804	836.5	0	?
[C <sub>8</sub> H <sub>9</sub> N]	533-35-7	3,4-Cyclopentenopyridine	930.5	962.4	2	pyridines
[C <sub>8</sub> H <sub>9</sub> N]	533-37-9	2,3-Cyclopentenopyridine	925.6	957.5	2	pyridines
[C <sub>8</sub> H <sub>9</sub> N]	696-18-4	Aziridine, 1-phenyl	895.7	926.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>9</sub> N]	496-15-1	2,3-Dihydroindole	926.3	957.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>9</sub> NO]	619-55-6	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	869.9	900.9	5	amides
[C <sub>8</sub> H <sub>9</sub> NO]	618-47-3	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	869.9	900.9	5	amides
[C <sub>8</sub> H <sub>9</sub> NO]	99-92-3	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	877.0	908.8	2	anilines
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ]	89-87-2	2,4-Dimethylnitrobenzene	798.5	831.0	0	?
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ]	619-45-4	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	853.0	883.9	5	esters
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ]	3424-93-9	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	869.4	900.3	5	amides
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ]	5813-86-5	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	869.9	900.9	5	amides
[C <sub>8</sub> H <sub>10</sub> ]	95-47-6	o-Xylene	768.3	796.0	16	aromatics
[C <sub>8</sub> H <sub>10</sub> ]	106-42-3	p-Xylene	766.8	794.4	16	aromatics
[C <sub>8</sub> H <sub>10</sub> ]	100-41-4	C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	760.3	788.0	16	toluene
[C <sub>8</sub> H <sub>10</sub> ]	108-38-3	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	786.2	812.1	22	87LI/STO
[C <sub>8</sub> H <sub>10</sub> ClN]	698-69-1	4-ClC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	896.4	922.9	20	anilines
[C <sub>8</sub> H <sub>10</sub> FN]	403-46-3	4-FC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	898.3	924.8	20	anilines
[C <sub>8</sub> H <sub>10</sub> F <sub>3</sub> NS]	#696	4-SF <sub>5</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	872.2	898.7	20	anilines
[C <sub>8</sub> H <sub>10</sub> F <sub>3</sub> NS]	#678	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> SF <sub>5</sub>	874.5	901.0	20	anilines
[C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ]	100-23-2	N,N-Dimethyl-4-nitroaniline	870.2	896.7	20	anilines
[C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ]	619-31-8	3-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	867.6	894.1	20	anilines
[C <sub>8</sub> H <sub>10</sub> O]	538-86-3	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OCH <sub>3</sub>	787.5	816.7	11	unsym ethers
[C <sub>8</sub> H <sub>11</sub> ClO]	17530-69-7	3-Chloro-5,5-dimethylcyclohexen-2-one	836.0	867.9	2	unsym ketones
[C <sub>8</sub> H <sub>11</sub> N]	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	909.2	941.1	2	anilines
[C <sub>8</sub> H <sub>11</sub> N]	587-02-0	3-C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	866.1	897.9	2	anilines
[C <sub>8</sub> H <sub>11</sub> N]	64-04-0	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>	902.3	936.2	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>8</sub> H <sub>11</sub> N]	696-30-0	4-(i-C <sub>3</sub> H <sub>7</sub> )-C <sub>3</sub> H <sub>4</sub> N	923.8	955.7	2	pyridines
[C <sub>8</sub> H <sub>11</sub> N]	622-39-9	2-(C <sub>3</sub> H <sub>7</sub> )-pyridine	923.8	955.7	2	pyridines
[C <sub>8</sub> H <sub>11</sub> N]	75981-47-4	2-(i-C <sub>3</sub> H <sub>7</sub> )-pyridine	924.6	956.4	2	pyridines
[C <sub>8</sub> H <sub>11</sub> N]	103-69-5	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub>	892.9	924.8	2	anilines
[C <sub>8</sub> H <sub>11</sub> OP]	10311-08-7	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> )PO	876.4	908.9	0	Rln(1/1)
[C <sub>8</sub> H <sub>11</sub> P]	672-66-2	C <sub>6</sub> H <sub>5</sub> P(CH <sub>3</sub> ) <sub>2</sub>	936.8	969.2	0	Rln(1/1)
[C <sub>8</sub> H <sub>12</sub> ]	822-93-5	(c-C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> C=CH <sub>2</sub>	875.8	904.7	12	propene
[C <sub>8</sub> H <sub>12</sub> ]	497-35-8	2-Methylenebicyclo[2.2.1]heptane	831.8	860.7	12	propene
[C <sub>8</sub> H <sub>12</sub> ]	694-92-8	2-Methylbicyclo[2.2.1]hept-2-ene	812.5	845	0	Rln(1/1)
[C <sub>8</sub> H <sub>12</sub> F <sub>3</sub> N]	#363	1-Azabicyclo[2.2.2]octane,4-trifluoromethyl-	916.8	947.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ]	26458-78-6	1-azabicyclo[2.2.2]octane, 4-cyano	902.3	933.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ]	51627-76-0	1-azabicyclo[2.2.2]octane, 3-cyano	904.6	935.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ]	90196-91-1	1-azabicyclo[2.2.2]octane, 2-cyano	895.6	926.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ]	99-98-9	4-H <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	928.4	955.0	20	anilines
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ]	5744-40-1	1,3-dimethyl-5-ethoxycarbonylpyrazole	893.1	924.9	2	pyridines

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ]	5744-51-4	1,5-dimethyl-3-ethoxycarbonylpyrazole	901.5	933.4	2	pyridines
[C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> ]	2578-58-7	his-gly	<b>955.5</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> ]	2489-13-6	gly-his	<b>955.5</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>12</sub> O]	4694-17-1	5,5-Dimethylcyclohex-2-ene-1-one	837.9	869.8	2	unsym ketones
[C <sub>8</sub> H <sub>12</sub> O]	10599-58-3	2,3,4,5-tetramethylfuran	884.8	915.5	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>13</sub> N]	#249	1-Azabicyclo[2.2.2]oct-2-ene, 3-methyl	950.8	981.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>13</sub> N]	22207-84-7	1-Azabicyclo[2.2.2]octane, 3-methylene	946.4	977.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>13</sub> N]	609-72-3	N,N,2-trimethylaniline	925.3	951.8	20	anilines
[C <sub>8</sub> H <sub>13</sub> NO]	873-95-0	3-Amino-5,5-dimethylcyclohex-2-enone	915.9	946.9	5	amide-like
[C <sub>8</sub> H <sub>14</sub> ]	72014-90-5	(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub>	841.0	869.9	12	propene
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	141665-17-0	1-methyl-5-t-butylpyrazole	907.3	939.2	2	pyridines
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	141665-16-9	1-methyl-3-t-butylpyrazole	912.5	944.4	2	pyridines
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	19616-52-5	1,5-diazabicyclo[4.4.0]dec-6-ene (DBD)	1014.0	1046.4	0	Rln(1/1)
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	96440-80-1	3(5)-methyl-5(3)-t-butylpyrazole	914.3	946.2	2	pyridines
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	13618-34-3	3,5-diethyl-4-methylpyrazole	919.2	952.8	-4	pyridines + Rln(1/2)
[C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> O <sub>5</sub> ]	637-84-3	tetraglycine	928.2	973.8	-44	93CHE/WU
[C <sub>8</sub> H <sub>14</sub> O]	502-49-8	cyclooctanone	819.6	849.4	9	sym ketones
[C <sub>8</sub> H <sub>14</sub> O]	823-76-7	c-C <sub>6</sub> H <sub>11</sub> COCH <sub>3</sub>	809.5	841.4	2	unsym ketones
[C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ]	4630-82-4	c-C <sub>6</sub> H <sub>11</sub> COOCH <sub>3</sub>	815.3	846.2	5	esters
[C <sub>8</sub> H <sub>15</sub> N]	5261-65-4	1-azabicyclo[2.2.2]-octane, 2-methyl	956.1	986.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>15</sub> N]	45651-41-0	1-azabicyclo[2.2.2]-octane, 4-methyl	948.6	979.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>15</sub> N]	35079-50-6	1,4,4-(CH <sub>3</sub> ) <sub>3</sub> -1,2,3,4-tetrahydropyridine	947.3	979.9	0	estimate
[C <sub>8</sub> H <sub>15</sub> N]	695-88-5	1-azabicyclo[2.2.2]-octane, 3-methyl	951.7	982.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>15</sub> NO]	17997-65-8	cis-3-Aminobicyclo[2.2.2]octan-2-ol	916.2	948.6	0	Rln(1/1)
[C <sub>8</sub> H <sub>15</sub> NO]	40335-14-6	trans-3-Aminobicyclo[2.2.2]octan-2-ol	899.2	933.1	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> ]	84030-20-6	7-methyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene	1030.2	1062.7	0	Rln(1/1)
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ]	14287-92-4	2,3-diazabicyclo[2.2.2]octane, 2,3-dimethyl	950.0	980.7	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ]	3661-15-2	Pyridazino[1,2-a]pyridazine, octahydro-	947.9	978.7	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ]	18389-95-2	1,1'-bipyrolidine	949.0	979.7	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	3303-45-5	ala-val	<b>874.1</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	27493-61-4	val-ala	<b>883.5</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> ]	13588-94-8	val-ser	<b>874.1</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>16</sub> O]	19752-94-4	C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> OCH <sub>3</sub>	801.6	833.5	2	unsym ketones
[C <sub>8</sub> H <sub>16</sub> O]	5857-36-3	i-C <sub>3</sub> H <sub>7</sub> CO(t-C <sub>4</sub> H <sub>9</sub> )	825.0	856.9	2	unsym ketones
[C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> ]	294-93-9	12-crown-4	890.5	927.2	-14	84SHA/BLA; 83MAU
[C <sub>8</sub> H <sub>17</sub> N]	27644-32-2	N,3,5-Trimethylpiperidine	947.2	978.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>17</sub> N]	1003-84-5	1,4,4-Trimethylpiperidine	934.7	965.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>17</sub> N]	98-94-2	c-C <sub>6</sub> H <sub>11</sub> N(CH <sub>3</sub> ) <sub>2</sub>	952.6	983.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>17</sub> NO]	26153-90-2	neo-C <sub>5</sub> H <sub>11</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	896.7	927.7	5	amides
[C <sub>8</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> ]	997-62-6	gly-lys	<b>945.6</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> ]	7563-03-3	lys-gly	<b>946.0</b>	NE	NE	not estimated
[C <sub>8</sub> H <sub>17</sub> P]	#181	(CH <sub>2</sub> ) <sub>2</sub> PCH <sub>3</sub>	947.2	979.7	0	Rln(1/1)
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ]	112752-57-5	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(i-C <sub>3</sub> H <sub>7</sub> )	1004.6	1037.0	0	Rln(1/1)
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ]	133835-17-3	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1,1-dimethylpropyl)	989.6	1022.0	0	Rln(1/1)
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ]	94793-23-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(n-C <sub>5</sub> H <sub>11</sub> )	985.5	1018.0	0	Rln(1/1)
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ]	147350-05-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> )	1005.9	1038.3	0	Rln(1/1)
[C <sub>8</sub> H <sub>18</sub> O]	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	818.3	845.7	17	sym ethers
[C <sub>8</sub> H <sub>18</sub> O]	6163-66-2	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	860.0	887.4	17	sym ethers
[C <sub>8</sub> H <sub>18</sub> O]	6863-58-7	(sec-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	838.5	865.9	17	sym ethers
[C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> ]	112-49-2	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> O] <sub>3</sub> CH <sub>3</sub>	892.4	946.6	-73	84SHA/BLA; 83MAU
[C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> ]	112-60-7	HO[CH <sub>2</sub> CH <sub>2</sub> O] <sub>4</sub> H	>910	NE	NE	not estimated
[C <sub>8</sub> H <sub>18</sub> S]	544-40-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	842.1	871.8	9	sym sulfides
[C <sub>8</sub> H <sub>18</sub> S]	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	864.0	893.8	9	sym sulfides
[C <sub>8</sub> H <sub>19</sub> N]	111-86-4	n-(C <sub>8</sub> H <sub>17</sub> )NH <sub>2</sub>	895.0	928.9	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>8</sub> H <sub>19</sub> N]	7087-68-5	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	963.5	994.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>19</sub> N]	111-92-2	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	935.3	968.5	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>8</sub> H <sub>19</sub> N]	110-96-3	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	925.1	958.1	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>8</sub> H <sub>19</sub> N]	626-23-3	(sec-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	947.5	980.7	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>8</sub> H <sub>19</sub> N]	21981-37-3	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	954.7	987.9	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>8</sub> H <sub>19</sub> N <sub>3</sub> ]	151328-45-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	1016.1	1048.5	0	Rln(1/1)
[C <sub>8</sub> H <sub>19</sub> N <sub>3</sub> ]	29166-71-0	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(i-C <sub>3</sub> H <sub>7</sub> )	1023.2	1055.6	0	Rln(1/1)
[C <sub>8</sub> H <sub>19</sub> N <sub>3</sub> ]	139033-04-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	1010.6	1057.7	-49	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>
[C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> ]	4267-00-9	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	935.3	964.3	11.5	Rln(4/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> ]	23337-88-4	Hydrazine, 1,2-dimethyl-1,2-dipropyl	941.2	971.9	5.8	Rln(2/1)
[C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> ]	111-51-3	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	992.7	1046.3	-71	80MAU/HAM
[C <sub>8</sub> H <sub>21</sub> NSi]	28247-29-2	(CH <sub>3</sub> ) <sub>3</sub> Si(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	949.4	980.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>8</sub> H <sub>21</sub> NSi]	66365-05-7	(CH <sub>3</sub> ) <sub>2</sub> (t-C <sub>4</sub> H <sub>9</sub> )SiN(CH <sub>3</sub> ) <sub>2</sub>	938.8	969.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>5</sub> F <sub>3</sub> ]	705-28-2	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH	773.8	806.2	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> ClO]	120136-29-0	3-Cl-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -CCH	839.5	871.9	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> ClS]	120136-30-3	3-Cl-4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>3</sub> -CCH	836.1	868.6	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> FO]	120136-28-9	3-F-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -CCH	839.5	871.9	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> ]	402-24-4	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>	781.8	810.7	12	propene
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O]	709-63-7	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	805.0	836.9	2	unsym ketones
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O]	349-76-8	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	803.7	835.6	2	unsym ketones
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ]	2967-66-0	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	796.5	827.5	5	esters
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ]	2557-13-3	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	795.7	826.6	5	esters
[C <sub>9</sub> H <sub>7</sub> MnO <sub>3</sub> ]	12108-13-3	(CH <sub>3</sub> C <sub>5</sub> H <sub>4</sub> )Mn(CO) <sub>3</sub>	801.3	833.8	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> N]	91-22-5	Quinoline	921.4	953.2	2	pyridines
[C <sub>9</sub> H <sub>7</sub> N]	119-65-3	Isoquinoline	919.9	951.7	2	pyridines
[C <sub>9</sub> H <sub>7</sub> NO]	1443-80-7	4-CN-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	795.0	826.8	2	unsym ketones
[C <sub>9</sub> H <sub>7</sub> NO]	6136-68-1	3-CN-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	795.4	827.2	2	unsym ketones
[C <sub>9</sub> H <sub>7</sub> NO]	1613-37-2	Quinoline-1-oxide	910.8	943.3	0	Rln(1/1)
[C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub> ]	13531-48-1	3-CN-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	786.5	817.4	5	esters
[C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub> ]	1129-35-7	4-CN-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	785.6	816.6	5	esters
[C <sub>9</sub> H <sub>8</sub> ]	766-82-5	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH	810.6	843.0	0	Rln(1/1)
[C <sub>9</sub> H <sub>8</sub> ]	95-13-6	indene	819.6	848.8	11	91MAU/SIE
[C <sub>9</sub> H <sub>8</sub> ]	766-97-2	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH	822.5	853.2	5.8	Rln(2/1)
[C <sub>9</sub> H <sub>8</sub> CrO <sub>3</sub> ]	41311-89-1	(C <sub>9</sub> H <sub>5</sub> )Cr(CO) <sub>3</sub> CH <sub>3</sub>	827.3	859.8	0	Rln(1/1)
[C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> ]	2458-26-6	3(5)-phenylpyrazole	882.3	914.2	2	pyridines
[C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> ]	10199-68-5	4-(C <sub>6</sub> H <sub>5</sub> )-pyrazole	871.8	906.0	-5.8	Rln(1/2)
[C <sub>9</sub> H <sub>8</sub> O]	768-60-5	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -CCH	855.7	886.4	5.8	Rln(2/1)
[C <sub>9</sub> H <sub>8</sub> O]	4265-25-2	2-methylbenzofuran	827.2	859.6	0	?
[C <sub>9</sub> H <sub>8</sub> O <sub>3</sub> ]	1571-08-0	4-HC(O)-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	801.9	832.9	5	esters
[C <sub>9</sub> H <sub>8</sub> S]	56041-85-1	4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -CCH	854.1	886.6	0	?
[C <sub>9</sub> H <sub>9</sub> Cl]	1712-70-5	4-ClC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	825.4	854.3	12	propene
[C <sub>9</sub> H <sub>9</sub> ClOS]	32467-66-6	3-Cl-4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	848.6	880.4	2	unsym ketones
[C <sub>9</sub> H <sub>9</sub> ClO <sub>2</sub> ]	37612-52-5	3-Cl-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	851.9	883.7	2	unsym ketones
[C <sub>9</sub> H <sub>9</sub> ClO <sub>2</sub> S]	105442-23-7	3-Cl-4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	825.4	856.3	5	esters
[C <sub>9</sub> H <sub>9</sub> ClO <sub>3</sub> ]	37908-98-8	3-Cl-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	827.5	858.4	5	esters
[C <sub>9</sub> H <sub>9</sub> F]	3825-81-8	3-FC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	810.8	839.7	12	propene
[C <sub>9</sub> H <sub>9</sub> F]	350-40-3	4-FC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	833.7	862.6	12	propene
[C <sub>9</sub> H <sub>9</sub> N]	6921-29-5	(HCCCH <sub>2</sub> ) <sub>3</sub> N	894.4	925.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> ]	64416-49-5	3-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	783.3	812.2	12	propene
[C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> ]	1830-68-8	4-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	786.5	815.4	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	873-49-4	c-C <sub>3</sub> H <sub>5</sub> -C <sub>6</sub> H <sub>5</sub>	802.4	834.9	0	Rln(1/1)
[C <sub>9</sub> H <sub>10</sub> ]	873-66-5	Benzene, trans-(2-methylethenyl)	805.3	834.2	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	611-15-4	Benzene, 1-ethenyl-2-methyl	826.3	855.2	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	766-90-5	Benzene, cis-(2-methylethenyl)	807.5	836.4	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	100-80-1	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>	820.5	849.4	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	622-97-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>	832.8	861.7	12	propene
[C <sub>9</sub> H <sub>10</sub> ]	98-83-9	C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>	835.3	864.2	12	propene
[C <sub>9</sub> H <sub>10</sub> CINO]	14062-80-7	4-Cl-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.9</b>	927.9	5	amides
[C <sub>9</sub> H <sub>10</sub> CINO]	24167-52-0	3-Cl-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.9</b>	927.9	5	amides
[C <sub>9</sub> H <sub>10</sub> FNO]	24167-56-4	4-F-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.9</b>	927.9	5	amides
[C <sub>9</sub> H <sub>10</sub> FNO]	33322-64-4	3-F-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.9</b>	927.9	5	amides
[C <sub>9</sub> H <sub>10</sub> F <sub>3</sub> N]	329-00-0	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	881.8	908.3	20	anilines
[C <sub>9</sub> H <sub>10</sub> F <sub>3</sub> N]	329-17-9	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	876.8	903.2	20	anilines
[C <sub>9</sub> H <sub>10</sub> F <sub>3</sub> NS]	#585	3-(SCF <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	887.7	914.2	20	anilines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	1197-19-9	1,4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> CN	862.6	889.1	20	anilines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	875-80-9	2,3-Dimethylimidazo(1,2-a)pyridine	966.4	998.2	2	pyridines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	6188-30-3	2,5-Dimethylimidazo(1,2-a)pyridine	964.5	996.4	2	pyridines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	3268-61-9	2,7-Dimethylimidazo(1,2-a)pyridine	968.6	1000.5	2	pyridines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	38803-30-4	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> CN	868.1	894.6	20	anilines
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ]	7291-02-3	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>869.9</b>	900.9	5	amides
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ]	7291-01-2	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>869.9</b>	900.9	5	amides
[C <sub>9</sub> H <sub>10</sub> O]	93-55-0	C <sub>6</sub> H <sub>5</sub> COC <sub>2</sub> H <sub>5</sub>	835.6	867.4	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> O]	103-79-7	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> COCH <sub>3</sub>	810.8	842.6	2	unsym ketones

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>9</sub> H <sub>10</sub> O]	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	843.6	875.5	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> O]	585-74-0	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	836.4	868.2	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> OS]	1441-99-2	3-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	834.7	866.6	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> OS]	1778-09-2	4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	856.3	888.2	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	99-75-2	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	830.6	861.5	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	100-06-1	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	863.7	895.6	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	586-37-8	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	839.3	871.2	2	unsym ketones
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	99-36-5	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	826.8	857.7	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	89-71-4	2-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	827.3	858.3	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> S]	90721-40-7	3-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	822.4	853.4	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> S]	3795-79-7	4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	833.3	864.3	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> ]	5368-81-0	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	825.8	856.7	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> ]	121-98-2	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	839.6	870.6	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>4</sub> S]	22821-70-1	4-CH <sub>3</sub> SO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	796.7	827.7	5	esters
[C <sub>9</sub> H <sub>10</sub> O <sub>4</sub> S]	22821-69-8	3-CH <sub>3</sub> SO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	799.5	830.5	5	esters
[C <sub>9</sub> H <sub>11</sub> ]	16804-70-9	C <sub>6</sub> H <sub>5</sub> C(CH <sub>3</sub> ) <sub>2</sub> radical	<b>809.7</b>	842.2	0	Rln(1/1)?
[C <sub>9</sub> H <sub>11</sub> ]	19019-92-2	C <sub>6</sub> H <sub>5</sub> (CHC <sub>2</sub> H <sub>5</sub> ) radical	<b>809.7</b>	842.2	0	?
[C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> ]	119044-60-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-bromophenyl)	948.9	981.3	0	Rln(1/1)
[C <sub>9</sub> H <sub>11</sub> N]	36556-06-6	Isoquinoline, 5,6,7,8-tetrahydro-	934.7	966.6	2	pyridines
[C <sub>9</sub> H <sub>11</sub> N]	1962-08-9	4-H <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	903.3	929.8	20	anilines
[C <sub>9</sub> H <sub>11</sub> N]	3334-89-2	Azetidine, 1-phenyl	902.4	933.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>11</sub> N]	10500-57-9	Quinoline, 5,6,7,8-tetrahydro-	934.1	966.0	2	pyridines
[C <sub>9</sub> H <sub>11</sub> NO]	100-10-7	4-CHOC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	898.3	924.8	20	anilines
[C <sub>9</sub> H <sub>11</sub> NO]	611-74-5	C <sub>6</sub> H <sub>5</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	901.8	932.7	5	amides
[C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> ]	603-71-4	2,4,6-Trimethylnitrobenzene	793.1	823.8	5.8	Rln(2/1)
[C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> ]	63-91-2	L-phenylalanine	888.9	922.9	-5	CH <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>
[C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub> ]	60-18-4	L-tyrosine	892.1	926	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>9</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> ]	74739-51-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-nitrophenyl)	917.8	950.2	0	Rln(1/1)
[C <sub>9</sub> H <sub>12</sub> ]	108-67-8	1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	808.6	836.2	16.2	86STO/XI
[C <sub>9</sub> H <sub>12</sub> ]	103-65-1	n-C <sub>3</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>	762.4	790.1	16	aromatics
[C <sub>9</sub> H <sub>12</sub> ]	98-82-8	i-C <sub>3</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>	763.9	791.6	16	aromatics
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> ]	56687-95-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-phenyl	951.3	983.8	0	Rln(1/1)
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> ]	494-97-3	3-(2-pyrrolidinyl)pyridine	931.0	964.0	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O]	33322-60-0	3-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>913.5</b>	944.4	5	amides
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O]	6331-71-1	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>925.9</b>	956.9	5	amides
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> ]	37687-24-4	3,5-dithoxycarbonylpyrazole	849.7	881.6	2	pyridines
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub> ]	58-96-8	Uridine	916.6	947.6	5	amides
[C <sub>9</sub> H <sub>12</sub> O <sub>3</sub> ]	621-23-8	1,3,5-C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>	898.2	926.7	13	aromatics
[C <sub>9</sub> H <sub>13</sub> N]	3978-81-2	4-(t-C <sub>4</sub> H <sub>9</sub> )-pyridine	925.8	957.7	2	pyridines
[C <sub>9</sub> H <sub>13</sub> N]	613-97-8	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )	912.4	939.0	20	anilines
[C <sub>9</sub> H <sub>13</sub> N]	103-83-3	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	937.4	968.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>13</sub> N]	121-72-2	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	915.7	942.1	20	anilines
[C <sub>9</sub> H <sub>13</sub> N]	5944-41-2	2-(t-C <sub>4</sub> H <sub>9</sub> )-pyridine	929.8	961.7	2	pyridines
[C <sub>9</sub> H <sub>13</sub> N]	99-97-8	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	918.1	950.0	2	anilines
[C <sub>9</sub> H <sub>13</sub> N]	935-28-4	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	940.4	972.3	2	pyridines
[C <sub>9</sub> H <sub>13</sub> NO]	701-56-4	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	922.4	949.1	20	anilines
[C <sub>9</sub> H <sub>13</sub> NO]	15799-79-8	3-Methoxy-N,N-dimethylbenzamine	894.1	920.6	20	anilines
[C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	951-77-9	Deoxycytidine	956.0	988.4	0	Rln(1/1)
[C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> ]	65-46-3	cytidine	950.0	982.5	0	Rln(1/1)
[C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>6</sub> ]	5627-05-4	5,6-Dihydrouridine	<b>841.7</b>	874.2	0	Rln(1/1)
[C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> ]	111062-19-2	1H-dimidazo[1,2-d:2',1'-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro (TTT)	> 1049	> 1081	0	Rln(1/1)
[C <sub>9</sub> H <sub>14</sub> O]	78-59-1	Isophorone	861.6	893.5	2	unsym ketones
[C <sub>9</sub> H <sub>14</sub> O <sub>2</sub> ]	4683-45-8	3-Methoxy-5,5-dimethylcyclohex-2-ene	890.1	922.6	0	?
[C <sub>9</sub> H <sub>15</sub> N]	102-70-5	(CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>3</sub> N	941.3	972.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>15</sub> N]	7148-07-4	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	988.4	1019.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	14379-76-1	gly-gly-pro	<b>915.5</b>	NE	NE	not estimated
[C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	7561-25-3	pro-gly-gly	<b>925.1</b>	NE	NE	not estimated
[C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	2441-63-6	gly-pro-gly	<b>915.5</b>	NE	NE	not estimated
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ]	6674-22-2	1,8-diazabicyclo [5.4.0]undec-7-ene	1015.5	1047.9	0	Rln(1/1)
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> ]	13433-04-0	asp-val	<b>874.1</b>	NE	NE	not estimated
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> ]	20556-16-5	val-asp	<b>874.1</b>	NE	NE	not estimated
[C <sub>9</sub> H <sub>16</sub> O]	3350-30-9	c-Nonanone	822.8	852.6	9	sym ketones
[C <sub>9</sub> H <sub>17</sub> N]	673-33-6	c-C <sub>5</sub> H <sub>10</sub> NCH=C(CH <sub>3</sub> ) <sub>2</sub>	949.4	978.2	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub> ]	#231	3,3-Dimethoxy-1-azabicyclo[2.2.2]octane	954.7	985.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>17</sub> N <sub>3</sub> ]	95510-44-4	7-ethyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ETBD)	1035.8	1068.2	0	Rln(1/1)
[C <sub>9</sub> H <sub>18</sub> NO]	2564-83-2	2,2,6,6-tetramethyl-1-piperidinyloxy radical	<b>849.8</b>	882.3	0	Rln(1/1)
[C <sub>9</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> ]	5874-90-8	tri-L-alanine	924.1	NE	NE	not estimated
[C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> ]	283-58-9	1,5-Diazabicyclo[3.3.3]undecane	940.1	971.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> ]	3459-75-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(c-hexyl)	987.9	1020.4	0	Rln(1/1)
[C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> ]	22766-69-4	1-Azabicyclo[2.2.2]octane,4-N,N-dimethylamino-	952.9	983.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>18</sub> O]	815-24-7	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CO	831.5	861.3	9	sym ketones
[C <sub>9</sub> H <sub>18</sub> O]	502-56-7	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CO	821.9	853.7	2	unsym ketones
[C <sub>9</sub> H <sub>18</sub> S]	54396-69-9	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CS	852.0	881.8	9	sym ketones
[C <sub>9</sub> H <sub>19</sub> N]	16607-80-0	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	944.7	975.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>19</sub> N]	10315-89-6	N-Isobutylpiperidine	943.5	974.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>19</sub> N]	768-66-1	2,2,6,6-Tetramethyl-piperidine	953.9	987.0	-1.9	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ]	85599-94-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl)	984.9	1017.4	0	Rln(1/1)
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ]	151328-44-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> )	1010.9	1043.3	0	Rln(1/1)
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ]	94793-24-5	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>5</sub> H <sub>11</sub> )	1002.1	1034.5	0	Rln(1/1)
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ]	151328-42-6	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>3</sub> H <sub>7</sub> )	1005.5	1037.9	0	Rln(1/1)
[C <sub>9</sub> H <sub>21</sub> N]	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	960.1	991.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>21</sub> N]	3733-36-6	(t-C <sub>4</sub> H <sub>9</sub> )C(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	951.4	982.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>21</sub> N]	58471-09-3	(t-C <sub>5</sub> H <sub>11</sub> )(t-C <sub>4</sub> H <sub>9</sub> )NH	958.2	991.4	-2	(CH <sub>3</sub> ) <sub>2</sub> NH
[C <sub>9</sub> H <sub>21</sub> N <sub>3</sub> ]	34331-58-3	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(t-C <sub>4</sub> H <sub>9</sub> )	1029.4	1061.8	0	Rln(1/1)
[C <sub>9</sub> H <sub>19</sub> N]	15673-04-8	(CH <sub>3</sub> ) <sub>3</sub> C(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	942.0	973.0	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>9</sub> H <sub>21</sub> N <sub>3</sub> ]	151328-47-1	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N-(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	1030.5	1077.5	-49	80MAU/HAM
[C <sub>9</sub> H <sub>21</sub> OP]	17513-58-5	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> PO	924.5	954.4	9.1	Rln(3/1)
[C <sub>9</sub> H <sub>21</sub> OP]	1496-94-2	OP(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub>	918.4	948.2	9.1	Rln(3/1)
[C <sub>9</sub> H <sub>24</sub> N <sub>3</sub> OP]	2327-88-0	OP(CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	965.2	997.7	0	Rln(1/1)
[C <sub>10</sub> H <sub>7</sub> CrO <sub>3</sub> ]	32984-97-7	(C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> )Cr(CO) <sub>3</sub>	819.9	852.4	0	Rln(1/1)
[C <sub>10</sub> H <sub>8</sub> ]	275-51-4	azulene	896	925.2	11	average
[C <sub>10</sub> H <sub>8</sub> ]	91-20-3	Naphthalene	779.4	802.9	30	88LI/STO
[C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> ]	55186-75-9	4-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )CH <sub>2</sub>	796.6	825.5	12	propene
[C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> ]	368-79-6	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	794.8	823.7	12	propene
[C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> N]	34060-81-6	3,5-(CF <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	858.4	884.9	20	anilines
[C <sub>10</sub> H <sub>9</sub> N]	134-32-7	1-Naphthalenamine	875.1	907.0	2	anilines
[C <sub>10</sub> H <sub>10</sub> ]	6366-06-9	3,5-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> .CCH	819.7	850.4	5.8	Rln(2/1)
[C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> NO]	25771-21-5	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>873.5</b>	904.5	5	amides
[C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> NO]	90238-10-1	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>876.2</b>	907.1	5	amides
[C <sub>10</sub> H <sub>10</sub> Fe]	102-54-5	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Fe	841.3	863.6	34	average
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ]	3463-27-2	1-methyl-5-phenylpyrazole	900.5	932.4	2	pyridines
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ]	3463-26-1	1-methyl-3-phenylpyrazole	900.8	932.6	2	pyridines
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ]	479-27-6	1,8-Diaminonaphthalene	912.1	944.5	0	?
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ]	3347-62-4	3(5)-methyl-5(3)-phenylpyrazole	900.2	932.1	2	pyridines
[C <sub>10</sub> H <sub>10</sub> Ni]	1271-28-9	Ni(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub>	907.3	935.7	13.4	Rln(5/1)
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ]	6781-42-6	3-CH <sub>3</sub> CO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	822.3	852.0	9	sym ketones
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ]	1009-61-6	4-CH <sub>3</sub> CO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	821.0	850.8	9	sym ketones
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ]	90843-31-5	1-(2,3-dihydro-5-benzofuranyl)-ethanone	870.7	902.6	2	unsym ketones
[C <sub>10</sub> H <sub>10</sub> O <sub>3</sub> ]	13031-43-1	4-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	821.3	853.2	2	unsym ketones
[C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> ]	1459-93-4	3-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	814.3	843.5	10.8	esters+Rln(2/1)
[C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> ]	120-61-6	4-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	812.3	843.2	5	esters
[C <sub>10</sub> H <sub>10</sub> Ru]	1287-13-4	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Ru	876.8	899.1	34	(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Fe
[C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> ]	119044-58-5	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-cyanophenyl)	919.8	952.2	0	Rln(1/1)
[C <sub>10</sub> H <sub>12</sub> ]	6921-43-3	Benzene, 1-cyclopropyl-4-methyl-	813.8	846.3	0	?
[C <sub>10</sub> H <sub>12</sub> ]	7399-49-7	Benzene, 1-methyl-2-(1-methylethenyl)-	828.9	857.8	12	propene
[C <sub>10</sub> H <sub>12</sub> ]	27546-46-9	Benzene, 1-cyclopropyl-2-methyl-	807.9	840.4	0	?
[C <sub>10</sub> H <sub>12</sub> ]	1195-32-0	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )CH <sub>2</sub>	852.9	881.8	12	propene
[C <sub>10</sub> H <sub>12</sub> ]	19714-73-9	Benzene, 1-cyclopropyl-3-methyl-	803.3	835.8	0	?
[C <sub>10</sub> H <sub>12</sub> ]	1124-20-5	Benzene, 1-methyl-3-(1-methylethenyl)-	838.7	867.6	12	propene
[C <sub>10</sub> H <sub>12</sub> ]	119-64-2	1,2,3,4-Tetrahydronaphthalene	782.1	809.7	16	aromatics
[C <sub>10</sub> H <sub>12</sub> ]	26444-18-8	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	842.4	871.3	12	propene
[C <sub>10</sub> H <sub>12</sub> CIN]	4280-30-2	Pyrrrolidine, 1-(4-chlorophenyl)	906.6	937.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>10</sub> H <sub>12</sub> NS]	74362-50-8	4-CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	917.4	946.2	12	propene
[C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> ]	34165-19-0	2,3,5-Trimethylimidazo(1,2-a)-pyridine	973.7	1005.5	2	pyridines
[C <sub>10</sub> H <sub>12</sub> O]	25108-57-0	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	843.7	872.6	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>10</sub> H <sub>12</sub> O]	2142-73-6	2,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	841.6	873.5	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O]	5379-16-8	3,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	844.2	876.0	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O]	3637-01-2	3,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	851.0	882.8	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O]	1712-69-2	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	882.2	911.1	12	propene
[C <sub>10</sub> H <sub>12</sub> O]	2142-76-9	2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	825.2	857.0	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O]	89-74-7	2,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	850.8	882.6	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O]	2142-71-4	2,3-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	842.7	874.6	2	unsym ketones
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	23617-71-2	2,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	837.2	868.2	5	esters
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	15012-36-9	2,3-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	832.7	863.6	5	esters
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	14920-81-1	2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	824.3	855.3	5	esters
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	38404-42-1	3,4-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> -CO <sub>2</sub> CH <sub>3</sub>	837.5	868.5	5	esters
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	13730-55-7	2,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	833.7	864.7	5	esters
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	25081-39-4	3,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	833.4	864.3	5	esters
[C <sub>10</sub> H <sub>12</sub> S]	#838	3-(CH <sub>3</sub> S)C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	850.6	879.5	12	propene
[C <sub>10</sub> H <sub>13</sub> N]	4096-21-3	N-Phenylpyrrolidine	915.1	941.6	20	anilines
[C <sub>10</sub> H <sub>13</sub> NO]	18992-80-8	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COCH <sub>3</sub>	901.5	928.0	20	anilines
[C <sub>10</sub> H <sub>13</sub> NO]	6935-65-5	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.0</b>	927.0	5	amides
[C <sub>10</sub> H <sub>13</sub> NO]	14062-78-3	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.0</b>	927.0	5	amides
[C <sub>10</sub> H <sub>13</sub> NO]	2124-31-4	4-[(CH <sub>3</sub> ) <sub>2</sub> N]-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	906.3	932.8	20	anilines
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	7290-99-5	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>896.0</b>	927.0	5	amides
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	1202-25-1	4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	894.1	920.6	20	anilines
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	16518-64-2	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	903.8	930.2	20	anilines
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	7291-00-1	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	<b>917.4</b>	948.3	5	amides
[C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> ]	118-00-3	guanosine	960.9	993.4	0	Rln(1/1)
[C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>3</sub> ]	958-09-8	Deoxyadenosine	959.1	991.5	0	Rln(1/1)
[C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	961-07-9	Deoxyguanosine	962.9	995.4	0	Rln(1/1)
[C <sub>10</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	58-61-7	adenosine	956.8	989.3	0	Rln(1/1)
[C <sub>10</sub> H <sub>14</sub> ]	527-53-7	1,2,3,5-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H <sub>2</sub>	816.5	845.6	11.4	86STO/XI
[C <sub>10</sub> H <sub>14</sub> ]	104-51-8	n-C <sub>4</sub> H <sub>9</sub> C <sub>6</sub> H <sub>5</sub>	764.2	791.9	16	aromatics
[C <sub>10</sub> H <sub>14</sub> BrN]	50638-54-5	N,N,2,6-Tetramethylaniline,4-bromo-	902.9	935.4	0	anilines-restricted
[C <sub>10</sub> H <sub>14</sub> CIN]	2873-89-4	4-ClC <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	899.2	931.0	2	anilines
[C <sub>10</sub> H <sub>14</sub> FN]	14994-35-5	N,N,2,6-Tetramethylaniline,4-fluoro	910.7	943.2	0	anilines-restricted
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	54-11-5	3-(2-(N-methylpyrrolidinyl))pyridine	932.6	963.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	119044-57-4	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NCH <sub>3</sub>	1000.9	1033.3	0	Rln(1/1)
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	27159-75-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(phenylmethyl)	981.7	1014.1	0	Rln(1/1)
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	56638-68-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-methylphenyl)	956.1	988.6	0	Rln(1/1)
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O]	59-26-7	N,N-diethylnicotinamide	909.0	940.9	2	pyridines
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ]	24558-36-9	N,N,2,6-Tetramethyl-4-nitroaniline	886.0	918.4	0	anilines-restricted
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S]	28809-04-3	S-(2-(4-pyrindyl)ethyl)cysteine	> 869	NE	NE	not estimated
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> ]	100852-80-0	1-methyl-3,5-diethoxycarbonylpyrazole	881.5	913.4	2	pyridines
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>5</sub> ]	50-89-5	Thymidine	915.9	948.3	0	Rln(1/1)
[C <sub>10</sub> H <sub>14</sub> O <sub>3</sub> ]	#997	3-Acetyl-5,5-dimethylcyclohexen-2-one	828.8	861.2	0	Rln(1/1)
[C <sub>10</sub> H <sub>15</sub> N]	769-06-2	N,N,2,6-Tetramethylaniline	923.2	954.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>10</sub> H <sub>15</sub> N]	4913-13-7	3,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	924.3	956.1	2	anilines
[C <sub>10</sub> H <sub>15</sub> N]	91-66-7	C <sub>6</sub> H <sub>5</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	927.9	959.8	2	anilines
[C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	7451-76-5	gly-gly-his	979.5	NE	NE	not estimated
[C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	32999-80-7	his-gly-gly	<b>946.0</b>	NE	NE	not estimated
[C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ]	7758-33-0	gly-his-gly	<b>955.5</b>	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ]	45214-22-0	gly-lys-gly	<b>955.5</b>	NE	NE	not estimated
[C <sub>10</sub> H <sub>16</sub> ]	16609-28-2	1,5,5-Trimethyl-3-methylenecyclohexene	874.2	904.9	6	propene-Rln2
[C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> ]	704-01-8	1,2-(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub>	950.2	982.6	0	?
[C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	20488-28-2	pro-pro	<b>944.8</b>	NE	NE	not estimated
[C <sub>10</sub> H <sub>16</sub> N <sub>4</sub> ]	111062-21-6	1H-dimidazo[1,2-d:2',1'-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro-1-methyl (MTTT)	> 1060	> 1091	0	Rln(1/1)
[C <sub>10</sub> H <sub>16</sub> O]	76-22-2	Camphor	827.3	859.2	2	unsym ketones
[C <sub>10</sub> H <sub>16</sub> S]	7519-74-6	thiocamphor	852.0	883.9	2	unsym ketones
[C <sub>10</sub> H <sub>17</sub> N]	768-94-5	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decane-1-amine	916.3	948.8	0	Rln(1/1)
[C <sub>10</sub> H <sub>17</sub> NO]	31039-88-0	3-(N,N-Dimethylamino)-5,5-dimethyl-cyclohex-2-en-1-one	952.9	983.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>10</sub> H <sub>17</sub> NO]	33540-02-2	tricyclo[4.4.0.0 <sup>3,8</sup> ]decan-4-ol-5-amino, stereoisomer	914.5	947.0	0	?
[C <sub>10</sub> H <sub>17</sub> NO]	33701-54-1	5-amino-tricyclo[4.4.0.0 <sup>3,8</sup> ]decan-4-ol	896.0	928.4	0	?
[C <sub>10</sub> H <sub>17</sub> NO]	52305-49-4	tricyclo[4.4.0.0 <sup>3,8</sup> ]decan-4-ol-5-amino, stereoisomer	916.6	949.0	0	?
[C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> ]	7093-67-6	pentaglycine	921	NE	NE	not estimated

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> ]	52899-09-9	pro-val	909.0	NE	NE	not estimated
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> ]	20488-27-1	val-pro	918.8	NE	NE	not estimated
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> ]	3062-07-5	val-glu	921	NE	NE	not estimated
[C <sub>10</sub> H <sub>19</sub> N]	31023-92-4	1-Azabicyclo[3.3.3]undecane (Manxine)	947.7	978.7	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>10</sub> H <sub>19</sub> NO]	29910-43-8	2-Naphthalenol, 3-aminodecahydro-(2,3 $\beta$ ,4 $\alpha$ , 8 $\alpha\beta$ )	914.5	947.0	0	?
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> ]	160172-95-2	7-isopropyl-1,5,7-triazabicyclo[4.4.0]dec-5-ene (ITBD)	1039.2	1071.6	0	Rln(1/1)
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ]	1187-50-4	leu-gly-gly	926.7	NE	NE	not estimated
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ]	2576-67-2	gly-leu-gly	921.8	NE	NE	not estimated
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ]	14857-82-0	gly-gly-leu	918.1	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> ]	6130-94-5	1,1'-bipiperidine	950.4	981.2	5.8	Rln(2/1)
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	14486-13-6	met-val	899.0	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	14486-09-0	val-met	909.0	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	3918-94-3	val-val	883.5	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ]	10236-53-0	gly-gly-lys	958.6	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ]	55488-08-9	lys-gly-gly	958.6	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> N <sub>6</sub> O <sub>4</sub> ]	54944-27-3	gly-gly-arg	1028.5	NE	NE	not estimated
[C <sub>10</sub> H <sub>20</sub> O <sub>5</sub> ]	33100-27-5	15-Crown-5	899.7	943.8	-39	84SHA/BLA
[C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> ]	107322-35-0	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(n-C <sub>5</sub> H <sub>11</sub> )	1005.5	1037.9	0	Rln(1/1)
[C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> ]	94793-26-7	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>6</sub> H <sub>13</sub> )	1000.9	1033.3	0	Rln(1/1)
[C <sub>10</sub> H <sub>22</sub> O]	693-65-2	(n-C <sub>5</sub> H <sub>11</sub> ) <sub>2</sub> O	825.3	852.7	17	sym ethers
[C <sub>10</sub> H <sub>22</sub> O <sub>5</sub> ]	143-24-8	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> O] <sub>4</sub> CH <sub>3</sub>	897.8	953.8	-79	84SHA/BLA
[C <sub>10</sub> H <sub>22</sub> O <sub>6</sub> ]	4792-15-8	HO[CH <sub>2</sub> CH <sub>2</sub> O] <sub>5</sub> H	>910	NE	NE	not estimated
[C <sub>10</sub> H <sub>23</sub> N]	2016-57-1	n-(C <sub>10</sub> H <sub>21</sub> )NH <sub>2</sub>	896.5	930.4	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> ]	68970-05-8	Hydrazine, 1,2-dimethyl-1,2-bis(2-methylpropyl)	949.0	979.7	5.8	Rln(2/1)
[C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> ]	116149-14-5	Hydrazine, 1,2-dibutyl-1,2-dimethyl	945.2	975.9	5.8	Rln(2/1)
[C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> ]	111-18-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>6</sub> N(CH <sub>3</sub> ) <sub>2</sub>	982.2	1035.8	-71	80MAU/HAM
[C <sub>11</sub> H <sub>9</sub> N]	939-23-1	4-phenyl-pyridine	907.8	939.7	2	pyridines
[C <sub>11</sub> H <sub>10</sub> ]	91-57-6	2-Methylnaphthalene	802.4	831.9	10	aromatics
[C <sub>11</sub> H <sub>10</sub> ]	90-12-0	1-methylnaphthalene	805.3	834.8	10	aromatics
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ]	10250-60-9	1,5-dimethyl-3-phenylpyrazole	922.4	954.3	2	pyridines
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ]	141665-22-7	3(5)-ethyl-5(3)-phenylpyrazole	903.8	935.6	2	pyridines
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ]	10250-58-5	1,3-dimethyl-5-phenylpyrazole	924.7	956.6	2	pyridines
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ]	73-22-3	L-tryptophan	915	948.9	-5	CH <sub>3</sub> NH <sub>2</sub>
[C <sub>11</sub> H <sub>13</sub> N]	4363-25-1	Benzoquinuclidine	948.8	979.8	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> ]	13012-16-3	N,N,2,6-Tetramethyl-4-cyanoaniline	886.8	913.3	20	anilines
[C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O]	119044-59-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-acetylphenyl)	947.3	979.8	0	Rln(1/1)
[C <sub>11</sub> H <sub>14</sub> O <sub>2</sub> ]	2282-84-0	2,4,6-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> -COOCH <sub>3</sub>	835.3	866.3	5	esters
[C <sub>11</sub> H <sub>14</sub> O <sub>2</sub> ]	13544-66-6	3,4,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> -CO <sub>2</sub> CH <sub>3</sub>	844.6	875.5	5	esters
[C <sub>11</sub> H <sub>15</sub> FSi]	140843-92-1	4-F-C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>	829.1	858.0	12	propene
[C <sub>11</sub> H <sub>15</sub> N]	54104-82-4	Pyrrolidine, 1-(4-methylphenyl)	879.4	910.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>11</sub> H <sub>15</sub> N]	35843-88-0	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	915.5	946.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>11</sub> H <sub>15</sub> N]	25108-56-9	4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	938.0	964.6	20	anilines
[C <sub>11</sub> H <sub>15</sub> N]	4096-20-2	Piperidine, 1-phenyl	926.4	952.9	20	anilines
[C <sub>11</sub> H <sub>15</sub> N]	23074-42-2	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decane-1-carbonitrile	803.8	834.4	6	nitriles
[C <sub>11</sub> H <sub>15</sub> NO]	54660-04-7	Pyrrolidine, 1-(4-methoxyphenyl)	930.4	961.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>11</sub> H <sub>16</sub> ]	700-12-9	(CH <sub>3</sub> ) <sub>5</sub> -C <sub>6</sub> H	823.5	850.7	17.6	86STO/XI
[C <sub>11</sub> H <sub>16</sub> ClN <sub>3</sub> ]	20815-38-7	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(4-ClC <sub>6</sub> H <sub>4</sub> )	995.5	1027.9	0	Rln(1/1)
[C <sub>11</sub> H <sub>16</sub> FN <sub>3</sub> ]	20815-37-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(4-FC <sub>6</sub> H <sub>4</sub> )	997.6	1030.0	0	Rln(1/1)
[C <sub>11</sub> H <sub>16</sub> N <sub>2</sub> ]	120235-03-2	(CH <sub>3</sub> ) <sub>2</sub> N-C(4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> )=NCH <sub>3</sub>	1005.5	1037.9	0	Rln(1/1)
[C <sub>11</sub> H <sub>16</sub> Si]	1923-01-9	C <sub>6</sub> H <sub>5</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>	832.0	860.9	12	propene
[C <sub>11</sub> H <sub>17</sub> N]	1129-69-7	2-C <sub>6</sub> H <sub>13</sub> (c-C <sub>3</sub> H <sub>4</sub> N)	931.7	963.6	2	pyridines
[C <sub>11</sub> H <sub>17</sub> N]	6832-21-9	2,6-(1-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> pyridine	947.2	979.0	2	pyridines
[C <sub>11</sub> H <sub>17</sub> N]	613-48-9	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	931.0	962.8	2	anilines
[C <sub>11</sub> H <sub>17</sub> N]	91-67-8	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	932.2	964.1	2	anilines
[C <sub>11</sub> H <sub>17</sub> NO]	5511-18-2	1-adamantyl-CONH <sub>2</sub>	880.9	912.8	2	amides
[C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> ]	2556-43-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-C <sub>6</sub> H <sub>5</sub>	1006.0	1038.4	0	Rln(1/1)
[C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub> ]	#41	N <sup>4</sup> -(4,6-dimethylpyrimidin-2-yl)ornithine	<1007	NE	NE	not estimated
[C <sub>11</sub> H <sub>18</sub> O]	10309-50-9	4-Methylcamphor	831.4	863.3	2	unsym ketones
[C <sub>11</sub> H <sub>18</sub> O]	19066-23-0	Adamantylmethylether	831.0	860.2	11	unsym ethers
[C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> ]	1132-14-5	3,5-di-t-butylpyrazole	920.8	952.7	2	pyridines
[C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> ]	3989-97-7	val-leu	883.5	NE	NE	not estimated
[C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> ]	13588-95-9	leu-val	883.5	NE	NE	not estimated



TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>11</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> ]	22677-62-9	val-lys	924.3	NE	NE	not estimated
[C <sub>11</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> ]	20556-11-0	lys-val	924.3	NE	NE	not estimated
[C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> ]	66226-75-3	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> O] <sub>3</sub> CH <sub>3</sub>	895.1	NE	NE	not estimated
[C <sub>12</sub> H <sub>8</sub> ]	259-79-0	Biphenylene	819.2	848.2	11.5	Rln(4/1)
[C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> ]	92-82-0	Phenazine	908.3	938.4	8	pyridines + Rln2
[C <sub>12</sub> H <sub>9</sub> NO]	5424-19-1	3-C <sub>6</sub> H <sub>5</sub> CO-pyridine	902.3	934.1	2	pyridines
[C <sub>12</sub> H <sub>10</sub> ]	83-32-9	Acenaphthene	821.0	851.7	5.8	Rln(2/1)
[C <sub>12</sub> H <sub>10</sub> ]	92-52-4	Biphenyl	782.9	813.6	5.8	Rln(2/1)
[C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ]	5932-30-9	3(5)-phenyl-5(3)-ethoxycarbonylpyrazole	867.8	899.7	2	pyridines
[C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> ]	20734-56-9	N,N'-Dimethyl-1,8-naphthalenediamine	930.9	960.3	10	
[C <sub>12</sub> H <sub>15</sub> Cl]	146558-43-2	$\alpha$ -t-butylstyrene,3-Cl	811.0	839.8	12	propene
[C <sub>12</sub> H <sub>15</sub> F]	146558-44-3	$\alpha$ -t-butylstyrene,3-F	809.9	838.8	12	propene
[C <sub>12</sub> H <sub>16</sub> ]	5676-29-9	$\alpha$ -t-butylstyrene	830.3	859.2	12	propene
[C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> ]	362-43-6	2',3'-O-Isopropylideneuridine	841.7	874.2	0	Rln(1/1)
[C <sub>12</sub> H <sub>16</sub> O]	943-27-1	4-t-C <sub>4</sub> H <sub>9</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	850.6	882.5	2	unsym ketones
[C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> ]	22524-51-2	2,3,5,6-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H-COOCH <sub>3</sub>	834.3	865.2	5	esters
[C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> ]	26537-19-9	4-t-C <sub>4</sub> H <sub>9</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	836.2	867.1	5	esters
[C <sub>12</sub> H <sub>17</sub> N]	40832-99-3	1-H-Azepine, hexahydro-1-phenyl	925.8	956.6	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>12</sub> H <sub>17</sub> NO <sub>2</sub> ]	56066-86-5	N,N,2,6-Tetramethylaniline,4-carboxylic acid, methyl ester	913.0	945.4	0	anilines-restricted
[C <sub>12</sub> H <sub>18</sub> ]	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	836.0	860.6	26.4	86STO/XIA
[C <sub>12</sub> H <sub>18</sub> O]	1660-04-4	Adamantylmethylketone	833.1	864.9	2	unsym ketones
[C <sub>12</sub> H <sub>18</sub> OSi]	107099-29-6	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>	874.0	902.9	12	propene
[C <sub>12</sub> H <sub>18</sub> O <sub>2</sub> ]	711-01-3	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decane-1-carboxylic acid, methyl ester	833.1	864.1	5	esters
[C <sub>12</sub> H <sub>18</sub> Si]	120093-92-7	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>	839.4	868.3	12	propene
[C <sub>12</sub> H <sub>18</sub> Si]	17920-24-0	4-((CH <sub>3</sub> ) <sub>3</sub> Si)C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	849.7	878.6	12	propene
[C <sub>12</sub> H <sub>18</sub> Si]	40595-34-4	3-((CH <sub>3</sub> ) <sub>3</sub> Si)C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>	849.7	878.6	12	propene
[C <sub>12</sub> H <sub>18</sub> Si]	94397-80-5	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>	848.1	877.0	12	propene
[C <sub>12</sub> H <sub>19</sub> N]	2217-07-4	C <sub>6</sub> H <sub>5</sub> N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>	931.1	963.0	2	anilines
[C <sub>12</sub> H <sub>19</sub> N]	22025-87-2	(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> (t-C <sub>4</sub> H <sub>9</sub> )	934.3	961.0	20	anilines
[C <sub>12</sub> H <sub>19</sub> NO]	3357-16-2	3-Pyrrolidino-5,5-dimethylcyclohex-2-enone	968.7	1001.2	0	Rln(1/1)
[C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> ]	20815-36-5	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-(4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> )	1011.9	1044.3	0	Rln(1/1)
[C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> O]	20815-35-4	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-(4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> )	1015.2	1047.7	0	Rln(1/1)
[C <sub>12</sub> H <sub>20</sub> N <sub>6</sub> O <sub>7</sub> ]	3887-13-6	hexaglycine	950	NE	NE	not estimated
[C <sub>12</sub> H <sub>20</sub> O]	4789-40-6	2,5-di-t-butylfuran	863.9	894.7	5.8	Rln(2/1)
[C <sub>12</sub> H <sub>20</sub> O]	90547-83-4	4-Ethylcamphor	833.3	865.1	2	unsym ketones
[C <sub>12</sub> H <sub>21</sub> N]	6321-40-0	(CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> ) <sub>3</sub> N	949.4	980.2	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>12</sub> H <sub>21</sub> N]	3717-40-6	N,N-Dimethyladamantylamine	963.0	993.9	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>12</sub> H <sub>21</sub> NO]	73495-63-3	3-Amino-tricyclo[7.3.0.0 <sup>4,8</sup> ]dodecan-2-ol	895.6	928.0	0	Rln(1/1)
[C <sub>12</sub> H <sub>21</sub> NO]	65115-73-3	3-(N,N-Diethylamino)-5,5-dimethylcyclohex-2-enone	968.7	1001.2	0	Rln(1/1)
[C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> ]	18712-47-5	3,5-di-t-butyl-4-methylpyrazole	933.8	967.5	-4	pyridines + Rln(1/2)
[C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> ]	141665-18-1	1-methyl-3,5-di-t-butylpyrazole	937.1	970.8	-4	pyridines + Rln(1/2)
[C <sub>12</sub> H <sub>22</sub> N <sub>4</sub> O <sub>5</sub> ]	926-79-4	tetra-L-alanine	944.6	NE	NE	not estimated
[C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> ]	71058-67-8	1,6-Diazabicyclo[4.4.4]tetradecane	916.3	947.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> ]	17455-13-9	18-crown-6	909.5	967.0	-84	84SHA/BLA
[C <sub>12</sub> H <sub>27</sub> N]	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	967.6	998.5	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>12</sub> H <sub>28</sub> N <sub>2</sub> ]	106376-59-4	Hydrazine, 1,2-dimethyl-1,2-dipentyl	946.4	977.2	5.8	Rln(2/1)
[C <sub>12</sub> H <sub>28</sub> N <sub>2</sub> ]	68970-09-2	Hydrazine, 1,2-bis(2,2-dimethylpropyl)-1,2-dimethyl	947.1	977.8	5.8	Rln(2/1)
[C <sub>12</sub> H <sub>30</sub> N <sub>3</sub> OP]	2622-07-3	OP(N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>3</sub>	942.2	974.7	0	Rln(1/1)
[C <sub>13</sub> H <sub>9</sub> N]	260-94-6	Acridine	940.7	972.6	2	pyridines
[C <sub>13</sub> H <sub>10</sub> ]	86-73-7	Fluorene	803.8	831.5	16	aromatics
[C <sub>13</sub> H <sub>10</sub> O]	119-61-9	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CO	852.5	882.3	9	sym ketones
[C <sub>13</sub> H <sub>12</sub> ]	643-93-6	3-Methylbiphenyl	795.5	828.0	0	?
[C <sub>13</sub> H <sub>12</sub> ]	643-58-3	2-Methylbiphenyl	783.4	815.9	0	?
[C <sub>13</sub> H <sub>12</sub> ]	101-81-5	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	769.5	802.0	0	
[C <sub>13</sub> H <sub>12</sub> ]	644-08-6	4-Methylbiphenyl	785.4	817.9	0	?
[C <sub>13</sub> H <sub>13</sub> OP]	2129-89-7	CH <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO	876.4	908.9	0	Rln(1/1)
[C <sub>13</sub> H <sub>13</sub> P]	1486-28-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> (CH <sub>3</sub> )P	939.7	972.1	0	Rln(1/1)
[C <sub>13</sub> H <sub>15</sub> F <sub>3</sub> ]	146558-45-4	$\alpha$ -t-butylstyrene,3-CF <sub>3</sub>	802.2	831.1	12	propene
[C <sub>13</sub> H <sub>15</sub> F <sub>3</sub> ]	22666-67-7	$\alpha$ -t-butylstyrene,4-CF <sub>3</sub>	796.5	825.3	12	propene

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> ]	20734-57-0	N,N,N'-Trimethyl-1,8-naphthalenediamine	951.8	984.3	0	?
[C <sub>13</sub> H <sub>17</sub> ClO]	146558-40-9	$\alpha$ -t-butylstyrene,4-CH <sub>3</sub> O, 3-Cl	854.2	883.0	12	propene
[C <sub>13</sub> H <sub>18</sub> ]	31006-98-1	$\alpha$ -t-butylstyrene,4-CH <sub>3</sub>	845.7	874.6	12	propene
[C <sub>13</sub> H <sub>18</sub> ]	146558-42-1	$\alpha$ -t-butylstyrene,3-CH <sub>3</sub>	838.5	867.4	12	propene
[C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> ]	84396-62-3	4-(1-adamantyl)-pyrazole	878.9	913.1	-5.8	Rln(1/2)
[C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> ]	92234-54-3	1-(1-adamantyl)pyrazole	922.4	954.5	2	pyridines
[C <sub>13</sub> H <sub>18</sub> O]	22666-53-1	$\alpha$ -t-butylstyrene, 4-methoxy	869.1	897.9	12	propene
[C <sub>13</sub> H <sub>18</sub> S]	146558-39-6	$\alpha$ -t-butylstyrene,4-CH <sub>3</sub> S	866.0	894.8	12	propene
[C <sub>13</sub> H <sub>21</sub> N]	585-48-8	2,6-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine	951	982.9	2	pyridines
[C <sub>13</sub> H <sub>21</sub> N]	29939-31-9	2,4-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine	952.0	983.8	2	pyridines
[C <sub>13</sub> H <sub>21</sub> NO]	13358-76-4	3-Piperidino-5,5-dimethylcyclohex-2-enone	968.3	1000.7	0	Rln(1/1)
[C <sub>13</sub> H <sub>21</sub> NO]	1502-00-7	1-adamantyl-CON(CH <sub>3</sub> ) <sub>2</sub>	917.6	949.4	2	amides
[C <sub>13</sub> H <sub>22</sub> N <sub>2</sub> ]	133835-18-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-Ad)	1001.0	1033.5	0	Rln(1/1)
[C <sub>13</sub> H <sub>23</sub> N]	#177	Adamantyl-CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	947.4	978.4	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> ]	69340-58-5	3,3,6,9,9-pentamethyl-2,10-diazabicyclo[4.4.0]dec-1-ene	1006.9	1039.3	0	Rln(1/1)
[C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> ]	141665-20-5	1,4-dimethyl-3,5-di-t-butylpyrazole	947.8	979.6	2	pyridines
[C <sub>13</sub> H <sub>25</sub> N]	75197-24-9	out-6H-1-Azabicyclo[4.4.4]tetradecane	864.5	897.0	0	Rln(3/3)
[C <sub>13</sub> H <sub>27</sub> N]	66922-18-7	2,6-Di-t-butylpiperidine	960.1	992.5	0	estimate
[C <sub>14</sub> H <sub>10</sub> ]	85-01-8	Phenanthrene	795.0	825.7	5.8	Rln(2/1)
[C <sub>14</sub> H <sub>10</sub> ]	120-12-7	Anthracene	846.6	877.3	5.8	Rln(2/1)
[C <sub>14</sub> H <sub>12</sub> ]	530-48-3	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C=CH <sub>2</sub>	856.9	885.7	12	propene
[C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> ]	75863-17-1	15,16-diazatricyclo[8.4.1.1 <sup>3,8</sup> ]hexadeca-1,3,5,7,9,11,13-heptaene	951.4	983.8	0	?
[C <sub>14</sub> H <sub>14</sub> ]	103-29-7	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	774.1	801.8	16	toluene
[C <sub>14</sub> H <sub>18</sub> ]	5325-97-3	1,2,3,4,5,6,7,8-Octahydrophenanthrene	815.5	846.2	5.8	Rln(2/1)
[C <sub>14</sub> H <sub>18</sub> ]	1079-71-6	1,2,3,4,5,6,7,8-Octahydroanthracene	814.7	845.4	5.8	Rln(2/1)
[C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> ]	20734-58-1	N,N,N',N'-Tetramethyl-1,8-naphthalenediamine	995.8	1028.2	0	?
[C <sub>14</sub> H <sub>20</sub> ]	146558-41-0	$\alpha$ -t-butylstyrene,3,5-dimethyl	845.5	874.3	12	propene
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	3918-90-9	phe-val	<b>893.6</b>	NE	NE	not estimated
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	3918-92-1	val-phe	<b>909.0</b>	NE	NE	not estimated
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> ]	3061-91-4	val-tyr	<b>909.0</b>	NE	NE	not estimated
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> ]	17355-09-8	tyr-val	<b>893.6</b>	NE	NE	not estimated
[C <sub>14</sub> H <sub>23</sub> N]	16245-79-7	4-(n-C <sub>8</sub> H <sub>17</sub> )C <sub>8</sub> H <sub>4</sub> NH <sub>2</sub>	862	894.5	0	86SUN/KUL
[C <sub>14</sub> H <sub>23</sub> N <sub>7</sub> O <sub>8</sub> ]	18861-82-0	heptaglycine	980.6	NE	NE	not estimated
[C <sub>14</sub> H <sub>24</sub> N <sub>2</sub> ]	151328-46-0	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N(1-Ad)	1018.4	1050.8	0	Rln(1/1)
[C <sub>14</sub> H <sub>28</sub> O <sub>7</sub> ]	33089-36-0	21-crown-7	>910	NE	NE	not estimated
[C <sub>14</sub> H <sub>29</sub> N]	64326-83-6	1-Methyl-2,6-t-butylpiperidine	980.3	1011.1	5.6	(CH <sub>3</sub> ) <sub>3</sub> N
[C <sub>15</sub> H <sub>12</sub> ]	779-02-2	9-Methylanthracene	865.8	896.5	5.8	Rln(2/1)
[C <sub>15</sub> H <sub>12</sub> ]	613-12-7	2-Methylanthracene	855.1	887.5	0	Rln(1/1)
[C <sub>15</sub> H <sub>12</sub> Fe <sub>2</sub> O <sub>3</sub> ]	76722-37-7	[(C <sub>5</sub> H <sub>5</sub> )(CO)Fe] <sub>2</sub> ( $\mu$ -CO)( $\mu$ -C=CH <sub>2</sub> )	<b>949.4</b>	981.8	0	Rln(1/1)
[C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> ]	1145-01-3	3,5-diphenylpyrazole	912.7	946.3	-3.8	pyridines+Rln(1/2)
[C <sub>15</sub> H <sub>16</sub> ]	34403-06-0	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub>	801.0	833.5	0	?
[C <sub>15</sub> H <sub>16</sub> ]	1081-75-0	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>5</sub>	787.6	821.0	0	?
[C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> ]	95935-55-0	9,5-metheno-5H,7H-pyrimido[1,6-a:3,4-a']bisazepine	898.7	931.1	0	?
[C <sub>15</sub> H <sub>17</sub> OP]	2959-75-3	i-C <sub>3</sub> H <sub>7</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO	<b>876.4</b>	908.9	0	Rln(1/1)
[C <sub>15</sub> H <sub>18</sub> ]	489-84-9	1,4-Dimethyl-7-isopropylazulene	950.6	983.1	0	Rln(1/1)
[C <sub>15</sub> H <sub>24</sub> ]	15181-11-0	1,3-di-(t-C <sub>4</sub> H <sub>9</sub> )-5-CH <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	826.0	853.7	16	aromatics
[C <sub>15</sub> H <sub>27</sub> N <sub>5</sub> O <sub>6</sub> ]	10183-34-3	penta-L-alanine	962	NE	NE	not estimated
[C <sub>16</sub> H <sub>10</sub> ]	206-44-0	Fluoranthene	800.9	828.6	16	aromatics
[C <sub>16</sub> H <sub>10</sub> ]	129-00-0	Pyrene	840.1	869.2	11.5	Rln(4/1)
[C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> ]	19311-79-6	1-methyl-3,5-diphenylpyrazole	927.0	958.9	2	pyridines
[C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> ]	95935-56-1	10,5-metheno-5H-bisazepino[1,2-d:2',1'-g][1,4]diazepine,7,8-dihydro	930.1	962.6	0	?
[C <sub>16</sub> H <sub>16</sub> ]	2919-20-2	(4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> C=CH <sub>2</sub>	871.4	900.2	12	propene
[C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> ]	95864-13-4	15,16-diazatricyclo[8.4.1.1 <sup>3,8</sup> ]hexadeca-1,3,5,7,9,11,13-heptaene,15,16-dimethyl	951.9	984.4	0	?
[C <sub>16</sub> H <sub>18</sub> ]	1083-56-3	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>5</sub>	779.8	822.0	-33	80MAU/HUN
[C <sub>16</sub> H <sub>19</sub> OP]	56598-35-7	t-C <sub>4</sub> H <sub>9</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO	<b>876.4</b>	908.9	0	Rln(1/1)
[C <sub>16</sub> H <sub>21</sub> N <sub>3</sub> O <sub>3</sub> ]	24587-37-9	val-trp	<b>909.0</b>	NE	NE	not estimated
[C <sub>16</sub> H <sub>26</sub> N <sub>8</sub> O <sub>9</sub> ]	38416-68-1	octaglycine	990.7	NE	NE	not estimated
[C <sub>16</sub> H <sub>27</sub> N]	2909-76-4	N,N-Dimethylbenzamine,2,4-di-t-butyl	942.4	973.3	5.6	(CH <sub>3</sub> ) <sub>3</sub> N

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[C <sub>17</sub> H <sub>20</sub> ]	1718-50-9	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	782.4	824.7	-33	80MAU/HUN
[C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> ]	95935-57-2	11,5-metheno-5H,7H-bisazepino[1,2-a:2',1'-d][1,5]diazocine,8,9-dihydro	942.0	974.5	0	Rln(1/1)
[C <sub>18</sub> H <sub>12</sub> ]	218-01-9	Chrysene	810.1	840.9	5.8	Rln(2/1)
[C <sub>18</sub> H <sub>12</sub> ]	92-24-0	Tetracene	876.5	905.5	11.5	Rln(4/1)
[C <sub>18</sub> H <sub>12</sub> ]	217-59-4	Triphenylene	791.2	819.2	14.9	Rln(6/1)
[C <sub>18</sub> H <sub>15</sub> As]	603-32-7	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> As	876.4	908.9	0	Rln(3/3)
[C <sub>18</sub> H <sub>15</sub> AsO]	1153-05-5	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> AsO	876.4	906.2	9.1	Rln(3/1)
[C <sub>18</sub> H <sub>15</sub> N]	603-34-9	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> N	876.4	908.9	0	Rln(3/3)
[C <sub>18</sub> H <sub>15</sub> OP]	791-28-6	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PO	876.4	906.2	9.1	Rln(3/1)
[C <sub>18</sub> H <sub>15</sub> P]	603-35-0	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P	940.4	972.8	0	Rln(3/3)
[C <sub>18</sub> H <sub>15</sub> PS]	3878-45-3	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PS	876.4	906.2	9.1	Rln(3/1)
[C <sub>18</sub> H <sub>15</sub> Sb]	603-36-1	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> Sb	813.1	845.5	0	Rln(3/3)
[C <sub>18</sub> H <sub>22</sub> ]	1087-49-6	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>6</sub> C <sub>6</sub> H <sub>5</sub>	783.8	826.1	-33	80MAU/HUN
[C <sub>18</sub> H <sub>20</sub> ]	21072-42-4	<i>trans</i> -1,4-diphenylcyclohexane	771.7	804.1	0	?
[C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> ]	120789-29-9	12,5-metheno-5H-bisazepino[1,2-a:2',1'-d][1,5]diazocine,7,8,9,10-tetrahydro	940.2	972.6	0	Rln(1/1)
[C <sub>18</sub> H <sub>30</sub> ]	1460-02-2	1,3,5-( <i>t</i> -C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	822.3	848.8	20	1,3,5-Me <sub>3</sub> C <sub>6</sub> H <sub>3</sub>
[C <sub>18</sub> H <sub>32</sub> N <sub>6</sub> O <sub>7</sub> ]	111652-29-0	hexa-L-alanine	981.3	NE	NE	not estimated
[C <sub>18</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ]	153841-62-4	gly-lys-lys-gly-gly	1008.4	NE	NE	not estimated
[C <sub>18</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ]	153841-63-5	gly-lys-gly-lys-gly	1010.8	NE	NE	not estimated
[C <sub>18</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ]	153841-64-6	lys-gly-gly-gly-lys	1026	NE	NE	not estimated
[C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> ]	123524-78-7	13,5-metheno-5H,7H-bisazepino[1,2-a:2',1'-d][1,5]diazocine,8,9,10,11-tetrahydro	961.8	994.3	0	?
[C <sub>20</sub> H <sub>12</sub> ]	198-55-0	Perylene	859.6	888.6	11.5	Rln(4/1)
[C <sub>20</sub> H <sub>20</sub> ]	4493-23-6	dodecahedrane	817.5	843.8	20.6	Rln(60/5)
[C <sub>20</sub> H <sub>24</sub> ]	128484-66-2	<i>trans</i> -1,4-dibenzylcyclohexane	773.3	805.7	0	?
[C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> ]	123524-79-8	14,5-metheno-5H-bisazepino[1,2-a:2',1'-d][1,5]diazacycloundecine,7,8,9,10,11,12-hexahydro	946	978.5	0	Rln(1/1)
[C <sub>20</sub> H <sub>32</sub> N <sub>10</sub> O]	76960-32-2	decaglycine	1004.6	NE	NE	not estimated
[C <sub>21</sub> H <sub>22</sub> ]	82400-17-7	Methyl-dodecahedrane	823.1	855.6	0	?
[C <sub>21</sub> H <sub>30</sub> O]	38256-01-8	(1-adamtyl) <sub>2</sub> CO	862.4	894.3	2	unsym ketones
[C <sub>21</sub> H <sub>30</sub> S]	73509-04-3	(1-adamtyl) <sub>2</sub> CS	882.4	912.1	9	sym ketones
[C <sub>22</sub> H <sub>12</sub> ]	191-24-2	1,12-Benzoperylene	845.2	876.0	5.8	Rln(2/1)
[C <sub>22</sub> H <sub>14</sub> ]	213-46-7	Picene	820.6	851.3	5.8	Rln(2/1)
[C <sub>22</sub> H <sub>24</sub> ]	77387-50-9	1,16-Dimethyldodecahedrane	844.0	876.5	0	?
[C <sub>24</sub> H <sub>12</sub> ]	191-07-1	Coronene	835.0	861.3	20.6	Rln(12/1)
[C <sub>26</sub> H <sub>54</sub> O <sub>8</sub> ]	3055-97-8	C <sub>12</sub> H <sub>25</sub> (OC <sub>2</sub> H <sub>4</sub> ) <sub>7</sub> OH	940.3	1006.7	-113.9	93LIN/ROC
[C <sub>60</sub> ]	99685-96-8	buchminsterfullerene	827.5	NE	NE	not estimated
[C <sub>70</sub> ]	115383-22-7	[5,6]Fullerene-C <sub>70</sub>	827.5	NE	NE	not estimated
[CaO]	1305-78-8	CaO	1162.3	1190.6	14	89GUR/VEY
[Cl]	22537-15-1	Cl	490.1	513.6	30.1	S(HS)-S(Cl)
[ClH]	7647-01-0	HCl	530.1	556.9	19	S(H <sub>2</sub> S)-S(HCl)
[ClLi]	7447-41-8	LiCl	800.5	827	20	linear-to-bent est.
[Co]	7440-48-4	Co	719.8	742.7	32	rot est (0.116)
[Cr]	7440-47-3	Cr	768.4	791.3	32	rot est (0.117)
[CsHO]	21351-79-1	CsOH	1092.2	1117.9	22.6	70DZI/KEB
[Cs <sub>2</sub> O]	20281-00-9	Cs <sub>2</sub> O	1412.2	1442.9	5.8	Rln(2/1)
[Cu]	7440-50-8	Cu	632.4	655.3	32	rot est (0.117)
[F]	14762-94-8	F	315.1	340.1	25	S(OH)-S(F)
[FH]	7664-39-3	HF	456.7	484	17.3	97EAS/SMI
[FO]	12061-70-0	OF	482.2	508.7	20	linear-to-bent est.
[F <sub>2</sub> ]	7782-41-4	F <sub>2</sub>	305.5	332	20	linear-to-bent est.
[F <sub>2</sub> O <sub>2</sub> S]	2699-79-8	F <sub>2</sub> SO <sub>2</sub>	580.5	605.5	25	93SZU/MCM
[F <sub>3</sub> HOSi]	91419-78-2	SiF <sub>3</sub> OH	611.5	641.9	7	CH <sub>3</sub> OH
[F <sub>3</sub> N]	7783-54-2	NF <sub>3</sub>	538.6	568.4	9.1	Rln(3/1)
[F <sub>3</sub> OP]	13478-20-1	OPF <sub>3</sub>	664.2	694.0	9.1	Rln(3/1)
[F <sub>3</sub> P]	7783-55-3	PF <sub>3</sub>	662.8	695.3	0	Rln(1/1)
[F <sub>4</sub> Si]	7783-61-1	SiF <sub>4</sub>	476.6	502.9	20.6	Rln(12/1)
[F <sub>6</sub> S]	2551-62-4	SF <sub>6</sub>	550.7	575.3	26.4	Rln(24/1)
[Fe]	7439-89-6	Fe	731.1	754	32	rot est (0.117)
[FeO]	1345-25-1	FeO	880.5	907	20	linear-to-bent est.

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[GeH <sub>4</sub> ]	7782-65-2	GeH <sub>4</sub>	<b>687.1</b>	713.4	20.6	Rln(12/1)
[HI]	10034-85-2	HI	601.3	627.5	21	HBr
[HKO]	1310-58-3	KOH	1075.4	1101.8	20.4	average
[HLi]	7580-67-8	LiH	996.4	1021.7	24	88DIX/GOL
[HLiO]	1310-66-3	LiOH	972.1	1000.1	14.9	70DZI/KEB
[HNO <sub>3</sub> ]	7697-37-2	HNO <sub>3</sub>	731.5	751.4	42	94CAC/ATT
[HNSi]	14515-04-9	SiNH	819.0	853.2	-5.8	Rln(1/2)
[HN <sub>3</sub> ]	7782-79-8	HNNN	<b>723.5</b>	756.0	0	Rln(1/1)
[HNa]	7646-69-7	NaH	1070.6	1095	27	88DIX/GOL
[HNaO]	1310-73-2	NaOH	1044.8	1071.8	18.2	70DZI/KEB
[HOSi]	71132-80-4:b	SiOH at O	700.1	732.6	0	?
[HOSi]	71132-80-4:a	SiOH at Si	742.8	775.3	0	Rln(1/1)
[HOSi]	97402-81-8:a	HSiO at O	777.5	810	0	Rln(1/1)
[HOSi]	97402-81-8:b	HSiO at Si	602.5	635	0	Rln(1/1)
[HOSr]	12141-14-9	SrOH	981.6	1019.4	-18	
[HO <sub>2</sub> ]	3170-83-0	HO <sub>2</sub> •	627.5	660	0	?
[HP]	13967-14-1	PH	639.6	670.3	5.8	Rln(2/1)
[H <sub>2</sub> ]	1333-74-0	H <sub>2</sub>	394.7	422.3	16.3	97EAS/SMI
[H <sub>2</sub> N]	15194-15-7	NH <sub>2</sub>	742.0	773.4	3.4	Rln(3/2)
[H <sub>2</sub> N <sub>2</sub> ]	3618-05-1	HN=NH	772.3	803	5.8	Rln(2/1)
[H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> ]	7782-94-7	H <sub>2</sub> N-NO <sub>2</sub>	<b>725.0</b>	757.4	0	?
[H <sub>2</sub> O]	7732-18-5	H <sub>2</sub> O	660.0	691	5	AUE; 97EAS/SMI
[H <sub>2</sub> OSi]	83892-34-6	HSiOH at Si	807.5	840	0	?
[H <sub>2</sub> OSi]	22755-01-7:a	H <sub>2</sub> SiO at O	808.5	841	0	?
[H <sub>2</sub> OSi]	22755-01-7:b	H <sub>2</sub> SiO at Si	295.5	328	0	Rln(1/1)
[H <sub>2</sub> O <sub>2</sub> ]	7722-84-1	H <sub>2</sub> O <sub>2</sub>	<b>643.8</b>	674.5	5.8	Rln(2/1)
[H <sub>2</sub> O <sub>4</sub> S]	7664-93-9	H <sub>2</sub> SO <sub>4</sub>	<b>666.9</b>	699.4	0	?
[H <sub>2</sub> P]	13765-43-0	PH <sub>2</sub>	675.7	709.2	-3.4	Rln(2/3)
[H <sub>2</sub> S]	7783-06-4	H <sub>2</sub> S	673.8	705	4.3	S(PH <sub>3</sub> )-S(H <sub>2</sub> S)
[H <sub>2</sub> Se]	7783-07-5	H <sub>2</sub> Se	676.4	707.8	3.8	S(AsH <sub>3</sub> )-S(H <sub>2</sub> Se)
[H <sub>2</sub> Si]	13825-90-6	SiH <sub>2</sub>	<b>804.1</b>	839.2	-9.1	Rln(2/6)
[H <sub>2</sub> Te]	7783-09-7	H <sub>2</sub> Te	704.5	735.9	3.8	H <sub>2</sub> Se
[H <sub>3</sub> N]	7664-41-7	NH <sub>3</sub>	819.0	853.6	-6.4	97EAS/SMI
[H <sub>3</sub> OSi]	113648-09-2:a	H <sub>2</sub> SiOH at O	705.5	738	0	?
[H <sub>3</sub> OSi]	113648-09-2:b	H <sub>2</sub> SiOH at Si	556.5	589	0	?
[H <sub>3</sub> OSi]	81429-20-1	H <sub>3</sub> SiO at O	667.5	700	0	?
[H <sub>3</sub> O <sub>3</sub> P]	10294-56-1	H <sub>3</sub> PO <sub>3</sub>	<b>788.8</b>	821.3	0	?
[H <sub>3</sub> P]	7803-51-2	PH <sub>3</sub>	750.9	785	-5.6	S(SiH <sub>4</sub> )-S(PH <sub>3</sub> )
[H <sub>4</sub> N <sub>2</sub> ]	302-01-2	H <sub>2</sub> NNH <sub>2</sub>	822.4	853.2	5.8	Rln(2/1)
[H <sub>4</sub> OSi]	14475-38-8	H <sub>3</sub> SiOH at O	713.9	746.4	0	Rln(1/1)
[H <sub>4</sub> Si]	7803-62-5	SiH <sub>4</sub>	613.4	639.7	20.6	Rln(12/1)
[H <sub>4</sub> OSi <sub>2</sub> ]	13597-73-4	H <sub>3</sub> SiOSiH <sub>3</sub>	718.3	749	5.8	Rln(2/1)
[He]	7440-59-7	He	148.5	177.8	10.5	S(H <sub>2</sub> )-S(He)+Rln2
[I]	14362-44-8	I	583.5	608.2	26	S(HI)-S(I)
[K <sub>2</sub> O]	12136-45-7	K <sub>2</sub> O	1311.8	1342.5	5.8	Rln(2/1)
[Kr]	7439-90-9	Kr	402.4	424.6	34.4	S(HBr)-S(Kr)
[La]	7439-91-0	La	991.9	1013	38	rot est (0.17)
[Li <sub>2</sub> ]	14452-59-6	Li <sub>2</sub>	1133.1	1162	12	88DIX/GOL
[Li <sub>2</sub> O]	12057-24-8	Li <sub>2</sub> O	1175.3	1206	5.8	Rln(2/1)
[Lu]	7439-94-3	Lu	970.6	992	37	rot est (0.16)
[Mg]	7439-95-4	Mg	<b>797.3</b>	819.6	34	rot est (0.136)
[MgO]	1309-48-4	MgO	959.4	988	13	89GUR/VEY
[Mg <sub>2</sub> ]	29904-79-8	Mg <sub>2</sub>	886.5	919	0	Rln(1/1)
[Mn]	7439-96-5	Mn	774.4	797.3	32	rot est (0.117)
[N]	17778-88-0	N	318.7	342.2	30	S(CH)-S(N)
[NO]	10102-43-9	NO	505.3	531.8	20	linear-to-bent est.
[NO <sub>2</sub> ]	10102-44-0	NO <sub>2</sub>	<b>560.3</b>	591.0	5.8	Rln(2/1)
[NP]	17739-47-8	PN	<b>757.0</b>	789.4	0	?
[N <sub>2</sub> ]	7727-37-9	N <sub>2</sub>	464.5	493.8	10.5	97EAS/SMI
[N <sub>2</sub> O]	10024-97-2:b	N <sub>2</sub> O at N	523.3	549.8	20	CO <sub>2</sub> -Rln(2/1)
[N <sub>2</sub> O]	10024-97-2:a	N <sub>2</sub> O at O	548.7	575.2	20	CO <sub>2</sub> -Rln(2/1)
[Na <sub>2</sub> ]	25681-79-2	Na <sub>2</sub>	1118.2	1146.8	13	88DIX/GOL
[Na <sub>2</sub> O]	1313-59-3	Na <sub>2</sub> O	1345.2	1375.9	5.8	Rln(2/1)

TABLE 1. Gas basicity, proton affinity and protonation entropy of Hill sorted bases—Continued

Formula	Reg No	Base	GB	PA	$\Delta S_p$	$\Delta S_p$ Reasons
[Ne]	7440-01-9	Ne	174.4	198.8	27	$S(\text{HF})-S(\text{Ne})$
[Ni]	7440-02-0	Ni	714.1	737	32	rot est (0.115)
[O]	17778-80-2	O	459.6	485.2	23	rot est (0.066)
[HO]	3352-57-6	OH	564.0	593.2	11	$S(\text{NH}_2)-S(\text{OH})$
[OP]	14452-66-5	PO	649.5	682	0	Rln(1/1)
[OSi]	10097-28-6:a	SiO at O	<b>750.4</b>	777.8	17	85BOT/ROS
[OSi]	10097-28-6:b	SiO at Si	500.5	533	0	Rln(1/1)
[OSr]	1314-11-0	SrO	1180.7	1209	14	89GUR/VEY
[O <sub>2</sub> ]	7782-44-7	O <sub>2</sub>	396.3	421	26	AUE; 84ADA/SMI
[O <sub>2</sub> S]	7446-09-5	SO <sub>2</sub>	643.3	672.3	11.5	AUE
[O <sub>3</sub> ]	10028-15-6	O <sub>3</sub>	595.9	625.5	9.5	91MER/QUE
[O <sub>3</sub> S]	7446-11-9	SO <sub>3</sub>	<b>560.3</b>	588.3	14.9	Rln(6/1)
[O <sub>4</sub> Os]	20816-12-0	OsO <sub>4</sub>	<b>650.6</b>	676.9	20.6	Rln(12/1)
[P]	7723-14-0	P	604.8	626.8	35	$S(\text{HSi})-S(\text{P})$
[PS]	12281-36-6	PS	665.5	698	0	?
[P <sub>4</sub> ]	12185-10-8	P <sub>4</sub>	714.3	742.3	14.9	Rln(12/2)
[Pd]	7440-05-3	Pd	673.4	696	33	rot est (0.13)
[Rh]	7440-16-6	Rh	745.4	768	33	rot est (0.13)
[Ru]	7440-18-8	Ru	751.4	774	33	rot est (0.13)
[S]	7704-34-9	S	640.2	664.3	28	rot est (0.104)
[SSi]	113443-18-8	SiS	<b>677.7</b>	710.2	0	Rln(1/1)
[SSi]	12504-41-5:b	SiS at Si	596.6	627	7	92BRU/GRE
[SSi]	12504-41-5:a	SiS at S	660.2	683	32.5	92BRU/GRE
[Sc]	7440-20-2	Sc	892.0	914	35	rot est (0.144)
[Si]	7440-21-3	Si	814.1	837	32	rot est (0.12)
[Ti]	7440-32-6	Ti	853.7	876	34	rot est (0.132)
[U]	7440-61-1	U	973.2	995.2	35	rot est (0.142)
[V]	7440-62-2	V	836.8	859.4	33	rot est (0.13)
[Xe]	7440-63-3	Xe	478.1	499.6	36.8	$S(\text{HI})-S(\text{Xe})$
[Y]	7440-65-5	Y	945.9	967	38	rot est (0.17)
[Zn]	7440-66-6	Zn	<b>586.0</b>	608.6	33	rot est (0.125)

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[Cs <sub>2</sub> O] 84BUT/KUD	20281-00-9	Cs <sub>2</sub> O See Refs.				1412.2			1442.9 1442.9			5.8	5.8
[Na <sub>2</sub> O] 84BUT/KUD	1313-59-3	Na <sub>2</sub> O See Refs.				1345.2			1375.9 1375.9			5.8	5.8
[K <sub>2</sub> O] 84BUT/KUD	12136-45-7	K <sub>2</sub> O See Refs.				1311.8			1342.5 1342.5			5.8	5.8
[BaO] 81MUR	1304-28-5	BaO See Refs.				1187.6			1215.4 1215.4			15.5	15.5
[OSr] 83MUR 81MUR	1314-11-0	SrO See Refs. See Refs.				1180.7			1209 1210.7 1207.3			14	14
[Li <sub>2</sub> O] 84BUT/KUD	12057-24-8	Li <sub>2</sub> O See Refs.				1175.3			1206 1206			5.8	5.8
[CaO] 83MUR 81MUR	1305-78-8	CaO See Refs. See Refs.				1162.3			1190.6 1193.7 1187.4			14	14
[Li <sub>2</sub> ] 88DIX/GOL	14452-59-6	Li <sub>2</sub> theory	300			1133.1			1162 1162			12	12
[Na <sub>2</sub> ] 88DIX/GOL	25681-79-2	Na <sub>2</sub> theory	300			1118.2			1146.8 1146.8			13	13
[CsHO] 72MCK/SAW 70DZI/KEB	21351-79-1	CsOH See Refs. See Refs.				1092.2			1117.9 1110.3 1117.9			22.6 42.3 22.6	22.6 42.3 22.6
[HKO] 82BUR/HAY 76DAV/KEB 70DZI/KEB	1310-58-3	KOH See Refs. See Refs. See Refs.				1075.4			1101.8 1100.6 1100.3 1104.5			20.4 21 23.7 16.6	20.4 21 23.7 16.6
[HN <sub>3</sub> ] 88DIX/GOL	7646-69-7	NaN <sub>3</sub> theory	300			1070.6			1095 1095			27	27
[C <sub>10</sub> H <sub>16</sub> N <sub>4</sub> ] 94RAC/MAR	111062-21-6 80-70-6	1H-diazepine, 2,3,5,6,8,9-hexahydro-1-methyl (MITT) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	<62.2	>1060 >1060			>1091			0	0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M) ΔS <sub>p</sub> (M)
[C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> ] 94RAC/MAR	111062-19-2 80-70-6	1H-dimidazo[1,2-d:2',1'-g][1,4]diazepine, 2,3,5,6,8,9-hexahydro (TTT) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	>51.2	>1049			>1081			0
[HNao] 82BUR/HAY 70DZJ/KEB	1310-73-2	NaOH See Refs. See Refs				1044.8			1071.8 1072.1 1071.5			18.2 18.2 18.2
[C <sub>10</sub> H <sub>10</sub> N <sub>5</sub> ] 94RAC/MAR	160172-95-2 80-70-6	7-isopropyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene (TTBD) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	42	1039.2			1071.6			0
[C <sub>9</sub> H <sub>17</sub> N <sub>3</sub> ] 94RAC/MAR	95510-44-4 80-70-6	7-ethyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene (ETBD) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	38.6	1035.8			1068.2			0
[C <sub>9</sub> H <sub>21</sub> N <sub>3</sub> ] 94RAC/MAR 93DEC/GAL	151328-47-1 80-70-6 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N-(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338 338	997.4 967.6	31.4 >61.1	1030.5 1030.5 >1016.3			1077.5			-49
[C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> ] 94RAC/MAR 93DEC/GAL	84030-20-6 80-70-6 102-82-9	7-methyl-1,5,7-triazabicyclo[4,4,0]dec-5-ene ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338 338	997.4 967.6	32.7 62.8	1030.2 1029.9 1030.6			1062.7			0
[C <sub>9</sub> H <sub>21</sub> N <sub>3</sub> ] 94RAC/MAR	34331-58-3 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(t-C <sub>4</sub> H <sub>9</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	32.2	1029.4 1029.4			1061.8			0
[C <sub>10</sub> H <sub>20</sub> N <sub>6</sub> O <sub>4</sub> ] 93WU/FEN	54944-27-3	gly-gly-arg kinetic method				1028.5 1028.5			NE NE			NE NE
[C <sub>16</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ] 93WU/FEN	153841-64-6	lys-gly-gly-gly-lys kinetic method				1028 1026			NE NE			NE NE
[C <sub>8</sub> H <sub>10</sub> N <sub>3</sub> ] 94RAC/MAR	29166-71-0 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(i-C <sub>3</sub> H <sub>7</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	26	1023.2 1023.2			1055.6			0
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> ] 94RAC/MAR 93DEC/GAL	5807-14-7 80-70-6 102-82-9	1,5,7-triazabicyclo [4,4,0]dec-5-ene ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338 338	997.4 967.6	25.5 53.8	1022.1 1022.7 1021.6			1054.6			0
[C <sub>7</sub> H <sub>17</sub> N <sub>3</sub> ] 94RAC/MAR	13439-88-8 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NC <sub>2</sub> H <sub>5</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	21.8	1019.0 1019.0			1051.4			0
[C <sub>14</sub> H <sub>24</sub> N <sub>2</sub> ] 93DEC/GAL	151328-46-0 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N(1-Ad) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	50.6	1018.4 1018.4			1050.8			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>8</sub> H <sub>19</sub> N <sub>3</sub> ] 93DEC/GAL	151328-45-9 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	48.3	1016.1 1016.1			1048.5			0
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 93DEC/GAL	6674-22-2 102-82-9	1,8-diazabicyclo[5,4,0]undec-7-ene (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	47.7	1015.5 1015.5			1047.9			0
[C <sub>8</sub> H <sub>15</sub> N <sub>3</sub> ] 94RAC/MAR	13439-84-4 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NCH <sub>3</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	18	1015.2 1015.2			1047.7			0
[C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> O] 94RAC/MAR	20815-35-4 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-(4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	18	1015.2 1015.2			1047.7			0
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ] 94RAC/MAR	19616-52-5 80-70-6	1,5-diazabicyclo[4,4,0]dec-6-ene (DBD) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	16.8	1014.0 1014.0			1046.4			0
[C <sub>12</sub> H <sub>19</sub> N <sub>3</sub> ] 94RAC/MAR	20815-36-5 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-(4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	14.7	1011.9 1011.9			1044.3			0
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ] 93DEC/GAL	151328-44-8 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	43.1	1010.9 1010.9			1043.3			0
[C <sub>18</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ] 93WU/FEN	153841-63-5	gly-lys-gly-lys-gly kinetic method				1010.8 1010.8			NE			NE
[C <sub>8</sub> H <sub>19</sub> N <sub>3</sub> ] 94RAC/MAR	139033-04-8 80-70-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	14.2	1010.6 1013.3			1057.7			-49
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92RAC/MAR	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	40.6	1010.2						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92RAC/MAR	147320-05-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> )	338	1005.9	2.1	1009.8						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92RAC/MAR	133835-18-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(1-Ad)	338	1001.0	7.9	1010.8						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92RAC/MAR	101398-58-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	996.4	10.9	1009.1						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92RAC/MAR	94793-19-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(t-C <sub>3</sub> H <sub>7</sub> )	338	999.2	9.6	1010.6						
[C <sub>18</sub> H <sub>35</sub> N <sub>7</sub> O <sub>6</sub> ] 93WU/FEN	153841-62-4	gly-lys-gly-gly kinetic method				1008.4 1008.4			NE			NE
[C <sub>11</sub> H <sub>18</sub> N <sub>4</sub> O <sub>2</sub> ] 93BUR/GAS	#41 74-79-3	N <sup>4</sup> -(4,6-dimethylpyrimidin-2-yl)ornithine L-Arginine		1006.6	<0	<1007 <1007			NE			NE
[C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> ] 93DEC/GAL	69340-58-5 102-82-9	3,3,6,9-pentamethyl-2,10- diazabicyclo[4.4.0]dec-1-ene (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	39.1	1006.9 1006.9			1039.3			0
[C <sub>8</sub> H <sub>14</sub> N <sub>4</sub> O <sub>2</sub> ] 93LI/HAR	74-79-3	L-Arginine kinetic method				1006.6			1051.0			-40
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> ] 92WU/FEN	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	350	967.6		1006.6						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
90ISA/OMO		kinetic method-relative order											
87BOJ		kinetic method-relative order											
86BOJ		kinetic method-relative order											
[C <sub>11</sub> H <sub>17</sub> N <sub>3</sub> ] 94RAC/MAR	2556-43-6 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N-C <sub>6</sub> H <sub>5</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	8.8	1006.0 1006.0			1038.4	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>7</sub> H <sub>17</sub> N <sub>2</sub> ] 93DEC/GAL	3001-72-7 102-82-9	1,5-diazabicyclo[4.3.0]non-5-ene (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	38.1	1005.9 1005.9			1038.3	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ] 93DEC/GAL	147350-05-8 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	38.1	1005.9 1005.9			1038.3	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ] 93DEC/GAL	151328-42-6 102-82-9	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>3</sub> H <sub>7</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	37.7	1005.5 1005.5			1037.9	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> ] 93DEC/GAL	107322-35-0 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(n-C <sub>5</sub> H <sub>11</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	37.7	1005.5 1005.5			1037.9	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>11</sub> H <sub>24</sub> N <sub>2</sub> ] 93DEC/GAL	120235-03-2 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> )=NCH <sub>3</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	37.7	1005.5 1005.5			1037.9	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>20</sub> H <sub>32</sub> N <sub>10</sub> O] 92WU/FEN2	76960-32-2	decaglycine kinetic method							NE	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	NE	NE
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ] 93DEC/GAL	112752-57-5 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>2</sub> H <sub>5</sub> )=N(i-C <sub>3</sub> H <sub>7</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	36.8	1004.6 1004.6			1037.0	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O] 93DEC/GAL	151328-41-5 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(CH <sub>2</sub> ) <sub>2</sub> OCH <sub>3</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	36	1003.8 1003.8			1036.2	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ] 93DEC/GAL	94793-24-5 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>3</sub> H <sub>7</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	34.3	1002.1 1002.1			1034.5	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
[C <sub>13</sub> H <sub>22</sub> N <sub>2</sub> ] 93DEC/GAL	133836-18-4 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-Ad) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	33.1	1001.0 1000.9			1033.5	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0
92RAC/MAR	101398-58-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	996.4	7.9	1004.3							
92RAC/MAR	151328-40-4	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NC <sub>2</sub> H <sub>5</sub>	338	996.7	4.6	1001.3							
92RAC/MAR	94793-19-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(i-C <sub>3</sub> H <sub>7</sub> )	338	999.2	1.7	1000.8							
92RAC/MAR	147350-05-8	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(t-C <sub>4</sub> H <sub>9</sub> )	338	1005.9	-5.0	1000.8							
91DEC/GAL	80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	2.5	999.7							
91DEC/GAL	133835-17-3	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1,1-dimethylpropyl)	338	989.6	9.6	999.2							
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ] 93DEC/GAL	119044-57-4 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(C <sub>6</sub> H <sub>5</sub> )=NCH <sub>3</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	33.1	1000.9 1000.9			1033.3	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	0	0

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>i</sub> sorted by gas basicity of M<sub>i</sub>—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>10</sub> H <sub>22</sub> N <sub>2</sub> ] 93DEC/GAL	94793-26-7 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>6</sub> H <sub>13</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	33.1	1000.9 1000.9	1033.3		1033.3			0
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ] 93DEC/GAL	94793-19-8 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(i-C <sub>3</sub> H <sub>7</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	31.4	999.2 999.2	1031.6		1031.6			0
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ] 93DEC/GAL	94793-20-1 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(n-C <sub>3</sub> H <sub>7</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	30.1	997.9 997.9	1030.3		1030.3			0
[C <sub>11</sub> H <sub>16</sub> FN <sub>3</sub> ] 94RAC/MAR	20815-37-6 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(4-FC <sub>6</sub> H <sub>4</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338	997.4	0.4	997.6 997.6	1030.0		1030.0			0
[C <sub>3</sub> H <sub>7</sub> N <sub>3</sub> ] 87TAF 86TAF/GAL	80-70-6 75-50-3 7664-41-7	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	350 350	918.1 819	78.7 172.3	997.4 997.4 991.2	1031.6		1031.6			-5.8
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ] 93DEC/GAL	151328-40-4 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NC <sub>2</sub> H <sub>5</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	28.9	996.7 996.7	1029.1		1029.1			0
[HLi] 88DIX/GOL	7580-67-8	LiH theory	300			996.4	1021.7 1021.7		1021.7 1021.7			24
[C <sub>7</sub> H <sub>17</sub> N <sub>3</sub> ] 93DEC/GAL 92RAC/MAR	101398-58-7 102-82-9 80-70-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338 338	967.6 997.4	27.6 0.4	996.4 995.4 997.6	1028.8		1028.8			0
[C <sub>14</sub> H <sub>18</sub> N <sub>2</sub> ] 83TAF 78LAU/SAL	133835-17-3 20734-58-1 87-85-4 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1,1-dimethylpropyl) N,N,N',N'-Tetramethyl-1,8- naphthalenediamine (CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub> NH <sub>3</sub>	338	989.6	6.3	995.9 995.8	1028.2		1028.2			0
[C <sub>11</sub> H <sub>16</sub> CIN <sub>3</sub> ] 94RAC/MAR	20815-38-7 80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=N(4-ClC <sub>6</sub> H <sub>4</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	350 650	836.0 819	159.7 177.7	997.0 994.5	1027.9		1027.9			0
[C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> ] 87TAF 83TAF2 79AUE/BOW	111-51-3 75-50-3 7664-41-7 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350 350 298	918.1 819 918.1	70.5 171.2 74.2	992.7 992.4 993.4 992.3	1046.3		1046.3			-71
[La] 89ELK/SUN	7439-91-0	La See Refs.				991.9	1013 1013±9		1013 1013±9			38
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ] 93DEC/GAL	151328-39-1 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=N(c-C <sub>3</sub> H <sub>5</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	23.9	991.7 991.7	1024.1		1024.1			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>3</sub> H <sub>12</sub> N <sub>2</sub> ] 93DEC/GAL	28504-67-8 102-82-9	(CH <sub>3</sub> ) <sub>2</sub> N-C(CH <sub>3</sub> )=NCH <sub>3</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	23	990.8 990.8			1023.2			0	
[C <sub>16</sub> H <sub>26</sub> N <sub>8</sub> O <sub>9</sub> ] 92WU/FEN2	38416-68-1	octaglycine kinetic method				990.7 990.7			NE			NE	
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> ] 95HER/ABB 95HER/ABB 95HER/ABB	673-46-1 110-95-2 111-51-3 80-70-6	N $\alpha$ ,N $\alpha$ -dimethylhistamine (CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	333 333 333	985.4 992.7 997.4	2.4 -0.6 -2.4	990.1 985.8 989.7 994.8			1022.0			2	
[C <sub>8</sub> N <sub>18</sub> N <sub>2</sub> ] 91DEC/GAL 91DEC/GAL	133835-17-3 3459-75-4 23314-06-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1,1-dimethylpropyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(t-C <sub>4</sub> H <sub>9</sub> )	338 338	987.9 988.3	1.7 1.3	989.6 989.6 989.6			1022.0			0	
[C <sub>9</sub> H <sub>16</sub> N] 79AUE/BOW	7148-07-4 75-50-3	Pyrrolidine,1-(1-cyclopenten-1-yl)- (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	70.3	988.4 988.4			1019.2 975.3			5.6	
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ] 93DEC/GAL 91DEC/GAL 91DEC/GAL 91DEC/GAL	23314-06-9 102-82-9 110-95-2 80-70-6 32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(t-C <sub>4</sub> H <sub>9</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338 338 338 338	967.6 985.4 997.4 981.0	19.9 3.3 -7.1 7.9	987.7 986.6 990.1 989.0			1020.8			0	
[C <sub>4</sub> H <sub>18</sub> N <sub>2</sub> ] 91DEC/GAL 91DEC/GAL	3459-75-4 23314-06-9 80-70-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(t-C <sub>4</sub> H <sub>9</sub> ) ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH	338 338	988.3 997.4	-1.3 -8.4	987.9 987.1 988.8			1020.4			0	
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O] 92RAC/MAR 92RAC/MAR 92RAC/MAR 92RAC/MAR	134166-62-4 23314-06-9 111-51-3 80-70-6 32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methoxyethyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(t-C <sub>4</sub> H <sub>9</sub> ) (CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> ((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> C=NH (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338 338 338 338	988.3 992.7 997.4 981.0	-0.4 -5.0 -10.0 4.6	987.9 985.0 987.2 985.6			1018.9			0	
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ] 91DEC/GAL 91DEC/GAL	85599-92-4 85599-94-6 134166-62-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylpropyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methoxyethyl)	338 338	984.9 986.4	1.7 -1.7	985.7 986.6 984.7			1018.1			0	
[C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> ] 93DEC/GAL 91DEC/GAL 91DEC/GAL	94793-23-4 102-82-9 85599-94-6 3717-82-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-C <sub>5</sub> H <sub>11</sub> ) (n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl) (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-butyl)	338 338 338	967.6 984.9 980.5	16.7 1.7 5.0	984.5 986.6 985.5			1018.0			0	
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ] 87TAF	110-95-2 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	64.5	985.4 985.8			1035.2			-58	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (M)
Yr/Squib	Reg No(R)	Base(R)											
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	165.2	986.8							
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	66.9	985.0							
[C <sub>9</sub> H <sub>20</sub> N <sub>2</sub> ]	85599-94-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-hexyl)				984.9			1017.4			0	
91DEC/GAL	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	>12.6	>980							
91DEC/GAL	80-70-6	((CH <sub>3</sub> ) <sub>2</sub> N) <sub>2</sub> =NH	338	997.4	-12.1	985.1							
91DEC/GAL	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338	981.0	3.8	984.8							
[C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> ]	111-18-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>6</sub> N(CH <sub>3</sub> ) <sub>2</sub>				982.2			1035.8			-71	
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	161.5	983.8							
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	62.4	980.5							
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	67161-18-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methylpropyl)				982.0			1014.5			0	
91DEC/GAL	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338	981.0	0.4	981.4							
91DEC/GAL	134166-62-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methoxyethyl)	338	986.4	-3.8	982.7							
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	27159-75-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(phenylmethyl)				981.7			1014.1			0	
92RAC/MAR	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338	981.0	0.4	981.4							
92RAC/MAR	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	976.3	4.6	980.9							
92RAC/MAR	134166-62-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-methoxyethyl)	338	986.4	-3.8	982.7							
[HOSF]	12141-14-9	SrOH				981.6			1019.4			-18	
76TAN/LIA		See Refs.							1019.4			-18	
[C <sub>18</sub> H <sub>32</sub> N <sub>6</sub> O <sub>7</sub> ]	111652-29-0	hexa-L-alanine kinetic method				981.3			NE			NE	
93WU/FEN						981.3							
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ]	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)				981.0			1013.5			0	
91DEC/GAL	109-55-7	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	338	975.3	8.4	981.4							
91DEC/GAL	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	976.3	3.8	980.0							
91DEC/GAL	110-95-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	985.4	-1.7	981.6							
[C <sub>14</sub> H <sub>22</sub> N <sub>7</sub> O <sub>8</sub> ]	18861-82-0	heptaglycine				980.6			NE			NE	
92WU/FEN2		See Refs.	350			980.6							
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ]	3717-82-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-butyl)				980.5			1013.0			0	
91DEC/GAL	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	976.3	5.0	981.3							
91DEC/GAL	32150-24-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(1-methylethyl)	338	981.0	-1.3	979.8							
[C <sub>14</sub> H <sub>26</sub> N]	64326-83-6	1-Methyl-2,6-t-butylpiperidine				980.3			1011.1			5.6	
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	61.8	979.9							
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	143.7	980.7							
[C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub> ]	7451-76-5	gly-gly-his kinetic method				979.5			NE			NE	
93WU/FEN						979.5							
96CAR/CAS	926-63-6;	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				932-960							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
	102-69-2											
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ] 9IDEDEC/GAL	32150-25-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-propyl)	338	976.3	2.1	979.2			1011.7			0
	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	980.5	-0.4	978.4						
	3717-82-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(n-butyl)				980.1						
[C <sub>3</sub> H <sub>12</sub> N <sub>2</sub> ] 9IDEDEC/GAL	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	971.1	1.7	976.3			1008.7			0
	1122-58-3	N,N-Dimethyl-4-pyridinamine	338	970.0	6.7	973.5						
	1609-01-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>3</sub>	338	975.3	2.9	976.7						
	109-55-7	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	338	975.3		976.0						
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ] 83TAF2	109-55-7	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> NH <sub>2</sub>	350	819	154.7	975.3			1025.0			-58
	7664-41-7	NH <sub>3</sub>	298	918.1	56.1	976.3						
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N				974.3						
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ] 9IDEDEC/GAL	133835-16-2	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(c-propyl)	338	970.0	3.3	973.8			1006.2			0
	1609-01-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>3</sub>	338	976.3	-2.1	973.4						
	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	976.3		974.2						
[C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> ] 87TAF	34165-19-0	2,3,5-Trimethylimidazo(1,2-a)-pyridine	350	918.1	55.4	973.7			1005.6			2
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N				973.7						
[U] 77ARM/HOD	7440-61-1	U reaction onset				973.2			995.2			35
[C <sub>6</sub> H <sub>13</sub> N] 8HELL/DIX	78733-72-9	(CH <sub>3</sub> ) <sub>2</sub> NC(CH <sub>3</sub> )=CHCH <sub>3</sub>				972.9			1005.4			0
	110-18-9;	(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> ;				971-975						
	109-55-7	(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>										
[C <sub>6</sub> H <sub>12</sub> N] 92RAC/MAR	60598-49-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-propenyl)	338	976.3	-2.9	972.3			1004.8			0
	74119-36-1	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-C <sub>2</sub> H <sub>5</sub>	338	963.4	7.9	973.3						
	32150-27-9	CH <sub>3</sub> C(N(CH <sub>3</sub> ) <sub>2</sub> )=NN(CH <sub>3</sub> ) <sub>2</sub>				971.3						
[HLiO] 70DZJ/KEB	1310-66-3	LiOH See Refs.				972.1			1000.1			14.9
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ] 91AUE/WEB	1122-58-3	N,N-Dimethyl-4-pyridinamine	300	898.1	74.7	971.1			997.6			20
	110-86-1	pyridine	350	918.1	51.3	972.8						
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	819	151.7	968.7						
	7664-41-7	NH <sub>3</sub>	350	819	152.4	969.3						
	7664-41-7	NH <sub>3</sub>	298	970.6	1.3	970.1						
	110-18-9	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	298	918.1	55.6	971.9						
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N				973.8						
[Lu] 89ELK/SUN	7439-94-3	Lu See Refs.				970.6			992			37
									992±15			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	110-18-9	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	350	918.1	49.9	970.6	1012.8		1012.8			-33
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	52.2	969.9			969.9			
75TAF	7664-41-7	NH <sub>3</sub>	350	819	151.0	971.3			971.3			
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ] 93DEC/GAL	1609-01-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>3</sub>	338	967.6	2.1	970.0	1002.5		1002.5			0
91DEC/GAL	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	971.1	-3.3	968.5			968.5			
91DEC/GAL	1122-58-3	N,N-Dimethyl-4-pyridinamine	338	967.6	2.1	969.9			969.9			
91DEC/GAL	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	975.3	-1.3	971.8			971.8			
[C <sub>12</sub> H <sub>19</sub> NO] 87TAF	3357-16-2	3-Pyrrolidino-5,5-dimethylcyclohex-2-enone	350	918.1	50.3	968.7	1001.2		1001.2			0
[C <sub>12</sub> H <sub>21</sub> NO] 87TAF	65115-73-3	3-(N,N-Diethylamino)-5,5-dimethylcyclohex-2-enone	350	918.1	50.3	968.7	1001.2		1001.2			0
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	3268-61-9	2,7-Dimethylimidazo(1,2-a)pyridine	350	918.1	50.3	968.6	1000.5		1000.5			2
[C <sub>9</sub> H <sub>21</sub> NO] 87TAF	13358-76-4	3-Piperidino-5,5-dimethylcyclohex-2-enone	350	918.1	49.9	968.3	1000.7		1000.7			0
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ] 93DEC/GAL	1606-49-1	1,4,5,6-tetrahydropyrimidine	338	967.6	-0.2	967.8	1002.0		1002.0			-5.8
[C <sub>12</sub> H <sub>27</sub> N] 87TAF	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	350	918.1	49.0	967.6	998.5		998.5			5.6
85BOL/HOU	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	323	967.6	0	967.6			967.6			
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	104.0	968.5			968.5			
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	875-80-9	2,3-Dimethylimidazo(1,2-a)pyridine	350	918.1	48.1	966.4	998.2		998.2			2
[C <sub>9</sub> H <sub>17</sub> N] 77ARN/CHA	6006-15-1	(i-C <sub>3</sub> H <sub>7</sub> )N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	298	971.1	-5.4	965.6	996.4		996.4			5.6
[C <sub>9</sub> H <sub>24</sub> N <sub>3</sub> OP] 85BOL/HOU	2327-88-0	OP(CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	323	960.1	4.2	964.4	997.7		997.7			0
85BOL/HOU	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	323	967.6	-1.7	966.0			966.0			
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	6188-30-3	2,5-Dimethylimidazo(1,2-a)pyridine	350	918.1	46.2	964.5	996.4		996.4			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>8</sub> H <sub>9</sub> N] 87TAF	7087-68-5	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	350	918.1	44.8	963.5	994.3		994.3			5.6
83TAF2	75-50-3 7664-41-7	(CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	350	819	145.5	963.0 963.9						
[C <sub>5</sub> H <sub>13</sub> N <sub>3</sub> ] 92RAC/MAR	32150-79-9	CH <sub>3</sub> C(N(CH <sub>3</sub> ) <sub>2</sub> )=NN(CH <sub>3</sub> ) <sub>2</sub>	338	960.1	2.5	963.4	995.8		995.8			0
92RAC/MAR	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	338	951	12.6	962.8						
92RAC/MAR	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	338	967.6	-4.2	963.6						
92RAC/MAR	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6		963.6						
[C <sub>12</sub> H <sub>21</sub> N] 87TAF	3717-40-6	N,N-Dimethyladamantylamine	350	918.1	44.8	963.0	993.9		993.9			5.6
90GRE/LIG	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1		963.0						
[C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> ] 90GRE/LIG	961-07-9	Deoxyguanosine kinetic method				962.9	995.4 995.4		995.4 995.4			0
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	874-39-5	7-Methylimidazo(1,2-a)pyridine	350	918.1	44.4	962.7	994.6		994.6			2
93WU/FEN	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1		962.7						
[C <sub>15</sub> H <sub>27</sub> N <sub>5</sub> O <sub>6</sub> ] 93WU/FEN	10183-34-3	penta-L-alanine kinetic method				962	NE		NE			NE
[C <sub>3</sub> H <sub>9</sub> N <sub>3</sub> ] 93DEC/GAL	51-45-6	Histamine	338	967.6	-6.5	961.9	999.8		999.8			-18
93DEC/GAL	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6		961.9						
[C <sub>19</sub> H <sub>20</sub> N <sub>2</sub> ] 89HOU/FEN	123624-78-7	13,5-metheno-6H,7H-bisazepino[1,2a:2',1'- d][1,5]diazacine,8,9,10,11-tetrahydro	313	967.6	1.3	968.9	994.3		994.3			0
89HOU/FEN	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	313	967.6		968.9						
89HOU/FEN	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	313	960.1	1.7	961.8						
89HOU/FEN	4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	313	947.9	2.1	950.0						
[C <sub>7</sub> H <sub>15</sub> N] 81ELL/DIX	78733-73-0	(CH <sub>3</sub> ) <sub>2</sub> NC(C <sub>2</sub> H <sub>5</sub> )=CHCH <sub>3</sub>				961	991.8		991.8			5.6
81ELL/DIX	121-44-8; 110-18-9	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N;(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>				951-971						
[C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>2</sub> ] 94LIG/NAP	118-00-3	guanosine kinetic method				960.9	993.4 993.4		993.4 993.4			0
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ] 92RAC/MAR	121508-72-3	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(2-propynyl)	338	967.6	-7.5	960.7	993.1		993.1			0
92RAC/MAR	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	970.0	-7.9	960.2						
92RAC/MAR	1609-01-4	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>3</sub>	338	963.4	-3.3	962.1						
92RAC/MAR	32150-27-9	CH <sub>3</sub> C(N(CH <sub>3</sub> ) <sub>2</sub> )=NN(CH <sub>3</sub> ) <sub>2</sub>	338	963.4		960.0						
[C <sub>9</sub> H <sub>21</sub> N] 91MAU/SMI	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	300	967.6	-9.6	960.1	991.0		991.0			5.6
87TAF	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	350	918.1	42.6	957.9	998.5		998.5			
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1		960.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	143.3	961.7						
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	124.0	961.1						
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	97.1	961.6						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	140.0	958.4						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	128.0	946.4						
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	100.1	964.6						
[C <sub>13</sub> H <sub>27</sub> N]	66922-18-7	2-6-Di- <i>t</i> -butylpiperidine				960.1			992.5			0
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	41.6	960.1						
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	121.3	958.6						
[MgO]	1309-48-4	MgO				959.4			988			13
81MUR		See Refs.							988			
[C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>3</sub> ]	958-09-8	Deoxyadenosine				959.1			991.5			0
90GRE/LIG		kinetic method							991.5			
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	934-37-2	2-Methylimidazo(1,2- <i>a</i> )pyridine				959.0			990.9			2
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	40.7	959.0						
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ]	10236-53-0	gly-gly-lys				958.6			NE			NE
96CAR/CAS	926-63-6;	(CH <sub>3</sub> ) <sub>2</sub> ( <i>n</i> -C <sub>3</sub> H <sub>7</sub> )N;				932-985						
	110-95-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>										
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ]	55488-08-9	lys-gly-gly				958.6			NE			NE
96CAR/CAS	926-63-6;	(CH <sub>3</sub> ) <sub>2</sub> ( <i>n</i> -C <sub>3</sub> H <sub>7</sub> )N;				932-985						
	110-95-2	(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>										
[C <sub>9</sub> H <sub>21</sub> N]	58471-09-3	( <i>t</i> -C <sub>3</sub> H <sub>11</sub> )( <i>t</i> -C <sub>4</sub> H <sub>9</sub> )NH				958.2			991.4			-2
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	40.0	958.2						
[C <sub>10</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> ]	58-61-7	adenosine				956.8			989.3			0
94LIG/NAP		kinetic method							989.3			
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	56638-68-7	(CH <sub>2</sub> ) <sub>2</sub> N-CH=N-(4-methylphenyl)				956.1			988.6			0
90BOR/HOU	102-69-2	( <i>n</i> -C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> N	313	960.1	1.3	961.4						
90BOR/HOU	4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ( <i>n</i> -C <sub>3</sub> H <sub>7</sub> )N	313	947.9	2.9	950.9						
[C <sub>8</sub> H <sub>15</sub> N]	5261-65-4	1-azabicyclo[2.2.2]-octane-2-methyl				956.1			986.9			5.6
86HEI/HON	4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ( <i>n</i> -C <sub>3</sub> H <sub>7</sub> )N	313	947.9	3.8	951.7						
86HEI/HON	102-69-2	( <i>n</i> -C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	313	960.1	-0.4	959.7						
[C <sub>9</sub> H <sub>13</sub> N <sub>5</sub> O <sub>4</sub> ]	951-77-9	Deoxycytidine				956.0			988.4			0
90GRE/LIG		kinetic method							988.4			
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> ]	2305-59-1	4,4-dimethyl-2-imidazoline				955.7			988.1			0



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
93DEC/GAL	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	338	967.6	-12.1	955.7						
[C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> ] 96CAR/CAS	2489-13-6 121-44-8; 102-69-2	gly-his (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				955.5 951-960			NE			NE
[C <sub>8</sub> H <sub>12</sub> N <sub>4</sub> O <sub>3</sub> ] 96CAR/CAS	2578-58-7 121-44-8; 102-69-2	his-gly (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				955.6 951-960			NE			NE
[C <sub>10</sub> H <sub>15</sub> N <sub>5</sub> O <sub>4</sub> ] 96CAR/CAS	7758-33-0 121-44-8; 102-69-2	gly-his-gly (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				955.5 951-960			NE			NE
[C <sub>10</sub> H <sub>20</sub> N <sub>4</sub> O <sub>4</sub> ] 96CAR/CAS	45214-22-0 121-44-8; 102-69-2	gly-lys-gly (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				955.5 951-960			NE			NE
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	933-69-7 75-50-3	5-Methylimidazo(1,2-a)pyridine (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	37.1	955.4 955.4			987.4			2
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ] 87TAF	45676-04-8 75-50-3	1-t-Butylimidazole (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	36.6	954.9 954.9			987.0			2
[C <sub>7</sub> H <sub>14</sub> Na <sub>2</sub> ] 79AUE/BOW	6238-14-8 75-50-3	3-Amino-1-azabicyclo[2.2.2]octane (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	36.6	954.7 954.7			985.7			5.6
[C <sub>9</sub> H <sub>17</sub> NO <sub>2</sub> ] 79AUE/BOW	#231 75-50-3	3,3-Dimethoxy-1-azabicyclo[2.2.2]octane (CH <sub>3</sub> ) <sub>2</sub> N	298	918.1	36.6	954.7 954.7			985.7			5.6
[C <sub>8</sub> H <sub>19</sub> N] 87TAF 83TAF2	21981-37-3 75-50-3 7664-41-7	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	350 350	918.1 819	35.7 136.4	954.7 954.2 955.2			987.9			-1.9
[C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ] 93CHE/WU 80MAU/HAM 79AUE/BOW 73AUE/WEB	110-60-1 142-84-7 75-50-3 107-10-8	1,4-butanediamine kinetic method (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH (CH <sub>3</sub> ) <sub>3</sub> N n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	330 298 298	929.3 918.1 883.9	22.6 36.1 71.3	954.3 953.7 954.3 955.1			1005.6 1004.5 1004.5			-63 -65 -61.7
[C <sub>9</sub> H <sub>19</sub> N] 84HOP/JAH 79AUE/BOW	768-66-1 29939-31-9 75-50-3	2,2,6,6-Tetramethyl-piperidine 2,4-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine (CH <sub>3</sub> ) <sub>3</sub> N	298 298	952.0 918.1	1.7 36.1	953.9 953.6 954.3			987.0			-1.9
[C <sub>3</sub> H <sub>9</sub> NO] 80KOP/COM	1184-78-7	(CH <sub>3</sub> ) <sub>3</sub> NO See Refs				953.5			983.2 983.2			9.1

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YsSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> ] 87TAF	22766-69-4 75-50-3	1-Azabicyclo[2.2.2]octane,4-N,N, dimethylamino- (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	34.8	952.9			983.9			5.6	5.6
[C <sub>10</sub> H <sub>17</sub> NO] 87TAF 86TAF/GAL	31039-88-0 75-50-3 7664-41-7	3-(N,N-Dimethylamino)-5,5-dimethyl- cyclohex-2-en-1-one (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	350 350	918.1 819	33.9 134.9	952.0 953.3			983.8			5.6	5.6
[C <sub>6</sub> H <sub>17</sub> N] 86TAF/GAL	98-94-2 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	134.2	952.6 952.6			983.6			5.6	5.6
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	1739-84-0 75-50-3	1,2-Dimethylimidazole (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	34.3	952.6 952.6			984.7			2	2
[C <sub>7</sub> H <sub>13</sub> N] 87TAF 86TAF/GAL 86HEI/HON 83TAF 80HOU/VOG 79AUE/BOW 77STA/TAA 75TAF 74STA/BEA2	100-75-5 75-50-3 7664-41-7 121-44-8 87-85-4 74-89-5 7664-41-7 7664-41-7 75-50-3	1-azabicyclo[2.2.2]-octane (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub> See Refs. CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350 350 313 350	918.1 819 951 836.0	35.7 136.1 1.3 116.7	952.5 953.8 954.5 952.3 953.7			983.3			5.6	5.6
[C <sub>4</sub> H <sub>8</sub> P] 87TAF 79AUE/BOW	554-70-1 75-50-3 75-50-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> P (CH <sub>3</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	350 298	918.1 918.1	31.1 36.1	952.0 949.5 954.3			984.5			0	0
[C <sub>13</sub> H <sub>21</sub> N] 84HOP/AH 84HOP/AH 76AUE/WEB2	29939-31-9 626-23-3 121-44-8 75-50-3	2,4-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine (sec-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	298 298	947.5 951	3.3 1.7	952.0 950.8 952.7 952.8			983.8			2	2
[C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> ] 89HOU/FEN	95864-13-4 121-44-8	15,16-diazatricyclo[8.4.1.1 <sup>3,8</sup> ]hexadeca- 1,3,5,7,9,11,13-heptaene,15,16-dimethyl (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	313	951	0.8	951.9 951.9			984.4			0	0
[C <sub>13</sub> H <sub>16</sub> N <sub>2</sub> ] 78LAU/SAL	20734-57-0 7664-41-7	N,N,N'-Trimethyl-1,8-naphthalenediamine NH <sub>3</sub>	600	819	134.7	951.8 951.8			984.3			0	0
[C <sub>8</sub> H <sub>15</sub> N] 86HEI/HON 86HEI/HON	695-88-6 102-69-2 4458-31-5	1-azabicyclo[2.2.2]-octane, 3-methyl (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	313 313	960.1 947.9	-5.9 -1.3	951.7 954.2 946.6			982.5			5.6	5.6

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	36.1	954.3						
[C <sub>7</sub> H <sub>17</sub> N]	57767-60-5	(i-C <sub>4</sub> H <sub>11</sub> )(CH <sub>3</sub> ) <sub>2</sub> N				951.5			982.5			5.6
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	33.4	951.5						
[C <sub>9</sub> H <sub>21</sub> N]	3733-36-6	(i-C <sub>4</sub> H <sub>9</sub> )C(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>				951.4			982.4			5.6
78SHE/GOB	7664-41-7	NH <sub>3</sub>	320	819	132.6	951.4						
[C <sub>14</sub> H <sub>12</sub> N <sub>2</sub> ]	75863-17-1	15,16-diazatricyclo[8.4.1.1 <sup>3,8</sup> ]hexadeca-				951.4			983.8			0
89HOU/FEN	6832-21-9	1,3,5,7,9,11,13-heptaene 2,6-(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> -pyridine	313	947.2	4.2	951.4						
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> ]	56687-95-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-phenyl				951.3			983.8			0
90BOR/HOU	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	313	960.1	-5.4	954.7						
90BOR/HOU	4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	313	947.9	0	947.9						
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ]	56-87-1	L-lysine				951.0			996			-42
96CAR/CAS	142-87-7; 121-44-8	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				929-951						
94WU/FEN		kinetic method							996			
93LI/HAR		kinetic method							942			
92GOR/SPE	109-89-7; 142-84-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	350			919-929						
90ISA/OMO		kinetic method-relative order										
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	21.5	942.0						
87BOJ		kinetic method-relative order										
86BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	123.1	943.9						
[C <sub>6</sub> H <sub>15</sub> N]	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				951			981.8			5.6
91MAU/SMI	102-82-9	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> N	602	967.6	-17.6	950.0		-22.6	975.9			
91MAU/SMI	102-69-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N	300	960.1	-12.1	948.0		-12.6	978.5			
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	33.4	951.5						
86MAU/LIE	110-86-1	pyridine	600	898.1	60.3	957.4						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	134.1	952.5						
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	131.8	950.2						
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	550	883.9	61.5	942.7						
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	33.7	951.8						
77STA/TAA	7664-41-7	NH <sub>3</sub>	320	819	119.2	938.0						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	130.4	948.8						
74STA/BEA2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	320	918.1	30.5	948.7						
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	88.8	953.3						
72ARN/ION	7664-41-7	NH <sub>3</sub>	350	819	132.3	950.7						
[C <sub>13</sub> H <sub>21</sub> N]	585-48-8	2,6-(i-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine				951			982.9			2
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	29.7	948.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: Squire	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
83TAFZ	7664-41-7	NH <sub>3</sub>	350	819	131.8	950.4						
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub>	350	836.0	111.7	948.9						
83MAU/SIE	110-86-1	pyridine	425	898.1	56.9	955.0						
76AUE/WEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	31.7	949.9						
75WOL/HAR	7664-41-7	NH <sub>3</sub>	350	819	129.1	947.6						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	136.4	955.0						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	124.7	943.3						
[C <sub>7</sub> H <sub>17</sub> F] 87TAF	3405-42-3 75-50-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> (CH <sub>3</sub> )P (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	32.5	950.9 950.9			983.5			0
[C <sub>8</sub> H <sub>13</sub> N] 79AUE/BOW	#249 75-50-3	1-Azabicyclo[2.2.2]oct-2-ene, 3-methyl (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	32.7	950.8 950.8			981.6			5.6
[C <sub>15</sub> H <sub>18</sub> ] 87TAF	489-84-9 75-50-3	1,4-Dimethyl-7-isopropylazulene (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	31.1	950.6 949.5			983.1			0
77WOL/ABB	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub>	350	836.0	114.4	951.7						
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> ] 88NEL/RUM	6130-94-5 121-44-8	1,1'-bipiperidine (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	1.3	950.4 952.2			981.2			5.8
88NEL/RUM	935-28-4	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	550	940.4	9.2	948.7						
[C <sub>9</sub> H <sub>9</sub> N <sub>3</sub> O <sub>2</sub> ] 96CAR/CAS	71-00-1 142-84-7; 121-	L-histidine (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				950.2 929-951			988			-18
94WU/FEN		kinetic method							988			-18
92GOR/SPE	110-86-1; 75-	pyridine; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>	350			898-900						
90ISA/OMO		kinetic method-relative order										
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	29.7	949.1						
87BOJ		kinetic method-relative order										
86BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	130.4	950.0						
[C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> ] 78LAU/SAL	704-01-8 7664-41-7	1,2-(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub> C <sub>2</sub> H <sub>4</sub> NH <sub>3</sub>	600	819	133.1	950.2 950.1			982.6			0
[C <sub>9</sub> H <sub>13</sub> N <sub>3</sub> O <sub>5</sub> ] 94LIGNAP	65-46-3	cytidine kinetic method				950.0			982.6 982.5			0
[C <sub>12</sub> H <sub>20</sub> N <sub>8</sub> O <sub>7</sub> ] 93ZHA/ZIM	3887-13-6 142-84-7; 111 92-2	hexaglycine (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	300			950			NE			NE
92WU/FEN2		kinetic method				929-935						
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ] 88NEL/RUM	14287-92-4 108-48-5	2,3-diazabicyclo[2.2.2]octane, 2,3-dimethyl 2-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	550	931.1	18.8	950.0 949.0			980.7			5.8
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	0	951.0						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[CH <sub>5</sub> N <sub>3</sub> ] 96AME/TOR	113-00-8 98-84-2	(NH <sub>2</sub> ) <sub>2</sub> C=NH c-C <sub>6</sub> H <sub>11</sub> (CH <sub>3</sub> ) <sub>2</sub>	338	952.6	-3.0	949.4	986.3		986.3			-14.9	
[C <sub>7</sub> N <sub>19</sub> NSi] 78SHE/GOB	100-76-5 23138-94-5 7664-41-7	1-azabicyclo[2.2.2]octane (CH <sub>3</sub> ) <sub>3</sub> Si(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	338 350	952.5 819	-4.9 131.0	948.4 949.4	980.4		980.4			5.6	
[C <sub>8</sub> H <sub>21</sub> NSi] 78SHE/GOB	28247-29-2 7664-41-7	(CH <sub>3</sub> ) <sub>3</sub> Si(CH <sub>2</sub> ) <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	131.0	949.4 949.4	980.4		980.4			5.6	
[C <sub>9</sub> H <sub>17</sub> N] 79AUE/BOW	673-33-6 75-50-3	c-C <sub>5</sub> H <sub>10</sub> NCH=C(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	31.2	949.4 949.4	978.2		978.2			12	
[C <sub>12</sub> H <sub>21</sub> N] 79AUE/BOW	6321-40-0 75-50-3	(CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	31.2	949.4 949.4	980.2		980.2			5.6	
[C <sub>15</sub> H <sub>12</sub> Fe <sub>2</sub> O <sub>3</sub> ] 89JAC	76722-37-7 108-18-9, 102-69-2	[(C <sub>5</sub> H <sub>5</sub> )(CO)Fe] <sub>2</sub> ( $\mu$ -CO)( $\mu$ -C=CH <sub>2</sub> ) (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				949.4 939-960	981.8		981.8			0	
[C <sub>10</sub> H <sub>2</sub> N <sub>2</sub> ] 88NEL/RUM	6897-05-8 935-28-4	Hydrazine, 1,2-dimethyl-1,2-bis(2-methylpropyl) 2-6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine				949.0 947.9	979.7		979.7			5.8	
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ] 88NEL/RUM	121-44-8 18389-95-2 935-28-4	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N 1-1'-bipyrrolidine 2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	550	940.4	8.4	949.0 947.0	979.7		979.7			5.8	
[C <sub>9</sub> H <sub>11</sub> BrN <sub>2</sub> ] 90BOR/HOU	121-44-8 119044-60-9 4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-bromophenyl) (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	550	951	0	951.0	981.3		981.3			0	
[C <sub>11</sub> H <sub>13</sub> N] 87TAF	75-50-3 7664-41-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N Benzoquinuclidine (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	313 350	947.9 918.1	-1.7 30.2	948.9 946.3	979.8		979.8			5.6	
[C <sub>8</sub> H <sub>15</sub> N] 86HEI/HON	121-44-8 45651-41-0 4458-31-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N 1-azabicyclo[2.2.2]octane, 4-methyl (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N	313	951	0	951.5	979.4		979.4			5.6	
[C <sub>8</sub> H <sub>15</sub> N] 87TAF	121-44-8 918-02-5 75-50-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N (CH <sub>3</sub> ) <sub>2</sub> (t-C <sub>4</sub> H <sub>9</sub> )N (CH <sub>3</sub> ) <sub>3</sub> N	313	951	0	951	979.6		979.6			5.6	
[C <sub>8</sub> H <sub>15</sub> N] 83TAF2	7664-41-7 75-50-3 7664-41-7	NH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub>	350 350	918.1 819	29.7 130.9	947.9 949.3	979.6		979.6			5.6	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>2</sub> H <sub>11</sub> N <sub>2</sub> ] 92RAC/MAR	134166-60-2 121-44-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> -CH <sub>2</sub> CN (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	338	951	-2.5	948.3			980.8			0	
92RAC/MAR	98-94-2	c-C <sub>6</sub> H <sub>11</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	952.6	-2.5	948.7							
92RAC/MAR	134166-59-9	(CH <sub>3</sub> ) <sub>2</sub> -CH=N-CH <sub>2</sub> CF <sub>3</sub>	338	933.8	12.1	950.3							
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ] 88NEL/RUM	3661-15-2 935-28-4	Pyridazino[1,2-a]pyridazine,octahydro- 2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	550	940.4	7.1	947.9			978.7			5.8	
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-1.7	946.6							
[C <sub>7</sub> H <sub>17</sub> N] 87TAF	4458-31-5 75-50-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	29.7	947.9			978.8			5.6	
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	90.3	954.8							
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ] 91AUE/WEBB	504-24-5 110-86-1	4-Pyridinamine pyridine	300	898.1	51.7	947.8			979.7			2	
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	32.0	949.9							
84CAT/PAZ	110-86-1	pyridine	320	898.1	47.7	950.3							
76AUE/WEBB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	26.8	945.8							
[C <sub>13</sub> H <sub>24</sub> N <sub>2</sub> ] 92ABB/CAB	141665-20-5 108-18-9	1,4-dimethyl-3,5-di-t-butylpyrazole (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	938.6	9.2	947.8			979.6			2	
92ABB/CAB	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	333	951	-3.3	947.7							
[C <sub>10</sub> H <sub>19</sub> N] 79AUE/BOW	31023-92-4 75-50-3	1-Azabicyclo[3.3.3]undecane(Mannixine) (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	31.7	947.7			978.7			5.6	
75AUE/WEBB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	81.0	949.9							
[C <sub>8</sub> H <sub>19</sub> N] 72AUE/WEBB	626-23-3 74-89-5	(sec-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH CH <sub>3</sub> NH <sub>2</sub>	298	864.5	83.0	945.5			980.7			-1.9	
[C <sub>13</sub> H <sub>23</sub> N] 87TAF	#177 75-50-3	Adamantyl-CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	29.3	947.5			978.4			5.6	
[C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> O] 90BOR/HOU	119044-59-6 121-44-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-acetylphenyl) (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	313	951	-3.8	947.4			979.8			0	
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ] 88NEL/RUM	5397-67-1 108-48-5	1H,5H-pyrazolo[1,2-a]pyrazole,tetrahydro 2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	550	931.1	16.3	947.3			978.0			5.8	
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-2.9	946.5							
[C <sub>8</sub> H <sub>15</sub> N] 80HOU/YOG	35079-50-6	1-4-4-(CH <sub>3</sub> ) <sub>3</sub> -1,2,3,4-tetrahydropyridine See Refs.				948.0			979.9			0	
[C <sub>8</sub> H <sub>17</sub> P] 87TAF	#181 75-50-3	(CH <sub>2</sub> ) <sub>7</sub> PCH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	28.8	947.2			979.7			0	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
[C <sub>11</sub> H <sub>17</sub> N]	6832-21-9	2,6-(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> -pyridine				947.2			979.0			2	
91MAU/SMI	585-48-8	2,6-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine	357	951	-5.0	946.0							
83MAU/SIE	110-86-1	pyridine	425	898.1	50.2	948.4							
[C <sub>8</sub> H <sub>17</sub> N]	27644-32-2	N <sub>3</sub> ,5-Trimethylpiperidine				947.2			978.1			5.6	
84HOP/AH	6832-21-9	2,6-(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> -pyridine	298	947.2	0	947.2							
[C <sub>12</sub> H <sub>28</sub> N <sub>2</sub> ]	68970-09-2	Hydrazine, 1,2-bis(2,2-dimethylpropyl)-1,2-dimethyl				947.1			977.8			5.8	
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-2.1	948.9							
88NEL/RUM	935-28-4	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	550	940.4	5.9	945.3							
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	110-70-3	CH <sub>3</sub> NHCH <sub>2</sub> -CH <sub>2</sub> NHCH <sub>3</sub>				946.9			989.2			-33	
90BOR/HOU	119044-59-6	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-acetylphenyl)	313	947.3	-0.8	946.9							
[C <sub>8</sub> H <sub>13</sub> N]	22207-84-7	1-Azabicyclo[2.2.2]octane, 3-methylene				946.4			977.2			5.6	
79AUE/BOW	750-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	28.3	946.4							
[C <sub>12</sub> H <sub>28</sub> N <sub>2</sub> ]	106376-59-4	Hydrazine, 1,2-dimethyl-1,2-dipentyl				946.4			977.2			5.8	
88NEL/RUM	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	550	931.1	15.5	945.7							
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-3.8	947.2							
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ]	462-94-2	1,5-Diaminopentane				946.2			999.6			-70	
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	26.2	944.4							
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	109.6	947.7							
73YAM/KEB	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	600	918.1	4.2	945.0							
73AUE/AWEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	64.1	947.9							
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	124-09-4	1,6-Diaminohexane				946.2			999.5			-70	
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	26.4	944.5							
73AUE/AWEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	64.1	947.9							
[C <sub>20</sub> H <sub>22</sub> N <sub>2</sub> ]	123524-79-8	14,5-metheno-5H-bisazepinol[1,2-a:2',1'-d][1,5]diazacycloundecene,7,8,9,10,11,12-hexahydro				946			978.5			0	
89HOU/FEN		See Refs.	313			946±7							
[C <sub>8</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> ]	7563-03-3	lys-gly				946.0			NE			NE	
96CAR/CAS	926-63-6; 102-69-2	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				932-960							
[C <sub>10</sub> H <sub>15</sub> N <sub>3</sub> O <sub>2</sub> ]	32999-80-7	his-gly-gly				946.0			NE			NE	
96CAR/CAS	926-63-6; 102-69-2	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> N				932-960							
[Y]	7440-65-6	Y				945.9			967			38	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
89ELK/SUN		See Refs.							967±6			
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	10447-93-6 75-50-3	1-5-Dimethylimidazole (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	27.5	945.8 945.8			977.6			2
[C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> ] 88NEL/RUM	14287-89-9 121-44-8	2,3-diazabicyclo[2.2.1]heptane,2,3-dimethyl (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-5.4	945.6 947.0			978.0			0
88NEL/RUM	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	550	931.1	12.6	944.2						
[C <sub>8</sub> H <sub>17</sub> N <sub>3</sub> O <sub>3</sub> ] 96CAR/CAS	997-62-6 626-67-5; 121-44-8	gly-lys 1-Methylpiperidine; (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				945.6 940-951			NE			NE
[C <sub>10</sub> H <sub>24</sub> N <sub>2</sub> ] 88NEL/RUM	116149-14-5 108-48-5	Hydrazine, 1,2-dibutyl-1,2-dimethyl 2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	550	931.1	13.8	945.2 944.0			976.9			5.8
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-4.6	946.3						
[C <sub>6</sub> H <sub>15</sub> N] 87TAF	921-04-0 75-50-3	(sec-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> ) <sub>2</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	27.0	945.1 945.1			975.9			5.6
[C <sub>7</sub> N <sub>16</sub> N <sub>2</sub> ] 73YAM/KEB	646-19-5 75-50-3	1,7-Diaminooheptane (CH <sub>3</sub> ) <sub>3</sub> N	600	918.1	3.8	944.9 944.9			998.6			-71
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	6338-45-0 75-50-3	1,4-Dimethylimidazole (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	26.5	944.9 944.9			976.7			2
[C <sub>10</sub> H <sub>16</sub> N <sub>2</sub> O <sub>5</sub> ] 96EWI/ZHA	20488-28-2 108-18-9; 121-44-8	pro-pro (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				944.8 939-951			NE			NE
[C <sub>9</sub> H <sub>19</sub> N] 87TAF	16607-80-0 75-50-3	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	26.5	944.7 944.7			975.6			5.6
[C <sub>12</sub> H <sub>22</sub> N <sub>4</sub> O <sub>5</sub> ] 93WU/FEN	926-79-4	tetra-L-alanine kinetic method				944.6 944.6			NE			NE
[C <sub>6</sub> H <sub>17</sub> NSi] 87TAF	18182-40-6 75-50-3	(CH <sub>3</sub> ) <sub>3</sub> SiCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	25.6	943.8 943.8			974.5			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	128.1	946.5						
78SHE/GOB	7664-41-7	NH <sub>3</sub>	320	819	116.7	935.5						
[C <sub>5</sub> H <sub>11</sub> N] 79AUE/BOW	1743-55-1 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> C=NC <sub>2</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	25.4	943.5 943.5			976.0			0
[C <sub>9</sub> H <sub>19</sub> N] 80HOU/VOG	10315-89-6	N-Isobutylpiperidine See Refs.				943.5			974.5 974.5			5.6



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ] 91AUE/WEBB	18437-57-5 110-86-1	N,N-Dimethyl-3-pyridinamine pyridine	300	898.1	46.4	943.1	969.6		969.6			20
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	24.3	944.5						
76AUE/AWEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	27.3	941.7						
[C <sub>16</sub> H <sub>27</sub> N] 87TAF	2909-76-4 75-50-3	N,N-Dimethylbenzenamine,2,4-di-t-butyl (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	24.3	942.4	973.3		973.3			5.6
[C <sub>12</sub> H <sub>30</sub> N <sub>3</sub> OP] 85BOL/HOU	2622-07-3 142-84-7	OP(N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> ) <sub>3</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	323	929.3	9.6	942.2	974.7		974.7			0
85BOL/HOU	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	323	951	-3.8	938.8						
85BOL/HOU	616-39-7	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N	323	940.0	0.4	947.4						
[C <sub>17</sub> H <sub>16</sub> N <sub>2</sub> ] 89HOU/FEN	95935-57-2 110-96-3	11,5-metheno-5H,7H-bisazepino[1,2-a:2',1'- d][1,5]diazocine,8,9-dihydro (i-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	313	925.1	0.8	942.0	974.5		974.5			0
89HOU/FEN	626-67-5	1-Methylpiperidine	313	940.1	2.9	925.9						
89HOU/FEN	935-28-4	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	313	940.4	0.4	943.1						
[C <sub>8</sub> H <sub>19</sub> N] 78SHE/GOB	15673-04-8 7664-41-7	(CH <sub>3</sub> ) <sub>3</sub> C(CH <sub>2</sub> ) <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	123.6	940.9	973.0		973.0			5.6
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> ] 91AUE/WEBB	5683-33-0 110-86-1	N,N-Dimethyl-2-pyridinamine pyridine	300	898.1	43.0	941.6	968.2		968.2			20
76AUE/AWEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	23.9	941.1						
[C <sub>9</sub> H <sub>15</sub> N] 87TAF	102-70-5 75-50-3	[CH <sub>2</sub> =CHCH <sub>2</sub> ] <sub>3</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	22.0	941.3	972.3		972.3			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	123.6	940.1						
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	24.4	942.0						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	120.8	942.5						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	110.5	939.2						
[C <sub>8</sub> H <sub>20</sub> N <sub>2</sub> ] 88NEL/RUM	3337-88-4 108-48-5	Hydrazine, 1,2-dimethyl-1,2-dipropyl 2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	550	931.1	10.9	941.2	971.9		971.9			5.8
88NEL/RUM	121-44-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	550	951	-9.6	941.1						
[C <sub>13</sub> H <sub>19</sub> N] 79MAU	260-94-6 107-10-8	Acridine n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	550	883.9	58.6	941.3	972.6		972.6			2
[C <sub>9</sub> H <sub>13</sub> N] 91MAU/SMI	935-28-4 6832-21-9	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine 2,6-(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> -pyridine	525	947.2	-7.1	940.4	972.3		972.3			2
83MAU/SIE	110-86-1	pyridine	425	898.1	42.7	940.1						
[C <sub>18</sub> H <sub>15</sub> P] [C <sub>8</sub> H <sub>5</sub> ] <sub>3</sub> P	603-35-0	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> P				940.8	972.8		972.8			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)
86TRA/MUN	108-18-9; 121-44-8	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH, (C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				939-951						
82IKU/KEB	594-09-2	(CH <sub>3</sub> ) <sub>3</sub> P	320	926.3	13.4	939.7						
[C <sub>26</sub> H <sub>54</sub> O <sub>8</sub> ] 93LIN/ROC	3055-97-8 121-69-7	(C <sub>12</sub> H <sub>25</sub> (OC <sub>2</sub> H <sub>4</sub> ) <sub>7</sub> OH C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	298	909.2	31.4	940.3 940.3	941.1	71.5	1006.7 1012.6	2	-133.9	-113.9 -131.9
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	274-76-0 75-50-3	Imidazo(1,2-a)pyridine (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	22.0	940.3 940.3			972.1			2
[C <sub>18</sub> H <sub>18</sub> N <sub>2</sub> ]	120789-29-9	12-5-metheno-5H-bisazepino[1,2-a:2',1'- d][1,5]diazonine,7,8,9,10-tetrahydro				940.2			972.6			0
89HOU/FEN	110-96-3	(i-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH	313	925.1	0.4	925.5						
89HOU/FEN	120-94-5	N-Methylpyrrolidine	313	934.8	5.4	940.3						
89HOU/FEN	935-28-4	2-6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	313	940.4	-0.4	940.0						
[C <sub>9</sub> H <sub>18</sub> N <sub>2</sub> ] 81ALD/ARR	283-58-9 7664-41-7	1,5-Diazabicyclo[3.3.3]undecane NH <sub>3</sub>	320	819	121.3	940.1 940.1			971.1			5.6
[C <sub>8</sub> H <sub>13</sub> N] 87TAF	626-67-5 75-50-3	1-Methylpiperidine (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	21.1	940.1 939.2			971.1			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	122.6	941.0						
76AUE/WEB	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	22.0	940.1						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	114.6	933.0						
[C <sub>3</sub> H <sub>13</sub> N] 87TAF	616-39-7 75-50-3	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	21.5	940.0 939.6			971.0			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	123.1	941.5						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	120.4	938.8						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	110.0	928.4						
[C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ] 80MAU/HAM	109-76-2 142-84-7	1,3-Diaminopropane (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	600	929.3	-2.8	940.0 940.6	962.3	24.3	987.0 986.5	-1.9	-45.2	-49 -47.1
80MAU/HAM	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	600	918.1	4.2	938.7	948.9	37.7	986.6	5.6	-55.6	-50
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	21.5	939.6						
73YAM/KEB	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	600	918.1	4.2	938.7	948.9	54.4	1003.3	5.6	-86.2	-80.6
73AUE/WEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	58.6	942.4						
[C <sub>13</sub> H <sub>13</sub> P] 82IKU/KEB	1486-28-8 594-09-2	(C <sub>2</sub> H <sub>5</sub> )(CH <sub>3</sub> )P (CH <sub>3</sub> ) <sub>3</sub> P	320	926.3	13.4	939.7 939.7			972.1			0
[C <sub>5</sub> H <sub>13</sub> N] 87TAF	996-35-0 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> (i-C <sub>3</sub> H <sub>7</sub> )N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	21.5	939.6 939.6			970.6			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	123.1	941.5						
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	75.1	939.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>7</sub> H <sub>17</sub> N] 87TAF	10076-31-0	(CH <sub>3</sub> ) <sub>2</sub> (neo-C <sub>5</sub> H <sub>11</sub> )N				939.5			970.5			5.6	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	20.6	938.7							
	83TAF2	NH <sub>3</sub>	350	819	121.7	940.1							
	78SHE/GOB	NH <sub>3</sub>	350	819	121.3	939.7							
[C <sub>8</sub> H <sub>17</sub> NSi] 78SHE/GOB	66365-05-7	(CH <sub>3</sub> ) <sub>2</sub> (i-C <sub>4</sub> H <sub>9</sub> )SiN(CH <sub>3</sub> ) <sub>2</sub>				938.8			969.8			5.6	
	7664-41-7	NH <sub>3</sub>	350	819	120.4	938.8							
[C <sub>8</sub> H <sub>15</sub> N] 87TAF	108-18-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH				938.6			971.9			-1.9	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	20.1	938.6							
	83TAF2	NH <sub>3</sub>	350	819	120.8	939.6							
	83LOC/MCI	NH <sub>3</sub>	350	819	120.8	939.6							
	79AUE/BOW	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	73.3	937.8							
	75ARN	NH <sub>3</sub>	350	819	106.7	925.5							
	72AUE/WEB	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	79.1	943.6							
[C <sub>7</sub> H <sub>11</sub> N] 79AUE/BOW	13929-94-7	1-Azabicyclo[2.2.2]oct-2-ene				938.6			969.4			5.6	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	20.5	938.6							
[C <sub>6</sub> H <sub>15</sub> N] 87TAF	927-62-8	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )N				938.2			969.2			5.6	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	20.1	938.3							
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> ] 96GON/MO	143-37-3	CH <sub>3</sub> C(=NH)NH <sub>2</sub>				938.2			970.7			0	
	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	929.3	8.0	937.2							
	120-94-5	N-Methylpyrrolidine	338	934.8	3.4	938.4							
	108-18-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	938.6	0.6	939.2							
	103-83-3	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	937.4	0.4	938.1							
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ] 84MAU/NEL	52598-10-4	(n-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub>				938.1			970.5			0	
	6415-12-9	(CH <sub>3</sub> ) <sub>2</sub> NN(CH <sub>3</sub> ) <sub>2</sub>	600	917.9	18.4	938.1							
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> ] 84MAU/NEL	6523-29-1	2-Methyl-1,2-diazabicyclo[2.2.2]-octane				938.1			968.9			5.6	
	6415-12-9	(CH <sub>3</sub> ) <sub>2</sub> NN(CH <sub>3</sub> ) <sub>2</sub>	600	917.9	20.1	938.1							
[C <sub>11</sub> H <sub>15</sub> N] 87TAF	25108-56-9	4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>				938.0			946.6			20	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	20.6	938.0							
[C <sub>8</sub> H <sub>15</sub> N] 87TAF	7239-24-9	(CH <sub>3</sub> ) <sub>2</sub> (i-C <sub>4</sub> H <sub>9</sub> )N				937.8			968.7			5.6	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	19.7	937.8							
[C <sub>9</sub> H <sub>13</sub> N] 87TAF	103-83-3	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>				937.4			968.4			5.6	
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	20.1	938.3							
	79AUE/BOW	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	18.5	936.6							
[C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> ] 87TAF	141665-18-1	1-methyl-3,5-di-t-butylpyrazole				937.1			970.8			-4	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
92ABB/CAB	594-39-8	t-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	5.7	909.2						
92ABB/CAB	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	929.3	6.9	936.3						
92ABB/CAB	108-18-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	938.6	-1.0	937.7						
92ABB/CAB	616-39-7	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N	333	940.0	-2.9	937.4						
[C <sub>8</sub> H <sub>11</sub> P] 82IKU/KEB	672-66-2 594-09-2	C <sub>6</sub> H <sub>5</sub> P(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> P	320	926.3	10.5	936.8 936.8			969.2			0
[C <sub>6</sub> H <sub>13</sub> P] 87TAF	39763-50-3 75-50-3	(CH <sub>2</sub> ) <sub>5</sub> PCH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	18.3	936.7 936.7			969.4			0
[C <sub>7</sub> H <sub>12</sub> FN] 79AUE/BOW	#321 75-50-3	3-Fluoro-1-azabicyclo[3.2.1]octane (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	18.6	936.7 936.7			967.5			5.6
[C <sub>6</sub> H <sub>13</sub> NO] 79AUE/BET	53687-79-9 75-50-3	c-C <sub>5</sub> H <sub>10</sub> N(2-OCH <sub>3</sub> ) (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	18.6	936.7 936.7			969.9			-2
[C <sub>7</sub> H <sub>18</sub> N <sub>2</sub> ] 84MAU/NEL	60678-73-1 108-48-5	(t-C <sub>4</sub> H <sub>9</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub> 2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	600	931.1	4.6	936.4 936.4			968.8			0
[C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> ] 88NEL/RUM 88NEL/RUM	49840-68-8 108-48-5 935-28-4	1H-1,2-diazepine,hexahydro-1,2-dimethyl 2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine 2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> pyridine	550 550 550	931.1 931.1 940.4	5.4 -2.9	936.6 936.6 936.6			966.8 966.8			5.8
[C <sub>8</sub> H <sub>15</sub> NSi] 83HEN/FRE	18135-05-2 109-89-7, 121-44-8	(CH <sub>3</sub> ) <sub>3</sub> SiN(CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH;(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N				936 919-951			966.8			5.6
[C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> ] 88NEL/RUM 88NEL/RUM 84MAU/NEL 84MAU/NEL	26163-37-1 935-28-4 108-48-5 613-48-9 108-48-5	Pyridazine, hexahydro-1,2-dimethyl 2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> pyridine 2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine 4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> 2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	550 550 600 600	940.4 931.1 931.0 931.1	-1.7 7.1 0.8 5.4	935.4 937.9 937.4 930.7 935.5			966.1			5.6
[C <sub>8</sub> H <sub>10</sub> N] 76AUE/AWEB 75ARN 72AUE/AWEB	111-92-2 74-89-5 7664-41-7 74-89-5	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub>	298 350 298	864.5 819 864.5	70.8 102.9 71.3	935.3 935.3 921.7 935.8			968.6			-1.9
[C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> ] 84MAU/NEL 84MAU/NEL	4267-00-9 613-48-9 589-93-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NN(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> 4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> 2,5-(CH <sub>3</sub> ) <sub>2</sub> pyridine	600 600	931.0 926.9	4.2 14.2	935.3 932.3 938.3			964.3			11.6
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ] 88CAT/CLA 88CAT/CLA	1632-83-3 108-18-9 598-56-1	1-methylbenzimidazole (t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH (CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	~300 ~300	938.6 929.1	-2.9 5.4	935.2 935.7 934.5			967.0			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (M)
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	16.9	935.2							
[C <sub>5</sub> H <sub>11</sub> N]	120-94-5	N-Methylpyrrolidine							965.6				5.6
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	16.0	934.8							
78TAA/WOL	110-86-1	pyridine	350	898.1	34.7	934.1							
76AUE/WEB	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	17.1	932.7							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	117.6	936.0							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	107.5	925.9							
73TAF/TAA	110-86-1	pyridine	350	898.1	38.0	935.9							
[C <sub>8</sub> H <sub>11</sub> N]	36556-06-6	Isoquinoline,5,6,7,8-tetrahydro-							966.6				2
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	16.6	934.7							
[C <sub>8</sub> N <sub>17</sub> N]	1003-84-5	1,4,4-Trimethylpiperidine							966.7				5.6
80HOU/VOG		See Refs.				934.7			965.7				
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ]	280-57-9	1,4-Diazabicyclo[2.2.2]octane							963.4				12
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	17.1	934.6							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	73.2	937.7							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	105.0	923.1							
74STA/BEA2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	320	918.1	15.9	933.9							
[C <sub>5</sub> H <sub>11</sub> N]	6163-56-0	CH <sub>3</sub> CH=CHN(CH <sub>3</sub> ) <sub>2</sub>							967.0				0
81ELL/DIX	616-47-7; 102-70-5	1H-methylimidazole; (CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>3</sub> N				934.5 928-941							
[C <sub>6</sub> H <sub>13</sub> N]	6906-32-7	(CH <sub>3</sub> ) <sub>2</sub> C=CHN(CH <sub>3</sub> ) <sub>2</sub>							967.0				0
81ELL/DIX	616-47-7; 108-18-9	1H-methylimidazole; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH				934.5 928-939							
[C <sub>12</sub> H <sub>19</sub> N]	22025-87-2	(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> (t-C <sub>4</sub> H <sub>9</sub> )							961.0				20
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	16.9	934.3							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	118.5	936.2							
[C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> ]	60678-65-1	(n-C <sub>3</sub> H <sub>7</sub> )(CH <sub>3</sub> )NN(CH <sub>3</sub> ) <sub>2</sub>							966.8				0
84MAU/NEL	6415-12-9	(CH <sub>3</sub> ) <sub>2</sub> NN(CH <sub>3</sub> ) <sub>2</sub>	600	917.9	14.6	934.3							
[C <sub>7</sub> H <sub>13</sub> CIN]	49665-74-9	c-C <sub>5</sub> H <sub>9</sub> N,2-CH <sub>2</sub> Cl,1-CH <sub>3</sub>							965.0				5.6
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	16.1	934.2							
[C <sub>9</sub> H <sub>11</sub> N]	10500-57-9	Quinoline,5,6,7,8-tetrahydro-							966.0				2
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	16	934.1							
[C <sub>12</sub> H <sub>22</sub> N <sub>2</sub> ]	18712-47-6	3,5-di-t-butyl-4-methylpyrazole							967.5				-4
92ABB/CAB	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	929.3	4.4	933.7							
92ABB/CAB	108-18-9	(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	938.6	-4.7	934.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
92ABB/CAB	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	333	931.1	2.4	933.7							
[C <sub>5</sub> H <sub>6</sub> F <sub>3</sub> N]	134166-59-9	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> CF <sub>3</sub>				933.8			966.2			0	
92RAC/MAR	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	929.3	3.8	933.0							
92RAC/MAR	120-94-5	N-Methylpyrrolidine	338	934.8	-0.4	934.6							
92RAC/MAR	139033-03-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-OCH <sub>3</sub>	338	915.8	>14	>930							
[CH <sub>2</sub> O]	19710-56-6	HCOH (hydroxymethylene)				933.4			965.9			0	
82PAU/HEH2	19961-27-4; 626-67-5	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> (i-C <sub>3</sub> H <sub>7</sub> )NH; N-methylpiperidine				927-940							
[C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> ]	23337-93-1	Hydrazine, 1,2-dieethyl-1,2-dimethyl				933.0			963.7			5.8	
88NEL/RUM	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	550	931.1	2.1	932.3							
88NEL/RUM	935-28-4	2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine	550	940.4	-5.9	933.6							
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> ]	54-11-5	3-(2-(N-methylpyrrolidinyl))pyridine				932.6			963.4			5.6	
91BER/DEC	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	929.3	3.1	932.1							
91BER/DEC	120-94-5	N-Methylpyrrolidine	338	934.8	-1.6	933.2							
[C <sub>11</sub> H <sub>17</sub> N]	91-67-8	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>	320	909.2	23.0	932.2			964.1			2	
85LIA/JAC	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>				932.2							
[C <sub>4</sub> H <sub>11</sub> NO]	13325-10-5	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>4</sub> OH				932.1			984.5			-67	
80MAU/HAM	110-86-1	pyridine	330	898.1	31.8	932.0	930	54	984	2	-67	-65	
[C <sub>3</sub> H <sub>7</sub> N]	926-63-6	(CH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )N				931.9			962.8			5.6	
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	13.7	931.9							
80HOU/VOG		See Refs.							959.4				
[C <sub>7</sub> H <sub>12</sub> BrN]	#364	3-Bromo-1-azabicyclo[2.2.2]octane				931.8			962.6			5.6	
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	13.7	931.8							
[C <sub>11</sub> H <sub>17</sub> N]	1129-69-7	2-C <sub>6</sub> H <sub>13</sub> (c-C <sub>3</sub> H <sub>4</sub> N)				931.7			963.6			2	
83MAU/SIE	110-86-1	pyridine	425	898.1	33.5	931.6							
[C <sub>7</sub> H <sub>9</sub> N]	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine				931.1			963.0			2	
92ABB/CAB	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	929.3	2.1	931.2							
91AUE/WEB	110-86-1	pyridine	300	898.1	32.7	930.8							
91MAU/SMI	585-48-8	2,6-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> pyridine	480	951	-20.1	930.9							
83MAU/SIE	110-86-1	pyridine	425	898.1	32.6	930.8							
76AUE/WEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	13.7	931.8							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	101.7	920.3							
[C <sub>12</sub> H <sub>19</sub> N]	2217-07-4	C <sub>6</sub> H <sub>5</sub> N(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub>				931.1			963.0			2	
85LIA/JAC	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	320	909.2	21.8	931.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0(R)$	$\Delta \Delta S_p^0(M,R)$	$\Delta S_p^0(M)$
[C <sub>3</sub> H <sub>7</sub> N <sub>2</sub> ] 91BER/DEC 91BER/DEC	494-97-3 123-75-1 120-94-5	3-(2-pyrrolidiny)pyridine Pyrrolidine N-Methylpyrrolidine	338 338	915.3 934.8	14.1 -2.5	931.0 929.4 932.6			964.0			-2
[C <sub>11</sub> H <sub>17</sub> N] 85LIA/JAC	613-48-9 121-69-7	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	320	909.2	21.8	931.0 931.0			962.8			2
[C <sub>12</sub> H <sub>14</sub> N <sub>2</sub> ] 78LAU/SAL	20734-56-9 7664-41-7	N,N'-Dimethyl-1,8-naphthalenediamine NH <sub>3</sub>	600	819	116.7	930.9 930.8			960.3			10
[C <sub>7</sub> H <sub>6</sub> N] 91AUE/WEB 76AUE/WEB2	108-47-4 110-86-1 75-50-3	2,4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine pyridine (CH <sub>3</sub> ) <sub>3</sub> N	300 298	898.1 918.1	32.7 12.7	930.8 930.8 930.8			962.9			2
[C <sub>8</sub> H <sub>9</sub> N] 79AUE/BOW	533-35-7 75-50-3	3,4-Cyclopentenopyridine (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	12.2	930.5 930.4			962.4			2
[C <sub>11</sub> H <sub>15</sub> NO] 88CAU/CER	54660-04-7	Pyrrolidine, 1-(4-methoxyphenyl) See Refs.				930.4 930.4			961.2			5.6
[C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> ] 89HOU/FEN 89HOU/FEN	95936-56-1 108-48-5 142-84-7	10,5-metheno-5H-bisazepino[1,2-d:2',1'- g][1,4]diazepine,7,8-dihydro 2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	313 313	931.1 929.3	-1.7 1.7	929.5 930.9			962.6			0
[C <sub>9</sub> H <sub>13</sub> N] 91MAU/SMI 91MAU/SMI 83MAU/SIE 79AUE/BOW	5944-41-2 585-48-8 6832-21-9 110-86-1 75-50-3	2-(t-C <sub>4</sub> H <sub>9</sub> )-pyridine 2,6-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> -pyridine 2,6-(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> -pyridine pyridine (CH <sub>3</sub> ) <sub>3</sub> N	397 485 425 298	951 947.2 898.1 918.1	-17.2 -19.2 31.0 10.3	929.8 933.8 927.9 929.1 928.4			961.7			2
[C <sub>8</sub> H <sub>7</sub> NO] 91AUE/WEB 87TAF 81TAA/SUM 76AUE/WEB2 75TAF 75ARN 72TAA/HEN	620-08-6 110-86-1 75-50-3 7664-41-7 75-50-3 7664-41-7 75ARN 110-86-1	4-(CH <sub>3</sub> O)-pyridine pyridine (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N NH <sub>3</sub> NH <sub>3</sub> pyridine	300 350 320 298 350 350 320	898.1 918.1 819 918.1 819 819 898.1	31.2 12.4 103.8 11.2 110.7 101.3 36.4	929.8 929.4 930.7 922.6 929.4 929.3 919.8 934.5			961.7			2
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	693-98-1 75-50-3	2-Methylimidazole (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	11.0	929.6 929.6			963.4			-4
[C <sub>6</sub> H <sub>16</sub> N <sub>3</sub> O] 85BOL/HOU 85BOL/HOU	7778-06-5 496-15-1 598-56-1	c-OP(N(CH <sub>3</sub> ) <sub>2</sub> N(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> )) 2,3-Dihydroindole (CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	323 323	926.3 929.1	0.4 2.5	929.3 926.8 931.7			961.7			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>6</sub> H <sub>15</sub> N] 87TAF	142-84-7 75-50-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	9.6	929.3			962.3			-1.9
83TAF	7664-41-7	NH <sub>3</sub>	350	819	111.2	928.1						
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	40.2	930.0						
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	13.2	923.3						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	111.2	931.3						
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	67.3	930.0						
						931.8						
[C <sub>4</sub> H <sub>11</sub> N] 87TAF	598-56-1 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	10.5	929.1			960.1			5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	112.1	928.7						
76AUE/WEB	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	11.2	930.5						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	109.4	929.4						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	100.0	927.8						
						918.4						
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> OP] 87TAF	680-31-9 75-50-3	OP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	10.1	928.7			958.6			9.1
84BOL/HOU	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	~323	929.3	0.4	928.0						
						929.4						
[C <sub>3</sub> H <sub>12</sub> N <sub>2</sub> ] 88NEL/RUM	38704-89-1 935-28-4	Pyrazolidine, 1,2-dimethyl 2,6-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> pyridine	550	940.4	-11.7	928.6			959.3			5.8
88NEL/RUM	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> pyridine	550	931.1	-0.8	927.8						
						929.4						
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> ] 87TAF	99-98-9 75-50-3	4-H <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	11.0	928.4			956.0			20
						928.4						
[C <sub>9</sub> H <sub>14</sub> N <sub>4</sub> O <sub>3</sub> ] 93ZHA/ZIM	637-84-3 109-06-8;	tetraglycine 2-CH <sub>3</sub> -C <sub>3</sub> H <sub>6</sub> N; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	300			928.2			973.8			-44
	109-89-7					917-919						
93WU/LEB	127-19-5;	CH <sub>3</sub> CON(CH <sub>3</sub> ) <sub>2</sub> ; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	300			877-884						
	107-10-8	kinetic method										
93CHE/WU		kinetic method				924.8						
92WU/FEN2												
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 89OSA/DEL	922-69-0 142-84-7	CH <sub>2</sub> =C(OCH <sub>3</sub> ) <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	313	929.3	-1.3	928.1			957.0			12
89OSA/DEL	110-89-4	Piperidine	313	921	6.3	927.8						
89OSA/DEL	598-56-1	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> )N	313	929.1	0.4	927.1						
						929.4						
[C <sub>10</sub> H <sub>15</sub> N] 85LIA/JAC	91-66-7 121-69-7	C <sub>6</sub> H <sub>5</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	325	909.2	17.6	927.9			959.8			2
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	112.5	926.8						
						929.0						
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ] 88CAT/CLA	616-47-7 111-49-9	1-methylimidazole Hexahydroazepine	~300	923.5	3.3	927.7			959.6			2
						926.9						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
88CAT/CLA	598-56-1	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> N	~300	929.1	-2.5	926.6						
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	8.2	926.5						
86MAU/LIE	121-44-8	(CH <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> N	600	951	-23.0	929.1						
86MAU/LIE	108-99-6	3-(CH <sub>3</sub> )-pyridine	600	911.6	19.7	931.3						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	114.9	933.4						
81ELL/DIX	142-84-7; 108-18-9	(C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH				929-939						
[C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> O]	73-40-5	Guanine				927.6			959.5			2
90GRE/LIG	124-40-3;	kinetic method							959.5			
75WIL/MCC	75-50-3	(CH <sub>3</sub> ) <sub>2</sub> NH; (CH <sub>3</sub> ) <sub>3</sub> N				896-918						
[C <sub>7</sub> H <sub>9</sub> N]	583-61-9	2,3-(CH <sub>3</sub> ) <sub>2</sub> -pyridine				927.0			958.9			2
91AUE/AWEB	110-86-1	pyridine	300	898.1	28.3	926.5						
76AUE/AWEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	9.3	927.4						
[C <sub>16</sub> H <sub>14</sub> N <sub>2</sub> ]	19311-79-6	1-methyl-3,5-diphenylpyrazole				927.0			958.9			2
92ABB/CAB	3978-81-2	4-(i-C <sub>4</sub> H <sub>9</sub> )-pyridine	333	925.8	2.2	928.0						
92ABB/CAB	142-84-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	929.3	-3.1	926.0						
[C <sub>7</sub> H <sub>9</sub> N]	589-93-5	2,5-(CH <sub>3</sub> ) <sub>2</sub> -pyridine				926.9			958.8			2
91AUE/AWEB	110-86-1	pyridine	300	898.1	28.3	926.5						
76AUE/AWEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	9.3	927.4						
[C <sub>2</sub> H <sub>11</sub> N]	2155-94-4	CH <sub>2</sub> =CHCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>				926.8			957.8			5.6
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	8.7	926.8						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	108.9	927.3						
[C <sub>3</sub> H <sub>5</sub> N]	19961-27-4	(C <sub>2</sub> H <sub>5</sub> )(i-C <sub>3</sub> H <sub>7</sub> )NH				926.7			960.0			-1.9
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	8.2	926.7						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	108.9	927.7						
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ]	1187-50-4	leu-gly-gly				926.7			NE			NE
93WU/FEN		kinetic method				926.7						
[C <sub>7</sub> H <sub>9</sub> NO]	23579-92-2	2-(CH <sub>3</sub> OCH <sub>2</sub> )-pyridine				926.4			958.3			2
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	8.3	926.4						
[C <sub>11</sub> H <sub>15</sub> N]	4096-20-2	Piperidine, 1-phenyl				926.4			952.9			20
88CAU/CER		See Refs.				926.7						
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	8.7	926.1						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	109.4	927.1						
[C <sub>8</sub> H <sub>9</sub> N]	496-15-1	2,3-Dihydroindole				926.3			957.1			5.6
85BOL/HOU	496-15-1	2,3-Dihydroindole	323	926.3	0	926.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>3</sub> H <sub>9</sub> P] 87TAF	594-09-2 75-50-3	(CH <sub>3</sub> ) <sub>3</sub> P (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	7.8	926.3			958.8			0
[C <sub>3</sub> H <sub>9</sub> P] 82IKU/KEB	594-09-2 7664-41-7	(CH <sub>3</sub> ) <sub>3</sub> P NH <sub>3</sub>	320	926.3	0	926.3			958.8			0
[C <sub>3</sub> H <sub>9</sub> P] 75TAF	7664-41-7 75-50-3	NH <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	819	107.1	925.8			958.8			0
[C <sub>3</sub> H <sub>9</sub> P] 74STA/BEA	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	320	918.1	6.7	924.9			958.8			0
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O] 94GRU/CAL	6331-71-1 110-89-4; 108-47-4	4-NH <sub>2</sub> -C <sub>8</sub> H <sub>16</sub> CON(CH <sub>3</sub> ) <sub>2</sub> piperidine; 2,4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine				925.9			956.9			5
[C <sub>9</sub> H <sub>13</sub> N] 92ABB/CAB	3978-81-2 142-84-7	4-(t-C <sub>4</sub> H <sub>9</sub> )-pyridine (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	333	929.3	-4.6	924.5			957.7			2
[C <sub>9</sub> H <sub>13</sub> N] 76AUE/WEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	8.8	926.9			957.7			2
[C <sub>12</sub> H <sub>17</sub> N] 88CAU/CER	40832-99-3	1-H-Azepine, hexahydro-1-phenyl See Refs.				925.8			956.6			5.6
[C <sub>8</sub> H <sub>9</sub> N] 79AUE/BOW	533-37-9 75-50-3	2,3-Cyclopentenopyridine (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	7.3	925.6			957.5			2
[C <sub>7</sub> H <sub>7</sub> N] 79AUE/BOW	56911-27-4 75-50-3	3,4-Cyclobutenopyridine (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	7.3	925.5			957.5			2
[C <sub>7</sub> H <sub>9</sub> N] 91AUE/WEB	583-58-4 110-86-1	3,4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine pyridine	300	898.1	27.3	925.5			957.3			2
[C <sub>3</sub> H <sub>5</sub> NO] 79AUE/BET	5264-35-7 75-50-3	c-C <sub>4</sub> H <sub>6</sub> N(2-OCH <sub>3</sub> ) (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	7.3	925.5			957.9			0
[C <sub>8</sub> H <sub>13</sub> N] 94BOH/DEC	609-72-3 110-89-4	N,N,2-trimethylaniline Piperidine	338	921	4.3	924.5			951.8			20
[C <sub>8</sub> H <sub>13</sub> N] 94BOH/DEC	109-06-8 142-84-7	2-(CH <sub>3</sub> )-pyridine (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	917.3	8.9	925.5			951.8			20
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ] 96EWI/ZHA	2578-57-6 110-89-4; 142-84-7	pro-gly Piperidine; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	338	929.3	-2.5	925.9			951.8			20
[C <sub>9</sub> H <sub>15</sub> N <sub>2</sub> O <sub>4</sub> ] 96EWI/ZHA	7561-25-3 110-89-4; 142-84-7	pro-gly-gly Piperidine; (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH				925.1			NE			NE
[C <sub>8</sub> H <sub>19</sub> N] 75ARN	110-96-3 7664-41-7	(i-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> NH NH <sub>3</sub>	350	819	105.4	925.1			958.1			-1.9
[C <sub>8</sub> H <sub>19</sub> N] 72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	61.5	926.0			958.1			-1.9

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	10250-58-5 3978-81-2 536-75-4	1,3-dimethyl-5-phenylpyrazole 4-(i-C <sub>4</sub> H <sub>9</sub> )-pyridine 4-(C <sub>2</sub> H <sub>5</sub> )-pyridine	333 333	925.8 919.2	-0.4 4.9	924.7 925.4 924.1	956.6		956.6			2
[C <sub>8</sub> H <sub>11</sub> N] 83MAU/SIE	75981-47-4 110-86-1	2-(i-C <sub>3</sub> H <sub>7</sub> )-pyridine pyridine	425	898.1	26.4	924.6 924.5	956.4		956.4			2
[C <sub>9</sub> H <sub>21</sub> OP] 85BOL/HOU 85BOL/HOU	17513-58-5 496-15-1 142-84-7	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> PO 2,3-Dihydroindole (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	323 323	926.3 929.3	-1.3 -5.0	924.5 925.0 924.0	954.4		954.4			9.1
[C <sub>6</sub> H <sub>6</sub> N] 81ELL/DIX	5763-87-1 110-89-4; 616-42-7	(CH <sub>3</sub> ) <sub>2</sub> NCH=CH <sub>2</sub> piperidine; 1-methylimidazole				924.4 921-928	956.8		956.8			0
[C <sub>11</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> ] 93GOR/AMS	20556-11-0 109-89-7; 142-84-7	lys-val (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH; (C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH	350			924.3 919-929	NE		NE			NE
[C <sub>11</sub> H <sub>23</sub> N <sub>3</sub> O <sub>3</sub> ] 93GOR/AMS	22677-62-9 109-89-7; 142-84-7	val-lys (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH; (C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> N	350			924.3 919-929	NE		NE			NE
[C <sub>10</sub> H <sub>15</sub> N] 85LIA/JAC	4913-13-7 121-69-7	3,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub>	320	909.2	15.1	924.3 924.3	956.1		956.1			2
[C <sub>9</sub> H <sub>17</sub> N <sub>3</sub> O <sub>4</sub> ] 93WU/FEN	5874-90-8	tri-L-alanine kinetic method				924.1 924.1	NE		NE			NE
[C <sub>8</sub> H <sub>11</sub> N] 89HOU/FEN	622-39-9 95935-56-1	2-(C <sub>3</sub> H <sub>7</sub> )-pyridine 10,5-metheno-5H-bisazepino[1,2-d:2',1'- g][1,4]diazepine,7,8-dihydro	313	930.1	-6.3	923.8 923.8	955.7		955.7			2
[C <sub>8</sub> H <sub>11</sub> N] 92ABB/CAB	696-30-0 10250-58-5	4-(i-C <sub>3</sub> H <sub>7</sub> )-C <sub>5</sub> H <sub>4</sub> N 1,3-dimethyl-5-phenylpyrazole	333	924.7	-0.9	923.8 923.8	956.7		956.7			2
[C <sub>6</sub> H <sub>13</sub> N] 87TAF	111-49-9 75-50-3	Hexahydroazepine (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	5.0	923.5 923.5	956.7		956.7			-1.9
[C <sub>7</sub> H <sub>9</sub> N] 91AUE/WEB 76AUE/WEB	591-22-0 110-86-1 74-89-5	3,5-(CH <sub>3</sub> ) <sub>2</sub> -pyridine pyridine CH <sub>3</sub> NH <sub>2</sub>	300 298	898.1 864.5	25.4 58.6	923.5 923.5 923.1	955.4		955.4			2
[C <sub>7</sub> H <sub>12</sub> CIN] 86HEI/HON	42332-45-6 110-89-4	3-Chloro-1-azabicyclo[2.2.2]octane Piperidine	313	921	1.3	923.5 922.2	954.3		954.3			5.6

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
	496-15-1	75-50-3	Base(R)	Base(M)										
86HEI/HON	496-15-1	75-50-3	2,3-Dihydroindole (CH <sub>3</sub> ) <sub>3</sub> N		313	926.3	-2.5	923.8						
79AUE/BOW	75-50-3				298	918.1	6.3	924.5						
[C <sub>6</sub> H <sub>7</sub> NS]	22581-72-2		4-(CH <sub>3</sub> S)-pyridine					923.3			955.2			2
91AUE/WEB	110-86-1		pyridine		300	898.1	24.9	923.0						
87TAF	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		350	918.1	5.0	923.3						
79AUE/BOW	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		298	918.1	5.8	923.9						
[C <sub>10</sub> H <sub>15</sub> N]	769-06-2		N,N,2,6-Tetramethylaniline					923.2			954.1			5.6
87TAF	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		350	918.1	5.0	923.2						
[C <sub>6</sub> H <sub>13</sub> N]	1611-12-7		n-C <sub>3</sub> H <sub>7</sub> CH=NC <sub>2</sub> H <sub>5</sub>					923.0			955.5			0
79AUE/BOW	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		298	918.1	4.9	923.0						
[C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> ]	462-08-8		3-Pyridinamine					922.6			954.4			2
91AUE/WEB	110-86-1		pyridine		300	898.1	24.4	922.6						
76AUE/WEB2	124-40-3		(CH <sub>3</sub> ) <sub>2</sub> NH		298	896.5	4.4	900.9						
[C <sub>9</sub> H <sub>13</sub> NO]	701-56-4		4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>					922.4			949.1			20
87TAF	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		350	918.1	5.0	922.4						
[C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> ]	92234-54-3		1-(1-adamanty)pyrazole					922.4			954.5			2
87TAF	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		350	918.1	4.1	922.4						
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ]	10250-60-9		1,5-dimethyl-3-phenylpyrazole					922.4			954.3			2
92ABB/CAB	696-30-0		4-(i-C <sub>3</sub> H <sub>7</sub> )-C <sub>3</sub> H <sub>4</sub> N		333	923.8	-0.5	923.3						
92ABB/CAB	536-75-4		4-(C <sub>2</sub> H <sub>5</sub> )-pyridine		333	919.2	2.3	921.6						
[C <sub>7</sub> H <sub>7</sub> N]	56911-25-2		2,3-Cyclobutenopyridine					922.0			953.9			2
79AUE/BOW	75-50-3		(CH <sub>3</sub> ) <sub>3</sub> N		298	918.1	3.9	922.0						
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ]	2576-67-2		gly-leu-gly					921.8			NE			NE
93WU/FEN			kinetic method					921.8						
[C <sub>9</sub> H <sub>7</sub> N]	91-22-5		Quinoline					921.4			953.2			2
91AUE/WEB	110-86-1		pyridine		300	898.1	26.4	924.5						
8IMCL/CAM	583-58-4		3,4-dimethylpyridine:kinetic method		425									
79MAU	107-10-8		n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>		535	883.9	36.0	918.2					-1.7	944.7
[C <sub>3</sub> H <sub>8</sub> Si]	4112-23-6		(CH <sub>3</sub> ) <sub>2</sub> Si=CH <sub>2</sub>					921.0			947.5			20
90ALL/MCM	110-89-4;		piperidine; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> NH					921.0						
	108-18-9							921-939						
82PIE/HEH	7664-41-7		NH <sub>3</sub>		350	819	102.5	920.2						
79PIE/POL	110-89-4;		piperidine; (C <sub>2</sub> H <sub>5</sub> )(i-C <sub>3</sub> H <sub>7</sub> )NH		320			921-927						
	19961-27-4													

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>10</sub> H <sub>17</sub> N <sub>3</sub> O <sub>6</sub> ] 93ZHA/ZIM	7093-67-6 109-06-8; 109-89-7	pentaglycine 2-CH <sub>3</sub> -C <sub>3</sub> H <sub>4</sub> N; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	300			921 917-919			NE			NE
93WU/LEB	78-81-9; 13952-84-6	i-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> ; s-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> See Refs.	300			891-896 947.4						
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>5</sub> ] 93GOR/AMS	3062-07-5 75-50-3; 109-89-7	val-glu (CH <sub>3</sub> ) <sub>3</sub> N, (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	350			921 918-919			NE			NE
[C <sub>5</sub> H <sub>11</sub> N] 87TAF	110-89-4 75-50-3	Piperidine (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	1.4	921 919.9			954.0			-1.9
83TAF	7664-41-7	NH <sub>3</sub>	350	819	102.1	920.8						
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	96.7	914.3						
76AUE/AWEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	56.1	920.6						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	102.1	920.8						
75AUE/AWEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	58.1	922.6						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	93.3	912.1						
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	102.5	920.2						
73AUE/AWEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	40.5	924.4						
71BOW/AUE	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	4.9	923.0						
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	822-36-6 7664-41-7	4-Methylimidazole NH <sub>3</sub>	350	819	105.3	920.9 923.8			952.8			2
86MAU/LIE	110-86-1	pyridine	600	898.1	19.9	918.0						
[C <sub>11</sub> H <sub>20</sub> N <sub>2</sub> ] 92ABB/CAB	1132-14-5 696-30-0	3,5-di-t-butylpyrazole 4-(i-C <sub>3</sub> H <sub>7</sub> )-C <sub>3</sub> H <sub>4</sub> N	333	923.8	-2.5	920.8 921.3			952.7			2
92ABB/CAB	536-75-4	4-(C <sub>2</sub> H <sub>5</sub> )-pyridine	333	919.2	1.1	920.3						
[C <sub>7</sub> H <sub>9</sub> N] 91AUE/AWEB	100-71-0 110-86-1	2-(C <sub>2</sub> H <sub>5</sub> )-pyridine pyridine	300	898.1	22.0	920.6 920.1			952.4			2
83MAU/SIE	110-86-1	pyridine	425	898.1	22.2	920.3						
76AUE/AWEB2	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	2.9	921.1						
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ] 84FLA/MAQ	51-17-2	Benzimidazole kinetic method				920.5 916			953.8			-3
83CAT/ELG		kinetic method				925						
[C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub> ] 86SUN/KUL	111-42-2	(HOCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NH See Refs.	300			920 920			953.0 954			-2 0
[C <sub>7</sub> H <sub>12</sub> CIN] 86HEI/HON	96943-88-3 496-15-1	1-azabicyclo[2.2.2]-octane, 2-chloro 2,3-Dihydroindole	313	926.3	-5.9	920.0 920.4			950.8			5.6
86HEI/HON	110-89-4	Piperidine	313	921	-1.3	919.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p^{\ddagger}(R)$	$\Delta \Delta S_p^{\ddagger}(M,R)$	$\Delta S_p^{\ddagger}(M)$	$\Delta S_p^{\ddagger}(M)$
[C <sub>9</sub> H <sub>7</sub> N] 91AUE/WEB 79MAU	119-65-3	Isoquinoline				919.9			951.7				2
	110-86-1	pyridine	300	898.1	25.9	924.0							
	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	33.5	915.7							
[C <sub>5</sub> H <sub>14</sub> N <sub>2</sub> ] 87TAF	51-80-9	(CH <sub>3</sub> ) <sub>2</sub> NCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>				919.8			952.2				0
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	1.4	919.8							
[C <sub>10</sub> H <sub>11</sub> N <sub>3</sub> ] 90BOR/HOU 90BOR/HOU 90BOR/HOU 90BOR/HOU	119044-58-5	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-cyanophenyl)				919.8			952.2				0
	109-89-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	313	919.4	-0.4	919.0							
	109-06-8	2-(CH <sub>3</sub> )-pyridine	313	917.3	3.3	920.6							
	110-89-4	Piperidine	313	921	-0.8	920.1							
	591-22-0	3,5-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	313	923.5	-4.2	919.4							
[C <sub>4</sub> H <sub>11</sub> N] 87TAF 87BIS/RUH 83TAF 79MAU 76AUE/WEB 75TAF 75AUE/WEB2 75ARN 72AUE/WEB 72ARN/JON	109-89-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH				919.4			952.4				-1.9
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	0.9	919.4			965±15				
	7664-41-7	appearance											
	107-10-8	NH <sub>3</sub>	350	819	100.7	919.5							
	74-89-5	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	550	883.9	31.8	914.9							
	7664-41-7	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	54.7	919.2							
	74-89-5	NH <sub>3</sub>	350	819	98.8	917.6							
	7664-41-7	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	57.1	921.6							
	74-89-5	NH <sub>3</sub>	350	819	90.4	909.1							
	7664-41-7	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	58.6	923.1							
[C <sub>4</sub> H <sub>11</sub> N] 90BOR/HOU	4747-21-1	CH <sub>3</sub> NH(i-C <sub>3</sub> H <sub>7</sub> )				919.4			952.4				-2
	119044-58-5	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-cyanophenyl)	313	919.8	-0.4	919.4							
[C <sub>7</sub> H <sub>9</sub> N] 91AUE/WEB 76AUE/WEB2	536-75-4	4(C <sub>2</sub> H <sub>5</sub> )-pyridine				919.2			951.1				2
	110-86-1	pyridine	300	898.1	20.5	918.6							
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	1.5	919.6							
[C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	13618-34-3	3,5-diethyl-4-methylpyrazole				919.2			952.8				-4
	536-75-4	4-(C <sub>2</sub> H <sub>5</sub> )-pyridine	333	919.2	0.6	920.0							
	108-89-4	4-(CH <sub>3</sub> )-pyridine	333	915.3	3.2	918.7							
[C <sub>6</sub> H <sub>13</sub> O <sub>3</sub> P] 80HOD/HOU 80HOD/HOU	7735-82-2	cis,cis-2-Methoxy-4,6-dimethyl-1,3,2-dioxaphosphorinane				919.1			951.6				0
	110-89-4	Piperidine	320	921	-0.8	920.1							
	108-89-4	4-(CH <sub>3</sub> )-pyridine	320	915.3	2.5	917.9							
[C <sub>5</sub> H <sub>15</sub> N <sub>2</sub> OP] 87TAF 84BOL/HOU	2511-17-3	OP(N(CH <sub>3</sub> ) <sub>2</sub> )(CH <sub>3</sub> )				918.9			951.3				0
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	0.5	918.9							
	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	~323	918.1	0.8	919.1							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> ] 93GOR/AMS	20488-27-1 75-50-3; 109-89-7	val-pro (CH <sub>3</sub> ) <sub>3</sub> N; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	350			918.8 918-919			NE				NE
[C <sub>7</sub> H <sub>12</sub> CIN] 87TAF	5960-95-2 75-50-3	1-azabicyclo[2.2.2]-octane, 4-chloro (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	0.5	918.6			949.4				5.6
86HEI/HON 86HEI/HON	75-50-3 109-89-7	(CH <sub>3</sub> ) <sub>3</sub> N (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	313 313	918.1 919.4	0.4 -0.4	918.5 918.9							
[C <sub>9</sub> H <sub>21</sub> OP] 87TAF	1496-94-2 75-50-3	OP(n-C <sub>3</sub> H <sub>7</sub> ) <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	0.5	918.4			948.2				9.1
84BOL/HOU	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	~323	918.1	0.4	918.5							
[C <sub>3</sub> H <sub>9</sub> N] 97EAS/SMI	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N theory	298			918.1			948.9				5.6
95SMI/RAD		theory	298						951.6				5.6
91MAU/SIE	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH pyridine	600	896.5	23.4	917.6		929.5	20.5				3.0
87TAF	110-86-1	NH <sub>3</sub>	600	898.1	20.1	917.1		930	22.2				-1.8
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	100.7	919.1							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	100.2	918.6							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	100.7	919.1							
80MAU/HAM	110-86-1	pyridine	330	898.1	18.4	916.4							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	52.7	917.2							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	97.9	916.3							
75AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	52.2	916.7							
74STA/BEA2	7664-41-7	NH <sub>3</sub>	350	819	89.5	907.9							
74STA/BEA	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	320	918.1	0	918.1							
72HEN/TAA	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	320	918.1	0	918.1							
72BRI/YAM	7664-41-7	NH <sub>3</sub>	350	819	99.8	918.2							
72AUE/WEB	7664-41-7	CH <sub>3</sub> NH <sub>2</sub>	600	819	97.5	912.9							
72ARN/JON	74-89-5	NH <sub>3</sub>	298	864.5	56.1	920.6							
71BOW/AUE	7664-41-7	(CH <sub>3</sub> ) <sub>3</sub> N	350	819	99.8	918.2							
[C <sub>9</sub> H <sub>13</sub> N] 87TAF	99-97-8 75-50-3	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	-0.5	918.1			950.0				2
85LIA/JAC	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	320	909.2	9.2	918.4							
[C <sub>10</sub> H <sub>19</sub> N <sub>3</sub> O <sub>4</sub> ] 93WU/FEN	14857-82-0	gly-gly-leu kinetic method				918.1			NE				NE
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O] 90GRE/LIG	71-30-7	Cytosine kinetic method				918.1			949.9				2
79MAU	109-89-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	535	919.4	-6.3	912.2			953.1				

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yfsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		PA(M)		$\Delta$ S <sub>p</sub> (M)	
						GB(M)	$\Delta$ GB(M,R,T)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)	$\Delta$ S <sub>p</sub> (M)
75WIL/MCC	124-40-3; 75-50-3	(CH <sub>3</sub> ) <sub>2</sub> NH; (CH <sub>3</sub> ) <sub>3</sub> N				896-918							
[C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> ]	6415-12-9	(CH <sub>3</sub> ) <sub>2</sub> NN(CH <sub>3</sub> ) <sub>2</sub>				917.9				948.7			5.8
84MAU/NEL	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	600	931.1	-142	915.8							
84MAU/NEL	108-99-6	3-(CH <sub>3</sub> )-pyridine	600	911.6	9.2	919.7							
84MAU/NEL	108-48-5	2,6-(CH <sub>3</sub> ) <sub>2</sub> -pyridine	550	931.1	-11.7	918.5							
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	3146-40-5	ala-gly-gly kinetic method				917.8				NE			NE
93WU/FEN						917.8							
[C <sub>9</sub> H <sub>11</sub> N <sub>3</sub> O <sub>2</sub> ]	74739-51-8	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-(4-nitrophenyl)				917.8				950.2			0
90BOR/HOU	123-75-1	Pyridoline	313	915.3	0.8	916.1							
90BOR/HOU	109-06-8	2-(CH <sub>3</sub> )-pyridine	313	917.3	2.1	919.4							
[C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> ]	1192-21-8	1-methyl-5-aminopyrazole				917.6				949.5			2
92ABB/CAB	108-99-6	3-(CH <sub>3</sub> )-pyridine	333	911.6	5.8	917.4							
92ABB/CAB	536-75-4	4-(C <sub>2</sub> H <sub>5</sub> )-pyridine	333	919.2	-1.3	917.9							
[C <sub>13</sub> H <sub>21</sub> NO]	1502-00-7	1-adamantyl-CON(CH <sub>3</sub> ) <sub>2</sub>				917.6				949.4			2
97HOM/HER	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	9.8	913.1							
97HOM/HER	108-99-6	3-(CH <sub>3</sub> )-pyridine	333	911.6	5.9	917.5							
97HOM/HER	108-89-4	4-(CH <sub>3</sub> )-pyridine	333	915.3	2.3	917.7							
[C <sub>6</sub> H <sub>10</sub> N <sub>3</sub> ]	1072-91-9	1,3,5-Trimethylpyrazole				917.4				949.3			2
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	-0.9	917.4							
[C <sub>6</sub> H <sub>6</sub> N]	2348-49-4	C <sub>6</sub> H <sub>5</sub> NH radical				917.4				949.8			0
82MAU	108-89-4; 109-89-7	4-CH <sub>3</sub> -pyridine; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH				915-919							
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	7291-00-1	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				917.4				948.3			5
94GRU/CAL	108-89-4; 109-89-7	4-CH <sub>3</sub> -pyridine; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH				915-919							
[C <sub>10</sub> H <sub>12</sub> NS]	74362-50-8	4-CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>				917.4				946.2			12
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	-0.5	917.4							
[C <sub>3</sub> H <sub>9</sub> NO]	156-87-6	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>3</sub> OH				917.3				962.5			-43
80MAU/HAM	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	330	918.1	-1.7	917.9				963.6			-43.4
79AUE/BOW	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	18.1	914.5			948.9	14.6	5.6	-49	
[C <sub>6</sub> H <sub>7</sub> N]	109-06-8	2-(CH <sub>3</sub> )-pyridine				917.3				949.1			2
91AUE/WEB	110-86-1	pyridine	300	898.1	16.1	914.3							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	107.1	925.7							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	107.1	925.7							



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ FPA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
83MAU/SIE 76AUE/WEB2	110-86-1 124-40-3	pyridine (CH <sub>3</sub> ) <sub>2</sub> NH	425 298	898.1 896.5	17.2 17.6	915.3 914.0							
[C <sub>8</sub> H <sub>12</sub> F <sub>3</sub> N] 87TAF	#363 7664-41-7	1-Azabicyclo[2.2.2]octane,4-trifluoromethyl- NH <sub>3</sub>	350	819	98.4	916.8 916.8			947.6			5.6	
[C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O <sub>4</sub> ] 98ZHA/ZIM	556-33-2 75-31-0, 110-86-1	triglycine (i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; C <sub>3</sub> H <sub>5</sub> N	300			916.8 889-898			966.8			-59	
93WU/LEB	127-19-5; 107-10-8	CH <sub>3</sub> CON(CH <sub>3</sub> ) <sub>2</sub> ; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>  kinetic method kinetic method	300			877-884			966.8			-59	
[C <sub>7</sub> H <sub>10</sub> CIN] 79AUE/BOW	#449 75-50-3	3-Chloro-1-azabicyclo[2.2.2]oct-2-ene (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	-1.5	916.7 916.7			947.5			5.6	
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>6</sub> ] 94LIG/NAP 75WIL/MCC	58-96-8 7664-41-7; 74-89-5	Uridine kinetic method NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				916.6 819-864			947.6 946.7			5	
[C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S] 93ABB/MO 93ABB/MO	2782-91-4 536-75-4 108-89-4	SC[N(CH <sub>3</sub> ) <sub>2</sub> ] <sub>2</sub> 4-(C <sub>2</sub> H <sub>5</sub> )-pyridine 4-(CH <sub>3</sub> )-pyridine	333 333	919.2 915.3	-2.1 1.1	916.6 917.0 916.3			947.6			5	
[C <sub>10</sub> H <sub>17</sub> NO] 83HOU/RUF	52305-49-4 108-89-4	tricyclo[4.4.0.0 <sup>3,5</sup> ]decan-4-ol-5-amino, stereoisomer 4-(CH <sub>3</sub> )-pyridine	1300	915.3	1.3	916.6			949.0			0	
[C <sub>10</sub> H <sub>17</sub> N] 89BRO/COO 87TAF	768-94-5 536-75-4 7664-41-7	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decan-1-amine 4-(C <sub>2</sub> H <sub>5</sub> )-pyridine NH <sub>3</sub>	300 350	919.2 819	-2.1 97.0	916.3 916.5 915.7			948.8			0	
[C <sub>6</sub> H <sub>11</sub> N] 87TAF 83TAF2	124-02-7 7664-41-7 7664-41-7	(CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>2</sub> NH NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	97.5 97.5	916.3 916.3 916.3			949.3			-2	
[C <sub>12</sub> H <sub>24</sub> N <sub>2</sub> ] 81ALD/ARR	71058-67-8 7664-41-7	1,6-Diazabicyclo[4.4.4]tetradecane NH <sub>3</sub>	320	819	97.5	916.3 916.2			947.1			5.6	
[C <sub>8</sub> H <sub>15</sub> NO] 83HOU/RUF	17997-65-8 108-89-4	cis-3-Aminobicyclo[2.2.2]octan-2-ol 4-(CH <sub>3</sub> )-pyridine	1300	915.3	0.8	916.2 916.2			948.6			0	
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	5519-42-6 7664-41-7	3,4,5-Trimethylpyrazole NH <sub>3</sub>	350	819	97.0	916.0 915.8			949.3			-3	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>8</sub> H <sub>13</sub> NO] 87TAF	873-95-0 7664-41-7	3-Amino-5,5-dimethylcyclohex-2-enone NH <sub>3</sub>	350	819	97.5	915.9			946.9			5
[C <sub>3</sub> H <sub>2</sub> ] 95CHY/SQU	16166-40-5 7664-41-7	cyclopropenyldiene NH <sub>3</sub>				915.9	853.6	97.5	951.1 951.1			-9.1
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> ] 90GRE/LIG 75WIL/MCC	50-89-5 7664-41-7; 74-89-5	Thymidine kinetic method NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				915.9			948.3 948.3			0
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O] 92RAC/MAR 92RAC/MAR	139033-03-7 123-75-1 109-89-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-OCH <sub>3</sub> Pyrrolidine (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	338 338	915.3 919.4	0 -2.9	915.8 915.2 916.4			948.3			0
[C <sub>6</sub> H <sub>15</sub> NO] 79AUE/BOW	4048-33-3 75-50-3	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>6</sub> OH (CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	-2.4	915.7 915.7			969.0			-70
[C <sub>9</sub> H <sub>13</sub> N] 87TAF 77POL/DEV	121-72-2 7664-41-7 62-53-3	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	350 350	819 850.6	97.9 65.4	915.7 915.6 915.1			942.1			20
[C <sub>3</sub> H <sub>9</sub> N <sub>3</sub> ] 92RAC/MAR 92RAC/MAR	134166-58-8 123-75-1 139033-03-7	(CH <sub>3</sub> ) <sub>2</sub> N-CH=N-CH <sub>2</sub> CN Pyrrolidine (CH <sub>3</sub> ) <sub>2</sub> N-CH=N-OCH <sub>3</sub>	338 338	915.3 915.8	0 0	915.5 915.2 915.8			948.0			0
[C <sub>7</sub> H <sub>9</sub> N] 91AUE/WEB 89BRO/COO 76AUE/WEB2	536-78-7 110-86-1 768-94-5 124-40-3	3-(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -pyridine pyridine Tricyclo[3.3.1.1 <sup>3,1'</sup> ]decane-1-amine (CH <sub>3</sub> ) <sub>2</sub> NH	300 300 298	898.1 916.3 896.5	17.1 -0.4 18.5	915.5 915.2 916.5 915.0			947.4			2
[C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ] 96EWI/ZHA	14379-76-1 108-99-6; 109-89-7	gly-gly-pro 3-(CH <sub>3</sub> ) <sub>2</sub> -pyridine; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH				915.5 912-919			NE			NE
[C <sub>9</sub> H <sub>15</sub> N <sub>3</sub> O <sub>4</sub> ] 96EWI/ZHA	2441-63-6 108-99-6; 109-89-7	gly-pro-gly 3-(CH <sub>3</sub> ) <sub>2</sub> -pyridine; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH				915.5 912-919			NE			NE
[C <sub>11</sub> H <sub>15</sub> N] 87TAF	35843-88-0 7664-41-7	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	97.0	915.5 915.4			946.2			5.6
[C <sub>6</sub> H <sub>7</sub> N] 91AUE/WEB 87TAF	108-89-4 110-86-1 7664-41-7	4-(CH <sub>3</sub> ) <sub>2</sub> -pyridine pyridine NH <sub>3</sub>	300 350	898.1 819	16.1 96.6	915.3 914.2 915.1			947.2			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
83TAF	7664-41-7	NH <sub>3</sub>	350	819	96.6	915.1							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	97.9	916.5							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	97.9	916.5							
72TAA/HEN	110-86-1	pyridine	320	898.1	22.6	920.7							
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ]	504-29-0	2-Pyridinamine				915.3			947.2			2	
91AUE/WEB	110-86-1	pyridine	300	898.1	16.6	914.7							
79AUE/BOW	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	-2.4	915.7							
[C <sub>4</sub> H <sub>8</sub> N]	123-75-1	Pyrrolidine				915.3			948.3			-2	
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	-3.2	915.3							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	97.5	916.3							
81TAA/SUM	7664-41-7	NH <sub>3</sub>	320	819	89.1	908.0							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	50.8	915.3							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	97.9	916.7							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	89.5	908.3							
71BOW/AUE	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	-1.3	916.9							
[C <sub>10</sub> H <sub>13</sub> N]	4096-21-3	N-Phenylpyrrolidine				915.1			941.6			20	
88CAU/CER		See Refs.				912.8							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	97.0	914.7							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	97.5	915.2							
[C <sub>4</sub> H <sub>14</sub> N <sub>3</sub> OP]	3732-36-3	OP(NH <sub>2</sub> )(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>2</sub>				915.0			947.5			0	
85BOL/HOU	109-06-8	2-(CH <sub>3</sub> )-pyridine	323	917.3	-1.7	915.6							
85BOL/HOU	109-89-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH	323	919.4	-5.0	914.4							
[C <sub>2</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub> ]	16606-18-1	c-P(O)CH <sub>3</sub> N(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>3</sub> )				915.0			947.5			0	
85BOL/HOU	108-89-4	4-(CH <sub>3</sub> )-pyridine	323	915.3	-1.7	913.7							
85BOL/HOU	109-06-8	2-(CH <sub>3</sub> )-pyridine	323	917.3	-0.8	916.5							
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ]	73-22-3	L-tryptophan				915			948.9			-5	
93LI/HAR		kinetic method							931				
92GOR/SPE	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918							
90ISA/OMO		kinetic method-relative order											
87TAF	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	350	918.1	0	918.7							
87BOJ		kinetic method-relative order											
86BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	100.7	919.6							
[C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> O <sub>4</sub> ]	19729-30-7	gly-gly-ala				914.8			NE			NE	
93WU/FEN		kinetic method				914.8							
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	110-85-0	Piperazine				914.7			943.7			11.5	
73AUE/WEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	30.8	914.7							



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
79MAU 75WIL/MCC	110-86-1 124-40-3; 75-	pyridine (CH <sub>3</sub> ) <sub>2</sub> NH; (CH <sub>3</sub> ) <sub>3</sub> N	570	898.1	10.5	907.3 896-918	930	6.7	936.7	2	6.7	8.7	8.7
[C <sub>9</sub> H <sub>13</sub> N] 78LAU/SAL 73YAM/KEB	613-97-8 7664-41-7 7664-41-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> ) NH <sub>3</sub> NH <sub>3</sub>	600 600	819 819	101.3 101.3	912.4 912.3 912.3			939.0			20	
[C <sub>7</sub> H <sub>7</sub> N] 91AUE/WEB 79AUE/BOW	100-43-6 110-86-1 75-50-3	4-Vinylpyridine pyridine (CH <sub>3</sub> ) <sub>3</sub> N	300 298	898.1 918.1	13.7 -5.4	912.3 911.8 912.8			944.1			2	
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> PS] 88WEB/HOU 88WEB/HOU	3732-82-9 108-89-4 108-99-6	SP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub> 4-(CH <sub>3</sub> )-pyridine 3-(CH <sub>3</sub> )-pyridine	313 313	915.3 911.6	-1.0 -1.3	912.2 914.2 910.2			942.0			9.1	
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ] 78LAU/SAL	479-27-6 110-89-4	1,8-Diaminonaphthalene Piperidine	600	921	-8.4	912.1 912.1			944.5			0	
[C <sub>6</sub> H <sub>7</sub> N] 91AUE/WEB 87TAF 86TAF/ANV 86MAU/LJE 83TAF2 76AUE/WEB2 76AUE/WEB	108-99-6 110-86-1 7664-41-7 108-99-6 110-86-1 7664-41-7 124-40-3 74-89-5	3-(CH <sub>3</sub> )-pyridine pyridine NH <sub>3</sub> 3-(CH <sub>3</sub> )-pyridine pyridine NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> NH CH <sub>3</sub> NH <sub>2</sub>	300 350 350 600 350 298 298	898.1 819 911.6 898.1 819 896.5 864.5	11.7 92.9 0 17.6 94.3 13.2 45.4	911.6 909.9 911.5 911.6 915.8 912.9 909.6 909.9			943.4			2	
[C <sub>3</sub> H <sub>8</sub> Pb] 82PIE/HEH	82065-01-8 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> Pb=CH <sub>2</sub> NH <sub>3</sub>	350	819	93.8	911.5 911.5			938.0			20	
[C <sub>6</sub> H <sub>7</sub> NO] 91AUE/WEB 87TAF 83TAF2 76AUE/WEB2	7295-76-3 110-86-1 7664-41-7 7664-41-7 124-40-3	3-(CH <sub>3</sub> O)-pyridine pyridine NH <sub>3</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> NH	300 350 350 298	898.1 819 819 896.5	10.3 94.7 95.6 11.7	910.9 908.4 913.3 914.2 908.2			942.7			2	
[C <sub>9</sub> H <sub>7</sub> NO] 79MAU	1613-37-2 107-10-8	Quinoline-1-oxide n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	526	883.9	28.0	910.8 910.8			943.3			0	
[C <sub>10</sub> H <sub>14</sub> FN] 87TAF	14994-35-5 7664-41-7	N,N,2,6-Tetramethylaniline,4-fluoro NH <sub>3</sub>	350	819	92.0	910.7 910.7			943.2			0	
[C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> ] 92LIO/BRO	112-60-7 17455-13-9	HO[CH <sub>2</sub> CH <sub>2</sub> O] <sub>4</sub> H 18-crown-6		909.5	>0	>910 >910			NE See Refs.			NE	
[C <sub>14</sub> H <sub>28</sub> O <sub>7</sub> ] 87TAF	33089-36-0	21-crown-7				>910			NE			NE	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
92LIO/BR0	17455-13-9	18-crown-6		909.5	>0	>910			See Refs.			
[C <sub>10</sub> H <sub>22</sub> O <sub>6</sub> ] 92LIO/BR0	4792-15-8 17455-13-9	HO[CH <sub>2</sub> CH <sub>2</sub> O] <sub>5</sub> H 18-crown-6		909.5	>0	>910			NE See Refs.			NE
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ] 88CAT/CLA	4838-00-0 7295-76-3	2-Methyl-2H-indazole 3-(CH <sub>3</sub> O)-pyridine	~300	910.9	-1.3	909.6			941.4			2
88CAT/CLA	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	~300	899.9	10.5	910.3						
88CAT/CLA	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	~300	903.6	4.2	907.8						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	92.0	910.6						
84FLA/MAQ		kinetic method				903.7						
[C <sub>3</sub> H <sub>9</sub> N] 87TAF	7223-38-3 7664-41-7	HCCCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	91.1	909.5			940.3			5.6
[C <sub>12</sub> H <sub>24</sub> O <sub>6</sub> ] 98LIO/BR0	17455-13-9	18-crown-6				909.5			967.0			-84
84SHA/BLA	372-48-5	kinetic method										
83MAU	110-86-1	2-F-pyridine	500	852.7	37.2	907.2		884.6	967.0	2	-86	-84
83MAU	289-80-5	pyridine	600	898.1	-11.3	912.6						
[C <sub>4</sub> H <sub>9</sub> N] 75AUE/WEB2	1190-79-0 74-89-5	CH <sub>3</sub> CH=NC <sub>2</sub> H <sub>5</sub> CH <sub>3</sub> NH <sub>2</sub>	600	877.1	3.8	908.4						
[C <sub>3</sub> H <sub>7</sub> N] 81ELL/DIX	4427-28-5	CH <sub>2</sub> =C(CH <sub>3</sub> )NH <sub>2</sub> See Refs.	298	864.5	44.9	909.4			941.9			0
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ] 88CAT/CLA	288-32-4 594-39-8	Imidazole t-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	~300	903.6	3.8	909.2						
88CAT/CLA	108-99-6	3-(CH <sub>3</sub> )-pyridine	~300	911.6	-2.5	909.1						
88CAT/CLA	1628-89-3	2-(CH <sub>3</sub> O)-pyridine	~300	902.8	7.5	910.3						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	91.5	910.4						
86TAF/ANV	1628-89-3	2-(CH <sub>3</sub> O)-pyridine	350	902.8	7.5	910.6						
86TAF/ANV	108-99-6	3-(CH <sub>3</sub> )-pyridine	350	911.6	-2.5	909.4						
86TAF/ANV	594-39-8	t-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	350	903.6	3.8	907.2						
86MAU/LJE	110-86-1	pyridine	600	898.1	3.1	903.0						
84FLA/MAQ		kinetic method										
[C <sub>8</sub> H <sub>11</sub> N] 87TAF	121-69-7 7664-41-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	90.6	909.2			941.1			2
85LIA/JAC	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	320	909.2	0	909.2						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	91.1	909.6						
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	90.6	909.2						
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	90.8	907.3						
77POL/DEV	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	350	850.6	57.2	907.8						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	91.1	909.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	90.8	907.3						
[C <sub>3</sub> H <sub>6</sub> N]	624-78-2	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NH				909.2			942.2			-2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	90.6	909.4						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	90.6	909.4						
76AUE/WEBB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	44.4	908.9						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	87.4	906.2						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	87.4	906.2						
[C <sub>10</sub> H <sub>18</sub> N <sub>2</sub> O <sub>3</sub> ]	52899-09-9	pro-val				909.0			NE			NE
93GOR/AMS	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918						
[C <sub>14</sub> H <sub>26</sub> N <sub>2</sub> O <sub>3</sub> ]	3918-92-1	val-phe				909.0			NE			NE
93GOR/AMS	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918						
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ]	14486-09-0	val-met				909.0			NE			NE
93GOR/AMS	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918						
[C <sub>14</sub> H <sub>26</sub> N <sub>2</sub> O <sub>4</sub> ]	3061-91-4	val-tyr				909.0			NE			NE
93GOR/AMS	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918						
[C <sub>16</sub> H <sub>24</sub> N <sub>3</sub> O <sub>3</sub> ]	24587-37-9	val-trp				909.0			NE			NE
93GOR/AMS	75-64-9; 75-50-3	(t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918						
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O]	59-26-7	N,N-diethylnicotinamide				909.0			940.9			2
91BER/DEC	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	338	909.2	0	909.2						
91BER/DEC	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	338	899.9	7.5	907.1						
91BER/DEC	108-89-4	4-(CH <sub>3</sub> )-pyridine	338	915.3	-5.0	910.3						
91BER/DEC	110-86-1	pyridine	338	898.1	11.3	909.4						
[C <sub>3</sub> H <sub>7</sub> N]	503-29-7	Azetidine				908.6			943.4			-7.8
92ABB/CAN	108-89-4	4-(CH <sub>3</sub> )-pyridine	333	915.3	-6.2	909.5						
92ABB/CAN	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	3.4	907.1						
92ABB/CAN	108-99-6	3-(CH <sub>3</sub> )-pyridine	333	911.6	-1.5	910.5						
76AUE/WEBB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	43.0	907.4						
75AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	44.4	908.9						
71BOW/AUE	75-50-3	(CH <sub>3</sub> ) <sub>3</sub> N	298	918.1	-10.3	907.9						
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	271-63-6	7-Azaindole				908.3			940.2			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	89.7	908.3						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YtSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>12</sub> H <sub>8</sub> N <sub>2</sub> ] 79MAU	92-82-0 107-10-8	Phenazine n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	514	883.9	27.2	908.3 908.3			938.4			8	
[C <sub>11</sub> H <sub>9</sub> N] 97SHE/STE	939-23-1	4-phenyl-pyridine See Refs.				907.8			939.7 939.7±2.1			2	
[C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> ] 87TAF	1004-36-0 7664-41-7	2,6-Dimethyl-4-pyrone NH <sub>3</sub>	350	819	88.3	907.3 907.3			941.5			-5.8	
[C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	141665-17-0 594-39-8 694-31-5	1-methyl-5-t-butylpyrazole t-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub> 1,5-Dimethylpyrazole	333 333	903.6 902.8	2.6 6.0	907.3 905.9 908.8			939.2			2	
[C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> ] 75WIL/MCC	2004-03-7 124-40-3; 75-50-3	6-Methylpurine (CH <sub>3</sub> ) <sub>2</sub> NH; (CH <sub>3</sub> ) <sub>3</sub> N				907.3 896-918			939.2			2	
[C <sub>10</sub> H <sub>10</sub> Ni] 81STE/BEA 76COR/BEA 76COR/BEA	1271-28-9 7664-41-7 109-89-7 75-50-3	Ni(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> NH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH (CH <sub>3</sub> ) <sub>3</sub> N	320 320 320	819 919.4 918.1	79.9 -6.7 -7.1	907.3 898.5 912.4 910.9			935.7			13.4	
[C <sub>6</sub> H <sub>15</sub> OP] 85BOL/HOU 85BOL/HOU	597-50-2 108-99-5 624-78-2	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> PO 3-(CH <sub>3</sub> )-pyridine (CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NH	323 323	911.6 909.2	-5.4 -1.3	906.8 906.0 907.7			936.6			9.1	
[C <sub>10</sub> H <sub>12</sub> CIN] 88CAU/CER	4280-30-2	Pyrrolidine, 1-(4-chlorophenyl) See Refs.				906.6 906.6			937.4			5.6	
[C <sub>10</sub> H <sub>13</sub> NO] 87TAF 86MIS/FUJ	2124-31-4 7664-41-7 98-86-2	4-[(CH <sub>3</sub> ) <sub>2</sub> N]-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	350 343	819 829.3	90.6 75.7	906.3 908.3 904.2			932.8			20	
[C <sub>6</sub> H <sub>7</sub> NS] 91AUE/WEBB 79AUE/BET 76AUE/WEB2	18438-38-5 110-86-1 74-89-5 124-40-3	2-(CH <sub>3</sub> S)-pyridine pyridine CH <sub>3</sub> NH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> NH	300 298 298	898.1 864.5 896.5	7.8 41.5 9.3	906.0 906.0 906.0 905.7			937.8			2	
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ] 93WU/FEN	1948-31-8	di-L-alanine kinetic method				905.6 905.6			NE			NE	
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> O <sub>3</sub> ] 96EWI/ZHA	704-15-4 108-91-8; 108-99-6	gly-pro c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub> ; 3-(CH <sub>3</sub> )-pyridine				905.6 900-912			NE			NE	



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> ]	1904-31-0	1-methyl-3-aminopyrazole				905.6			937.4			2	
92ABB/CAB	108-99-6	3-(CH <sub>3</sub> )-pyridine	333	911.6	-4.6	907.0							
92ABB/CAB	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	0.7	904.0							
[C <sub>7</sub> H <sub>11</sub> NO]	3731-38-2	1-Azabicyclo[2.2.2]octan-3-one				905.2			936.0			5.6	
79AUE/BOW	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	8.8	905.2							
[CH <sub>2</sub> Fe]	95260-85-4	FeCH <sub>2</sub>				905.2			937.7			0	
89JAC/GOR	110-86-1; 100-43-6	pyridine; 4-vinylpyridine				898-912							
[CH <sub>2</sub> Co]	116492-58-1	CoCH <sub>2</sub>				905.2			937.7			0	
89JAC/GOR	110-86-1; 100-43-6	pyridine; 4-vinylpyridine				898-912							
[C <sub>7</sub> H <sub>11</sub> F <sub>2</sub> N]	#524	3,3-Difluoro-1-azabicyclo[2.2.2]octane				904.8			935.6			5.6	
79AUE/BOW	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	8.3	904.8							
[C <sub>6</sub> H <sub>7</sub> NS]	18794-33-7	3-(CH <sub>3</sub> S)-pyridine				904.7			936.5			2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	86.0	904.6							
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ]	51627-76-0	1-azabicyclo[2.2.2]-octane, 3-cyano				904.6			935.4			5.6	
86HEI/HON	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	313	903.6	-0.4	903.0							
86HEI/HON	624-78-2	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NH	313	909.2	-2.9	906.2							
[C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> ]	253-66-7	Cinnoline				904.4			936.3			2	
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	22.2	904.4							
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> PSe]	7422-73-3	SeP(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>				904.3			934.1			9.1	
88WEB/HOU	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	313	903.6	0.4	903.8							
88WEB/HOU	108-91-8	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	313	899.6	5.4	904.8							
[C <sub>3</sub> H <sub>7</sub> N]	1072-44-2	N-Methylaziridine				904.1			934.8			5.6	
75AUE/AWEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	39.5	904.1							
[C <sub>11</sub> H <sub>12</sub> N <sub>2</sub> ]	141665-22-7	3(5)-ethyl-5(3)-phenylpyrazole				903.8			935.6			2	
92ABB/CAB	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	5.8	905.4							
92ABB/CAB	110-86-1	pyridine	333	898.1	6.0	904.1							
92ABB/CAB	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	-1.5	901.8							
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	16518-64-2	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>				903.8			930.2			20	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	86.0	903.7							
[C <sub>5</sub> H <sub>13</sub> N]	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>				903.6			837.8			-6	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	87.9	906.8							
86TAF/ANV	7664-41-7	NH <sub>3</sub>	350	819	80.3	899.3							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	40.0	904.5						
[C <sub>9</sub> H <sub>11</sub> N] 87TAF	1962-08-9 7664-41-7	4-H <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	85.6	903.3 903.3			929.8			20
[C <sub>4</sub> H <sub>12</sub> NO] 87TAF	50663-05-3 7664-41-7	OP(N(CH <sub>3</sub> ) <sub>2</sub> )(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	84.7	903.0 903.3			935.5			0
84BOL/HOU	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	~323	899.9	2.9	902.7						
[C <sub>10</sub> H <sub>14</sub> BrN] 87TAF	50638-54-5 7664-41-7	N,N,2,6-Tetramethylaniline,4-bromo- NH <sub>3</sub>	350	819	84.2	902.9 902.9			935.4			0
[C <sub>6</sub> H <sub>7</sub> NO] 91AUE/WEB	1628-89-3 110-86-1	2-(CH <sub>3</sub> O)-pyridine pyridine	300	898.1	4.4	902.8 902.5			934.7			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	83.3	901.9						
86TAF/ANV	7664-41-7	NH <sub>3</sub>	350	819	76.1	894.7						
79AUE/BET	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	38.1	902.6						
76COOK/KAT	7664-41-7	NH <sub>3</sub>	350	819	86.0	904.6						
76AUE/WEB2	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	5.9	902.3						
[C <sub>6</sub> H <sub>7</sub> NO] 92MIS/TER	1003-73-2 694-59-7	3-methyl-pyridine-1-oxide pyridine-1-oxide	343	892.9	9.6	902.8 902.8			935.2			0
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	694-31-5 7664-41-7	1,5-Dimethylpyrazole NH <sub>3</sub>	350	819	84.2	902.8 902.7			934.3			3
[C <sub>9</sub> H <sub>11</sub> N] 88CAU/CER	3334-89-2	Azetidine, 1-phenyl See Refs.				902.4 902.4			933.2			5.6
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ] 87TAF	26458-78-6 7664-41-7	1-azabicyclo[2.2.2]-octane,4-cyano NH <sub>3</sub>	350	819	84.7	902.3 903.1			933.1			5.6
86HEI/HON	624-78-2	(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NH	313	909.2	-5.9	903.2						
86HEI/HON	594-39-8	t-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	313	903.6	-2.6	900.5						
86HEI/HON	50663-05-3	OP(N(CH <sub>3</sub> ) <sub>2</sub> )(CH <sub>3</sub> ) <sub>2</sub>	313	903.0	-0.4	902.5						
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	694-48-4 7664-41-7	1,3-Dimethylpyrazole NH <sub>3</sub>	350	819	83.7	902.3 902.3			933.9			3
[C <sub>8</sub> H <sub>11</sub> N] 87TAF	64-04-0 7664-41-7	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub>	350	819	83.3	902.3 902.2			936.2			-5
[C <sub>12</sub> H <sub>9</sub> NO] 91BER/DEC	5424-19-1	3-C <sub>6</sub> H <sub>5</sub> CO-pyridine				902.3			934.1			2
91BER/DEC	13952-84-6	sec-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	338	895.7	6.9	902.3						
91BER/DEC	110-86-1	pyridine	338	898.1	4.1	902.2						
91BER/DEC	108-91-8	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	338	899.6	3.0	902.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
[C <sub>4</sub> H <sub>8</sub> S] 89OSA/DEL	51102-74-0	CH <sub>2</sub> =C(SCH <sub>3</sub> ) <sub>2</sub>				902.2			931.1			12	
89OSA/DEL	108-91-8	c-C <sub>4</sub> H <sub>11</sub> NH <sub>2</sub>	313	899.6	0.8	900.2							
89OSA/DEL	108-99-6	3-(CH <sub>3</sub> )-pyridine	313	911.6	-6.3	905.2							
89OSA/DEL	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	313	899.9	1.7	901.3							
[C <sub>8</sub> H <sub>7</sub> N] 87TAF	120-72-9 7664-41-7	Indole NH <sub>3</sub>	350	819	83.3	901.9 901.8			933.4			3	
[C <sub>9</sub> H <sub>11</sub> NO] 94GRU/CAL	611-74-5	C <sub>6</sub> H <sub>5</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				901.8			932.7			5	
	103-69-5; 108-45-2	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub> ; 1,3-(NH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				893-899							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	83.3	901.7							
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O] 92ABB/CAB	5744-51-4	1,5-dimethyl-3-ethoxycarbonylpyrazole				901.5			933.4			2	
92ABB/CAB	694-31-5	1,5-Dimethylpyrazole	333	902.8	-1.4	901.4							
92ABB/CAB	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	2.1	901.7							
[C <sub>3</sub> H <sub>11</sub> NO <sub>2</sub> S] 93LJ/HAR	63-68-3	L-Methionine				901.5			935.4			-5	
92GOR/SPE	110-86-1; 75-64-9	kinetic method-See Refs. pyridine; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>	350			898-900			920.5			-1.3	
90ISA/OMO		kinetic method-relative order											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	82.4	901.3							
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	82.4	901.3							
[C <sub>10</sub> H <sub>13</sub> NO] 87TAF	18992-80-8 7664-41-7	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COCH <sub>3</sub> NH <sub>3</sub>	350	819	83.7	901.5 901.4			928.0			20	
[C <sub>7</sub> H <sub>13</sub> N] 79AUE/BOW	31002-73-0 124-40-3	Bicyclo[2.2.1]heptan-2-amine,endo (CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	4.9	901.3 901.3			935.3			-5	
[C <sub>7</sub> H <sub>13</sub> N] 79AUE/BOW	7242-92-4 124-40-3	Bicyclo[2.2.1]heptan-2-amine,exo (CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	4.9	901.3 901.3			935.3			-5	
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ] 92ABB/CAB	3463-26-1	1-methyl-3-phenylpyrazole				900.8			932.6			2	
92ABB/CAB	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	1.9	901.5							
92ABB/CAB	5813-64-9	neo-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333	894.0	6.3	900.0							
[C <sub>3</sub> S] 92MAC/SUD	109545-35-9	C <sub>3</sub> S theory	298			900.5			933 933			0	
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ] 92ABB/CAB	3463-27-2	1-methyl-5-phenylpyrazole				900.5			932.4			2	
92ABB/CAB	594-39-8	t-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	-3.5	899.8							
92ABB/CAB	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	1.5	901.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		PA(M)		$\Delta S_p$ (M)	$\Delta S_p$ (M)
						GB(M)	$\Delta$ GB(M,R,T)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (M,R)		
[C <sub>10</sub> H <sub>10</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	3347-62-4	3(5)-methyl-5(3)-phenylpyrazole				900.2					932.1		2
	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	0.7	900.3					933.9		
	694-31-5	1,5-Dimethylpyrazole	333	902.8	-2.7	900.1					932.1		
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB 92ABB/CAB 87TAF	67-51-6	3,5-dimethylpyrazole				900.1					933.5		-3
	110-86-1	pyridine	333	898.1	1.8	900.1					933.5		
	594-39-8	t-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333	903.6	-5.9	897.6					933.9		
	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	0.3	900.1					935.4		
	7664-41-7	NH <sub>3</sub>	350	819	83.7	902.6					937.9		
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ] 93LI/HAR 92GOR/SPE	56-85-9	L-Glutamine				900					937.8		-18
	110-86-1;	kinetic method									938		
	75-64-9	pyridine; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>	350			898-900					938		
		kinetic method-relative order											
90ISA/OMO 87TAF 87BOJ 83LOC/MCI	7644-41-7	NH <sub>3</sub>	350	819	68.6	888.2							
	7664-41-7	kinetic method-relative order											
		kinetic method-relative order											
[C <sub>3</sub> H <sub>9</sub> O <sub>3</sub> P] 80HOD/MCD 80HOD/MCD	121-45-9	P(OCH <sub>3</sub> ) <sub>3</sub>				899.9					929.7		9.1
	108-91-8	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	300	899.6	0.4	900.0					929.7		
	110-86-1	pyridine	300	898.1	1.7	899.8					929.7		
[C <sub>4</sub> H <sub>11</sub> N] 93SZU/MCM 91MAU/SIE 91MAU/SIE 91MAU/SIE 87TAF 83TAF 83LOC/MCI 80MAU 79MAU 76AUE/WEB 75TAF 75ARN 72HENTAA 72AUE/WEB 72ARN/JON	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>				899.9					934.1		-6
	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	111.7	895.1			802.1	131.8	933.9	20	-33.5
	75-31-0	1-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	600	889.0	15.1	903.4			923.8	10.0	933.9	-8	8.4
	110-86-1	pyridine	600	898.1	-0.4	900.1			930	5.4	935.4	2	-9.2
	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	600	878	27.2	905.5			912.0	25.9	937.9	-5.1	2.1
	7664-41-7	NH <sub>3</sub>	350	819	81.5	900.4					937.9		-3.0
	7664-41-7	NH <sub>3</sub>	350	819	81.5	900.4					937.9		
	7664-41-7	NH <sub>3</sub>	350	819	81.5	900.4					937.9		
	7664-41-7	NH <sub>3</sub>	550	819	70.7	889.6					937.9		
	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	514	883.9	13.8	897.9					937.9		
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	35.1	899.6					937.9		
	7664-41-7	NH <sub>3</sub>	350	819	78.3	897.2					937.9		
	7664-41-7	NH <sub>3</sub>	350	819	78.3	897.2					937.9		
	7664-41-7	NH <sub>3</sub>	350	819	80.5	899.5					937.9		
74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	34.2	898.7					937.9			
7664-41-7	NH <sub>3</sub>	350	819	80.5	899.5					937.9			
[C <sub>10</sub> H <sub>20</sub> O <sub>3</sub> ] 92LIO/BRO 84SHA/BLA 83MAU 83MAU	33100-27-5	15-Crown-5				899.7					943.8		-39
	372-48-5	kinetic method									943.8		
	289-80-5	2-F-pyridine	500	852.7	33.9	894.8			884.6	54.0	938.5	2	-41
	110-86-1	Pyridazine pyridine	600	877.1	7.5	898.7					938.5		-39

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$ $\Delta S_p(R)$
[C <sub>6</sub> H <sub>13</sub> N] 89TOM/ABB	108-91-8 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub> NH <sub>3</sub>	298	819	75.7	899.6			934.4		-8
87TAF	7664-41-7	NH <sub>3</sub>	350	819	80.1	899.2					
83TAF	7664-41-7	NH <sub>3</sub>	350	819	80.1	899.2					
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	35.1	899.6					
75TAF	7664-41-7	NH <sub>3</sub>	350	819	80.1	899.2					
75ARN	7664-41-7	NH <sub>3</sub>	350	819	80.1	899.2					
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	81.6	901.1					
[C <sub>3</sub> H <sub>12</sub> N <sub>2</sub> O] 87TAF	632-22-4 7664-41-7	[(CH <sub>3</sub> ) <sub>2</sub> N] <sub>2</sub> C=O NH <sub>3</sub>	350	819	81.0	899.6			930.6		5
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	81.1	899.6					
[C <sub>6</sub> H <sub>11</sub> NO] 90WOL/GRU	23135-18-4 110-86-1	2-propenamide,N,N-dimethyl- pyridine	320	898.1	0.8	899.4			930.3		5
90WOL/GRU	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	320	899.9	0.2	899.9					
[C <sub>8</sub> H <sub>15</sub> NO] 83HOU/RUF	40335-14-6 108-91-8	trans-3-Aminobicyclo[2.2.2]octan-2-ol c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	1300	899.6	-0.4	899.2			933.1		-5
[C <sub>10</sub> H <sub>14</sub> CIN] 85LIA/JAC	2873-89-4 121-69-7	4-ClC <sub>6</sub> H <sub>4</sub> N(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	320	909.2	-10.0	899.2			931.0		2
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ] 81LAU/NIS	108-45-2 62-53-3	1,3-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	51.0	899.2			929.9		5.8
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	82.4	897.8					
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ] 93GOR/AMS	14486-13-6 110-86-1; 75-64-9	met-val C <sub>3</sub> H <sub>5</sub> N; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>	350			899.0 898-900			NE		NE
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S] 87TAF	96-50-4 7664-41-7	2-Aminothiazole NH <sub>3</sub>	350	819	80.1	898.7 898.7			930.6		2
[C <sub>4</sub> H <sub>5</sub> NS] 87TAF	3581-87-1 7664-41-7	2-Methylthiazole NH <sub>3</sub>	350	819	80.1	898.7 898.6			930.6		2
[C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> ] 89TOM/ABB	13351-73-0 108-91-8	1-methylbenzotriazole c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	298	899.6	0.8	898.7			931.2		0
89TOM/ABB	110-86-1	pyridine	298	898.1	-1.3	900.5 896.9					
[C <sub>15</sub> H <sub>12</sub> N <sub>2</sub> ] 89HOU/FEN	95935-55-0 110-86-1	9,5-metheno-5H,7H-pyrimidol[1,6-a:3,4- a']bisazepine	313	898.1	0.4	898.7			931.1		0
[C <sub>9</sub> H <sub>11</sub> NO] 924.8	100-10-7	4-CHOC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>				898.6			924.8		20

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
87TAF	7664-41-7	NH <sub>3</sub>	350	819	80.5	898.2						
[C <sub>8</sub> H <sub>10</sub> FN]	403-46-3	4-FC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>				898.3			924.8			20
87TAF	7664-41-7	NH <sub>3</sub>	350	819	80.5	898.2						
[C <sub>7</sub> H <sub>5</sub> N]	2510-22-7	4-ethynyl-pyridine				898.2			930.1			2
97SHE/SIE		See Refs.							930.1 ± 4.6			
[C <sub>3</sub> H <sub>7</sub> N]	38697-07-3	(CH <sub>3</sub> ) <sub>2</sub> C=NH				898.2			932.3			-5.8
81ELL/DIX	124-40-3; 75-64-9	(CH <sub>3</sub> ) <sub>2</sub> NH; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>				896-900						
[C <sub>6</sub> H <sub>11</sub> OSi]	1833-53-0	CH <sub>2</sub> =(CH <sub>3</sub> )OSi(CH <sub>3</sub> ) <sub>3</sub>				898.2			930.6			0
82HEN/WEI	124-40-3; 75-64-9	(CH <sub>3</sub> ) <sub>2</sub> NH; t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>				896-900						
[C <sub>9</sub> H <sub>12</sub> O <sub>3</sub> ]	621-23-8	1,3,5-C <sub>6</sub> H <sub>3</sub> (OCH <sub>3</sub> ) <sub>3</sub>				898.2			926.7			13
87TAF	7664-41-7	NH <sub>3</sub>	350	819	80.1	898.1						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	80.1	898.1						
[C <sub>5</sub> H <sub>5</sub> N]	110-86-1	pyridine				898.1			930			2
97EAS/SMI		theory	298									2.2
95SMI/RAD		theory	298						929.8			
95CHY/SQU	7664-41-7	NH <sub>3</sub>	298						853.6	78.7		
91MAU/SIE	75-31-0	i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	600	889.0	10.9	896.9			923.8	5.9	7.5	-0.5
91MAU/SIE	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	600	878	23.8	899.7			912.0	15.9	13.0	7.9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	80.5	899.1						
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	80.5	899.1						
86MAU/LIE	110-86-1	pyridine	600	898.1	0	898.1						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	81.0	899.6						
83MAU/SIE	110-86-1	pyridine	425	898.1	0	898.1						
83MAU	110-86-1	pyridine	600	898.1	0	898.1						
80MAU/HAM	110-86-1	pyridine	600	898.1	0	898.1						
80MAU	7664-41-7	NH <sub>3</sub>	550	819	72.4	889.3						
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	520	883.9	12.6	894.9						
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	73.6	890.1						
77COO/KRU		relative order-See Refs.										
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	33.7	898.2						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	77.8	896.4						
75AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	31.2	895.7						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	77.8	896.4						
72BRJ/YAM	7664-41-7	NH <sub>3</sub>	600	819	77.8	894.3						
[C <sub>10</sub> H <sub>2</sub> O <sub>5</sub> ]	143-24-8	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> O] <sub>1</sub> CH <sub>3</sub>				897.8			953.8			-79
92LJO/BRO		kinetic method										
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	28.9	897.8			884.6	69.0	2	-81

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>6</sub> H <sub>18</sub> N <sub>3</sub> P] 85BOL/HOU	1608-26-0	P(N(CH <sub>3</sub> ) <sub>2</sub> ) <sub>3</sub>	323	896.5	1.3	897.7			930.1			0	
	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH											
[C <sub>3</sub> H <sub>5</sub> NO] 91AUE/WEB	109-00-2	3-(OH)-pyridine	300	898.1	-0.5	897.7			929.5			2	
	110-86-1	pyridine											
[C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> ] 87TAF	52096-24-9	n-Butylpyrazole	350	819	78.7	897.3			928.8			3	
	7664-41-7	NH <sub>3</sub>											
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O] 94GRU/CAL	2835-68-9	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>	350	819	78.7	896.9			927.9			5	
	13952-84-6; 110-86-1	2-butylamine; C <sub>5</sub> H <sub>5</sub> N											
[C <sub>9</sub> H <sub>10</sub> FNO] 94GRU/CAL	33322-64-4	3-F-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.7	896.9			927.9			5	
	13952-84-6; 110-86-1	2-butylamine; C <sub>5</sub> H <sub>5</sub> N											
[C <sub>9</sub> H <sub>10</sub> FNO] 94GRU/CAL	24167-56-4	4-F-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.3	896.9			927.9			5	
	13952-84-6; 110-86-1	2-butylamine; C <sub>5</sub> H <sub>5</sub> N											
[C <sub>9</sub> H <sub>10</sub> ClNO] 94GRU/CAL	24167-52-0	3-Cl-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.3	896.9			927.9			5	
	13952-84-6; 110-86-1	2-butylamine; C <sub>5</sub> H <sub>5</sub> N											
[C <sub>9</sub> H <sub>10</sub> ClNO] 94GRU/CAL	14062-80-7	4-Cl-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.3	896.9			927.9			5	
	13952-84-6; 110-86-1	2-butylamine; C <sub>5</sub> H <sub>5</sub> N											
[C <sub>2</sub> H <sub>7</sub> NO] 80MAU/HAM	141-43-5	NH <sub>2</sub> (CH <sub>2</sub> ) <sub>2</sub> OH	600	896.5	0	896.8			930.3	-2	-1.3	-3.3	-3.3
	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH											
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	1072-68-0	1,4-Dimethylpyrazole	350	819	78.3	896.8			928.4			3	
	7664-41-7	NH <sub>3</sub>											
[C <sub>8</sub> H <sub>17</sub> NO] 87TAF	26153-90-2	neo-C <sub>5</sub> H <sub>11</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.3	896.7			927.7			5	
	7664-41-7	NH <sub>3</sub>											
[C <sub>10</sub> H <sub>23</sub> N] 79AUE/BOW	2016-57-1	n-(C <sub>10</sub> H <sub>21</sub> )NH <sub>2</sub>	298	896.5	0	896.5			930.4			-5	
	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH											
[C <sub>2</sub> H <sub>7</sub> N] 97EAS/SMI 93SZU/MCM	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	0	896.5			929.5			-2	-1.9
	75-64-9	theory t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>											
			600	899.9	-3.3	895.3	934.1	-3.8	930.4	-6	0.8	-5.2	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y:SQUB	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
93SMI/RAD		theory	298						931.7			
93SMI/RAD		theory	0						925.9			
93SMI/RAD		theory	600						936.4			
91MAU/SIE	110-86-1	pyridine	600	898.1	-4.2	895.2	930	0.8	930.8	2	-7.5	-5.5
91MAU/SIE	75-31-0	i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	600	889.0	7.9	895.1	923.8	5.0	928.8	-8	5.0	-3.0
87TAF	7664-41-7	NH <sub>3</sub>	350	819	78.3	897.0		955±15				
87BIS/RUH		appearance										
83TAF	7664-41-7	NH <sub>3</sub>	350	819	78.3	897.0						
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.7						
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	32.2	896.7						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.7						
75AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	31.7	896.2						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.7						
72HENTAA	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.7						
72BRI/YAM	7664-41-7	NH <sub>3</sub>	600	819	76.6	894.2						
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	33.3	897.7						
72ARN/JON	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.7						
[C <sub>8</sub> H <sub>10</sub> CIN]	698-69-1	4-ClC <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>	350	819	78.7	896.4			922.9			20
87TAF	7664-41-7	NH <sub>3</sub>				896.4						
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ]	7290-99-5	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				896.0			927.0			5
94GRU/CAL	103-69-5; 108-45-2	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub> ; 1,3-(NH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				893-899						
[C <sub>10</sub> H <sub>13</sub> NO]	6935-65-5	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				896.0			927.0			5
94GRU/CAL	103-69-5; 108-45-2	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub> ; 1,3-(NH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				893-899						
[C <sub>10</sub> H <sub>13</sub> NO]	14062-78-3	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				896.0			927.0			5
94GRU/CAL	103-69-5; 108-45-2	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub> ; 1,3-(NH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				893-899						
[C <sub>10</sub> H <sub>8</sub> ]	275-51-4	azulene				896			925.2			11
91MAU/SIE	110-86-1	pyridine	600	898.1	1.3	896.7	930	-4.2	925.8	2	9.2	11.2
91MAU/SIE	121-69-7	C <sub>6</sub> H <sub>5</sub> N(CH <sub>3</sub> ) <sub>2</sub>	600	909.2	-8.4	898.1	941.1	-18.0	923.1	2	16.3	18.3
91MAU/SIE	75-31-0	i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	600	889.0	10.0	893.3	923.8	0.4	924.2	-8	15.9	7.9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	108.5	926.6						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	108.5	926.6						
80MAU	110-86-1	pyridine	550	898.1	0	895.9						
77WOL/ABB	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub>	350	836.0	82.8	919.6						
75WOL/HAR	7664-41-7	NH <sub>3</sub>	350	819	103.3	921.5						
[C <sub>10</sub> H <sub>17</sub> NO]	33701-54-1	5-amino-tricyclo[4.4.0.0 <sup>3,6</sup> ]decan-4-ol				896.0			928.4			0
83HOU/RUF	110-86-1	pyridine	300	898.1	-2.1	896.1						
83HOU/RUF	108-91-8	c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	300	899.6	-3.8	895.8						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/squb	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
[C <sub>7</sub> H <sub>15</sub> N] 87TAF	3218-02-8 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub>	350	819	77.3	895.8 895.7			926.6			5.6
[C <sub>4</sub> H <sub>11</sub> N] 76AUE/WEB 72AUE/WEB	13952-84-6 74-89-5 74-89-5	sec-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub>	298 298	864.5 864.5	31.2 29.3	895.7 893.8			929.7			-5
[C <sub>8</sub> H <sub>9</sub> N] 88CAU/CER	696-18-4	Aziridine, 1-phenyl see Refs.				895.7 895.7			926.5			5.6
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> ] 86HEI/HON 86HEI/HON	90196-91-1 110-86-1 108-91-8	1-azabicyclo[2.2.2]-octane, 2-cyano pyridine c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>	313 313	898.1 899.6	-2.5 -3.8	895.6 895.6 895.6			926.4			5.6
[C <sub>12</sub> H <sub>21</sub> NO] 83HOU/RUF 83HOU/RUF 83HOU/RUF	73495-63-3 110-86-1 108-91-8 13952-84-6	3-Amino-tricyclo[7.3.0.0 <sup>4,8</sup> ]dodecan-2-ol pyridine c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub> sec-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	1300 1300 1300	898.1 899.6 895.7	-2.1 -3.8 -0.8	895.6 896.1 895.8 894.9			928.0			0
[C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	2820-37-3 5813-64-9 110-86-1	3(5),4-dimethylpyrazole neo-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub> pyridine	333 333	894.0 898.1	2.2 -3.3	895.4 895.9 894.9			927.3			2
[C <sub>7</sub> H <sub>15</sub> NO] 97HOM/HER 97HOM/HER	24331-71-3 110-86-1 5813-64-9	t-C <sub>4</sub> H <sub>9</sub> CON(CH <sub>3</sub> ) <sub>2</sub> pyridine neo-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333 333	898.1 894.0	-2.4 1.0	895.2 895.8 894.7			927.1			2
[C <sub>11</sub> H <sub>24</sub> O <sub>4</sub> ] 92LIO/BRO	66226-75-3 294-93-9; 33100-27-5	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> O] <sub>3</sub> CH <sub>3</sub> 12-crown-4; 15-Crown-5				895.1 891-900			NE			NE
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S] 93ABB/MO 93ABB/MO	534-13-4 75-64-9 110-58-7	SC(NHCH <sub>3</sub> ) <sub>2</sub> t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> n-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333 333	899.9 889.5	-3.0 4.4	895.1 896.5 893.6			926.0			5
[C <sub>8</sub> H <sub>19</sub> N] 79AUE/BOW	111-86-4 124-40-3	n-(C <sub>8</sub> H <sub>17</sub> )NH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	-1.5	895.0 895.0			928.9			-5
[C <sub>6</sub> H <sub>7</sub> NO] 87TAF 79AUE/BET 76COO/KAT	694-85-9 7664-41-7 74-89-5 110-86-1	1-Methyl-2-pyridinone NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub> pyridine	350 298 350	819 864.5 898.1	76.4 31.7 -4.6	894.8 894.9 896.2 893.4			925.8			5
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ] 91AUE/WEB	2459-09-8 110-86-1	Pyridine-4-carboxylic acid, methyl ester pyridine	300	898.1	-0.5	894.7 897.7			926.6			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: S, N, O	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
87TAF	7664-41-7	NH <sub>3</sub>	350	819	73.2	891.8							
[C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ] 87TAF	57-14-7	(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub>				894.7			927.1				0
84MAU/NEL	7664-41-7	NH <sub>3</sub>	350	819	77.3	896.0							
83TAF2	110-86-1	pyridine	600	898.1	-5.4	893.3							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	76.9	895.6							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	74.1	892.8							
	7664-41-7	NH <sub>3</sub>	350	819	74.1	892.8							
[C <sub>3</sub> H <sub>9</sub> NO] 73AUE/WEB	109-85-3	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>				894.6			928.6				-5.1
	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	10.7	894.6							
[C <sub>6</sub> H <sub>11</sub> NO] 87TAF	4030-18-6	Acetylpyrrolidine				894.4			925.4				5
	7664-41-7	NH <sub>3</sub>	350	819	76.0	894.4							
[C <sub>6</sub> H <sub>13</sub> NO] 87TAF	685-91-6	CH <sub>3</sub> CON(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub>				894.4			925.4				5
	7664-41-7	NH <sub>3</sub>	350	819	76.0	894.4							
[C <sub>9</sub> H <sub>9</sub> N] 87TAF	6921-29-5	(HCCCH <sub>2</sub> ) <sub>3</sub> N				894.4			925.2				5.6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	76.0	894.4							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	76.0	894.4							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	73.2	891.6							
	7664-41-7	NH <sub>3</sub>	350	819	73.2	891.6							
[C <sub>4</sub> H <sub>9</sub> NS] 93ABB/MO	631-67-4	CH <sub>3</sub> C(S)N(CH <sub>3</sub> ) <sub>2</sub>				894.4			925.3				5
93ABB/MO	110-86-1	pyridine	333	898.1	-2.0	896.1							
93ABB/MO	6921-29-5	(HCCCH <sub>2</sub> ) <sub>3</sub> N	333	894.4	0.9	895.3							
93ABB/MO	110-58-7	n-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub>	333	889.5	2.5	891.7							
[C <sub>10</sub> H <sub>13</sub> NO <sub>2</sub> ] 87TAF	1202-25-1	4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>				894.1			920.6				20
	7664-41-7	NH <sub>3</sub>	350	819	76.4	894.1							
[C <sub>9</sub> H <sub>13</sub> NO] 87TAF	15799-79-8	3-Methoxy-N,N-dimethylbenzenamine				894.1			920.6				20
	7664-41-7	NH <sub>3</sub>	350	819	76.4	894.1							
[C <sub>7</sub> H <sub>6</sub> O] 77DIT/NIB	502-87-4	4-Methylene-2,5-cyclohexadiene-1-one				894.0			923.8				9
	7664-41-7	NH <sub>3</sub>	~300	819	75	894			See Refs.				
[C <sub>2</sub> H <sub>13</sub> N] 87TAF	5813-64-9	neo-C <sub>2</sub> H <sub>11</sub> NH <sub>2</sub>				894.0			928.3				-6
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	74.6	893.6							
76AUE/WEB	7664-41-7	NH <sub>3</sub>	350	819	73.7	892.7							
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	29.8	894.3							
[C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> ] 87TAF	27258-04-4	Di(1-pyrazolyl)methane				893.9			924.7				5.8
	7664-41-7	NH <sub>3</sub>	350	819	75.5	893.9							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr:Squb	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ] 91BER/DEC	93-60-7	methylnicotinate				893.8			925.6			2	
91BER/DEC	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	338	883.9	9.8	893.5							
91BER/DEC	110-86-1	pyridine	338	898.1	-4.9	893.3							
91BER/DEC	110-91-8	Morpholine	338	891.2	1.0	892.1							
91AUE/WEB	110-86-1	pyridine	300	898.1	-0.5	897.7							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	73.7	892.3							
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>4</sub> ] 93GOR/AMS	17355-09-8	tyr-val				893.6			NE			NE	
	75-31-0;	(t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; C <sub>5</sub> H <sub>5</sub> N	350			889-898							
	110-86-1												
[C <sub>14</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ] 93GOR/AMS	3918-90-9	phe-val				893.6			NE			NE	
	75-31-0;	(t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; C <sub>5</sub> H <sub>5</sub> N	350			889-898							
	110-86-1												
[C <sub>6</sub> H <sub>15</sub> N] 79AUE/BOW	111-26-2	n-C <sub>6</sub> H <sub>13</sub> NH <sub>2</sub>				893.5			927.5			-5	
73AUE/WEB	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	-2.9	893.5							
	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	4.9	888.8							
[C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ] 92ABB/CAB	5744-40-1	1,3-dimethyl-5-ethoxycarbonylpyrazole				893.1			924.9			2	
92ABB/CAB	5813-64-9	neo-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	894.0	0.2	893.9							
92ABB/CAB	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	886.6	4.8	891.1							
92ABB/CAB	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	-5.5	894.1							
[C <sub>8</sub> H <sub>11</sub> N] 81MCL/CAM	103-69-5	C <sub>6</sub> H <sub>5</sub> NHC <sub>2</sub> H <sub>5</sub>				892.9			924.8			2	
81MCL/CAM	13952-84-6	sec-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	425						925.1	-4.6			
81MCL/CAM	111-26-2	n-C <sub>6</sub> H <sub>13</sub> NH <sub>2</sub>	425						927.5	-2.9			
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	77.0	893.5							
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	77.0	893.5							
[C <sub>2</sub> H <sub>5</sub> NO] 92MIS/TER	694-59-7	pyridine-1-oxide				892.9			923.6			5.8	
79MAU	7664-41-7	NH <sub>3</sub>	343	819	72.4	890.9							
	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	550	883.9	13.4	894.6							
[C <sub>4</sub> H <sub>9</sub> O <sub>3</sub> P] 80HOD/HOU	31131-06-9	2-Methoxy-1,3,2-dioxaphosphorinane				892.8			925.3			0	
	110-86-1	pyridine	320	898.1	-5.4	892.7							
[C <sub>4</sub> H <sub>8</sub> Se <sub>2</sub> ] 89OSA/DEL	99030-02-1	CH <sub>2</sub> =C(SeCH <sub>3</sub> ) <sub>2</sub>				892.6			921.5			12	
	110-58-7;	n-C <sub>3</sub> H <sub>11</sub> NH <sub>2</sub> ; CH <sub>3</sub> CH(NH <sub>2</sub> )C <sub>2</sub> H <sub>5</sub>	313			890-896							
	13952-84-6												
[C <sub>6</sub> H <sub>11</sub> NO] 79AUE/BOW	931-20-4	c-C <sub>5</sub> H <sub>9</sub> N(2-O)1-CH <sub>3</sub>				892.6			924.4			2	
79AUE/BET	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	-3.9	892.6							
76COO/KAT	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	28.3	892.8							
	7664-41-7	NH <sub>3</sub>	350	819	71.4	890.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta \Delta S_p$ (M)
[C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> ] 92LIO/BRO	112-49-2	CH <sub>3</sub> O[CH <sub>2</sub> CH <sub>2</sub> O] <sub>3</sub> CH <sub>3</sub> kinetic method-relative order only				892.4			946.6			-73	
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	20.9	888.6	884.6	56.1	940.6	2	-71	-69	
83MAU	289-80-5	Pyridazine	600	877.1	-6.3	895.1	907.2	38.1	945.3	7.8	-74	-66.2	
83MAU	372-47-4	3-F-pyridine	600	870.1	0.4	893.0	902.0	51.0	953.0	2	-85	-83	
[C <sub>3</sub> H <sub>7</sub> N] 79AUE/BOW	75-55-8 124-40-3	2-Methylaziridine (CH <sub>3</sub> ) <sub>2</sub> NH	298	896.5	-4.4	892.1			925.1			-2	
[C <sub>9</sub> H <sub>11</sub> NO <sub>3</sub> ] 93LI/HAR	60-18-4	L-tyrosine kinetic method				892.1			926			-5	
92GOR/SPE	75-31-0; 110-86-1	(i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; pyridine	350			889-898			926			-3.7	
90ISA/OMO		kinetic method-relative order											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	86.5	905.4							
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	86.5	905.4							
[C <sub>6</sub> H <sub>10</sub> F <sub>3</sub> N] 87TAF	657-36-3 7664-41-7	4-Trifluoromethylpiperidine NH <sub>3</sub>	350	819	73.2	892.0			925.1			-2	
[Sc] 89ELK/SUN	7440-20-2	Sc				892.0			914			35	
84TOL/BEA		See Refs. See Refs.							914±9 907.5				
[C <sub>6</sub> H <sub>13</sub> NO] 97HOM/HER	21678-37-5 107-10-8	i-C <sub>3</sub> H <sub>7</sub> CON(CH <sub>3</sub> ) <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	883.9	7.8	891.8			923.7			2	
97HOM/HER	5813-64-9	neo-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	894.0	-1.5	892.2							
[C <sub>3</sub> H <sub>6</sub> NO] 87TAF	872-50-4 7664-41-7	1-Methyl-2-pyrrolidinone NH <sub>3</sub>	350	819	71.8	891.6			923.5			2	
79AUE/BET	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	28.3	890.4							
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> ] 93LI/HAR	70-47-3	L-Asparagine kinetic method-See Refs.	350			891.5			929			-17	
92GOR/SPE	75-31-0; 110-86-1	(i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; pyridine	350			889-898			929			-17	
90ISA/OMO		kinetic method-relative order											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	75.1	894.6							
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	75.1	894.6							
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S] 93ABB/MO	96-45-7	2-imidazolinethione				891.2			921.9			5.8	
93ABB/MO	75-64-9	t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	899.9	-7.2	892.3							
93ABB/MO	110-58-7	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	889.5	-0.1	889.1							
93ABB/MO	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	883.9	8.7	892.3							

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSub	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>4</sub> H <sub>9</sub> NO] 73AUE/WEB	110-91-8 107-10-8	Morpholine n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	7.3	891.2 891.2			924.3			-2
[C <sub>7</sub> H <sub>6</sub> O] 83CAS/FRE	539-80-0 107-10-8, 110-86-1	2,4,6-Cycloheptatriene-1-one C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> ; pyridine				891.0 884-898			920.8			9
77DIT/NIB	7664-41-7	NH <sub>3</sub>	~300	819	92	911						
[C <sub>5</sub> H <sub>7</sub> N <sub>2</sub> ] 92ABB/CAB	15802-80-9 109-73-9	3(5)-t-butylpyrazole n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	886.6	4.1	891.0 890.4			922.8			2
92ABB/CAB	5813-64-9	neo-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	894.0	-2.1	891.6						
[C <sub>4</sub> H <sub>11</sub> N] 76AUE/WEB	78-81-9 74-89-5	i-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub>	298	864.5	26.4	890.8 890.8			924.8			-5
75ARN	7664-41-7	NH <sub>3</sub>	350	819	78.3	897.2						
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	23.4	887.9						
[C <sub>6</sub> H <sub>13</sub> NO] 87TAF	760-79-2 7664-41-7	n-C <sub>5</sub> H <sub>7</sub> CON(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	72.3	890.8 890.7			921.7			5
[C <sub>8</sub> H <sub>16</sub> O <sub>4</sub> ] 92LIO/BRO	294-93-9	12-crown-4 kinetic method				890.5			927.2			-14
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	31.4	887.3	884.6	45.6	930.2	2	-29	-27
83MAU	110-86-1	pyridine	600	898.1	-11.5	891.4	930	-5.0	925.0	2	-11	-9
83MAU	289-80-5	Pyridazine	600	877.1	6.0	889.7	907.2	13.8	921.0	7.8	-13	-5.2
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ] 88CAT/CLA	13436-48-1 657-36-3	1-methylindazole 4-Trifluoromethylpiperidine	~300	892.0	-1.3	890.5 890.8			922.4			2
88CAT/CLA	1628-89-3	2-(CH <sub>3</sub> O)-pyridine	~300	902.8	-10.5	892.3						
88CAT/CLA	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	~300	886.6	3.3	890.0						
87TAF	7664-41-7	NH <sub>3</sub> kinetic method	350	819	71.4	890.0 ~891.2						
[C <sub>7</sub> H <sub>9</sub> N] 78LAU/SAL	100-61-8 7664-41-7	C <sub>6</sub> H <sub>5</sub> NHCH <sub>3</sub> NH <sub>3</sub>		819	63.2	890.1 890.1			916.6			20
72BRU/YAM	7664-41-7	NH <sub>3</sub>		819	63.2	890.1						
[C <sub>9</sub> H <sub>14</sub> O <sub>2</sub> ] 87TAF	4683-45-8 7664-41-7	3-Methoxy-5,5-dimethylcyclohex-2-enone NH <sub>3</sub>	350	819	71.4	890.1 890.1			922.6			0
[C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> ] 92ABB/CAB	1820-80-0 5813-64-9	3(5)-aminopyrazole neo-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>	333	894.0	-3.4	889.6 890.4			921.5			2
92ABB/CAB	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	886.6	2.6	888.9						
[C <sub>5</sub> H <sub>13</sub> N] 9233.5	110-58-7	n-C <sub>5</sub> H <sub>11</sub> NH <sub>2</sub>				889.5			923.5			-5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	3.3	887.2							
79AUE/BET	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	27.3	891.8							
77COO/KRU		relative order-See Refs.											
[C <sub>4</sub> H <sub>6</sub> NO] 87TAF	1187-58-2 7664-41-7	C <sub>2</sub> H <sub>5</sub> CONHCH <sub>3</sub> NH <sub>3</sub>	350	819	70.9	889.4 889.4			920.4			5	
[C <sub>6</sub> H <sub>6</sub> CIN] 79AUE/BOW	3678-62-4 74-89-5	2-Cl-4-(CH <sub>3</sub> )-pyridine CH <sub>3</sub> NH <sub>2</sub>	298	864.5	24.9	889.4 889.4			921.2			2	
[C <sub>7</sub> H <sub>17</sub> N] 73AUE/WEB	111-68-2 107-10-8	n-C <sub>7</sub> H <sub>15</sub> NH <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	5.4	889.3 889.3			923.2			-5	
[C <sub>3</sub> H <sub>9</sub> N] 91MAU/SIE	75-31-0	i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	600	878	13.0	889.0			923.8			-8	
91MAU/SIE	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	600	872.1		891.8		12.1	924.1		1.7	-3.4	
91MAU/SIE	288-47-1	thiazole	600	870.1		891.1		904	932.0				
91MAU/SIE	372-47-4	3-F-pyridine	600	870.1		891.1		902.0	927.9				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	70.5	889.6							
86MAU/LIE	110-86-1	pyridine	600	898.1	-14.4	886.7							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	70.5	889.6							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	25.9	890.4							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	70.5	889.6							
72HEN/TAA	7664-41-7	NH <sub>3</sub>	350	819	70.5	889.6							
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	23.9	888.4							
72ARN/JON	7664-41-7	NH <sub>3</sub>	350	819	70.5	889.6							
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ] 93L/HAR	63-91-2	L-phenylalanine				888.9			922.9				
92GOR/SPE	75-31-0; 110-86-1	kinetic method (i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub> ; pyridine	350			889-898			915				
90ISA/OMO		kinetic method-relative order											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	76.4	895.4							
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	76.4	895.4							
79MAU/HUN	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	570	886.6	-3.8	882.1							
79MAU/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	500	850.6	25.9	877.9							
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ] 87TAF	107-97-1 7664-41-7	Sarcosine NH <sub>3</sub>	350	819	70.0	888.7			921.2			0	
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	70.0	888.7							
[C <sub>4</sub> H <sub>6</sub> NO <sub>3</sub> ] 93L/HAR	72-19-5	L-threonine				888.5			922.5				
92GOR/SPE	110-86-1; 75-64-9	kinetic method pyridine; (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub>	350			898-900			911				
90ISA/OMO		kinetic method-relative order											

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
87TAF	7664-41-7	NH <sub>3</sub>	350	819	69.6	888.5							
87BOJ	7664-41-7	kinetic method-relative order NH <sub>3</sub>	350	819	69.6	888.5							
83LOC/MCI	120-73-0	Purine	515	883.9	5.9	888.2			920.1			2	
[C <sub>3</sub> H <sub>4</sub> N <sub>4</sub> ]	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				888.2							
79MAU	74-89-5;	CH <sub>3</sub> NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>2</sub> NH				864-896							
75WIL/MCC	124-40-3												
[C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> ]	26629-33-4	CH <sub>3</sub> CONHCH(CH <sub>3</sub> )COOCH <sub>3</sub>				888.0			938.6			-61	
83MAU	372-47-4	3-F-pyridine	600	870.1	0.8	889.8		40.2	942.1	2	-65.7	-63.7	
83MAU	372-48-5	2-F-pyridine	600	852.7	14.6	886.2		51.5	936.0	2	-61.5	-59.5	
[C <sub>3</sub> H <sub>8</sub> F <sub>3</sub> NS]	#585	3-(SCF <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub>				887.7			914.2			20	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	70.0	887.7							
[C <sub>4</sub> H <sub>3</sub> NO]	145355-49-3	CH <sub>3</sub> NCCCCO				887.5			920			0	
94FLA/HAV		theory							920				
[C <sub>8</sub> H <sub>9</sub> N]	625-84-3	2,5-Dimethylpyrrole				887.1			918.7			3	
86MAU/LIE	110-86-1	pyridine	600	898.1	-10.5	887.4							
86MAU/LIE	372-47-4	3-F-pyridine	600	870.1	16.7	886.5							
[C <sub>3</sub> H <sub>8</sub> FN]	462-41-9	FCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>				886.9			920.9			-5	
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	22.5	886.9							
[C <sub>11</sub> H <sub>14</sub> N <sub>2</sub> ]	13012-16-3	N,N',2,6-Tetramethyl-4-cyanoaniline				886.8			913.3			20	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	69.1	886.8							
[C <sub>4</sub> H <sub>11</sub> N]	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>				886.6			921.5			-8	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	66.8	885.9							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	66.8	885.9							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	67.7	886.8							
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	515	883.9	2.1	886.6							
77COO/KRU		relative order-See Refs.											
76AUE/AWEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	23.9	888.4							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	66.4	885.4							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	66.4	885.4							
72AUE/AWEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	22.0	886.5							
[Mg <sub>2</sub> ]	29904-79-8	Mg <sub>2</sub>				886.5			919			0	
77PO/POR		See Refs.							919±30				
[C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> ]	6620-95-7	ser-ser				886.4			NE			NE	

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
94MCK/BEL	107-10-8; 75-31-0	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> ; i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				884-889						
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>4</sub> ] 94MCK/BEL	7361-43-5 107-10-8; 75-31-0	ser-gly n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> ; i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				886.4 884-889			NE			NE
[C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O] 91BER/DEC 91BER/DEC	98-92-0 78-81-9 127-19-5	nicotinamide i-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> Dimethylacetamide	338 338	890.8 877.0	-0.8 5.8	886.4 889.8 883.0			918.3			2
[C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O] 87TAF	80-73-9 7664-41-7	1,3-Dimethyl-2-imidazolidinone NH <sub>3</sub>	350	819	67.3	886.0 886.0			918.4			0
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> ] 87TAF	24558-36-9 7664-41-7	N,N',2,6-Tetramethyl-4-nitroaniline NH <sub>3</sub>	350	819	67.3	886.0 886.0			918.4			0
[C <sub>3</sub> H <sub>6</sub> NO <sub>2</sub> ] 96EWI/ZHA	147-85-3 110-86-1; 108-91-8	L-proline pyridine; c-C <sub>6</sub> H <sub>11</sub> NH <sub>2</sub>				886.0 898-900			920.5			-7
93LI/HAR 92GOR/SPE	75-64-9; 75- 50-3	kinetic method-See Refs. (t-C <sub>4</sub> H <sub>9</sub> )NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>3</sub> N	350			900-918			920.5			-7
90ISA/OMO 87BOJ		kinetic method-relative order										
83LOC/MCI 79MAU/HUN 79MAU/HUN 73YAM/KEB	7664-41-7 75-64-9 109-73-9 7664-41-7	NH <sub>3</sub> t-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> NH <sub>3</sub>	350 570 570 600	819 899.9 886.6 819	92.0 -0.4 10.5 46.0	911.0 899.7 896.8 865.2						
[C <sub>4</sub> H <sub>6</sub> BrN] 91AUE/WEB 76AUE/WEB2	1120-87-2 110-86-1 74-89-5	4-Br-pyridine pyridine CH <sub>3</sub> NH <sub>2</sub>	300 298	898.1 864.5	-12.2 21.5	886.0 885.9 886.0			917.8			2
[C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> ] 92MOR/MAR 92MOR/MAR	22157-30-8 109-73-9 107-10-8	CH <sub>3</sub> C(OCH <sub>3</sub> )=CHCOOCH <sub>3</sub> n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	338 338	886.6 883.9	-1.2 3.1	885.8 885.0 886.7			916.8			5
[C <sub>6</sub> H <sub>6</sub> CINO] 79AUE/BET	17228-63-6 74-89-5	6-Chloro-1-methyl-2(1H)pyridinone CH <sub>3</sub> NH <sub>2</sub>	298	864.5	21.0	885.6 885.5			918.5			-1.9
[C <sub>8</sub> H <sub>12</sub> O] 85HOU/ROL 85HOU/ROL 85HOU/ROL	10599-58-3 107-10-8 109-73-9 75-31-0	2,3,4,5-tetramethylfuran n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> i-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	313 313 313	883.9 886.6 889.0	0.4 -1.7 -3.3	884.8 884.2 884.8 885.5			915.5			5.8



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
[C <sub>2</sub> H <sub>7</sub> NO]	350-03-8	3-(CH <sub>3</sub> CO)-pyridine				884.3			916.2			2	
91BER/DEC	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	338	886.6	1.0	887.2							
91BER/DEC	127-19-5	Dimethylacetamide	338	877.0	6.8	883.9							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	63.2	881.7							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	63.2	881.7							
[C <sub>4</sub> H <sub>9</sub> CIN]	626-61-9	4-Cl-pyridine				884.2			916.1			2	
91AUE/WEB	110-86-1	pyridine	300	898.1	-12.7	885.5							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	65.0	883.6							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	65.9	884.5							
76AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	21.0	885.5							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	64.5	883.1							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	64.5	883.1							
[C <sub>3</sub> H <sub>9</sub> N]	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				883.9			917.8			-5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	64.5	883.5							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	64.5	883.5							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	65.9	884.8							
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	0	883.9							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	21.5	886.0							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	63.6	882.5							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	63.6	882.5							
73AUE/WEB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	298	883.9	0	883.9							
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	19.0	883.5							
[C <sub>4</sub> H <sub>9</sub> N]	2878-14-0	CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> NH <sub>2</sub>				883.6			917.5			-5	
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	19.0	883.5							
[C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> ]	3989-97-7	val-leu				883.6			NE			NE	
93GOR/AMS	75-04-7; 75-31-0	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			878-889							
[C <sub>11</sub> H <sub>22</sub> N <sub>2</sub> O <sub>3</sub> ]	13588-95-9	leu-val				883.5			NE			NE	
93GOR/AMS	75-04-7; 75-31-0	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			878-889							
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	27493-61-4	val-ala				883.5			NE			NE	
93GOR/AMS	75-04-7; 75-31-0	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			878-889							
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	73-32-5	L-isoleucine				883.6			917.4			-5	
93LI/HAR		kinetic method							912				
92GOR/SPE	75-04-7; 75-31-0	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (t-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			878-889							
90ISA/OMO	7664-41-7	kinetic method-relative order				890.3							
87TAF		NH <sub>3</sub>	350	819	71.4	890.3							

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^{\ddagger}$ (R)	$\Delta\Delta S_p^{\ddagger}$ (M,R)	$\Delta S_p^{\ddagger}$ (M)	$\Delta S_p^{\ddagger}$ (M)
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	71.4	890.3							
[C <sub>10</sub> H <sub>20</sub> N <sub>2</sub> O <sub>3</sub> ] 93GOR/AMS	3918-94-3 75-04-7; 75-31-0	val-val C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			883.5 878-889			NE				NE
[C <sub>7</sub> H <sub>7</sub> NO]	1122-54-9	1-(4-Pyridinyl)-ethanone				882.9			914.7				2
91AUE/WEB	110-86-1	pyridine	300	898.1	-14.6	883.5							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	63.2	881.7							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	64.1	882.6							
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	19.0	883.5							
[C <sub>2</sub> H <sub>30</sub> S]	73509-04-03	(1-adamantyl) <sub>2</sub> CS				882.4			912.1				9
93ABB/MO	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	883.9	-1.1	882.3							
93ABB/MO	107-11-9	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	333	875.5	7.4	882.4							
[C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> ] 92ABB/CAB	2458-26-6 109-73-9	3(5)-phenylpyrazole n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	886.6	-4.1	882.3 882.2			914.2				2
92ABB/CAB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	883.9	-1.3	882.4							
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O] 96KIN/RID	598-41-4 75-04-7; 109-73-9	H <sub>2</sub> NCH <sub>2</sub> CONH <sub>2</sub> (glycinamide) C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>				882.3 878-887			NE				NE
[C <sub>4</sub> H <sub>11</sub> NO] 83BAR/BAS	3710-84-7 107-10-8	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NOH n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	300	883.9	-1.7	882.2 882.2			914.7				0
[C <sub>10</sub> H <sub>12</sub> O] 87TAF	1712-69-2 7664-41-7	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	64.1	882.2 882.1			911.1				12
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	64.1	882.1							
[C <sub>4</sub> H <sub>8</sub> Cl <sub>3</sub> N] 87TAF	36726-94-0 7664-41-7	CCl <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	63.6	882.0 882.0			912.8				5.6
[C <sub>8</sub> H <sub>7</sub> N] 92MIS/ARI	14235-81-5 536-74-3	4-H <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	80.8	882.0 882.0			912.7				5.8
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> ] 93ZHA/ZIM	556-50-3 107-11-9; 100-46-9	diglycine CH <sub>2</sub> CHCH <sub>2</sub> NH <sub>2</sub> ; C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub>	300			882 876-879			NE				NE
93WU/LEB	107-11-9; 127-19-5	CH <sub>2</sub> =CHCH <sub>2</sub> NH <sub>2</sub> ; CH <sub>3</sub> CON(CH <sub>3</sub> ) <sub>2</sub>	300			876-877							
92WU/FEN2	593-67-9; 75-04-7	kinetic method CH <sub>2</sub> =CHNH <sub>2</sub> ; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>				890 866-878							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>3</sub> H <sub>10</sub> F <sub>3</sub> N] 87TAF	329-00-0 7664-41-7	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	64.1	881.8 881.7			908.3			20	
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> ] 92ABB/CAB 92ABB/CAB	100852-80-0 1122-54-9 289-80-5	1-methyl-3,5-diethoxycarbonylpyrazole 1-(4-Pyridinyl)-ethanone Pyridazine	333 333	882.9 877.1	-0.8 3.9	881.5 882.1 881.2			913.4			2	
[C <sub>5</sub> H <sub>4</sub> FN] 91AUE/WEB 87TAF 81TAA/SUM 79AUE/BOW 75TAF	694-52-0 110-86-1 7664-41-7 7664-41-7 74-89-5 7664-41-7	4-F-pyridine pyridine NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub>	300 350 320 298 350	898.1 819 819 864.5 819	-15.6 61.3 56.9 16.6 62.2	881.2 882.5 879.9 875.7 881.1 880.8			913.1			2	
[C <sub>7</sub> H <sub>9</sub> NO] 81LAU/NIS	536-90-3 62-53-3	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	30.5	881.1 881.1			913.0			2	
[C <sub>3</sub> H <sub>7</sub> N <sub>2</sub> O <sub>4</sub> ] 94MCK/BEL	687-63-8 75-04-7; 107-10-8	gly-ser C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				880.9 878-884			NE			NE	
[C <sub>11</sub> H <sub>17</sub> NO] 97HOM/HER 97HOM/HER	5511-18-2 289-80-5 107-10-8	1-adamantyl-CONH <sub>2</sub> Pyridazine n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333 333	877.1 883.9	3.8 -2.9	880.9 881.2 880.8			912.8			2	
[C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> ] 93LI/HAR 92GOR/SPE	56-45-1 74-89-5; 372-47-4	L-Serine kinetic method CH <sub>3</sub> NH <sub>2</sub> ; 3-F-pyridine				880.7 864-870			914.6 904			-5	
90ISA/OMO 87TAF 87BOJ 83LOC/MCI	7664-41-7 7664-41-7 108-44-1; 372-47-4 61-90-5	kinetic method-relative order NH <sub>3</sub> kinetic method-relative order NH <sub>3</sub> 3-CH <sub>3</sub> -aniline; 3-F-pyridine	350 350 350	819 819 819	61.3 61.3	880.3 880.3 864-870							
[C <sub>4</sub> H <sub>3</sub> NO <sub>2</sub> ] 93LI/HAR 92GOR/SPE	75-04-7; 75- 31-0 7664-41-7	L-leucine kinetic method C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; (i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>	350			880.6 878-889			914.6 909			-5	
90ISA/OMO 87TAF 87BOJ 83LOC/MCI 79MAU/HUN 79MAU/HUN	7664-41-7 7664-41-7 109-73-9 75-04-7	kinetic method-relative order NH <sub>3</sub> kinetic method-relative order NH <sub>3</sub> n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350 350 570 520	819 819 886.6 878	67.3 67.3 -4.6 -0.4	886.2 886.2 881.2 877.6							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
79MAU/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	500	850.6	25.1	877.1						
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ] 92MIS/TER	14188-94-4 694-59-7	1-(3-pyridinyl-1-oxide)ethanone pyridine-1-oxide	343	892.9	-12.6	880.6 880.6			913.1			0
[C <sub>6</sub> H <sub>11</sub> NO] 90WOL/GRU	6976-91-6 100-46-9	2-propenamide, N,N,2-trimethyl- C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub>	320	879.4	1.4	880.6 880.6			911.5			5
[C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> ] 84SHA/BLA	13179-96-9 372-48-5	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>4</sub> OCH <sub>3</sub> 2-F-pyridine	500	852.7	15.1	880.6 880.6	884.6	46.4	931.5 931.0	2	-64	-62 -62
[FeO] 84CAS/FRE	1345-25-1 107-10-8; 110-86-1	FeO n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> ; pyridine				880.5 884-898			907			20
80MUR		See Refs.							907			
[C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O] 75WIL/MCC	68-94-0 74-89-5; 124-40-3	Hypoxanthine CH <sub>3</sub> NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>2</sub> NH				880.5 864-896			912.3			2
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> S] 75WIL/MCC	2001-93-6 74-89-5; 124-40-3	Dithiouracil CH <sub>3</sub> NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>2</sub> NH				880.5 864-896			911.4			5
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ] 88CAT/CLA	930-36-9 109-73-9	1-methylpyrazole n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	300	886.6	-6.3	880.1 880.4			912.0			2
88CAT/CLA 87TAF	75-04-7 7664-41-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> NH <sub>3</sub>	300 350	878 819	2.9 60.4	880.9 879.0						
[C <sub>3</sub> H <sub>11</sub> NOS] 93ABB/MO 93ABB/MO	#638 107-10-8 289-80-5	C <sub>2</sub> H <sub>5</sub> OC(S)N(CH <sub>3</sub> ) <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> Pyridazine	333 333	883.9 877.1	-3.4 2.9	880.0 880.1 880.1			911.0			5
[C <sub>3</sub> H <sub>6</sub> OP] 87TAF 84BOL/HOU 84BOL/HOU	676-96-0 7664-41-7 107-10-8 75-04-7	OP(CH <sub>3</sub> ) <sub>3</sub> NH <sub>3</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350 ~323 ~323	819 883.9 878	60.9 -2.5 2.1	880.0 879.1 881.1 879.8			909.7			9.1
[C <sub>3</sub> H <sub>2</sub> N] 95BOU/SAL	18295-52-8 107-11-9; 107-10-8	vinylimine CH <sub>2</sub> =CHNH <sub>2</sub> ; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				879.7 876-884			912.1			0
[C <sub>6</sub> H <sub>15</sub> O <sub>4</sub> P] 87TAF 84BOL/HOU 84BOL/HOU	78-40-0 7664-41-7 75-04-7 107-10-8	OP(OC <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> NH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	350 ~323 ~323	819 878 883.9	60.9 0.4 -2.1	879.6 879.1 878.1 881.5			909.3			9.1

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
80HOD/MCD	75-04-7; 621-23-8	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> ; 1,3,5-(CH <sub>3</sub> O) <sub>3</sub> C <sub>6</sub> H <sub>3</sub>	300			878-898							
[C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> ] 84SHA/BLA	111-89-7 372-48-5	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>5</sub> OCH <sub>3</sub> 2-F-pyridine	500	852.7	13.4	879.5 879.5	884.6	46.4	931.3 931.0	2	-67	-6.5 -65	
[C <sub>7</sub> H <sub>7</sub> N] 90PEE/ING	16118-22-2 765-30-0; 75-31-0	C <sub>6</sub> H <sub>5</sub> CH=NH c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> ; (i-C <sub>3</sub> H <sub>7</sub> )NH <sub>2</sub>				879.4 870-889			911.9			0	
[C <sub>11</sub> H <sub>15</sub> N] 88CAU/CER	54104-82-4	Pyrrolidine, 1-(4-methylphenyl) See Refs.				879.4 879.4			910.2			5.6	
[C <sub>7</sub> H <sub>9</sub> N] 87TAF 83TAF2 79AUE/BOW	100-46-9 7664-41-7 7664-41-7 74-89-5	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub>	350 350 298	819 819 864.5	60.4 60.4 27.3	879.4 879.3 879.3 891.8			913.3			-5	
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	4395-98-6 7664-41-7	4-Cyanopiperidine NH <sub>3</sub>	350	819	60.4	879.2 879.2			912.3			-2	
[C <sub>3</sub> H <sub>9</sub> NO <sub>4</sub> ] 92GOR/SPE	56-86-0 75-50-3; 109-89-7	L-Glutamic Acid (CH <sub>3</sub> ) <sub>2</sub> N; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NH kinetic method-relative order NH <sub>3</sub> kinetic method-relative order NH <sub>3</sub>	350			879.1 918-919			913.0			-5	
90ISA/OMO 87TAF 87BOJ 83LOC/MCI	7664-41-7 7664-41-7		350 350	819 819	59.9 59.9	878.9 878.9							
[C <sub>13</sub> H <sub>18</sub> N <sub>2</sub> ] 94NOT/HER 94NOT/HER 94NOT/HER	84396-62-3 289-80-5 107-11-9 107-10-8	4-(1-adamantyl)-pyrazole Pyridazine H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub> n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333 333 333	877.1 875.5 883.9	1.2 3.3 -5.0	878.9 878.7 878.8 878.9			913.1			-5.8	
[C <sub>7</sub> H <sub>7</sub> NO] 87TAF	556-18-3 7664-41-7	4-NH <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub>	350	819	59.9	878.6 878.5			910.4			2	
[C <sub>5</sub> H <sub>4</sub> BrN] 91AUE/WEB 79AUE/BET 76AUE/WEB2	626-55-1 110-86-1 74-89-5 74-89-5	3-Br-pyridine pyridine CH <sub>3</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub>	300 298 298	898.1 864.5 864.5	-20.0 13.7 13.7	878.2 878.1 878.2 878.2			910.0			2	
[C <sub>6</sub> H <sub>6</sub> CINO] 79AUE/BET	17228-64-7 74-89-5	2-Cl-6-(CH <sub>3</sub> O)-pyridine CH <sub>3</sub> NH <sub>2</sub>	298	864.5	11.7	878.0 878.0			909.9			2	
[C <sub>2</sub> H <sub>7</sub> N] 87TAF	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>				878			912.0			-5.1	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr: Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
97EAS/SMI		theory	298										-5.1
95SMI/RAD		theory	298						914				
94DEC/EXN	765-30-0	c-C <sub>3</sub> H <sub>3</sub> NH <sub>2</sub>	338	869.9	5.9	875.7							
91MAU/SIE	372-47-4	3-F-pyridine	600	870.1	5.9	878.1	902.0	10.0	912.0	2	-6.7		-4.7
87TAF	7664-41-7	NH <sub>3</sub>	350	819	57.7	876.6							
87BIS/RUH		Appearance							940±15				
86TAF/ANV	7664-41-7	NH <sub>3</sub>	350	819	52.7	871.7							
86TAF/ANV	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350	878	0	878							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	58.1	877.1							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	58.1	877.1							
80MAU	7664-41-7	NH <sub>3</sub>	550	819	50.2	868.9							
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	535	878	0	878							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	14.6	879.1							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	58.1	877.1							
75AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	13.2	877.7							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	58.1	877.1							
74STA/BEA	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	320	878	0	878							
72HEN/TAA	7664-41-7	NH <sub>3</sub>	350	819	58.6	877.5							
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	13.2	877.7							
72ARN/ION	7664-41-7	NH <sub>3</sub>	350	819	58.6	877.5							
[C <sub>2</sub> H <sub>5</sub> P]	676-59-5	(CH <sub>3</sub> ) <sub>2</sub> PH				877.9			912.0				-5.8
87TAF	7664-41-7	NH <sub>3</sub>	350	819	59.0	878.0							
74STA/BEA	7664-41-7	NH <sub>3</sub>	320	819	54.0	873.0							
[C <sub>3</sub> H <sub>8</sub> O]	1487-15-6	5-Methyl-2,3-dihydrofuran				877.9			910.3				0
86BOU/DJA	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	313	878	-2.1	875.8							
86BOU/DJA	626-55-1	3-Br-pyridine	313	878.2	1.7	879.9							
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> ]	289-80-5	Pyridazine				877.1			907.2				7.8
87TAF	7664-41-7	NH <sub>3</sub>	350	819	58.1	876.4							
86TAF/ANV	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350	878	0	877.4							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	62.2	880.5							
79MAU	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	535	883.9	-3.3	877.5							
[C <sub>4</sub> H <sub>9</sub> NO]	127-19-5	Dimethylacetamide				877.0			908.0				5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	58.6	877.0							
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	58.7	877.1							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	58.6	877.0							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	61.3	879.8							
[C <sub>8</sub> H <sub>9</sub> NO]	99-92-3	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				877.0			908.8				2
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	47.7	877.0							
[C <sub>8</sub> H <sub>7</sub> N]	6921-28-4	(HCCCH <sub>2</sub> ) <sub>2</sub> NH				876.9			910.0				-2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	58.1	876.9							

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	58.1	876.9						
[C <sub>10</sub> H <sub>10</sub> Ru] 81STE/BEA	1287-13-4 7664-41-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> Ru NH <sub>3</sub>	320	819	58.6	876.8 876.8			899.1			34
[C <sub>9</sub> H <sub>10</sub> F <sub>3</sub> N] 87TAF	329-17-9 7664-41-7	4-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	59.0	876.8 876.7			903.2			20
[C <sub>3</sub> H <sub>11</sub> NO <sub>2</sub> ] 93LI/HAR	72-18-4	L-valine kinetic method				876.7			910.6			-5
92GOR/SPE	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878			907.2			
90ISA/OMO		kinetic method-relative order										
87BOJ		kinetic method-relative order										
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	62.2	881.2						
79MAU/HUN	109-73-9	n-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	520	886.6	-8.4	877.6						
79MAU/HUN	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	520	878	-1.7	876.3						
79MAU/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	520	850.6	22.6	874.7						
[C <sub>18</sub> H <sub>12</sub> ] 80MAU	92-24-0 7664-41-7	Tetralene NH <sub>3</sub>	550	819	61.9	876.5 876.4			905.5			11.5
[C <sub>18</sub> H <sub>15</sub> As] 86TRAMUN	603-32-7 109-09-1; 107-10-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> As 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0
[C <sub>18</sub> H <sub>15</sub> AsO] 86TRAMUN	1153-05-5 109-09-1; 107-10-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> AsO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			906.2			9.1
[C <sub>18</sub> H <sub>15</sub> N] 86TRAMUN	603-34-9 109-09-1; 107-10-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> N 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0
[C <sub>18</sub> H <sub>15</sub> PS] 86TRAMUN	3878-45-3 109-09-1; 107-10-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PS 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			906.2			9.1
[C <sub>18</sub> H <sub>15</sub> OP] 86TRAMUN	791-28-6 109-09-1; 107-10-8	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> PO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			906.2			9.1
[C <sub>13</sub> H <sub>15</sub> OP] 86TRAMUN	2129-89-7 109-09-1; 107-10-8	CH <sub>3</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>4</sub> H <sub>11</sub> OP] 86TRA/MUN	10311-08-7 109-09-1; 107-10-8	(CH <sub>3</sub> ) <sub>2</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0
[C <sub>16</sub> H <sub>19</sub> OP] 86TRA/MUN	56598-35-7 109-09-1; 107-10-8	t-C <sub>4</sub> H <sub>9</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0
[C <sub>15</sub> H <sub>17</sub> OP] 86TRA/MUN	2959-75-3 109-09-1; 107-10-8	i-C <sub>3</sub> H <sub>7</sub> (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> PO 2-Cl-pyridine; n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>				876.4 869-884			908.9			0
[C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> NO] 94GRU/CAL	90238-10-1 109-04-6; 100-46-9	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub> 2-Br-pyridine; C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub>				876.2 873-879			907.1			5
[C <sub>8</sub> H <sub>6</sub> CIN] 91AUE/WEB 79AUE/BOW	18368-63-3 110-86-1 124-40-3	2-Cl-6-(CH <sub>3</sub> )-pyridine pyridine (CH <sub>3</sub> ) <sub>2</sub> NH	300 298	898.1 896.5	-22.0 -6.3	876.2 876.2 890.1			908.0			2
[C <sub>8</sub> H <sub>12</sub> ] 87TAF 79AUE/BOW 77WOL/ABB	822-93-5 7664-41-7 74-89-5 87-85-4	(c-C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> C=CH <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub> (CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350 298 350	819 864.5 836.0		875.8 875.7 883.0 876.5	57.7 18.6 39.8		904.7			12
[C <sub>3</sub> H <sub>7</sub> N] 87TAF 83TAF2 80AUE/WEB 76AUE/WEB 75ARN	107-11-9 7664-41-7 7664-41-7 151-564 74-89-5 7664-41-7	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub> Azuridine CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub>	350 350 298 298 350	819 819 872.5 864.5 819	56.7 56.3 2.7 11.7 54.9	875.5 875.7 875.2 875.2 876.2 873.9			909.5			-5.1
[C <sub>3</sub> H <sub>5</sub> NS] 94DEC/EXN 94DEC/EXN 94DEC/EXN 94DEC/EXN 93ABB/MO 93ABB/MO	758-16-7 75-04-7 288-47-1 74-89-5 765-30-0 107-11-9 289-80-5	(CH <sub>3</sub> ) <sub>2</sub> NC(=S)H C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> thiazole CH <sub>3</sub> NH <sub>2</sub> c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub> Pyridazine	338 338 338 338 333 333	878 872.1 864.5 869.9 875.5 877.1	-2.8 4.9 11.4 5.4 0.1 -1.6	875.5 874.8 876.9 875.4 874.8 875.3 875.6			906.4			5
[C <sub>10</sub> H <sub>9</sub> N] 78LAU/SAL	134-32-7 7664-41-7	1-Naphthalenamine NH <sub>3</sub>	600	819	58.6	875.1 875.1			907.0			2
[C <sub>4</sub> H <sub>7</sub> NO <sub>4</sub> ] 92GOR/SPE	56-84-8 74-89-5; 372-47-4	L-aspartic acid CH <sub>3</sub> NH <sub>2</sub> ; 3-F-pyridine	350			875 864-870			908.9			-5



TABLE 2. Summary of proton transfer thermochemical data for each base  $M_i$ , sorted by gas basicity of  $M_i$ —Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
90ISA/OMO		kinetic method										
87TAF	7664-41-7	NH <sub>3</sub>	350	819	60.9	879.8						
87BOJ		kinetic method										
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	60.9	879.8						
[C <sub>3</sub> H <sub>10</sub> S]	38381-24-7	( <i>c</i> -C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CS				874.5			904.3			9
93ABB/MO	107-11-9	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	333	875.5	-0.6	874.4						
93ABB/MO	1453-58-3	3(5)-methylpyrazole	333	874.2	0.0	874.0						
93ABB/MO	7554-65-6	4-methylpyrazole	333	873.4	1.6	874.6						
[C <sub>8</sub> H <sub>10</sub> F <sub>3</sub> NS]	#678	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> SF <sub>5</sub>				874.5			901.0			20
87TAF	7664-41-7	NH <sub>3</sub>	350	819	56.7	874.4						
[C <sub>10</sub> H <sub>16</sub> ]	16609-28-2	1,5,5-Trimethyl-3-methylenecyclohexene				874.2			904.9			6
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	9.8	874.2						
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	1453-58-3	3(5)-methylpyrazole				874.2			906.0			2
92ABB/CAB	289-80-5	Pyridazine	333	877.1	-3.0	874.3						
92ABB/CAB	765-30-0	<i>c</i> -C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	333	869.9	3.3	872.9						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	56.7	875.3						
[C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> ]	686-43-1	val-gly				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>4</sub> ]	13588-94-8	val-ser				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub> ]	1963-21-9	gly-val				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	3303-45-5	ala-val				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	13433-04-0	asp-val				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub> ]	20556-16-5	val-asp				874.1			NE			NE
93GOR/AMS	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350			870-878						
[C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> ]	106-50-3	1,4-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>				874.0			905.9			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	23.4	874.0							
[C <sub>3</sub> H <sub>6</sub> N <sub>3</sub> ]	28466-26-4	4-NH <sub>2</sub> -pyrazole				874.0			907.6				
94NOT/HER	289-80-5	Pyridazine	333	877.1	-2.6	874.9							
94NOT/HER	107-11-9	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	333	875.5	-1.7	873.8							
94NOT/HER	7554-65-6	4-methylpyrazole	333	873.4	-0.4	873.1							
[C <sub>12</sub> H <sub>18</sub> OSi]	107099-29-6	4-CH <sub>3</sub> -O-C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>				874.0			902.9				12
92MIS/AR12	109-09-1	2-Cl-pyridine	308	869	4.6	873.5							
92MIS/AR12	127-19-5	Dimethylacetamide	308	877.0	-2.5	874.5							
[C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> ]	91-19-0	Quinoxaline				873.7			903.8				8
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	535	878	-1.3	873.7							
[C <sub>10</sub> H <sub>10</sub> F <sub>3</sub> NO]	25771-21-5	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				873.5			904.5				5
94GRU/CAL	109-04-6; 106-50-3	2-Br-pyridine; 1,4-(NH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				873.5 873-874							
[C <sub>8</sub> H <sub>8</sub> ]	502-86-3	1,4-C <sub>6</sub> H <sub>4</sub> (=CH <sub>2</sub> ) <sub>2</sub>	350			873.5			900.6				18
81POL/RAI	109-09-1; 75-04-7	2-Cl-pyridine; C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>				869-878							
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O]	96-31-1	OC(NHCH <sub>3</sub> ) <sub>2</sub>				873.5			903.3				9
93ABB/MO	107-11-9	H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	333	875.5	-1.3	873.7							
93ABB/MO	765-30-0	c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	333	869.9	3.9	873.2							
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> ]	7554-65-6	4-methylpyrazole				873.4			906.8				-3
92ABB/CAB	765-30-0	c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	333	869.9	2.5	872.2							
92ABB/CAB	289-80-5	Pyridazine	333	877.1	-3.6	873.9							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	55.4	874.2							
[C <sub>3</sub> H <sub>9</sub> NO]	2680-03-7	2-propenamide, N,N-dimethyl				873.4			904.3				5
90WOL/GRU	100-46-9	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> NH <sub>2</sub>	320	879.4	-5.8	873.4							
[C <sub>7</sub> H <sub>9</sub> NO]	90-04-0	2-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				873.3			905.2				2
78LAU/SAL	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	600	864.5	7.1	868.9							
73YAM/KEB	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	27.2	877.8							
[C <sub>3</sub> H <sub>4</sub> BrN]	109-04-6	2-Br-pyridine				873.0			904.8				2
91AUE/WEB	110-86-1	pyridine	300	898.1	-23.4	874.7							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	52.6	871.2							
79AUE/BET	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	10.3	874.8							
76AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	10.3	874.7							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	49.4	868.0							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	49.4	868.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>i</sub>, sorted by gas basicity of M<sub>i</sub>—Continued

[Formula] YrsQuib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (M)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>4</sub> H <sub>5</sub> NO] 91AUE/WEB 79AUE/BOW	872-85-5 110-86-1 74-89-5	4-Pyridinecarboxaldehyde pyridine CH <sub>3</sub> NH <sub>2</sub>	300 298	898.1 864.5	-25.4 8.3	872.8 872.8 872.8			904.6			2
[C <sub>2</sub> H <sub>5</sub> N] 83TAF2 80AUE/WEB 80AUE/WEB 80AUE/WEB 80AUE/WEB 80AUE/WEB 76AUE/WEB 75TAF 75AUE/WEB2 75ARN	151-56-4 7664-41-7 75-04-7 765-30-0 626-60-8 372-47-4 74-89-5 7664-41-7 74-89-5 7664-41-7	Aziridine NH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> 3-Cl-pyridine 3-F-pyridine CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub>	350 298 298 298 298 298 350 298 350	819 878 869.9 871.5 870.1 864.5 819 864.5 819	53.1 -5.6 -4.4 -1.0 2.4 9.3 54.5 8.3 54.5	872.5 871.9 872.4 865.5 870.6 872.6 873.8 873.2 872.8 873.2			905.5			-2
[C <sub>8</sub> H <sub>10</sub> F <sub>3</sub> N] 87TAF	#696 7664-41-7	4-SF <sub>2</sub> C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	54.5	872.2 872.1			898.7			20
[C <sub>3</sub> H <sub>3</sub> NS] 94DEC/EXN 91MAU/SIE 91MAU/SIE 87TAF 86MAU/LIE	288-47-1 765-30-0 74-89-5 372-48-5 7664-41-7 110-86-1	thiazole c-C <sub>3</sub> H <sub>3</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub> 2-F-pyridine NH <sub>3</sub> pyridine	338 600 600 350 600	869.9 864.5 852.7 819 898.1	0 47.1 -31.7	872.1 869.5 865.7 866.5	899.0 884.6	6.3 18.8	905.3 903.4			2
[C <sub>3</sub> H <sub>8</sub> F <sub>3</sub> N] 87TAF 83TAF 79AUE/BOW	819-06-7 7664-41-7 7664-41-7 74-89-5	CF <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub>	350 350 298	819 819 864.5	53.5 54.0 6.8	871.9 871.9 872.4 871.3			902.7			5.6
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> ] 94NOT/HER 94NOT/HER	10199-68-5 765-30-0 107-11-9	4-(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> -pyrazole c-C <sub>3</sub> H <sub>3</sub> NH <sub>2</sub> H <sub>2</sub> C=CHCH <sub>2</sub> NH <sub>2</sub>	333 333	869.9 875.5	1.5 -3.1	871.8 871.3 872.4			906.0			-5.8
[C <sub>8</sub> H <sub>8</sub> ] 81POL/RAI	32796-95-5 626-60-8; 819-06-7	1,2-C <sub>6</sub> H <sub>4</sub> (=CH <sub>2</sub> ) <sub>2</sub> 3-Cl-pyridine; CF <sub>3</sub> CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>	350			871.7 872-872			898.8			18
[C <sub>3</sub> H <sub>4</sub> CIN] 91AUE/WEB 87TAF 86TAF/ANV 83LOC/MCI 80MAU 76AUE/WEB2	626-60-8 110-86-1 7664-41-7 626-60-8 7664-41-7 7664-41-7 74-89-5	3-Cl-pyridine pyridine NH <sub>3</sub> 3-Cl-pyridine NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub>	300 350 350 350 550 298	898.1 819 871.5 819 819 864.5	-22.9 52.6 0 52.6 48.1 10.7	871.5 875.2 871.2 871.5 871.2 865.0 875.2			903.4			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
75TAF	7664-41-7	NH <sub>3</sub>	350	819	52.6	871.2						
[C <sub>16</sub> H <sub>16</sub> ]	2919-20-2	(4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> ) <sub>2</sub> C=CH <sub>2</sub>				871.4			900.2			12
87TAF	7664-41-7	NH <sub>3</sub>	350	819	53.1	871.2						
77WOL/ABB	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub>	350	836.0	34.8	871.5						
[C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> ]	4901-75-1	c-C(CH <sub>3</sub> )(C <sub>2</sub> H <sub>5</sub> )NHNH				871.3			903.8			0
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	6.8	871.3						
[C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ]	111-96-6	CH <sub>3</sub> (OCH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> OCH <sub>3</sub>				870.9			918.8			-52
84SHA/BLA	372-48-5	2-F-pyridine	500	852.7	6.3	869.8	884.6	33.1	917.6	2	-54	-52
83MAU	289-80-5	Pyridazine	600	877.1	-23.5	871.5	907.2	5.9	913.1	7.8	-49	-41.2
83MAU	372-47-4	3-F-pyridine	600	870.1	-15.6	870.8	902.0	23.8	925.8	2	-66	-64
83MAU	372-48-5	2-F-pyridine	600	852.7	2.4	871.3	884.6	35.6	920.1	2	-55	-53
[C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ]	4027-57-0	3(5)-methyl-5(3)-ethoxycarbonylpyrazole				870.8			902.6			2
92ABB/CAB	1453-58-3	3(5)-methylpyrazole	333	874.2	-4.0	870.2						
92ABB/CAB	7554-65-6	4-methylpyrazole	333	873.4	-2.2	871.1						
92ABB/CAB	107-10-8	n-C <sub>3</sub> H <sub>7</sub> NH <sub>2</sub>	333	883.9	-13.0	870.7						
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ]	90843-31-5	1-(2,3-dihydro-5-benzofuranyl)-ethanone				870.7			902.6			2
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	41.4	870.7						
[C <sub>7</sub> H <sub>9</sub> NS]	1783-81-9	3-CH <sub>3</sub> SC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				870.3			902.1			2
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	19.7	870.3						
[C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ]	100-23-2	N,N-Dimethyl-4-nitroaniline				870.2			896.7			20
87TAF	7664-41-7	NH <sub>3</sub>	350	819	51.3	868.9						
84ROL/HOU	626-60-8	3-Cl-pyridine	320	871.5	-1.3	869.9						
84ROL/HOU	109-04-6	2-Br-pyridine	320	873.0	-0.8	871.8						
[C <sub>2</sub> H <sub>4</sub> FN]	372-47-4	3-F-pyridine				870.1			902.0			2
91MAU/SIE	116-11-0	CH <sub>2</sub> =C(CH <sub>3</sub> )OCH <sub>3</sub>	600	866.1		866.1	894.9	8.4	903.3	12	-10.5	1.5
91MAU/SIE	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	600	864.5	12.1	873.9	899.0	4.6	903.6	-7	12.6	5.6
91MAU/SIE	288-47-1	thiazole	600	872.1		870.8	904	1.7	905.7			
91AUE/WEB	110-86-1	pyridine	300	898.1	-27.3	870.8						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	49.0	867.5						
86MAU/LJE	110-86-1	pyridine	600	898.1	-27.7	870.4						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	48.5	867.1						
76AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	6.3	870.8						
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ]	7291-02-3	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				869.9			900.9			5
94GRU/CAL	95-55-6; 109-04-6	2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH, 2-Br-pyridine				867-873						
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> O <sub>3</sub> ]	7291-01-2	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				869.9			900.9			5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(R)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (R)
94GRU/CAL	95-55-6; 109-04-6	2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH; 2-Br-pyridine				867-873						
[C <sub>8</sub> H <sub>9</sub> NO] 94GRU/CAL	619-55-6 95-55-6; 109-04-6	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH; 2-Br-pyridine				869.9 867-873			900.9			5
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ] 94GRU/CAL	5813-86-5 95-55-6; 109-04-6	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH; 2-Br-pyridine				869.9 867-873			900.9			5
[C <sub>8</sub> H <sub>9</sub> NO] 94GRU/CAL	618-47-3 95-55-6; 109-04-6	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH; 2-Br-pyridine				869.9 867-873			900.9			5
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O] 94GRU/CAL	3544-24-9 95-55-6; 109-04-6	3-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 2-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> OH; 2-Br-pyridine				869.9 867-873			900.9			5
[C <sub>3</sub> H <sub>7</sub> N] 94DEC/EXN 87TAF 79AUE/BOW	765-30-0 74-89-5 7664-41-7 74-89-5	c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub>	338 350 298	864.5 819 864.5	5.8 51.3 4.4	869.9 870.3 870.3 868.9			904.7			-7.9
[C <sub>7</sub> H <sub>11</sub> N] 94BOH/DEC 94BOH/DEC	87-62-7 765-30-0 95-53-4	2,6-dimethylamine c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub> 2-methylamine	338 338	869.9 859.1	1.1 10	869.8 870.6 869.1			901.7			2
[C <sub>5</sub> H <sub>4</sub> CINO] 92MIS/TER	1851-22-5 694-59-7	3-chloro-pyridine-1-oxide pyridine-1-oxide	343	892.9	-23.4	869.7 869.7			902.2			0
[C <sub>4</sub> H <sub>8</sub> F <sub>3</sub> N] 87TAF 83TAF2 79AUE/BOW 75TAF 75ARN	819-46-6 7664-41-7 7664-41-7 74-89-5 7664-41-7 7664-41-7	CF <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350 298 350 350	819 819 864.5 819 819	49.9 49.9 5.9 49.0 49.0	869.6 868.8 868.8 870.3 867.9 867.9			903.5			-5
[C <sub>8</sub> H <sub>9</sub> NO <sub>2</sub> ] 94GRU/CAL	3424-93-9 95-54-5; 109-04-6	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 1,2-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub> ; 2-Br-pyridine				869.4 866-873			900.3			5
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> S] 93LI/HAR 92GOR/SPE	52-90-4 109-97-7; 372-48-5	L-Cysteine knetic method pyrrole, 2-F-pyridine	350			869.3 844-853			903.2 898			-5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta GB(M,R,T)$	GB(M)	PA(R)	$\Delta PA(M,R)$	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
90ISA/OMO		kinetic method-relative order											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	49.9	868.8							
87BOJ		kinetic method-relative order											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	49.9	868.8							
[C <sub>13</sub> H <sub>18</sub> O]	22666-53-1	$\alpha$ -t-butylstyrene, 4-methoxy				869.1			897.9			12	
92NAK/NOM	127-19-5	Dimethylacetamide	343	877.0	-5.9	870.9							
92NAK/NOM	109-09-1	2-Cl-pyridine	343	869	0	868.6							
92NAK/NOM	626-60-8	3-Cl-pyridine	343	871.5	-3.3	867.8							
[C <sub>10</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> S]	28809-04-3	S-(2-(4-pyridyl)ethyl)cysteine							NE			NE	
93BUR/GAS	52-90-4	L-Cysteine		869.3		>869			NE			NE	
						See Refs.							
[C <sub>3</sub> H <sub>4</sub> CIN]	109-09-1	2-Cl-pyridine				869			900.9			2	
91AUE/WEB	110-86-1	pyridine	300	898.1	-27.3	870.8							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	50.3	868.9							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	50.3	868.9							
80MAU	7664-41-7	NH <sub>3</sub>	350	819	50.3	868.9							
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	550	819	46.0	862.9							
76AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	546	878	-4.2	872.1							
75TAF	7664-41-7	NH <sub>3</sub>	298	864.5	6.3	870.8							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	49.4	868.0							
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	118-92-3	2-NH <sub>2</sub> -benzoic acid				869.0			901.5			0	
95TAN/ISB	108-44-1; 106-50-3	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; 1,4-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub>				864-874							
[C <sub>4</sub> H <sub>9</sub> NOS]	16703-45-0	CH <sub>3</sub> OC(S)N(CH <sub>3</sub> ) <sub>2</sub>				869.0			900.0			5	
93ABB/MO	765-30-0	c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	333	869.9	-1.0	868.4							
93ABB/MO	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	864.0	5.4	869.6							
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	271-44-3	1H-Indazole				868.9			900.8			2	
88CAT/CLA	3796-24-5	4-(CF <sub>3</sub> )-pyridine	~300	862.0	7.5	869.6							
88CAT/CLA	109-09-1	2-Cl-pyridine	~300	869	-0.8	868.2							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	50.3	868.9							
84FLA/MAQ		kinetic method											
[C <sub>7</sub> H <sub>9</sub> NO]	104-94-9	4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				868.5			900.3			2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	49.9	868.5							
81TAA/SUM	7664-41-7	NH <sub>3</sub>	320	819	45.6	864.4							
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	3.9	868.4							
77SUM/POL	7664-41-7	NH <sub>3</sub>	350	819	49.9	868.5							
[C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> ]	38803-30-4	3-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> CN				868.1			894.6			20	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	50.3	868.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>2</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> ] 92ABB/CAB	5932-30-9 765-30-0	3(5)-phenyl-5(3)-ethoxycarbonylpyrazole c-C <sub>3</sub> H <sub>2</sub> NH <sub>2</sub>	333	869.9	-1.4	867.8			899.7			2	
92ABB/CAB	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	864.0	2.9	867.2							
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ] 93LU/HAR	56-41-7	L-alanine kinetic method				867.7			901.6			-5	
92GOR/SPE	372-47-4; 75-04-7	3-F-pyridine; C <sub>2</sub> H <sub>3</sub> NH <sub>2</sub>	350			870-878			897				
90ISA/OMO	7664-41-7	kinetic method-relative order NH <sub>3</sub>	350	819	50.3	869.3							
87TAF													
87BOJ	7654-41-7	kinetic method-relative order NH <sub>3</sub>	350	819	50.3	869.3							
83LOC/MCI	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	500	850.6	25.9	877.9							
79MAU/HUN	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	520	864.5	0.4	864.5	882.5	17.6	900.0	2	9.2	11.2	
79MAU/HUN													
[C <sub>2</sub> H <sub>4</sub> FNO] 92MIS/TER	695-37-4 694-56-7	3-fluoro-pyridine-1-oxide pyridine-1-oxide	343	892.9	-25.5	867.6			900.1			0	
[C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> ] 87TAF	619-31-8 7664-41-7	3-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> N(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	49.9	867.6			894.1			20	
[C <sub>3</sub> H <sub>8</sub> Sn] 82PIE/HEH	82065-00-7 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> Sn=CH <sub>2</sub> NH <sub>3</sub>	350	819	49.4	867.1			893.6			20	
[C <sub>4</sub> H <sub>9</sub> NO] 92DEC/EXN	625-50-3 765-30-0	Acetamide, N-ethyl- c-C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	338	869.9	-2.6	867.0			898.0			5	
92DEC/EXN	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	338	864.5	3.2	867.3							
[C <sub>6</sub> H <sub>7</sub> NO] 81LAU/NIS	95-55-6 62-53-3	2-(OH)C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	16.3	866.9			898.9			2	
[C <sub>6</sub> H <sub>7</sub> NO] 81LAU/NIS	591-27-6 62-53-3	3-(OH)C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	16.3	866.9			898.8			2	
[C <sub>8</sub> H <sub>9</sub> O <sub>3</sub> P] 80HOD/HOU	281-33-4 107-47-1	2,8,9-Trioxa-1-phosphadamtane (t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	320	864.0	0.4	866.8			899.3			0	
80HOD/HOU	109-09-1	2-Cl-pyridine	320	869	-0.4	868.6							
[C <sub>2</sub> H <sub>5</sub> N] 81ELL/DIX	593-67-9 108-44-1; 109-09-1	CH <sub>2</sub> =CHNH <sub>2</sub> 3-CH <sub>3</sub> -aniline; 2-Cl-pyridine				866.5			898.9			0	
[CH <sub>6</sub> N <sub>2</sub> ] 80AUE/WEB	60-34-4 151-56-4	CH <sub>3</sub> NHNH <sub>2</sub> Aziridine	298	872.5	-7.2	866.4			898.8			0	
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	2.9	867.4							

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>8</sub> H <sub>11</sub> N] 81LAU/NIS	587-02-0 62-53-3	3-C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	15.5	866.1 866.1			897.9				2
[C <sub>4</sub> H <sub>6</sub> O] 91MAU/SIE	116-11-0 372-48-5	CH <sub>2</sub> =C(CH <sub>3</sub> )OCH <sub>3</sub> 2-F-pyridine	600	852.7	16.3	866.1	884.6	10.0	894.9	2	11.3	12	13.3
91MAU/SIE	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	600	864.5		866.0	899.0	-6.7	892.3	-7	23.8	16.8	16.8
91MAU/SIE	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	600	878		865.5	912.0	-23.0	889.0	-5.1	31.0	25.9	25.9
88MAQ/JOR	372-47-4	3-F-pyridine	~300	870.1	-4.6								
[C <sub>13</sub> H <sub>18</sub> S] 92NAK/NOM	146558-39-6 512-56-1	$\alpha$ -t-butylstyrene, 4-CH <sub>3</sub> S OP(OCH <sub>3</sub> ) <sub>3</sub>	343	860.8	5.4	866.0			894.8			12	12
92NAK/NOM	106-49-0	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	343	864.8	2.9	866.1			894.6			13.3	13.3
92NAK/NOM	109-09-1	2-Cl-pyridine	343	869	-4.2	867.3			892.3			16.8	16.8
[C <sub>6</sub> H <sub>10</sub> ] 79AUE/BOW	3664-56-0 74-89-5	1,3,3-Trimethylcyclopropene CH <sub>3</sub> NH <sub>2</sub>	298	864.5	1.5	865.9 865.9			895.4			10	10
[C <sub>15</sub> H <sub>12</sub> ] 80MAU	779-02-2 109-09-1	9-Methylanthracene 2-Cl-pyridine	588	869	-3.8	865.8			896.5			5.8	5.8
80MAU	626-60-8	3-Cl-pyridine	608	871.5	-2.9	864.1			896.5			5.8	5.8
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> ] 81LAU/NIS	95-54-5 62-53-3	1,2-C <sub>6</sub> H <sub>4</sub> (NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	16.3	865.8			896.5			5	5
[C <sub>3</sub> H <sub>11</sub> NO <sub>2</sub> ] 83TAF2	687-48-9 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> NCOOC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	47.1	865.6 865.6			896.6			20	20
[C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> ] 84ROL/HOU	100-15-2 372-47-4	N-Methyl-4-nitroaniline 3-F-pyridine	320	870.1	-4.6	865.1			891.6			0	0
[C <sub>3</sub> H <sub>9</sub> As] 75HOD/BEA	593-88-4 74-89-5	(CH <sub>3</sub> ) <sub>3</sub> As CH <sub>3</sub> NH <sub>2</sub>	320	864.5	0.4	864.9 864.8			897.3			2	2
[C <sub>7</sub> H <sub>9</sub> N] 87TAF	106-49-0 7664-41-7	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> NH <sub>3</sub>	350	819	46.2	864.8			896.7			0	0
81TAA/SUM	7664-41-7	NH <sub>3</sub>	320	819	42.3	864.8			896.7			2	2
77SUM/POL	7664-41-7	NH <sub>3</sub>	350	819	46.2	861.1			896.7			0	0
75ARN	7664-41-7	NH <sub>3</sub>	350	819	49.0	864.8			896.7			2	2
[C <sub>13</sub> H <sub>25</sub> N] 81ALD/ARR	75197-24-9 7664-41-7	out-6H-1-Azabicyclo[4,4,4]tetradecane NH <sub>3</sub>	320	819	45.6	864.5 864.5			897.0			0	0
[CH <sub>5</sub> N] 97EAS/SMI	74-89-5	CH <sub>3</sub> NH <sub>2</sub> theory	298			864.5			899.0			-7	-7
93SZU/MCM	124-40-3	(CH <sub>3</sub> ) <sub>2</sub> NH theory	600	896.5	-33.5	864.5	929.5	-29.7	899.8	-2	-5.9	-6.6	-6.6
93SMI/RAD			0			864.5			895			-7.9	-7.9



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
93SM/RAD		theory	298						901				
93SM/RAD		theory	600						906				
91MAU/SIE	372-48-5	2-F-pyridine	600	852.7	6.7	862.1	884.6	16.3	900.9	2	-16.3		-14.3
87TAF	7664-41-7	NH <sub>3</sub>	350	819	44.8	863.9							
87BIS/RUH		Appearance							930±15				
83TAF	7664-41-7	NH <sub>3</sub>	350	819	44.8	863.9							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	44.8	863.9							
79LOC/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	382	850.6	11.1	862.4							
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	41.8	861.0							
76AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	0	864.5							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	44.8	863.9							
75HOD/BEA	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	320	864.5	0	864.5							
75AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	0	864.5							
72HEN/TAA	7664-41-7	NH <sub>3</sub>	350	819	46.2	865.3							
72BRJ/YAM	7664-41-7	NH <sub>3</sub>	600	819	45.2	864.4							
72AUE/WEB	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	0	864.5							
72ARN/JON	7664-41-7	NH <sub>3</sub>	350	819	46.2	865.3							
[C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> ]	35520-41-3	trans-dimethylamino acrylonitrile				864.3			896.8				0
93BER/HEL	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	~338	864.0	0	864.4							
93BER/HEL	78-59-1	isophorone	~338	861.6	2.5	864.2							
[C <sub>3</sub> H <sub>8</sub> S]	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S				864.0			893.8				9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	45.8	864.0							
86TAF/ANV	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	350	864.0	0	864.0							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	45.3	863.5							
[C <sub>7</sub> H <sub>7</sub> O]	88170-17-6	4-OH-benzyl				864			896.5				0
94HOK/YAN		kinetic method				864							
[C <sub>7</sub> H <sub>9</sub> N]	108-44-1	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				864.0			896.8				2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	45.8	864.3							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	45.8	864.3							
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	12.6	863.1							
77SUM/POL	7664-41-7	NH <sub>3</sub>	350	819	46.2	864.8							
77POL/DEV	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	350	850.6	13.7	864.3							
77COO/KRU		relative order- See Refs.											
75TAF	7664-41-7	NH <sub>3</sub>	350	819	46.2	864.8							
[C <sub>12</sub> H <sub>20</sub> O]	4789-40-6	2,5-di-t-butylfuran				863.9			894.7				5.8
85HOU/ROL	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	313	864.5	-0.4	863.9							
[CH <sub>4</sub> N <sub>2</sub> S]	62-56-6	SC(NH <sub>2</sub> ) <sub>2</sub>				863.9			893.7				9
93ABB/MO	765-30-0	c-C <sub>4</sub> H <sub>9</sub> NH <sub>2</sub>	333	869.9	-4.8	864.5							
93ABB/MO	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	864.0	-1.1	862.9							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^{\ddagger}(R)$	$\Delta\Delta S_p^{\ddagger}(M,R)$	$\Delta S_p^{\ddagger}(M)$	$\Delta S_p^{\ddagger}(R)$	$\Delta\Delta S_p^{\ddagger}(M,R)$
[C <sub>3</sub> H <sub>10</sub> O <sub>2</sub> ] 87TAF 86MIS/FUJ	100-06-1	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				863.7			895.6					2
	7664-41-7	NH <sub>3</sub>	350	819	45.3	863.9								
	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	33.9	863.2								
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ] 87TAF	3034-42-2	1-Methyl-5-nitroimidazole	350	819	44.8	863.5			895.3					2
	7664-41-7	NH <sub>3</sub>				863.4								
[C <sub>3</sub> H <sub>7</sub> O <sub>3</sub> P] 80HOD/HOU 80HOD/HOU	3741-36-4	2-Methoxy-1,3,2-dioxaphospholane				862.7			896.1					0
	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	320	864.0	0.4	864.6								
	109-09-1	2-Cl-pyridine	320	869	-8.4	860.7								
[C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> ] 87TAF	1197-19-9	1,4-(CH <sub>3</sub> ) <sub>2</sub> NC <sub>6</sub> H <sub>4</sub> CN	350	819	44.8	862.6			889.1					20
	7664-41-7	NH <sub>3</sub>				862.5								
[C <sub>21</sub> H <sub>30</sub> O] 93ABB/MO 93ABB/MO	38256-01-8	(1-adamantyl) <sub>2</sub> CO				862.4			894.3					2
	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	864.0	-2.1	862.2								
	372-48-5	2-F-pyridine	333	852.7	10.0	862.7								
[C <sub>2</sub> H <sub>7</sub> O <sub>3</sub> P] 82PIE/HEH2	868-85-9	(CH <sub>3</sub> O) <sub>2</sub> PHO				862.4			894.8					0
	512-56-1; 108-44-1	(CH <sub>3</sub> O) <sub>3</sub> PO; 3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				861-864								
	3710-43-8	2,4-dimethylfuran	313	864.5	-2.1	862.3			894.7					0
85HOU/ROL	74-89-5	CH <sub>3</sub> NH <sub>2</sub>												
[C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> N] 91AUE/WEB 87TAF 86TAF/ANV 83TAF 76AUE/WEB2 75TAF 75ARN 72TAA/HEN	3796-24-5	4-(CF <sub>3</sub> )-pyridine				862.0			893.9					2
	110-86-1	pyridine	300	898.1	-35.6	862.5								
	7664-41-7	NH <sub>3</sub>	350	819	43.0	861.6								
	3796-24-5	4-(CF <sub>3</sub> )-pyridine	350	862.0	0	862.0								
	7664-41-7	NH <sub>3</sub>	350	819	43.0	861.6								
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-2.4	862.0								
	7664-41-7	NH <sub>3</sub>	350	819	42.6	861.1								
7664-41-7	NH <sub>3</sub>	350	819	42.6	861.1									
110-86-1	pyridine	320	898.1	-49.0	849.2									
[C <sub>14</sub> H <sub>23</sub> N] 86SUN/KUL	16245-79-7	4-(n-C <sub>8</sub> H <sub>17</sub> )C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				862			894.5					0
		See Refs.	300			862			895.4					
[C <sub>3</sub> H <sub>14</sub> O] 87TAF	78-59-1	Isophorone				861.6			893.5					2
	7664-41-7	NH <sub>3</sub>	350	819	43.0	861.6								
[C <sub>7</sub> H <sub>7</sub> NO] 94GRU/CAL	55-21-0	C <sub>6</sub> H <sub>5</sub> CONH <sub>2</sub>				861.2			892.1					5
	68-12-2; 95-54-5	HCON(CH <sub>3</sub> ) <sub>2</sub> ; 1,2-(NH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub>				857-866								
[C <sub>2</sub> H <sub>9</sub> NO <sub>3</sub> ] 1117-77-7	CH <sub>3</sub> CONHCH <sub>2</sub> COOCH <sub>3</sub>					861			892.0					5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
83MAU		See Refs.				861							
[C <sub>3</sub> H <sub>5</sub> O <sub>4</sub> P]	512-56-1	OP(OCH <sub>3</sub> ) <sub>3</sub>				860.8			890.6			9.1	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	42.6	860.8							
86TAF/ANV	512-56-1	OP(OCH <sub>3</sub> ) <sub>3</sub>	350	860.8	0	860.8							
82PIE/HEH						845.2							
80HOD/MCD	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	300	850.6	5.9	856.5							
[C <sub>4</sub> H <sub>4</sub> F <sub>3</sub> N]	3796-23-4	3-(CF <sub>3</sub> )-pyridine				860.7			892.5			2	
91AUE/WEB	110-86-1	pyridine	300	898.1	-37.1	861.0							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	41.6	860.2							
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-3.4	861.1							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	42.1	860.7							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	42.1	860.7							
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ]	288-13-1	Pyrazole				860.5			894.1			-3.8	
88CAT/CLA	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	300	864.0	-4.2	859.8							
88CAT/CLA	78-59-1	Isophorone	300	861.6	-0.8	860.8							
88CAT/CLA	3796-24-5	4-(CF <sub>3</sub> )-pyridine	300	862.0	-0.8	861.2							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	41.6	860.5							
86TAF/ANV	3796-24-5	4-(CF <sub>3</sub> )-pyridine	350	862.0	-0.8	861.5							
86TAF/ANV	107-47-1	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	350	864.0	-4.2	860.5							
86TAF/ANV	512-56-1	OP(OCH <sub>3</sub> ) <sub>3</sub>	350	860.8	-2.5	859.0							
86MAU/LIE	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	52.2	859.5							
84FLA/MAQ		kinetic method											
[CTe]	12012-15-6	CTe at C				860.4			892			3	
85JAS/STE		theory							892				
[C <sub>8</sub> H <sub>18</sub> O]	6163-66-2	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O				860.0			887.4			17	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	42.1	859.9							
[C <sub>7</sub> H <sub>5</sub> NO]	273-53-0	benzoxazole				859.8			891.6			2	
88MAQ/JOR	116-11-0	CH <sub>2</sub> =C(CH <sub>3</sub> )OCH <sub>3</sub>	~300	866.1	-6.3	859.8							
[C <sub>4</sub> H <sub>6</sub> S]	7594-44-7	CH <sub>2</sub> =C(CH <sub>3</sub> )-SCH <sub>3</sub>				859.7			888.6			12	
89OSA/DEL	372-48-5	2-F-pyridine	313	852.7	4.2	856.8							
89OSA/DEL	116-11-0	CH <sub>2</sub> =C(CH <sub>3</sub> )OCH <sub>3</sub>	313	866.1	-3.8	862.3							
89OSA/DEL	4789-40-6	2,5-di-t-butylfuran	313	863.9	-4.2	859.7							
[C <sub>20</sub> H <sub>12</sub> ]	198-55-0	Perylene				859.6			888.6			11.5	
80MAU	109-09-1	2-Cl-pyridine	520	869	-5.9	861.1							
80MAU	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	525	850.6	9.6	858.1							
[C <sub>7</sub> H <sub>9</sub> N]	95-53-4	2-methylaniline				859.1			890.9			2	
94BOH/DEC	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	338	853.5	6	859.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^{\ddagger}(R)$	$\Delta \Delta S_p^{\ddagger}(M,R)$	$\Delta S_p^{\ddagger}(M)$
94BOH/DEC	1121-37-5	( <i>c</i> -C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CO	338	850.6	8.1	859.0						
[C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> ]	17081-21-9	CH <sub>3</sub> O(CH <sub>2</sub> ) <sub>3</sub> OCH <sub>3</sub>				858.6			897.2			-20.6
83MAU	372-47-4	3-F-pyridine	600	870.1	-20.9	856.0	902.0	-3.3	898.6	2	-29.3	-27.3
83MAU	372-48-5	2-F-pyridine	600	852.7	1.3	860.8	884.6	15.1	899.6	2	-23	-21
83MAU	544-40-1	( <i>n</i> -C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	600	842.1	8.2	859.1	871.8	21.8	893.6	9	-22.6	-13.6
[C <sub>10</sub> H <sub>9</sub> F <sub>6</sub> N]	34060-81-6	3,5-(CF <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>				858.4			884.9			20
87TAF	7664-41-7	NH <sub>3</sub>	350	819	40.7	858.4						
[C <sub>2</sub> H <sub>6</sub> FN]	406-34-8	CH <sub>2</sub> FCH <sub>2</sub> NH <sub>2</sub>				858.0			892.0			-5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	39.4	858.3						
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-8.3	856.2						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	39.8	858.7						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	39.8	858.7						
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	105-40-8	CH <sub>3</sub> NHCOOC <sub>2</sub> H <sub>5</sub>				857.8			888.8			5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	39.4	857.8						
[C <sub>7</sub> H <sub>12</sub> ]	1000-86-8	(CH <sub>3</sub> ) <sub>2</sub> C=CHC(CH <sub>3</sub> )=CH <sub>2</sub>				857.6			886.5			12
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	38.6	857.6						
[C <sub>3</sub> H <sub>7</sub> NO]	79-16-3	Acetamide, N-methyl				857.6			888.5			5
92DEC/EXN	765-30-0	<i>c</i> -C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>	338	869.9	-9.2	860.2						
92DEC/EXN	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	338	864.5	-2.7	861.4						
92DEC/EXN	372-48-5	2-F-pyridine	338	852.7	5.4	858.0						
92ABB/CAN	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	0.2	853.3						
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	2.3	854.9						
[C <sub>4</sub> H <sub>7</sub> N <sub>2</sub> ]	39687-97-3	N'-cyano-N,N-dimethyl formamidine				857.3			889.7			0
93BER/HEL	16584-00-2	2-methyl-2H-benzotriazole	338	855.9	-2.1	853.6						
93BER/HEL	78-59-1	Isophorone	338	861.6	-3.3	858.4						
93BER/HEL	107-47-1	( <i>t</i> -C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	338	864.0	-4.6	859.8						
[C <sub>5</sub> H <sub>11</sub> NO]	754-10-9	<i>t</i> -C <sub>4</sub> H <sub>9</sub> CONH <sub>2</sub>				857.2			889.0			2
97HOM/HER	687-48-9	(CH <sub>3</sub> ) <sub>2</sub> NCOOC <sub>2</sub> H <sub>5</sub>	333	865.6	3.1	868.8						
97HOM/HER	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	3.3	856.5						
97HOM/HER	107-47-1	( <i>t</i> -C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	864.0	-6.5	857.8						
[C <sub>6</sub> H <sub>12</sub> ]	530-48-3	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> C=CH <sub>2</sub>				856.9			885.7			12
87TAF	7664-41-7	NH <sub>3</sub>	350	819	38.0	856.1						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	38.6	857.6						
77WOL/ABB	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	18.8	855.5						
75WOF/HAR	7664-41-7	NH <sub>3</sub>	350	819	38.9	857.0						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	37.5	855.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[C <sub>6</sub> H <sub>6</sub> ] 79AUE/BOW	15082-13-0 7664-41-7	1-Methyl-3-methylenecyclobutene NH <sub>3</sub>	298	819	37.1	856.9 856.9	891.0		891.0			-5.8	
[C <sub>3</sub> H <sub>7</sub> NO] 92ABB/CAB 87TAF	68-12-2 372-48-5 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> NCHO 2-F-pyridine NH <sub>3</sub>	333 350	852.7 819	2.9 36.6	856.6 855.5 855.0	887.5		887.5			5	
79LOC/HUN 79AUE/BOW 75TAF	62-53-3 79-89-5 7664-41-7	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> CH <sub>3</sub> NH <sub>2</sub> NH <sub>3</sub>	382 298 350	850.6 864.5 819	4.0 -5.4 36.6	854.3 859.1 855.0							
[C <sub>9</sub> H <sub>10</sub> OS] 87TAF 86MIS/FUJ	1778-09-2 7664-41-7 98-86-2	4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	350 343	819 829.3	37.5 27.2	856.3 856.1 856.5	888.2		888.2			2	
[C <sub>4</sub> H <sub>7</sub> NO] 90WOL/GRU 90WOL/GRU	23350-58-5 68-12-2 119-61-9	2-butenamide (CH <sub>3</sub> ) <sub>2</sub> NCHO (C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CO	320 320	856.6 852.5	0.4 2.7	857.0 855.3	887.1		887.1			5	
[C <sub>3</sub> H <sub>6</sub> N] 79AUE/BOW 75AUE/WEB2	19540-05-7 7664-41-7 75-07-0	1-Azabicyclo[1,1,0]butane NH <sub>3</sub> CH <sub>3</sub> CHO	298 298	819 736.5	37.1 100.4	856.1 856.1 836.9	886.9		886.9			5.6	
[C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> ] 89TOM/ABB 89TOM/ABB	16584-00-2 68-12-2 288-13-1	2-methyl-2H-benzotriazole (CH <sub>3</sub> ) <sub>2</sub> NCHO Pyrazole	298 298	856.6 860.5	-0.4 -5.0	855.9 856.1 855.5	890.1		890.1			-5.8	
[C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> ] 86MAU/LIE	288-88-0 60-29-7	1,2,4-Triazole (C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> O	600	801	52.2	855.9 855.9	886.0		886.0			8	
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ] 87TAF 86TAF/ANV 83TAF2 79MAU	289-95-2 7664-41-7 100-48-1 7664-41-7 75-04-7	Pyrimidine NH <sub>3</sub> 4-Pyridinecarbonitrile NH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350 350 350 510	819 848.8 819 878	36.6 5.9 36.6 -17.6	855.7 854.9 854.3 854.9 857.7	885.8		885.8			7.8	
[C <sub>9</sub> H <sub>8</sub> O] 92MIS/ARI 85MAR/MOD	768-60-5 536-74-3 7664-41-7	4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH NH <sub>3</sub>	323 300	801.3 819	54.4 24.7	855.7 855.7 843.7	886.4		886.4			5.8	
[C <sub>6</sub> H <sub>4</sub> F <sub>3</sub> N] 91AUE/WEB 87TAF 75TAF	368-48-9 110-86-1 7664-41-7 7664-41-7	2-(CF <sub>3</sub> )-pyridine pyridine NH <sub>3</sub> NH <sub>3</sub>	300 350 350	898.1 819 819	-43.0 36.6 36.6	855.2 855.2 855.2 855.2	887.1		887.1			2	
[C <sub>15</sub> H <sub>12</sub> ] 80MAU	613-12-7 62-53-3	2-Methylanthracene C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	544	850.6	0.4	855.1 851.5	887.5		887.5			0	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M)		Base(M)		T(K)	GB(R)	ΔGB(M,R,T)	PA(M)		ΔS <sub>p</sub> (M)
	Reg No(R)	Reg No(M)	Base(R)	Base(M)				PA(R)	ΔPA(M,R)	
80MAU	109-09-1		2-Cl-pyridine		544	869	-10.9	858.6		
[C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ]	110-63-4		HO(CH <sub>2</sub> ) <sub>2</sub> OH					854.9		-95
95CHE/STO	98-86-2		C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>		600	829.3	-5.5	852.9	861.1	2
95CHE/STO	534-22-5		2-methylfuran		600	833.5	-5.1	856.9	865.9	0
79AUE/BOW	74-89-5		CH <sub>3</sub> NH <sub>2</sub>		298	864.5	-37.6	826.9		-101.3
[C <sub>2</sub> H <sub>5</sub> N]	#804		•CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>					854.5		0
89HOL/LOS					298			887		887
[C <sub>13</sub> H <sub>17</sub> ClO]	146558-40-9		α-t-butylstyrene, 4-CH <sub>3</sub> O, 3-Cl					854.2		12
92NAK/NOM	62-53-3		C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>		343	850.6	3.3	853.5		
92NAK/NOM	372-48-5		2-F-pyridine		343	852.7	2.5	854.8		
[C <sub>9</sub> H <sub>8</sub> S]	56041-85-1		4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>4</sub> -CCH					854.1		0
92MIS/ARI	536-74-3		C <sub>6</sub> H <sub>5</sub> -CCH		323	801.3	52.7	854.1		886.6
[CH <sub>3</sub> H <sub>9</sub> O <sub>3</sub> PS]	152-18-1		SP(OCH <sub>3</sub> ) <sub>3</sub>					853.9		9.1
80HOD/MCD	123-11-5		4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CHO		300	849.3	4.6	853.9		
[Ti]	7440-32-6		Ti					853.7		34
88ELK/ARM			See Refs.					876±11		
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> ]	926-64-7		NCCH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub>					853.7		5.6
87TAF	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
83TAF2	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
75ARN	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
[C <sub>3</sub> H <sub>6</sub> OS]	67-68-5		(CH <sub>3</sub> ) <sub>2</sub> SO					863.7		5.8
87TAF	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
83TAF	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
79LAU	7664-41-7		NH <sub>3</sub>		650	819	38.5	853.3		
77MCA	67-56-1; 64-17-5		CH <sub>3</sub> OH; C <sub>2</sub> H <sub>5</sub> OH					725-746		
75TAF	7664-41-7		NH <sub>3</sub>		350	819	35.2	853.6		
[C <sub>3</sub> H <sub>5</sub> N]	2450-71-7		HCCCH <sub>2</sub> NH <sub>2</sub>					853.5		-5
92ABB/CAB	372-48-5		2-F-pyridine		333	852.7	2.5	855.5		
87TAF	7664-41-7		NH <sub>3</sub>		350	819	33.9	852.8		
83TAF2	7664-41-7		NH <sub>3</sub>		350	819	33.9	852.8		
79AUE/BOW	74-89-5		CH <sub>3</sub> NH <sub>2</sub>		298	864.5	-12.7	851.8		
[C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> N]	460-39-9		CF <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub>					853.2		-5
87TAF	7664-41-7		NH <sub>3</sub>		350	819	33.9	852.8		
83TAF2	7664-41-7		NH <sub>3</sub>		350	819	33.9	852.8		
79AUE/BOW	74-89-5		CH <sub>3</sub> NH <sub>2</sub>		298	864.5	-11.2	853.3		

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^{\circ}$ (R)	$\Delta \Delta S_p^{\circ}$ (M,R)	$\Delta S_p^{\circ}$ (M)
YrSquib		Base(R)										
75TAF	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.9						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.9						
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	5057-98-7	cis-1,2-cyclopentanediol				853.1	853 6	32	885.6			0
89MEX/BUR	7664-41-7	NH <sub>3</sub>							885.6			
[C <sub>7</sub> H <sub>7</sub> O]	155174-22-4	3-OH-benzyl kinetic method				853			885.5			0
94HOK/YAN						853						
[C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> ]	619-45-4	4-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				853.0			883.9			5
86MIS/FUI2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	33.5	853.0						
[C <sub>10</sub> H <sub>12</sub> ]	1195-32-0	4-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )CH <sub>2</sub>				852.9			881.8			12
89GAL/SPE						849.4						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	34.8	852.9						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	34.8	852.9						
[C <sub>2</sub> H <sub>5</sub> NS]	62-55-5	CH <sub>3</sub> CSNH <sub>2</sub>				852.8			884.6			2
94DEC/EXN	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	338	853.5	-1.8	851.4						
94DEC/EXN	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	338	864.5	-9.3	854.8						
93ABB/MO	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	333	864.5	-10.4	853.8						
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	-1.7	851.0						
[C <sub>5</sub> H <sub>4</sub> FN]	372-48-5	2-F-pyridine				852.7			884.6			2
91MAU/SIE	109-97-7	pyrrole	600	843.8	10.5	854.5	875.4	8.8	884.2	2.8	2.5	5.3
91MAU/SIE	288-42-6	oxazole	600	844.5	9.2	853.7	876.4	8.8	885.2	2	-0.4	1.6
91MAU/SIE	107-25-5	CH <sub>2</sub> =CH-OCH <sub>3</sub>	600	830.3	19.2	852.6	859.2	29.7	888.9	12	-17.2	-5.2
91MAU/SIE	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	4.6	855.2	882.5	2.1	884.5	2	3.8	5.8
91AUE/WEB	110-86-1	pyridine	300	898.1	-46.9	851.3						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	33.9	852.4						
86MAU/LIE	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	44.2	849.7						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	33.9	852.4						
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	33.4	852.0						
79LOC/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	382	850.6	1.5	852.1						
76AUE/WEB2	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-8.3	856.2						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.5						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.5						
[C <sub>2</sub> H <sub>5</sub> N]	20729-41-3	CH <sub>3</sub> CH=NH				852.6			885.1			0
81ELL/DIX	108-42-9;	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; 2-ClC <sub>3</sub> H <sub>4</sub> N				836-869						
109-09-1												
79ELL/EAD	108-42-9;	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; 2-ClC <sub>3</sub> H <sub>4</sub> N				836-869						
109-09-1												
[C <sub>13</sub> H <sub>10</sub> O]	119-61-9	(C <sub>6</sub> H <sub>5</sub> ) <sub>2</sub> CO				852.5			882.3			9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	33.9	852.1						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
85VAN/LEA 83TAF	7664-41-7	See Refs. NH <sub>3</sub>	350	819	34.3	852.6							
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ] 94MCK/BEL	56-40-6 109-97-7; 62-53-3	glycine pyrrole; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>				852.2 844-851			886.5				-6
93ZHA/ZIM	109-97-7; 62-53-3	pyrrole; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	300			844-851							
93WU/LEB	62-53-3; 68- 12-2	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> ; HCON(CH <sub>3</sub> ) <sub>2</sub>	300			851-857							
93LJ/HAR		kinetic method											
92GOR/SPE	98-86-2; 109-97-7	acetophenone; pyrrole	350			829-844			884.6				
90ISA/OMO 87TAF	7664-41-7	kinetic method NH <sub>3</sub>	350	819	37.5	856.5							
87BOJ		kinetic method											
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	37.5	856.5							
79MAU/HUN	100-70-9	2-Pyridinecarboxitrile	570	841	7.9	851.1							
79MAU/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	500	850.6	0	852.2	882.5	0	882.5	2	0	2	2
79LOC/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	382	850.6	5.0	856.3							
[C <sub>7</sub> H <sub>5</sub> N] 90PEE/TNG	1761-67-7 62-53-3; 67- 68-5	CH <sub>2</sub> =NCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>2</sub> SO				852.1 851-854			884.6				0
[C <sub>10</sub> H <sub>16</sub> S] 93ABB/MO	7519-74-6	thiocamphor (CH <sub>3</sub> ) <sub>2</sub> NCOOCH <sub>3</sub>	333	847.3	2.5	852.0			883.9				2
93ABB/MO	7541-16-4	2-F-pyridine	333	852.7	-3.5	849.2							
93ABB/MO	290-37-9	Pyrazine	333	847.0	4.3	851.5							
93ABB/MO	1121-37-5	( <i>c</i> -C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CO	333	850.6	6.0	856.8							
[C <sub>9</sub> H <sub>18</sub> S] 93ABB/MO	54396-69-9	( <i>t</i> -C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CS				852.0			881.8				9
93ABB/MO	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	-2.4	850.6							
93ABB/MO	372-48-5	2-F-pyridine	333	852.7	-0.4	852.1							
93ABB/MO	290-37-9	Pyrazine	333	847.0	6.4	853.4							
[C <sub>7</sub> H <sub>7</sub> O] 94HOK/YAN	3174-48-9	4-Me-phenoxy kinetic method				852 852			884.5				0
[C <sub>9</sub> H <sub>9</sub> ClO <sub>2</sub> ] 86MIS/FUJ	37612-52-5 98-86-2	3-Cl-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	22.6	851.9 851.9			883.7				2
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ] 86MIS/FUJ	99-93-4 98-86-2	4-HO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	22.6	851.9 851.9			883.7				2
[C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> ] 94HOK/YAN	110-13-4	CH <sub>3</sub> COCH <sub>2</sub> CH <sub>2</sub> COCH <sub>3</sub>				851.8			892.0				-26



TABLE 2. Summary of proton transfer thermochemical data for each base  $M_1$ , sorted by gas basicity of  $M_1$ —Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
YrSquib	Reg No(R)	Base(R)											
87BOU/HOP	372-48-5	2-F-pyridine	313	852.7	-3.8	849.3							
87BOU/HOP	100-48-1	4-Pyridinecarboxitrile	313	848.8	2.9	852.0							
83MAU	372-48-5	2-F-pyridine	600	852.7	-10.5	850.7	884.6	10.9	895.5	2	-35.6	-33.6	
83MAU	109-97-7	pyrrole	600	843.8	2.3	854.7	875.4	16.3	891.7	2.8	-23.4	-20.6	
[C <sub>5</sub> H <sub>5</sub> O <sub>2</sub> Rh]	12192-97-1	(C <sub>5</sub> H <sub>5</sub> )Rh(CO) <sub>2</sub>				851.8			882.5			5.8	
81STE/BEA	7664-41-7	NH <sub>3</sub>	320	819	33	851.8							
[C <sub>4</sub> H <sub>9</sub> N]	4923-79-9	Azetidine, N-methyl-				851.7			882.5			5.6	
92ABB/CAN	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	-0.2	852.9							
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	-2.3	850.3							
[C <sub>6</sub> H <sub>5</sub> ]	2396-01-2	phenyl radical				851.5			884			0	
88LJA/BAR									884				
87KIN/BUR	7732-18-5	H <sub>2</sub> O		660.0			691	163	884				
87KIN/BUR	67-56-1	CH <sub>3</sub> OH		724.5			754.3	118	854				
87KIN/BUR	7664-41-7	NH <sub>3</sub>		819			853.6	21	872.3				
[C <sub>4</sub> H <sub>7</sub> NO]	2679-13-2	N-methyl-2-azetidinone				851.3			882.2			5	
92ABB/CAN	290-37-9	Pyrazine	333	847.0	4.9	851.9							
92ABB/CAN	372-48-5	2-F-pyridine	333	852.7	-2.0	850.6							
[C <sub>10</sub> H <sub>12</sub> O]	3637-01-2	3,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	320	843.6	6	849.6			882.8			2	
93KUK/STR	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	308	829.3	23.0	852.3							
92MIS/KAN	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>											
[C <sub>10</sub> H <sub>12</sub> O]	89-74-7	2,4-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>	320	843.6	7	850.8			882.6			2	
93KUK/STR	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				850.6							
[C <sub>12</sub> H <sub>16</sub> O]	943-27-1	4,4-C <sub>4</sub> H <sub>9</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				850.6			882.5			2	
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	21.3	850.6							
[C <sub>10</sub> H <sub>12</sub> S]	#838	3-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>				850.6			879.6			12	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	32.5	850.6							
[C <sub>7</sub> H <sub>10</sub> O]	1121-37-5	( <i>c</i> -C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CO				850.6			880.4			9	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.2							
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> C <sub>6</sub>	350	836.0	13.3	850.1							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	41.0	823.1							
[C <sub>6</sub> H <sub>7</sub> N]	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>				850.6			882.5			2	
91MAU/SIE	765-43-5	<i>c</i> -C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600	823	24.3	847.3			874.5	2	7.9	2	9.9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	31.6	850.2							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	31.6	850.2							
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	0	850.6							
80MAU	7664-41-7	NH <sub>3</sub>	550	819	24.3	841.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Sqib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
79MAU/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	500	850.6	0	850.6							
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	550	878	-21.8	854.5							
79LOC/HUN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	382	850.6	0	850.6							
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	28.9	845.3							
77POL/DEV	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	350	850.6	0	850.6							
77COO/KRU		relative order-See Refs.											
76LAU/KEB	71-43-2	C <sub>5</sub> H <sub>6</sub>	600	725.4	107.1	839.4							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.5							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	32.9	851.5							
72BRI/YAM	7664-41-7	NH <sub>3</sub>	600	819	37.2	853.7							
[C <sub>4</sub> H <sub>6</sub> Se] 89OSA/DEL	114659-08-4 372-48-5	CH <sub>2</sub> =C(CH <sub>3</sub> )-SeCH <sub>3</sub> 2-F-pyridine	313	852.7	-2.1	850.5			879.4			12	
[C <sub>3</sub> H <sub>3</sub> O <sub>3</sub> P] 80HOD/HOU	1449-91-8 430-67-1; 107-47-1	4-Methyl-2,6,7-trioxa-1- phosphabicyclo[2.2.2]octane CF <sub>2</sub> HCH <sub>2</sub> NH <sub>2</sub> ; (t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	320			837-864			882.8			0	
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ] 90GRE/LIG 79MAU 75WIL/MCC	65-71-4 75-04-7 7664-41-7; 74-89-5	Thymine kinetic method C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>	550	878	-27.6	847.9 819-864			880.9 880.9			5	
[C <sub>9</sub> H <sub>18</sub> NO] 95CHE/KAS	2564-83-2 290-37-9; 372-48-5	2,2,6,6-tetramethyl-1-piperidinyloxy radical Pyrazine(1,4-Diazine); 2-F-pyridine				849.8 847-853			882.3			0	
[C <sub>6</sub> H <sub>12</sub> O] 85GUE/HOU	823-18-7 110-63-4	cis-1,3-cyclohexandiol HO(CH <sub>2</sub> ) <sub>4</sub> OH	323	854.9	-3	849.7 849.7			882.2			0	
[C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> O <sub>4</sub> ] 92ABB/CAB 92ABB/CAB	37687-24-4 2450-71-7 372-48-5	3,5-diethoxycarbonylpyrazole HCCCH <sub>2</sub> NH <sub>2</sub> 2-F-pyridine	333 333	853.5 852.7	-4.5 -2.1	849.7 848.7 850.6			881.6			2	
[C <sub>12</sub> H <sub>18</sub> Si] 87TAF	17920-24-0 7664-41-7	4-((CH <sub>3</sub> ) <sub>3</sub> Si)C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	31.6	849.7 849.7			878.6			12	
[C <sub>12</sub> H <sub>18</sub> Si] 87TAF	40595-34-4 7664-41-7	3-((CH <sub>3</sub> ) <sub>3</sub> Si)C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	31.6	849.7 849.7			878.6			12	
[C <sub>6</sub> H <sub>8</sub> O] 87BOU/HOP 87BOU/HOP 87BOU/HOP	504-02-9 372-48-5 928-55-2 141-79-7	c-hexane-1,3-dione 2-F-pyridine C <sub>2</sub> H <sub>5</sub> OCH=CHCH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH(C=O)CH <sub>3</sub>	313 313 313	852.7 847.7 846.9	-2.1 1.3 1.3	849.4 850.6 849.1 848.1			881.2			2	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)
	372-48-5	109-97-7	Base(R)	Base(M)										
83MAU	372-48-5	109-97-7	2-F-pyridine		600	852.7	7.5	860.3						
83MAU	109-97-7		pyrrole		600	843.8	14.2	858.3						
[C <sub>4</sub> H <sub>7</sub> NO]	79-39-0		2-propanamide, 2-methyl-					849.4			880.4			5
90WOL/GRU	62-53-3		C <sub>6</sub> N <sub>5</sub> NH <sub>2</sub>		320	850.6	-1.3	849.2						
90WOL/GRU	122-00-9		4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>		320	843.6	5.9	849.5						
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	123-11-5		4-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CHO					849.3			881.1			2
87TAF	7664-41-7		NH <sub>3</sub>		350	819	30.7	849.2						
83TAF2	7664-41-7		NH <sub>3</sub>		350	819	45.3	863.9						
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ]	100-48-1		4-Pyridinecarbonitrile					848.8			880.6			2
91AUE/WEB	110-86-1		pyridine		300	898.1	-49.3	848.8						
87TAF	7664-41-7		NH <sub>3</sub>		350	819	29.7	848.3						
86TAF/ANV	100-48-1		4-Pyridinecarbonitrile		350	848.8	0	848.8						
76AUE/WEB2	74-89-5		CH <sub>3</sub> NH <sub>2</sub>		298	864.5	-14.2	850.3						
75TAF	7664-41-7		NH <sub>3</sub>		350	819	29.7	848.3						
75ARN	7664-41-7		NH <sub>3</sub>		350	819	29.7	848.3						
[C <sub>9</sub> H <sub>9</sub> ClOS]	32467-66-6		3-Cl-4-CH <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>					848.6			880.4			2
92MIS/KAN	98-86-2		C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>		308	829.3	18.8	848.1						
[C <sub>12</sub> H <sub>16</sub> Si]	94397-80-5		4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>					848.1			877.0			12
92MIS/AR12	100-70-9		2-Pyridinecarbonitrile		308	841	7.9	848.9						
92MIS/AR12	100-48-1		4-Pyridinecarbonitrile		308	848.8	-0.8	847.8						
92MIS/AR12	100-54-9		3-Pyridinecarbonitrile		308	845.1	2.5	847.5						
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	5806-90-6		Acetamide, N-methoxy					848.0			879.0			5
92DEC/EXN	109-97-7		pyrrole		338	843.8	4.0	847.7						
92DEC/EXN	68-12-2		(CH <sub>3</sub> ) <sub>2</sub> NCHO		338	856.6	-7.7	848.9						
[C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N]	2730-67-8		CF <sub>3</sub> CH <sub>2</sub> NHCH <sub>3</sub>					848.0			881.1			-2
87TAF	7664-41-7		NH <sub>3</sub>		350	819	28.8	847.6						
79AUE/BOW	74-89-5		CH <sub>3</sub> NH <sub>2</sub>		298	864.5	-16.1	848.4						
75TAF	7664-41-7		NH <sub>3</sub>		350	819	28.8	847.6						
[C <sub>5</sub> H <sub>10</sub> O]	4696-26-8		trans-CH <sub>3</sub> CH=CH-OC <sub>2</sub> H <sub>5</sub>					848.0			876.9			12
89OSA/DEL	114659-08-4		CH <sub>2</sub> =C(CH <sub>3</sub> )-SeCH <sub>3</sub>		313	850.5	-2.5	848.0						
[C <sub>5</sub> H <sub>10</sub> O]	928-55-2		C <sub>2</sub> H <sub>5</sub> OCH=CHCH <sub>3</sub>					847.7			876.6			12
86BOU/DJA	141-79-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH(C=O)CH <sub>3</sub>		313	846.9	1	847.7						
[C <sub>3</sub> O]	11127-17-6		CCCO					847.7			880.2			0
93MAC/SUD			theory		298						880.2			
89BOT			theory		298						885±5			

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: SQUIB	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)
[C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> ]	288-36-8	1,2,3-triazole				847.4			879.3			2
88CAT/CLA	372-48-5	2-F-pyridine	~300	852.7	-6.7	846.0						
88CAT/CLA	68-12-2	(CH <sub>3</sub> ) <sub>2</sub> NCHO	~300	856.6	-7.1	849.5						
88CAT/CLA	100-54-9	3-Pyridinecarbonitrile	~300	845.1	1.7	846.8						
[C <sub>4</sub> H <sub>9</sub> NO]	6281-94-3	n-C <sub>3</sub> H <sub>7</sub> NHCHO	298	864.5	-17.1	847.4			878.4			5
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>				847.4						
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ]	7541-16-4	(CH <sub>3</sub> ) <sub>2</sub> NCOOCH <sub>3</sub>	350	819	28.8	847.3			878.3			5
87TAF	7664-41-7	NH <sub>3</sub>				847.3						
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O]	14906-64-0	3-cyano-pyridine-1-oxide	343	892.9	-46.0	847.1			879.6			0
92MIS/TER	694-59-7	pyridine-1-oxide				847.1						
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ]	290-37-9	Pyrazine				847.0			877.1			7.8
86TAF	7664-41-7	NH <sub>3</sub>	350	819	25.9	844.2						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	27.9	846.2						
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	550	878	-25.1	849.7						
[C <sub>6</sub> H <sub>10</sub> O]	141-79-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH(C=O)CH <sub>3</sub>	313	848.8	-1.7	846.9			878.7			2
88BOU/DJA	100-48-1	4-Pyridinecarbonitrile				847.1						
88BOU/DJA	372-48-5	2-F-pyridine	313	852.7	-6.3	846.4						
86KAM/YOU	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	333	828.1	8.6	837.2						
[C <sub>6</sub> H <sub>6</sub> N]	626-01-7	3-I-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>	600	850.6	-3.8	846.8			878.7			2
81LAU/NIS	62-53-3	C <sub>3</sub> H <sub>5</sub> NH <sub>2</sub>				846.8						
[C <sub>4</sub> H <sub>9</sub> NO]	563-83-7	i-C <sub>3</sub> H <sub>7</sub> CONH <sub>2</sub>				846.7			878.6			2
97HOM/HER	100-48-1	4-Pyridinecarbonitrile	333	848.8	1.5	850.2						
97HOM/HER	100-70-9	2-Pyridinecarbonitrile	333	841	-1.1	839.9						
97HOM/HER	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	-3.2	850.0						
97HOM/HER	678-48-9	(CH <sub>3</sub> ) <sub>2</sub> NCOOC <sub>2</sub> H <sub>5</sub>	333	865.6	-3.4	862.3						
[C <sub>6</sub> H <sub>14</sub> S]	625-80-9	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S				846.6			876.4			9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	28.4	846.6						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	28.4	846.6						
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-18.1	846.4						
[C <sub>14</sub> H <sub>10</sub> ]	120-12-7	Anthracene				846.6			877.3			5.8
85VAN/LEA		See Refs.										
80MAU	151-18-8	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN	482	832.5	1.3	831.8						
80MAU	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	482	850.6	-3.3	846.6						
[C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> ]	37622-90-5	4-(C <sub>2</sub> H <sub>5</sub> COO)-pyrazole				846.5			880.7			-5.8
94NOT/HER	2450-71-7	HCCCH <sub>2</sub> NH <sub>2</sub>	333	853.5	-7.5	846.0						
94NOT/HER	372-48-5	2-F-pyridine	333	852.7	-6.3	846.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsqub	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
	544-40-1	824-76-9 106-47-8; 62-53-3	Base(R)	Base(M)				GB(M)	GB(M)						
94NOT/HER	544-40-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S			333	842.1	3.8	846.3	846.3			877.2			5
[C <sub>7</sub> H <sub>6</sub> FNO] 94GRU/CAL	824-76-9 106-47-8; 62-53-3	4-F-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 4-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>						846.3 842-851	846.3			877.2			5
[C <sub>7</sub> H <sub>6</sub> CINO] 94GRU/CAL	619-56-7 106-47-8; 62-53-3	4-Cl-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 4-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>						846.3 842-851	846.3			877.2			5
[C <sub>7</sub> H <sub>6</sub> CINO] 94GRU/CAL	618-48-4 106-47-8; 62-53-3	3-Cl-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 4-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>						846.3 842-851	846.3			877.2			5
[C <sub>7</sub> H <sub>6</sub> FNO] 94GRU/CAL	455-37-8 106-47-8; 62-53-3	3-F-C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> 4-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>						846.3 842-851	846.3			877.2			5
[C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> ] 93BER/HEL 93BER/HEL	1530-87-6 544-40-1 290-37-9	Piperidine, 1-carbonitrile- (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S Pyrazine			~338 ~338	842.1 847.0	2.1 0.8	846.1 844.3 847.9	846.1			876.7			6
[C <sub>7</sub> H <sub>7</sub> O] 94HOK/YAN	155174-21-3	2-OH-benzyl kinetic method						846 846	846			878.5			0
[C <sub>13</sub> H <sub>18</sub> ] 92NAK/NOM 92NAK/NOM	31006-98-1 100-48-1 100-54-9	$\alpha$ -t-butylstyrene, 4-CH <sub>3</sub> 4-Pyridinecarbonitrile 3-Pyridinecarbonitrile			343 343	848.8 845.1	-2.1 0.8	845.7 846.2 845.5	845.7			874.6			12
[C <sub>2</sub> H <sub>5</sub> N <sub>3</sub> ] 89ATT/CAC	871-31-8	CH <sub>3</sub> CH <sub>2</sub> NNN See Refs.			358			845.5	845.5			878	878±21		0
[C <sub>14</sub> H <sub>20</sub> ] 92NAK/NOM 92NAK/NOM	146558-41-0 100-54-9 123-54-6	$\alpha$ -t-butylstyrene, 3,5-dimethyl 3-Pyridinecarbonitrile CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>			343 343	845.1 836.8	1.3 9.6	845.5 845.9 845.3	845.5			874.3			12
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ] 92DEC/EXN 92DEC/EXN	13115-24-7 289-95-2 109-97-7	Acetamide, N-hydroxy-N-methyl Pyrimidine pyrrole			338 338	855.7 843.8	-10.1 1.3	845.3 845.6 845.1	845.3			876.2			5
[C <sub>3</sub> H <sub>7</sub> NO] 97HOM/HER 97HOM/HER 97HOM/HER 97HOM/HER 97HOM/HER	79-05-0 111-47-7 1121-37-5 290-37-9 625-80-9 372-48-5	C <sub>2</sub> H <sub>5</sub> CONH <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S (c-C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> CO Pyrazine (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S 2-F-pyridine			333 333 333 333 333	834.9 850.6 847.0 846.6 852.7	6.7 0.9 -3.7 -1.0 -9.0	845.3 841.7 851.7 843.4 845.8 843.7	845.3			876.2			5

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>1</sub>, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (R)
[C <sub>22</sub> H <sub>12</sub> ] 80MAU 80MAU	191-24-2	1,12-Benzoperylene				845.2			876.0			5.8	
	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	508	850.6	0	849.8							
	7664-41-7	NH <sub>3</sub>	550	819	24.7	840.6							
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> ] 91AUE/WEB 87TAF 83TAF2 76AUE/WEB2 75TAF 75ARN	100-54-9	3-Pyridinecarbonitrile				845.1			877.0			2	
	110-86-1	pyridine	300	898.1	-52.7	845.4							
	7664-41-7	NH <sub>3</sub>	350	819	26.1	844.7							
	7664-41-7	NH <sub>3</sub>	350	819	25.6	844.2							
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-19.5	845.0							
	7664-41-7	NH <sub>3</sub>	350	819	27.0	845.6							
7664-41-7	NH <sub>3</sub>	350	819	27.0	845.6								
[C <sub>7</sub> H <sub>7</sub> O] 94HOK/YAN	41115-75-7	3-Me-phenoxy kinetic method				845			877.5			0	
	845					845							
[C <sub>11</sub> H <sub>14</sub> O <sub>2</sub> ] 96DEC/EXN 96DEC/EXN 96DEC/EXN	13544-66-6	3,4,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> -CO <sub>2</sub> CH <sub>3</sub>				844.6			875.5			5	
	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	338	850.6	-5	845.5							
	23617-71-2	2,4-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>	338	837.2	7.3	844.5							
	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	8.6	843.7							
[C <sub>3</sub> H <sub>3</sub> O] 91MAU/SIE 91MAU/SIE 91MAU/SIE 91MAU/SIE 86MAU/LIE	288-42-6	oxazole				844.5			876.4			2	
	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-3.8	846.8			873.2	-9.2	9.2	11.2	
	372-48-5	2-F-pyridine	600	852.7	-9.2	843.5			882.5	-8.8	0.4	2.4	
	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600	823	19.7	842.7			884.6	17.6	3.3	5.3	
	109-97-7	pyrrole	600	843.8	3.3	847.4			854.9	0.4	4.2	7.0	
	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	36.4	841.9			875.4	2.8			
[C <sub>10</sub> H <sub>12</sub> O] 93KUK/STR 86MIS/FUJ	5379-15-8	3,5-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>				844.2			876.0			2	
	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	320	843.6	-1	842.6							
	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	15.9	845.2							
[C <sub>22</sub> H <sub>24</sub> ] 86SAN/BAL	77387-50-9	1,16-Dimethyldecahedrane				844.0			876.5			0	
	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	31.4	844.0							
[C <sub>4</sub> H <sub>5</sub> N] 97EAS/SMI 93SZU/MCM 93SZU/MCM 91MAU/SIE 91MAU/SIE 86MAU/LIE 81HOU/SCH	109-97-7	pyrrole theory	298			843.8			875.4			2.8	
	7664-41-7	NH <sub>3</sub>	600	819	29.7	845.6			877.4	23.8	-6.4	3.2	
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	600	864.5	-15.9	845.6			899.0	-7	16.3	9.3	
	7664-41-7	NH <sub>3</sub>	600	819	28.5	844.7			853.6	20.9	-6.4	6.2	
	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600	823	15.9	838.7			854.9	20.9		-5.9	
	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	35.1	840.4							
	7664-41-7;	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864							
	74-89-5												
79MAU 79LAU	75-04-7 7664-41-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub> NH <sub>3</sub>	550 650	878 819	-26.8 25.4	849.2 841.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	25.4	844.4						
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	29.9	846.2						
[C <sub>7</sub> H <sub>8</sub> S] 87TAF	100-68-5 7664-41-7	C <sub>6</sub> H <sub>5</sub> SCH <sub>3</sub> NH <sub>3</sub>	350	819	25.6	843.7 843.7			872.6			12
[C <sub>10</sub> H <sub>12</sub> O] 87TAF	25108-57-0 7664-41-7	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	25.6	843.7 843.7			872.6			12
[C <sub>9</sub> H <sub>10</sub> O] 87TAF	122-00-9 7664-41-7	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub>	350	819	25.2	843.6 843.7			875.5			2
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	16.3	845.6						
81BRO/ABB	7664-41-7	NH <sub>3</sub>	320	819	22.2	841.0						
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O] 92MIS/TER	14906-59-3 694-59-7	4-cyano-pyridine-1-oxide pyridine-1-oxide	343	892.9	-50.2	842.7 842.7			873.4			5.8
[C <sub>10</sub> H <sub>12</sub> O] 93KUK/STR	2142-71-4 122-00-9	2,3-(CH <sub>3</sub> )=C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub> 4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	320	843.6	-1	842.7 842.6			874.6			2
[C <sub>6</sub> H <sub>10</sub> ] 87TAF	4663-22-3 7664-41-7	c-C <sub>3</sub> H <sub>5</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	25.2	842.7 843.2			871.6			12
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	25.6	843.7						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	22.0	841.0						
[C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ] 91AUE/WEB	1122-61-8 110-86-1	4-(NO <sub>2</sub> )-pyridine pyridine	300	898.1	-56.1	842.5 842.0			874.3			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	22.9	841.5						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	22.9	841.5						
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-19.5	845.0						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	23.8	842.4						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	23.8	842.4						
72TAA/HEN	110-86-1	pyridine	320	898.1	-75.7	822.4						
[C <sub>10</sub> H <sub>12</sub> ] 87TAF	26444-18-8 7664-41-7	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	24.3	842.4 842.3			871.3			12
[C <sub>8</sub> H <sub>18</sub> S] 87TAF	544-40-1 7664-41-7	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S NH <sub>3</sub>	350	819	23.8	842.1 842.0			871.8			9
[C <sub>7</sub> H <sub>7</sub> O] 94HOK/YAN	3174-49-0	2-Me-phenoxy kinetic method				842 842			874.5			0
[C <sub>6</sub> H <sub>6</sub> CIN] 87TAF	106-47-8 7664-41-7	4-ClC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> NH <sub>3</sub>	350	819	23.3	842.0 841.9			873.8			2
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	23.3	841.9						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
YrSquib	Reg No(R)	Base(R)										
77SUM/POL	7664-41-7	NH <sub>3</sub>	350	819	24.7	843.3						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	24.7	843.3						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	24.7	843.3						
[C <sub>12</sub> H <sub>16</sub> N <sub>2</sub> O <sub>6</sub> ]	362-43-6	2',3'-O-isopropylideneuridine				841.7			874.2			0
75WIL/MCC	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>9</sub> H <sub>14</sub> N <sub>2</sub> O <sub>4</sub> ]	5627-05-4	5,6-Dihydrouridine				841.7			874.2			0
75WIL/MCC	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>5</sub> H <sub>3</sub> CIN <sub>4</sub> ]	87-42-3	6-Chloropurine				841.7			873.6			2
75WIL/MCC	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O]	557-01-7	2(1H)-Pyrimidinone				841.7			872.7			5
75WIL/MCC	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	66-22-8	Uracil				841.7			872.7			5
75WIL/MCC	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>10</sub> H <sub>12</sub> O]	2142-73-6	2,5-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub>				841.6			873.5			2
93KUK/STR	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	320	843.6	-2	841.6						
[C <sub>7</sub> H <sub>10</sub> O]	17348-59-3	(i-C <sub>3</sub> H <sub>7</sub> )O(t-C <sub>4</sub> H <sub>9</sub> )				841.5			870.7			11
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-22.9	841.5						
[C <sub>6</sub> H <sub>6</sub> BrN]	591-19-5	3-BrC <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				841.4			873.2			2
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-9.2	841.4						
[C <sub>10</sub> H <sub>10</sub> Fe]	102-54-5	(C <sub>3</sub> H <sub>5</sub> ) <sub>2</sub> Fe				841.3			863.6			34
89MAU	372-48-5	2-F-pyridine	600	852.7	0.4	843.5	884.6	-15.1	869.5	2	25.9	27.9
89MAU	109-97-7	pyrrole	600	843.8	5.0	839.5	875.4	-9.2	866.2	2.8	23.4	26.2
88IKO/SUN	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	500	829.3	19.2	842.1	861.1	-2.5	858.6	2	43.5	45.5
88IKO/SUN	626-60-8	3-Cl-pyridine	500	871.5	-25.1	840.0	903.4	-36.0	867.4	2	35	37
88IKO/SUN	68-12-2	(CH <sub>3</sub> ) <sub>2</sub> NCHO	500	856.6	-7.1	843.7						
88IKO/SUN	109-97-7	pyrrole	500	843.8	7.9	845.5						
75FOS/BEA2	4143-41-3; 74-89-5	(E)-CH <sub>3</sub> N=NCH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				834-864						34.2
[C <sub>8</sub> H <sub>14</sub> ]	72014-90-5	(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub>				841.0			869.9			12
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	22.0	841.0						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squb	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta\Delta S_p$ (M,R)	$\Delta\Delta S_p$ (M)
[C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> ] 86SUN/KUL	3068-00-6	HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> CH <sub>2</sub> OH See Refs.	300			841 841			905.9 904		-109
[C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> ] 91AUE/WEB	100-70-9	2-Pyridinecarbonitrile				841			872.9		2
87TAF	110-86-1	pyridine	300	898.1	-56.1	842.0					
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	20.1	838.7					
79MAU/HUN	7664-41-7	NH <sub>3</sub>	320	819	18.0	836.8					
76AUE/WEB2	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	350	850.6	-8.7	841.9					
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-22.5	842.0					
[C <sub>2</sub> S] 92MAC/SUD	12602-41-4	C <sub>2</sub> S theory	298			840.7			869.9 869.6		12
[C <sub>4</sub> H <sub>8</sub> O] 94KOP/ANV	109-92-2	C <sub>2</sub> H <sub>5</sub> OCH=CH <sub>2</sub>				840.4			870.1		9.5
94KOP/ANV	544-40-1	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	373	842.1	-0.4	841.6					
91MAU/SIE	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	373	834.9	3.3	838.3					
91MAU/SIE	288-42-6	oxazole	600	844.5	-0.4	841.8	876.4	-4.6	871.8	2	7.5
86BOU/DIA	372-48-5	2-F-pyridine	600	852.7	-10.5	840.0	884.6	-15.1	869.5	2	7.1
	622-97-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>	313	832.8	0	832.9					9.1
[C <sub>10</sub> H <sub>10</sub> ] 85VAN/LEA	129-00-0	Pyrene				840.1			869.2		11.5
80MAU	151-18-8	See Refs. H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN	549	832.5	9.6	838.0					
80MAU	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	514	850.6	-6.3	842.3					
[CHCl] 85LLA/KAR	2108-20-5	CHCl				839.9			874.1		-5.8
	98-86-2; 62-53-3	CH <sub>3</sub> COC <sub>6</sub> H <sub>5</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>				829-851					
[C <sub>3</sub> H <sub>5</sub> NO] 90WOL/GRU	79-06-1	2-propenamide				839.8			870.7		5
90WOL/GRU	122-00-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	320	843.6	-3.4	840.2					
	98-83-9	C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>	320	835.3	3.9	839.3					
[C <sub>6</sub> H <sub>6</sub> FN] 87TAF	371-40-4	4-F-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				839.7			871.5		2
81TAA/SUM	7664-41-7	NH <sub>3</sub>	350	819	21.1	839.6					
75TAF	7664-41-7	NH <sub>3</sub>	320	819	19.2	838.1					
75ARN	7664-41-7	NH <sub>3</sub>	350	819	22.9	841.5					
	7664-41-7	NH <sub>3</sub>	350	819	22.9	841.5					
[C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> ] 86MIS/FUI2	121-98-2	4-CH <sub>3</sub> -O-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				839.6			870.6		5
	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	20.1	839.6					
[C <sub>9</sub> H <sub>7</sub> ClO] 92MIS/ARI	120136-29-0	3-Cl-4-CH <sub>3</sub> -O-C <sub>6</sub> H <sub>3</sub> -CCH				839.5			871.9		0
	536-74-3	C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	38.1	839.5					
[C <sub>9</sub> H <sub>7</sub> FO] 120136-28-9	120136-28-9	3-F-4-CH <sub>3</sub> -O-C <sub>6</sub> H <sub>3</sub> -CCH				839.5			871.9		0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (R)
92MIS/ARI	536-74-3	C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	38.1	839.5							
[C <sub>12</sub> H <sub>14</sub> Si]	120093-92-7	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>							868.3			12	
92MIS/ARI2	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	308	836.8	2.5	839.1							
92MIS/ARI2	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	308	828.1	10.0	838.2							
92MIS/ARI2	100-70-9	2-Pyridinecarbonitrile	308	841	0	840.9							
[C <sub>3</sub> H <sub>10</sub> O <sub>2</sub> ]	586-37-8	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				839.3			871.2			2	
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	10.0	839.3							
[C <sub>10</sub> H <sub>12</sub> ]	1124-20-5	Benzene, 1-methyl-3-(1-methylethenyl)- See Refs.							867.6			12	
[C <sub>8</sub> H <sub>18</sub> O]	6863-58-7	(sec-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O				838.5			865.9			17	
82MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	810.5	28.0	838.5							
[C <sub>13</sub> H <sub>18</sub> ]	146558-42-1	$\alpha$ -t-butylstyrene, 3-CH <sub>3</sub>				838.5			867.4			12	
92NAK/NOM	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	343	836.8	3.8	839.5							
92NAK/NOM	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	343	828.1	9.2	837.6							
[C <sub>3</sub> H <sub>9</sub> N]	7188-38-7	t-C <sub>4</sub> H <sub>9</sub> NC				838.3			870.7			0.1	
86MAU/KAR	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	335	850.6	-9.2	841.5							
86MAU/KAR	109-97-7	pyrrole	335	843.8	-3.8	840.1							
86MAU/KAR	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	828.1	4.6	833.3							
[C <sub>6</sub> H <sub>8</sub> O]	20843-07-6	3,4-dimethylfuran				838.3			869.0			5.8	
85HOU/ROL	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	1.7	838.3							
[C <sub>8</sub> H <sub>12</sub> O]	4694-17-1	5,5-Dimethylcyclohex-2-ene-1-one							869.8			2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	19.2	837.8							
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	19.4	837.9							
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	38404-42-1	3,4-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -CO <sub>2</sub> CH <sub>3</sub>				837.5			868.5			5	
96DEC/EXN	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	1.4	836.5							
96DEC/EXN	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	338	836.8	2.4	838.5							
96DEC/EXN	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	9	837.6							
[C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> O <sub>3</sub> ]	1124-33-0	4-(NO <sub>2</sub> )-pyridine-1-oxide				837.3			868.0			5.8	
92MIS/TER	694-59-7	pyridine-1-oxide	343	892.9	-55.6	837.3							
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	23617-71-2	2,4-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>				837.2			868.2			5	
93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	9.3	837.9							
93DEC/ERT	111-47-1	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	1.5	836.6							
[C <sub>2</sub> H <sub>8</sub> O]	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>				836.8			873.5			-14	
93DEC/ERT	89-71-4	2-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	338	827.3	7	835.0							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
87TAF	7664-41-7	NH <sub>3</sub>	350	819	16.9	836.3							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	18.5	837.9							
83MAU	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	600	834.9	-2.5	839.3	864.7	5.0	869.7	9	-12.6	-3.6	
83MAU	109-97-7	pyrrole	600	843.8	-10.7	838.1	875.4	-0.4	875.0	2.8	-17.2	-14.4	
83CAS/KIM	111-43-3	(N-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	23.8	835.1							
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-27.3	837.1							
[V]	7440-62-2	V				836.8			859.4			33	
85ELK/ARM						859±6							
[C <sub>2</sub> H <sub>5</sub> F <sub>2</sub> N]	430-67-1	CF <sub>2</sub> HCH <sub>2</sub> NH <sub>2</sub>				836.6			870.5			-5.1	
86TAF	7664-41-7	NH <sub>3</sub>	320	819	17.2	836.1							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	18.3	837.2							
79AUE/BOW	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-27.8	836.7							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	19.2	838.2							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	19.2	838.2							
[C <sub>3</sub> H <sub>10</sub> O]	585-74-0	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				836.4			868.2			2	
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	7.1	836.4							
[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> P]	280-45-5	2,6,7-Trioxa-1-phosphabicyclo[2.2.2]octane				836.4			868.8			0	
80HOD/HOU	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	320	836.0	0	836.5							
80HOD/HOU	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	320	836.8	0	836.6							
[C <sub>6</sub> H <sub>8</sub> CIN]	108-42-9	3-Cl-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				836.3			868.1			2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	18.8	837.3							
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-13.0	837.6							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	17.7	833.7							
77SUM/POL	7664-41-7	NH <sub>3</sub>	350	819	18.3	835.9							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	20.6	839.2							
[C <sub>3</sub> H <sub>6</sub> O]	34314-83-5	4-Methyl-2,3-dihydrofuran				836.2			868.6			0	
86BOU/DJA	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	-0.5	836.2							
[C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> ]	26537-19-9	4-t-C <sub>4</sub> H <sub>9</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				836.2			867.1			5	
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	17.2	836.7							
[C <sub>3</sub> H <sub>7</sub> CIS]	120136-30-3	3-Cl-4-CH <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> -CCH				836.1			868.6			0	
92MIS/ARI	536-74-3	C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	34.7	836.1							
[C <sub>8</sub> H <sub>11</sub> ClO]	17530-69-7	3-Chloro-5,5-dimethylcyclohexen-2-one				836.0			867.9			2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	17.4	836.0							
[C <sub>12</sub> H <sub>18</sub> ]	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>				836.0			860.6			26.4	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	19.7	837.0							
86STO/LI	527-53-7	1,2,3,5-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H <sub>2</sub>	300	816.5	19.2	835.8	845.6	14.6	860.2	11.4	16.1	27.5	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(M,R)		$\Delta S_p^{\ddagger}(R)$	$\Delta \Delta S_p^{\ddagger}(M,R)$	$\Delta S_p^{\ddagger}(M)$	
						GB(M)	PA(M)	PA(R)	$\Delta$ PA(M,R)			$\Delta S_p^{\ddagger}(M)$	$\Delta S_p^{\ddagger}(M)$
86STO/LI	700-12-9	(CH <sub>3</sub> ) <sub>5</sub> -C <sub>6</sub> H	300	823.5	11.3	834.8	850.7	859.5	17.6	7.7	25.3		
83TAF	7664-41-7	NH <sub>3</sub>	350	819	19.2	836.6							
77WOL/ABB	630-08-0	CO	350			836.8							
76WOL/DEV	71-43-2	C <sub>6</sub> H <sub>6</sub>	320	725.4	105.0	830.4							
75WOL/HAR	7664-41-7	NH <sub>3</sub>	350	819	22.0	839.3							
[C <sub>6</sub> H <sub>10</sub> ]	1118-58-7	CH <sub>3</sub> CH=CHC(CH <sub>3</sub> )=CH <sub>2</sub>				836		864.9			12		
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	17.1	836.1							
[C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> NO]	1801-10-1	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>				836.0		866.9			5		
94GRU/CAL	108-20-3; 109-97-7	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O; pyrrole				828-844							
[C <sub>7</sub> H <sub>5</sub> N]	931-54-4	C <sub>6</sub> H <sub>5</sub> NC				836.0		868.4			0		
86MAU/KAR	108-20-3; 109-97-7	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O, pyrrole	335			828-844							
[C <sub>9</sub> H <sub>10</sub> O]	93-55-0	C <sub>6</sub> H <sub>5</sub> COC <sub>2</sub> H <sub>5</sub>				835.6		867.4			2		
87TAF	7664-41-7	NH <sub>3</sub>	350	819	16.9	835.5							
[C <sub>4</sub> H <sub>6</sub> FN]	372-19-0	3-F-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				836.6		867.3			2		
87TAF	7664-41-7	NH <sub>3</sub>	350	819	16.0	834.6							
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-13.4	837.2							
77SUMPOL	7664-41-7	NH <sub>3</sub>	350	819	16.0	834.6							
[C <sub>9</sub> H <sub>10</sub> ]	98-83-9	C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>				835.3		864.2			12		
87TAF	7664-41-7	NH <sub>3</sub>	350	819	16.0	834.1							
86SAN/BAL	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	828.1	8.4	837.1							
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	28.9	840.0							
78TAF/WOL	7664-41-7	NH <sub>3</sub>	320	819	15.1	833.7							
77WOL/ABB	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	-4.6	832.2							
75WOL/HAR	7664-41-7	NH <sub>3</sub>	350	819	16.5	834.6							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	16.5	834.6							
[C <sub>11</sub> H <sub>14</sub> O <sub>2</sub> ]	2282-84-0	2,4,6-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>2</sub> -COOCH <sub>3</sub>				836.3		866.3			5		
93DEC/EFT	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	-0.2	834.9							
93DEC/EFT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	7.1	835.7							
[C <sub>6</sub> H <sub>8</sub> O]	625-86-5	2,5-dimethylfuran				835.2		865.9			5.8		
86MAU		See Refs.	600			843.5							
85HOU/ROL	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	1.3	837.9							
83MAU	109-97-7	pyrrole	600	843.8	-10.0	832.9							
[C <sub>21</sub> H <sub>12</sub> ]	191-07-1	Coronene				835.0		861.3			20.6		
80MAU	151-18-8	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN	548	832.5	4.6	830.7							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y+Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
80MAU	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	547	850.6	-6.7	839.3						
[C <sub>6</sub> H <sub>14</sub> S]	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S				834.9			864.7			9
96DEC/EXN	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	338	850.6	-13.8	836.5						
86TAF	7664-41-7	NH <sub>3</sub>	320	819	14.6	833.3						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	14.2	832.4						
[C <sub>3</sub> H <sub>3</sub> CIN <sub>2</sub> ]	15965-31-8	4-Cl-pyrazole				834.9			868.5			-3.8
94NOT/HER	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	333	836.8	-1.6	834.9						
94NOT/HER	544-40-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S	333	842.1	-7.2	835.3						
[C <sub>2</sub> H <sub>6</sub> B <sub>4</sub> ]	20693-67-8	1,6-C <sub>2</sub> B <sub>4</sub> H <sub>6</sub>				834.8			863.8			11.5
80DIX	7664-41-7; 62-53-3	NH <sub>3</sub> ; C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>				819-851						
[C <sub>9</sub> H <sub>10</sub> OS]	1441-99-2	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				834.7			866.6			2
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	5.4	834.7						
[C <sub>6</sub> H <sub>10</sub> O]	1567-72-2	3-methyl-3-penten-2-one(Z)				834.5			866.4			2
88BOU/DIA	110-87-2	2H-Pyran, 3, 4-dihydro-	313	833.4	0.4	833.7						
88BOU/DIA	625-86-5	2,5-dimethylfuran	313	835.2	-2.1	833.2						
88BOU/DIA	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	0	836.6						
[C <sub>4</sub> H <sub>6</sub> O]	1191-99-7	2,3-Dihydrofuran				834.4			866.9			0
86BOU/DIA	622-97-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>	313	832.8	-0.4	832.6						
86BOU/DIA	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	-0.4	836.3						
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ]	4143-41-3	(E)-CH <sub>3</sub> N=NCH <sub>3</sub>				834.4			865.1			5.8
92GAR/RUT		theory							883			
74FOS/WIL	430-67-1	CF <sub>2</sub> HCH <sub>2</sub> NH <sub>2</sub>	320	836.6	-2.1	834.3						
72FOS/BEA	7664-41-7; 74-89-5	NH <sub>3</sub> ; CH <sub>3</sub> NH <sub>2</sub>				819-864						
[C <sub>12</sub> H <sub>16</sub> O <sub>2</sub> ]	22524-51-2	2,3,5,6-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H-COOCH <sub>3</sub>				834.3			865.2			5
93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	5.5	834.1						
93DEC/ERT	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	5.3	834.5						
[C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ]	100-01-6	4-Nitroaniline				834.2			866.0			2
84ROL/HOU	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	320	828.1	4.6	833.0						
84ROL/HOU	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	320	836.8	-1.3	835.3						
[C <sub>6</sub> H <sub>10</sub> O]	4376-23-2	3-hexen-2-one(E)				833.8			865.6			2
88BOU/DIA	20843-07-6	3,4-dimethylfuran	313	838.3	-4.6	833.7						
88BOU/DIA	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	-2.1	834.5						
88BOU/DIA	625-86-5	2,5-dimethylfuran	313	835.2	-4.6	830.7						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Ysquire	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 93DEC/ERT	13730-55-7 93-58-3	2,5-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	338	819.5	5.6	833.7	864.7		864.7			5	
93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	5.7	834.3							
93DEC/ERT	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	-1.9	833.2							
[C <sub>9</sub> H <sub>9</sub> F] 87TAF	350-40-3 7664-41-7	4-FC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	15.6	833.7	862.6		862.6			12	
87TAF2	7664-41-7	NH <sub>3</sub>	350	819	15.6	833.6							
[C <sub>8</sub> H <sub>8</sub> ] 86SAN/BAL	277-10-1 98-83-9	Cubane C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>	428	835.3	-2.9	833.6	859.9		859.9			20.6	
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	25.9	836.0							
[C <sub>5</sub> H <sub>6</sub> O] 86MAU/LIE	534-22-5 109-97-7	2-methylfuran pyrrole	600	843.8	-7.5	833.5	865.9		865.9			0	
86MAU/LIE	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	28.9	835.0							
85HOU/ROL	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	828.1	0	828.4							
[C <sub>5</sub> H <sub>6</sub> O] 86BOU/HAN	110-87-2 20843-07-6	2H-Pyran, 3, 4-dihydro- 3,4-dimethylfuran	313	838.3	-3.8	833.4	865.8		865.8			0	
86BOU/HAN	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	828.1	4.2	832.6							
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 96DEC/EXN	25081-39-4 111-47-7	3,5-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	-2.2	833.4	864.3		864.3			5	
96DEC/EXN	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	338	835.8	-1.2	834.9							
96DEC/EXN	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	5.4	834.0							
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	12.1	831.6							
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> S] 86MIS/FUJ2	3795-79-7 93-58-3	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	13.8	833.3	864.3		864.3			5	
[C <sub>7</sub> H <sub>14</sub> S] 87TAF	7133-37-1 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> SCH <sub>3</sub> NH <sub>3</sub>	350	819	14.6	833.3	864.5		864.5			4	
[C <sub>12</sub> H <sub>26</sub> O] 87TAF	90547-83-4 7664-41-7	4-Ethylcamphor NH <sub>3</sub>	350	819	14.6	833.3	865.1		865.1			2	
[C <sub>4</sub> H <sub>7</sub> F <sub>2</sub> NO] 87TAF	667-50-5 7664-41-7	CF <sub>2</sub> HCON(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	14.6	833.1	864.1		864.1			5	
82PIE/HEH2							867		867				
[C <sub>12</sub> H <sub>18</sub> O <sub>2</sub> ] 87TAF	711-01-3 7664-41-7	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decane-1-carboxylic acid, methyl ester NH <sub>3</sub>	350	819	14.6	833.1	864.1		864.1			5	
[C <sub>12</sub> H <sub>18</sub> O] 87TAF	1660-04-4	Adamantylmethylketone	350	819	14.6	833.1	864.9		864.9			2	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (R)
97HOM/HER	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	333	829.3	6.9	836.1							
97HOM/HER	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	333	828.1	4.7	833.4							
97HOM/HER	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	333	834.9	-2.0	833.2							
97HOM/HER	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	333	836.8	-3.6	832.6							
87TAF	7664-41-7	NH <sub>3</sub>	350	819	11.4	830.0							
[C <sub>9</sub> H <sub>10</sub> ]	622-97-9	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>				832.8			861.7				12
89GAL/SPE						831.8							
84HAR/HOU	7664-41-7	NH <sub>3</sub>	323	819	14.2	832.8							
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ]	15012-36-9	2,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>				832.7			863.6				5
93DEC/ERT	89-71-4	2-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	338	827.3	6.3	833.6							
93DEC/ERT	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	3.2	832.4							
93DEC/ERT	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	338	834.9	-3.6	831.5							
93DEC/ERT	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	338	836.8	-2.3	833.8							
93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	3.5	832.1							
[C <sub>2</sub> H <sub>5</sub> NO]	60-35-5	CH <sub>3</sub> CONH <sub>2</sub>				832.6			863.6				5
73YAM/KEB	7664-41-7	NH <sub>3</sub>	320	819	13.8	832.6							
[C <sub>3</sub> H <sub>8</sub> O]	625-33-2	CH <sub>3</sub> CH=CHC(=O)CH <sub>3</sub>				832.5			864.3				2
84BOU/HOP	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	828.1	4.2	832.7							
84BOU/HOP	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	323	836.8	-4.2	832.3							
[C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> ]	99-76-3	4-HO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				832.5			863.4				5
86MIS/FUI2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	13.0	832.5							
[C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> ]	151-18-8	H <sub>2</sub> N(CH <sub>2</sub> ) <sub>2</sub> CN				832.5			866.4				-5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	11.9	830.8							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	11.9	830.8							
80MAU	7664-41-7	NH <sub>3</sub>	550	819	10.0	828.7							
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	550	878	-40.2	837.8							
75ARN	7664-41-7	NH <sub>3</sub>	350	819	14.6	833.6							
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	150-13-0	4-NH <sub>2</sub> -benzoic acid				832.3			864.7				0
95TAN/ISB	98-86-2; 98-83-9	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub> ; C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>				829-835							
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ]	99-05-8	3-NH <sub>2</sub> -benzoic acid				832.3			864.7				0
95TAN/ISB	98-86-2; 98-83-9	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub> ; C <sub>6</sub> H <sub>5</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub>				829-835							
[C <sub>11</sub> H <sub>16</sub> Si]	1923-01-9	C <sub>6</sub> H <sub>5</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>				832.0			860.9				12
92MIS/ARI2	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	308	836.8	-3.8	832.9							
92MIS/ARI2	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	308	828.1	2.9	831.1							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,7)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>8</sub> H <sub>6</sub> F <sub>3</sub> NO] 94GRU/CAL	1891-90-3	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>				831.8			862.8			5
	108-20-3; 372-19-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O; 3-F-C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub>				828-835						
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ] 86MIS/FUJ	121-71-1	3-HO-C <sub>5</sub> H <sub>4</sub> -COCH <sub>3</sub>				831.8			863.6			2
	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	2.5	831.8						
[C <sub>8</sub> H <sub>12</sub> ] 79AUE/BOW	497-35-8	2-Methylenecyclo[2.2.1]heptane				831.8			860.7			12
	74-89-5	CH <sub>3</sub> NH <sub>2</sub>	298	864.5	-32.7	831.8						
[C <sub>4</sub> H <sub>9</sub> OS] 93ABB/MO 93ABB/MO 93ABB/MO	926-67-0	CH <sub>3</sub> C(S)OC <sub>2</sub> H <sub>5</sub>				831.8			863.6			2
	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	333	836.8	-5.6	830.8						
	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	333	828.1	4.0	832.6						
	352-93-2	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S	333	827.0	5.2	832.4						
[C <sub>3</sub> H <sub>8</sub> S <sub>2</sub> ] 83CAS/KIM	2168-84-5	CH <sub>3</sub> C(=S)SCH <sub>3</sub>				831.5			860.7			11
	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	20.9	831.5						
[C <sub>9</sub> H <sub>18</sub> O] 87TAF 82PIE/HEH2	815-24-7	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CO				831.5			861.3			9
	7664-41-7	NH <sub>3</sub>	350	819	13.3	831.5			864			
[C <sub>11</sub> H <sub>18</sub> O] 87TAF	10309-50-9	4-Methylcamphor				831.4			863.3			2
	7664-41-7	NH <sub>3</sub>	350	819	12.8	831.4						
[C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> ] 78FAR/MCM	540-80-7	t-C <sub>4</sub> H <sub>9</sub> ONO				831.4			863.9			0
	7664-41-7; 109-97-7	NH <sub>3</sub> ; pyrrole				819-844						
[C <sub>11</sub> H <sub>18</sub> O] 87TAF	19066-23-0	Adamantylmethylether				831.0			860.2			11
	7664-41-7	NH <sub>3</sub>	350	819	12.8	830.9						
[C <sub>3</sub> H <sub>6</sub> OS <sub>2</sub> ] 93ABB/MO 93ABB/MO	19708-81-7	CH <sub>3</sub> OC(S)SCH <sub>3</sub>				830.8			862.6			2
	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	333	836.8	-5.7	830.7						
	108-20-3	(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	333	828.1	2.2	830.9						
[C <sub>7</sub> H <sub>14</sub> S] 87TAF	6572-99-2	Heptamethylenesulfide				830.7			860.5			9
	7664-41-7	NH <sub>3</sub>	350	819	12.4	830.6						
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF 83TAF2	5616-32-0	CH <sub>3</sub> NHCH <sub>2</sub> CN				830.7			863.8			-2
	7664-41-7	NH <sub>3</sub>	350	819	11.9	830.7						
	7664-41-7	NH <sub>3</sub>	350	819	11.9	830.7						
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ] 96DEC/EXN 96DEC/EXN	99-75-2	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				830.6			861.6			5
	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	338	836.8	-4.1	832.0						
	108-20-3	(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	2.2	830.8						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
96DEC/EXN	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	338	820.5	9.7	830.4							
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	9.6	829.1							
[C <sub>3</sub> H <sub>6</sub> O]	107-25-5	CH <sub>2</sub> =CH-OCH <sub>3</sub>				830.3			859.2			12	
95SMI/RAD		theory	298						849.2				
91MAU/SIE	753-90-2	CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	600	812.9	23.8	831.6	846.8	13.0	859.8	-5	18.4	13.4	
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600	819			853.6	0.8	854.4				
89OSA/DEL	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	-5.9	830.6							
89OSA/DEL	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	828.1	0.4	828.6							
[C <sub>12</sub> H <sub>16</sub> ]	5676-29-9	$\alpha$ -t-butylstyrene				830.3			859.2			12	
92NAK/NOM	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	343	836.8	-4.6	831.1							
92NAK/NOM	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	343	828.1	1.3	829.6							
92NAK/NOM	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	343	823	7.5	830.1							
[C <sub>3</sub> H <sub>3</sub> FN <sub>2</sub> ]	35277-02-2	4-fluoropyrazole				829.4			863.0			-4	
92ABB/CAB	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	333	836.8	-6.9	829.6							
92ABB/CAB	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	333	828.1	0.7	829.5							
[C <sub>3</sub> H <sub>6</sub> S]	1822-74-8	CH <sub>2</sub> =CH-SCH <sub>3</sub>				829.3			858.2			12	
89OSA/DEL	123-54-6	CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>	313	836.8	-5.4	831.1							
89OSA/DEL	107-25-5	CH <sub>2</sub> =CH-OCH <sub>3</sub>	313	830.3	-1.3	829.0							
89OSA/DEL	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	828.1	-0.4	827.8							
[C <sub>8</sub> H <sub>8</sub> O]	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>				829.3			861.1			2	
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600	819	12.1	828.6	853.6	8.8	862.4	-6.4	4.6	-1.8	
91MAU/SIE	95-13-6	indene	600	819.6	8.4	830.7	848.8	10.9	859.7	11	-4.2	6.8	
91MAU/SIE	100-42-5	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	600	809.2	20.5	831.3	839.5	23.0	862.5	7.4	-4.2	3.2	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	7.8	826.4							
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	8.0	826.5							
85VAN/LEA		See Refs.											
83TAF	7664-41-7	NH <sub>3</sub>	350	819	7.8	826.4							
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-19.7	830.9							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	37.2	819.5							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	9.1	825.1							
[C <sub>11</sub> H <sub>15</sub> F <sub>5</sub> S]	140843-92-1	4-F-C <sub>6</sub> H <sub>4</sub> -C(Si(CH <sub>3</sub> ) <sub>3</sub> )=CH <sub>2</sub>				829.1			858.0			12	
92MIS/AR12	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	308	828.1	1.3	829.4							
92MIS/AR12	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	308	820.5	8.4	828.8							
[C <sub>10</sub> H <sub>12</sub> ]	7399-49-7	Benzene, 1-methyl-2-(1-methylethenyl)-				828.9			857.8			12	
89GAL/SPE						828.9							
[C <sub>10</sub> H <sub>14</sub> O <sub>3</sub> ]	#997	3-Acetyl-5,5-dimethylcyclohexen-2-one				828.8			861.2			0	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	10.1	828.7							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M) PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M) ΔS <sub>p</sub> (M)
[CCl <sub>2</sub> ]	1605-72-7	CCl <sub>2</sub>				828.5			861			0
91PAU/SQU	107-12-0;	threshold value	298						861			
85LIA/KAR	109-74-0	C <sub>2</sub> H <sub>5</sub> CN; n-C <sub>3</sub> H <sub>7</sub> CN				763-768						
78AUS/LIA2	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	801			<801						
[C <sub>3</sub> HNO]	145798-71-6	HNCCCO				828.5			861			0
94FLA/HAV		theory							861			
[C <sub>6</sub> H <sub>14</sub> O]	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				828.1			855.5			17
87TAF	7664-41-7	NH <sub>3</sub>	350	819	9.2	827.0						
86SAN/BAL	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	428	820.5	8.8	828.3						
86SAN/BAL	693-65-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	825.3	4.2	829.5						
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	20.5	831.0						
83CAS/KIM	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	16.3	826.8						
82MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	810.5	16.3	826.8						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	40.6	822.6						
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	45.6	821.3						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	11.2	830.2						
[C <sub>60</sub> ]	99685-96-8	buckminsterfullerene				827.5			NE			NE
91MCE/CAL	7664-41-7;	NH <sub>3</sub> ; 1,2,3,4,5,6-(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>				819-836						
	87-85-4											
[C <sub>70</sub> ]	115383-22-7	[5,6]Fullerene-C <sub>70</sub>				827.5			NE			NE
91MCE/CAL	7664-41-7;	NH <sub>3</sub> ; 1,2,3,4,5,6-(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>				819-836						
	87-85-4											
[C <sub>9</sub> H <sub>8</sub> CrO <sub>3</sub> ]	37908-98-8	3-Cl-4-CH <sub>3</sub> O-C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub>				827.5			858.4			5
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	7.9	827.5						
[C <sub>10</sub> H <sub>16</sub> O]	76-22-2	Camphor				827.3			859.2			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	8.7	827.3						
[C <sub>9</sub> H <sub>8</sub> CrO <sub>3</sub> ]	41311-89-1	(C <sub>3</sub> H <sub>5</sub> )Cr(CO) <sub>3</sub> CH <sub>3</sub>				827.3			859.8			0
81STE/BEA	7664-41-7	NH <sub>3</sub>	320	819	8.4	827.3						
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> ]	89-71-4	2-CH <sub>3</sub> -C <sub>5</sub> H <sub>4</sub> COOCH <sub>3</sub>				827.3			858.3			5
93DEC/ERT	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	338	819.5	9.4	828.9						
93DEC/ERT	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	-2.6	826.6						
93DEC/ERT	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	338	820.5	5.8	826.5						
93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	-1.3	827.3						
[C <sub>9</sub> H <sub>8</sub> O]	4265-25-2	2-methylbenzofuran				827.2			859.6			0
88BOU/DJA	107-86-8	3-methyl-2-butenal	313	825.0	2.1	827.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
[C <sub>6</sub> H <sub>5</sub> O] 94HOK/YAN 80DEF/MCI	2122-46-5	C <sub>6</sub> H <sub>5</sub> O radical kinetic method (i-C <sub>3</sub> H <sub>7</sub> )OC <sub>2</sub> H <sub>5</sub> , (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S				827 827 814-827			857.7				5.8
[C <sub>4</sub> H <sub>10</sub> S] 87TAF 83TAF2 79AUE/BOW	352-93-2 7664-41-7 7664-41-7 7664-41-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S NH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350 298	819 819 819	7.3 7.3 9.3	827.0 825.6 825.6 828.3			856.7				9
[C <sub>6</sub> H <sub>14</sub> O] 87TAF 83TAF2	637-92-3 7664-41-7 7664-41-7	C <sub>2</sub> H <sub>5</sub> O(t-C <sub>4</sub> H <sub>9</sub> ) NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	8.7 8.7	826.9 826.8 826.8			856.0				11
[C <sub>4</sub> H <sub>6</sub> ] 79AUE/BOW	3100-04-7 7664-41-7	1-Methylcyclopropene NH <sub>3</sub>	298	819	7.8	826.9 826.8			856.0				11
[C <sub>5</sub> H <sub>10</sub> ] 79AUE/BOW	16906-27-7 7664-41-7	1-ethenyl-1-methylcyclopropane NH <sub>3</sub>	298	819	7.8	826.9 826.8			856.7				12
[C <sub>9</sub> H <sub>10</sub> O] 96DEC/EXN 96DEC/EXN 96DEC/EXN 86MIS/FUJ2	99-36-5 123-54-6 108-20-3 565-80-0 93-58-3	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub> (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	338 338 338 343	836.8 828.1 820.5 819.5	-7.7 -1.7 5.8 5.9	826.8 828.4 826.9 826.5 825.4			857.7				5
[C <sub>8</sub> H <sub>7</sub> FO] 86MIS/FUJ	403-42-9 98-86-2	4-F-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-2.5	826.8 826.8			858.6				2
[CH <sub>2</sub> N <sub>2</sub> ] 94HOR/GLA 94GLU/SZU 84BEA/EYE 72FOS/BEA	334-88-3 7664-41-7; 4143-41-3	CH <sub>2</sub> NN theory theory See Refs. NH <sub>3</sub> ; (E)-CH <sub>3</sub> N=NCH <sub>3</sub>	298			826.7			858.9 883 883.7 841-866				1
[C <sub>3</sub> H <sub>6</sub> S] 86MAU 83MAU	554-14-3 765-43-5	2-Methylthiophene See Refs. c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600 600		2.9	826.5 826.5			859.0				0
[C <sub>9</sub> H <sub>10</sub> ] 89GAL/SPE	611-15-4	Benzene, 1-ethenyl-2-methyl				826.3 826.3			855.2				12
[C <sub>5</sub> H <sub>10</sub> S] 87TAF	1613-51-0 7664-41-7	Tetrahydrothiopyran NH <sub>3</sub>	350	819	7.8	826.0 826.0			855.8				9

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,7)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>15</sub> H <sub>34</sub> ] 91BUK/GRU	15181-11-0 7664-41-7	1,3-di-(t-C <sub>4</sub> H <sub>9</sub> )-5-CH <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> NH <sub>3</sub>	300	819	7	826.0 826			853.7			16
[C <sub>3</sub> H <sub>8</sub> O] 95CHE/STO	504-63-2 108-67-8	HO(CH <sub>2</sub> ) <sub>2</sub> OH 1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	600	808.6	-6.3	825.9 825.1	836.2	42.7	876.2 878.9	16.2	-81.6	-60 -65.4
[C <sub>9</sub> H <sub>9</sub> Cl] 87TAF	100-42-5 98-86-2	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	600	809.2	-3.9	825.5 827.0	839.5	34.7	874.2 879.1	7.4	-64.4	-57.0 -62.9
[C <sub>9</sub> H <sub>10</sub> O <sub>3</sub> ] 86MIS/FUJ2	5368-81-0 93-58-3	3-CH <sub>3</sub> O-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	6.3	825.8 825.8			856.7			5
[C <sub>9</sub> H <sub>9</sub> Cl] 87TAF	1712-70-5 7664-41-7	4-ClC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	7.3	825.4 825.4			854.3			12
[C <sub>9</sub> H <sub>9</sub> Cl] 83TAF2	7664-41-7	NH <sub>3</sub>	350	819	7.3	825.4						
[C <sub>9</sub> H <sub>9</sub> ClO <sub>2</sub> S] 86MIS/FUJ2	105442-23-7 93-58-3	3-Cl-4-CH <sub>3</sub> S-C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	5.9	825.4 825.4			856.3			5
[C <sub>10</sub> H <sub>22</sub> O] 86SAN/BAL	693-65-2 93-58-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	428	819.5	6.3	825.3 824.2			852.7			17
[C <sub>10</sub> H <sub>22</sub> O] 86SAN/BAL	565-80-0 111-43-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	820.5	4.2	823.7 826.8						
[C <sub>10</sub> H <sub>22</sub> O] 79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	7.3	826.3						
[C <sub>10</sub> H <sub>12</sub> O] 93KUK/STR	2142-76-9 98-86-2	2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	320	829.3	-4	825.2 825.3			857.0			2
[C <sub>7</sub> H <sub>6</sub> F <sub>3</sub> N] 81LAU/NIS	98-16-8 62-53-3	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> NH <sub>2</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-25.5	825.1 825.1			856.9			2
[C <sub>5</sub> H <sub>8</sub> O] 88BOU/DJA	107-86-8 502-49-8	2-methyl-2-butenal cyclooctanone	313	819.6	2.5	825.0 822.2			856.9			2
[C <sub>5</sub> H <sub>8</sub> O] 88BOU/DJA	693-65-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	825.3	2.1	827.6						
[C <sub>8</sub> H <sub>16</sub> O] 87TAF	5857-36-3 7664-41-7	i-C <sub>3</sub> H <sub>7</sub> CO(t-C <sub>4</sub> H <sub>9</sub> ) NH <sub>3</sub>	350	819	6.4	825.0 825.0			856.9			2
[C <sub>8</sub> H <sub>7</sub> ClO] 87TAF	99-91-2 7664-41-7	4-Cl-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub>	350	819	4.6	824.8 823.2			856.6			2
[C <sub>8</sub> H <sub>7</sub> ClO] 86MIS/FUJ	7664-41-7 98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-2.9	826.4						
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 93DEC/ERT	14920-81-1 93-58-3	2,6-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>3</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	338	819.5	-0.8	824.3 818.7			855.3			5
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 93DEC/ERT	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	338	820.5	4.8	825.5						
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 93DEC/ERT	108-20-3	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	-1.7	826.9						
[C <sub>10</sub> H <sub>12</sub> O <sub>2</sub> ] 93DEC/ERT	89-71-4	2-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub>	338	827.3	-1	826.3						

TABLE 2. Summary of proton transfer thermochemical data for each base  $M_i$ , sorted by gas basicity of  $M_i$ —Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>4</sub> H <sub>7</sub> N] 86MAU/KAR	627-36-1 565-80-0; 108-20-3	i-C <sub>3</sub> H <sub>7</sub> NC (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335			824.3 821-828			856.8			0
[C <sub>6</sub> H <sub>5</sub> NO] 80REE/FRE	586-96-9 7664-41-7; 108-20-3	Nitrosobenzene NH <sub>3</sub> , (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				823.6 819-828			854.3			5.8
[C <sub>11</sub> H <sub>16</sub> ] 86STO/LI 86STO/LI	700-12-9 108-67-8 527-53-7	(CH <sub>3</sub> ) <sub>5</sub> -C <sub>6</sub> H 1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> 1,2,3,5-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H <sub>2</sub>	300 300	808.6 816.5	15.1 6.8	823.5 823.7 823.3	836.2 845.6	14.8 5.2	850.7 851.0 850.7	16.2 11.4	1.1 5.3	17.6 17.3 16.7
[C <sub>6</sub> H <sub>10</sub> ] 79AUE/BOW	4549-74-0 7664-41-7	CH <sub>3</sub> CH=C(CH <sub>3</sub> )CH=CH <sub>2</sub> NH <sub>3</sub>	298	819	4.4	823.4 823.4			852.3			12
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> ] 94GRU/CAL	645-09-0 142-96-1; 108-20-3	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				823.2 818-828			854.2			5
[C <sub>7</sub> H <sub>12</sub> ] 86SAN/BAL	82400-17-7 111-43-3	Methylidodecahydride (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	10.5	823.1 823.1			855.6			0
[C <sub>3</sub> H <sub>5</sub> NO <sub>2</sub> ] 92DEC/EXN 92DEC/EXN	546-88-3 108-20-3 110-01-0	Acetamide,N-hydroxy (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O c-C <sub>4</sub> H <sub>8</sub> S	338 338	828.1 819.3	-4.6 2.3	823.0 824.0 821.8			854.0			5
[C <sub>5</sub> H <sub>8</sub> O] 93SZU/MCM 91MAU/SIE 91MAU/SIE 86MAU/LIE 83TAF	765-43-5 115-11-7 753-90-2 7664-41-7 60-29-7 7664-41-7	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O NH <sub>3</sub>	600 600 600 600 350	775.6 812.9 819 801 819	40.2 11.7	823 821.2 822.5 827.3 821.8	802.1 846.8 853.6	52.3 7.9 3.8	854.9 854.4 854.8 857.4	20 -5	-20.1 5.9	2 -0.1 0.9
[C <sub>9</sub> H <sub>16</sub> O] 87TAF	3350-30-9 7664-41-7	c-Nonanone NH <sub>3</sub>	350	819	4.6	822.8 822.8			852.6			9
[C <sub>9</sub> H <sub>8</sub> ] 92MIS/ARI 85MAR/MOD	766-97-2 536-74-3 7664-41-7	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH NH <sub>3</sub>	323 ~300	801.3 819	23.0 1.7	822.5 824.3 820.7			853.2			5.8
[H <sub>4</sub> N <sub>2</sub> ] 84MAU/NEL 84MAU/NEL 84MAU/NEL 75ARN	302-01-2 111-43-3 765-43-5 109-97-7 7664-41-7	H <sub>2</sub> NNH <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub> pyrrole NH <sub>3</sub>	600 600 600 350	810.5 823 843.8 819	8.8 -0.4 -19.7 18.3	822.4 822.6 821.4 823.2 836.7			853.2			5.8

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> S] 86MIS/FUJ2	90721-40-7 93-58-3	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	2.9	822.4 822.4			853.4			5
[C <sub>18</sub> H <sub>30</sub> ] 91BUK/GRU	1460-02-2 123-39-7	1,3,5-(t-C <sub>4</sub> H <sub>9</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub> HCONHCH <sub>3</sub>	300	820.3	2	822.3 822.3			848.8			20
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ] 94DEC/EXN2	6781-42-6 111-43-3	3-CH <sub>3</sub> CO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	810.5	9.6	822.3 820.4			852.0			9
94DEC/EXN2	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	338	818.3	4.3	822.9						
94DEC/EXN2	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	-5.5	823.5						
[C <sub>3</sub> H <sub>8</sub> Ge] 82PIE/HEH	82064-99-1 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> Ge=CH <sub>2</sub> NH <sub>3</sub>	350	819	4.1	822.2 822.2			851.1			12
[C <sub>3</sub> H <sub>6</sub> Se] 89OSA/DEL	76573-19-8 108-20-3	CH <sub>2</sub> =CH-SeCH <sub>3</sub> (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	828.1	-4.6	822.0 823.6			850.9			12
89OSA/DEL	502-49-8	cyclooctanone	313	819.6	0.4	820.0						
[C <sub>6</sub> H <sub>10</sub> O] 94HOK/YAN	2145-21-3	4-F-phenoxy kinetic method				822 822			854.5			0
[C <sub>9</sub> H <sub>18</sub> O] 87TAF	502-56-7 7664-41-7	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> CO NH <sub>3</sub>	350	819	3.2	821.9 821.8			853.7			2
[C <sub>3</sub> H <sub>5</sub> NO] 92ABB/CAN	930-21-2 565-80-0	2-Azetidinone (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	333	820.5	-0.9	821.7 819.7			852.6			5
92ABB/CAN	352-93-2	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> S	333	827.0	-3.7	823.4						
92ABB/CAN	76-22-2	Camphor	333	827.3	-5.0	822.2						
[C <sub>3</sub> H <sub>6</sub> O] 85HOU/ROL	930-27-8 142-96-1	3-methylfuran (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	313	818.3	0.8	821.5 819.3			854.0			0
85HOU/ROL	693-65-2	(n-C <sub>3</sub> H <sub>11</sub> ) <sub>2</sub> O	313	825.3	-2.1	823.4						
[C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> ] 87TAF	1467-79-4 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> NCN NH <sub>3</sub>	350	819	7.3	821.4 825.7			852.1			6
86MAR/TOP	74-90-8	HCN	300	681.6	136.4	818.0						
86MAR/TOP	78-82-0	1-C <sub>3</sub> H <sub>7</sub> CN	300	772.8	48.1	821.0						
[C <sub>10</sub> H <sub>10</sub> O <sub>3</sub> ] 87TAF	13031-43-1 7664-41-7	4-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub>	350	819	2.3	821.3 820.9			853.2			2
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-7.5	821.7						
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ] 93DEC/EXN2	1009-61-6 142-96-1	4-CH <sub>3</sub> CO-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	338	818.3	2.3	821.0 820.9			850.8			9
94DEC/EXN2	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	-7.5	821.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
94DEC/EXN2	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	338	811.2	6.8	817.8							
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-5.0	824.0							
[C <sub>12</sub> H <sub>10</sub> ] 80MAU	83-32-9 7664-41-7	Acenaphthene NH <sub>3</sub>	550	819	5.0	821.0			851.7				5.8
[C <sub>22</sub> H <sub>14</sub> ] 80MAU	213-46-7 7664-41-7	Picene NH <sub>3</sub>	550	819	4.6	820.6			851.3				5.8
[C <sub>9</sub> H <sub>10</sub> ] 89GAL/SPE	100-80-1	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CH=CH <sub>2</sub>				820.6			849.4				12
[C <sub>7</sub> H <sub>4</sub> O] 87TAF	565-80-0 7664-41-7	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO NH <sub>3</sub>	350	819	1.8	820.5			850.3				9
86SAN/BAL	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	428	819.5	1.7	820.7							
86SAN/BAL	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	428	818.3	2.1	821.4							
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	12.1	823.6							
83TAF	87-85-4	(CH <sub>3</sub> ) <sub>6</sub> -C <sub>6</sub>	350	836.0	-17.8	819.0							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	33.9	816.0							
[C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ] 90WOL/GRU	623-43-8 110-71-4	CH <sub>3</sub> CH=CHCOOCH <sub>3</sub> CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OCH <sub>3</sub>	320	820.2	0.6	820.4			851.3				5
[C <sub>7</sub> H <sub>8</sub> ] 86HOU/SCH	121-46-0 7664-41-7	Bicyclo[2.2.1]hepta-2,5-diene NH <sub>3</sub>	323	819	1.7	820.3			849.3				11.5
[C <sub>2</sub> H <sub>5</sub> NO] 81BRO/ABB	123-39-7 67-64-1	HCONHCH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	38.1	820.3			851.3				5
[C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ] 84SHA/BLA	110-71-4	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OCH <sub>3</sub>				820.2							
83MAU	372-48-5	2-F-pyridine	500	852.7	-33.9	822.8			858.0				-18
83MAU	624-89-5	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub>	600	815.3	-1.5	820.4			861.2				-19
83MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	600	810.5	-3.3	817.7			854.0				-11
[C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> ] 86SUN/KUL	56-81-5	HOCH <sub>2</sub> CH(OH)CH <sub>2</sub> OH See Refs.	300			820			874.8				-75
[C <sub>8</sub> H <sub>8</sub> O] 87TAF	104-87-0 7664-41-7	4-(CH <sub>3</sub> )C <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub>	350	819	1.4	820.0			851.8				2
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	1.4	820.0							
[C <sub>10</sub> H <sub>7</sub> CrO <sub>3</sub> ] 81STE/BEA	32984-97-7 7664-41-7	(C <sub>8</sub> H <sub>5</sub> CH <sub>2</sub> )Cr(CO) <sub>3</sub> NH <sub>3</sub>	320	819	1	819.9			852.4				0
[C <sub>10</sub> H <sub>10</sub> ] 92MIS/ARI	6366-06-9 536-74-3	3,6-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>3</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	18.4	819.7			850.4				5.8

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(R)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(R)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (R)
[C <sub>9</sub> H <sub>8</sub> ]	95-13-6	indene				819.6			848.8			11
91MAU/SIE	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	14.2	820.6	836.8	11.3	848.1	9	5.0	14.0
91MAU/SIE	100-42-5	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	600	809.2	12.1	820.3	839.5	15.1	854.5	7.4	-5.0	2.4
89KAF/MAU	100-42-5	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	570	809.2	11	819.2	839.5	15.1	854.6	7.4	-5	2.4
89KAF/MAU	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	570	807	12.7	819.2	836.8	11.3	848.1	9	5	14
89KAF/MAU	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	570	829.3	-7.8	819.0	861.1	-10.8	850.3	2	3.8	5.8
[C <sub>8</sub> H <sub>14</sub> O]	502-49-8	cyclooctanone				819.6			849.4			9
84BOU/HOU	502-42-1	cycloheptanone	300	815.9	3.8	819.6						
[C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> ]	290-87-9	1,3,5-Triazine				819.6			848.8			11
79MAU	75-04-7	C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	550	878	-54.4	819.6						
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>				819.5			850.5			5
93DEC/ERT	108-20-3	(t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	828.1	-9.5	819.1						
93DEC/ERT	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	338	829.3	-9	820.2						
93DEC/ERT	565-80-0	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	338	820.5	-1.9	818.8						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-2.7	815.7						
86SAN/BAL	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	428	818.3	0.8	820.6						
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	10.5	822.5						
86SAN/BAL	598-98-1	t-C <sub>4</sub> H <sub>9</sub> -COOCH <sub>3</sub>	428	814.2	5.4	819.7						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	29.7	811.9						
[C <sub>6</sub> H <sub>10</sub> F <sub>3</sub> NO]	400-59-9	CF <sub>3</sub> CONH(n-C <sub>4</sub> H <sub>9</sub> )				819.4			850.3			5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	0.9	819.3						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	0.9	819.3						
[C <sub>4</sub> H <sub>8</sub> S]	110-01-0	c-C <sub>4</sub> H <sub>9</sub> S				819.3			849.1			9
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	5.9	817.1						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	2.3	820.5						
83CAS/KIM	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	9.6	820.3						
[C <sub>12</sub> H <sub>8</sub> ]	259-79-0	Biphenylene				819.2			848.2			11.5
80MAU	7664-41-7	NH <sub>3</sub>	550	819	4.6	819.1						
[C <sub>8</sub> H <sub>8</sub> O <sub>3</sub> ]	19438-10-9	3-HO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				819.1			850.0			5
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-0.8	818.7						
[HNSI]	14515-04-9	SINH				819.0			853.2			-5.8
88WLO/ROD	7664-41-7	NH <sub>3</sub>	295	819	0	819.0						
[H <sub>3</sub> N]	7664-41-7	NH <sub>3</sub>				819			853.6			-6.4
97EAS/SMI		theory	298						853.1			-6.4
96MAR/LEE		theory	298						853.6			
93SMI/RAD		theory	298									



TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
93SMU/RAD		theory	600						858.8				
93SMU/RAD		theory	0						847.4				
93DEL		theory	298						852.3				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	0	819							
87POP/CUR		theory	298										
86TAF/GAL	7664-41-7	NH <sub>3</sub>	300	819	0	819							
84JEN/MOR		Sec Refs.	298						857.7				
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	0	819							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	0	819							
83LOC/MCI	7664-41-7	NH <sub>3</sub>	350	819	0	819							
82PIE/HEH	7664-41-7	NH <sub>3</sub>	350	819	0	819							
80MAU	7664-41-7	NH <sub>3</sub>	550	819	0	819							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	34.7	811.4							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	0	819			851.8				
79CEY/TIE		threshold value											
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	0	819							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	0	819							
75TAF	7664-41-7	NH <sub>3</sub>	350	819	0	819							
73YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	0	819							
72HEN/TAA	7664-41-7	NH <sub>3</sub>	350	819	0	819							
72ARN/JON	7664-41-7	NH <sub>3</sub>	350	819	0	819							
[C <sub>3</sub> H <sub>5</sub> N]	624-79-3	C <sub>2</sub> H <sub>5</sub> NC				818.9			851.3			0	
86MAU/KAR	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	335	818.3	0	818.9							
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ]	765-87-7	c-hexane-1,2-dione				818.9			849.6			5.8	
87BOU/HOP	502-49-8	cyclooctanone	313	819.6	-3.8	815.9							
87BOU/HOP	693-65-2	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	825.3	-2.5	822.9							
87BOU/HOP	108-94-1	cyclohexanone	313	811.2	3.8	815.0							
87BOU/HOP	1634-04-4	t-C <sub>4</sub> H <sub>9</sub> OCH <sub>3</sub>	313	812.4	1.3	813.7							
83MAU	111-47-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> S	600	834.9	-15.9	820.0							
83MAU	624-89-5	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub>	600	815.3	10.5	825.2							
[CH <sub>3</sub> N]	2053-29-4	CH <sub>2</sub> =NH				818.7			852.9			-5.8	
96BOU/SAL2	108-20-3;	(i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O; CH <sub>3</sub> COCH <sub>2</sub> COCH <sub>3</sub>				828-837							
	123-54-6												
	100-42-5;	C <sub>6</sub> H <sub>5</sub> CH=CH <sub>2</sub> ; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				809-828							
	108-20-3												
83TAF2													
[C <sub>4</sub> H <sub>12</sub> O]	1003-17-4	2,2-Dimethyltetrahydrofuran				818.5			847.7			11	
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	36.4	818.5							
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ]	54210-33-2	1-methyl-5-nitropyrazole				818.4			850.3			2	
92ABB/CAB	110-01-0	c-C <sub>4</sub> H <sub>6</sub> S	333	819.3	-2.3	817.3							
92ABB/CAB	108-94-1	cyclohexanone	333	811.2	7.3	818.7							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
92ABB/CAB	123-19-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO	333	815.3	3.7	819.2							
[C <sub>8</sub> H <sub>18</sub> O]	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O				818.3			845.7			17	
86SAN/BAL	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	428	811.2	8.4	818.0							
86SAN/BAL	598-98-1	t-C <sub>4</sub> H <sub>9</sub> -COOCH <sub>3</sub>	428	814.2	4.2	816.9							
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	9.6	820.1							
82MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	810.5	5.9	816.3							
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	1.0	820.0							
[C <sub>4</sub> H <sub>6</sub> F <sub>3</sub> NO]	1547-87-1	CF <sub>3</sub> CON(CH <sub>3</sub> ) <sub>2</sub>				818.0			849.0			5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-0.5	818.0							
[CH <sub>3</sub> P]	593-54-4	CH <sub>3</sub> PH <sub>7</sub>				817.6			851.5			-5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-1.4	817.6							
74STA/BEA	7664-41-7	NH <sub>3</sub>	320	819	-1.3	817.7							
[C <sub>20</sub> H <sub>20</sub> ]	4493-23-5	dodecahedrane				817.5			843.8			20.6	
86SAN/BAL	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	428	819.5	-1.7	815.8							
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	8.8	818.8							
[C <sub>3</sub> H <sub>6</sub> ]	3907-06-0	3,3-Dimethylcyclopropene				817.1			847.8			5.8	
76AUE/DAV	7664-41-7	NH <sub>3</sub>	298	819	-2.0	817.1							
[C <sub>6</sub> H <sub>10</sub> O]	279-49-2	Bicyclo[2.2.1]heptane,7-oxa				816.8			844.2			17	
86HOU/SCH	7664-41-7	NH <sub>3</sub>	323	819	-1.7	816.8							
[C <sub>3</sub> H <sub>3</sub> NO]	288-14-2	Isooxazole				816.8			848.6			2	
86MAU/LIE	60-29-7	(C <sub>2</sub> H <sub>3</sub> ) <sub>2</sub> O	600	801	11.3	816.8							
[C <sub>3</sub> H <sub>6</sub> OS]	21119-13-1	CH <sub>3</sub> C(=S)OCH <sub>3</sub>				816.5			846.0			10	
83CAS/KIM	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	5.9	816.5							
[C <sub>10</sub> H <sub>14</sub> ]	527-53-7	1,2,3,5-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H <sub>2</sub>				816.5			845.6			11.4	
86STO/LI	108-67-8	1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	300	808.6	7.9	816.5		9.2	845.4	16.2	-4.5	11.7	
[C <sub>6</sub> H <sub>18</sub> OSi <sub>2</sub> ]	107-46-0	(CH <sub>3</sub> ) <sub>3</sub> SiOSi(CH <sub>3</sub> ) <sub>3</sub>				816.2			846.4			7.8	
87LI/STO	527-53-7	1,2,3,5-(CH <sub>3</sub> ) <sub>4</sub> -C <sub>6</sub> H <sub>2</sub>	300	816.5	0.8	817.3		0	845.6	11.4	-2	9.4	
87LI/STO	108-67-8	1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	300	808.6	7.3	815.9		10.5	846.6	16.2	-10.5	5.7	
87LI/STO	108-38-3	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	300	786.2	29.3	815.5		33.5	845.6	22	-13.8	8.2	
75PIT/BUR	60-29-7; 108-20-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				801-828							
[C <sub>7</sub> H <sub>12</sub> O]	502-42-1	cycloheptanone				815.9			845.6			9	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-5.0	813.2							
84BOU/HOU	142-96-1	(n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O	300	818.3	0.2	818.5							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/sqib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
[C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	54210-32-1 565-80-0 108-94-1	1-methyl-3-nitropyrazole (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO cyclohexanone	333 333	820.5 811.2	-5.2 4.4	815.7 815.5 815.8			847.6			2
[C <sub>6</sub> H <sub>10</sub> O] 89KEN/PAC	286-20-4 75-97-8; 765-43-5	Cyclohexene oxide pinacolone; c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>				815.6 808-823			848.1			0
[C <sub>7</sub> H <sub>16</sub> O] 86HOU/SCH	497-38-1 7664-41-7	Bicyclo[2.2.1]heptan-2-one NH <sub>3</sub>	323	819	-3.3	815.5 815.5			847.4			2
[C <sub>14</sub> H <sub>18</sub> ] 80MAU	5325-97-3 7664-41-7	1,2,3,4,5,6,7,8-Octahydrophenanthrene NH <sub>3</sub>	523	819	-0.8	815.5 815.4			846.2			5.8
[C <sub>7</sub> H <sub>14</sub> O] 92ABB/CAB 87TAF	123-19-3 108-94-1 7664-41-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO cyclohexanone NH <sub>3</sub>	333 350	811.2 819	3.3 -2.3	815.3 814.6 815.9			845.0			9
[C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> ] 87TAF 83TAF	4630-82-4 7664-41-7 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> COOCH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-3.2 -3.2	815.3 815.2 815.2			846.2			5
[C <sub>3</sub> H <sub>8</sub> S] 87TAF 83TAF 79AUE/BOW	624-89-5 7664-41-7 7664-41-7 7664-41-7	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350 298	819 819 819	-4.1 -4.1 -2.9	815.3 814.4 814.4 816.1			846.5			4
[C <sub>8</sub> H <sub>7</sub> ClO] 86MIS/FUJ	99-02-5 98-86-2	3-Cl-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-14.2	815.1 815.1			846.9			2
[C <sub>3</sub> H <sub>6</sub> CINO] 87TAF	96-30-0 7664-41-7	ClCON(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	-3.7	814.8 814.8			845.8			5
[C <sub>14</sub> H <sub>18</sub> ] 80MAU	1079-71-6 7664-41-7	1,2,3,4,5,6,7,8-Octahydroanthracene NH <sub>3</sub>	519	819	-1.7	814.7 814.7			845.4			5.8
[C <sub>4</sub> H <sub>12</sub> OSi] 75PIT/BUR	1825-61-2 60-29-7; 108-20-3	(CH <sub>3</sub> ) <sub>2</sub> SiOCH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				814.6 801-828			847.0			0
[C <sub>4</sub> H <sub>4</sub> Si <sub>2</sub> ] 75PIT/BUR	3277-26-7 60-29-7; 108-20-3	((CH <sub>3</sub> ) <sub>2</sub> SiH) <sub>2</sub> O (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				814.6 801-828			845.3			5.8
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O <sub>3</sub> ] 87TAF	619-80-7	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CONH <sub>2</sub>				814.4			845.3			5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
94GRU/CAL	111-43-3; 142-96-1	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O; (n-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> O				810-818							
[C <sub>10</sub> H <sub>10</sub> O <sub>4</sub> ]	1459-93-4	3-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				814.3			843.5			10.8	
94DEC/EXN2	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	338	811.2	2	812.9							
94DEC/EXN2	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	810.5	4.9	815.6							
[C <sub>2</sub> H <sub>12</sub> O <sub>2</sub> ]	598-98-1	i-C <sub>4</sub> H <sub>9</sub> -COOCH <sub>3</sub>				814.2			845.2			5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-7.3	811.1							
86SAN/BAL	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	428	811.2	3.3	814.5							
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	5.0	817.0							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-7.3	811.1							
[Si]	7440-21-3	Si				814.1			837			32	
84ELK/ARM		See Refs.							837±4				
[C <sub>10</sub> H <sub>12</sub> ]	6921-43-3	Benzene, 1-cyclopropyl-4-methyl-				813.8			846.3			0	
89GAL/SPE						813.8							
[C <sub>8</sub> H <sub>7</sub> FO]	455-36-7	3-F-C <sub>6</sub> H <sub>4</sub> COCH <sub>3</sub>				813.8			845.7			2	
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-15.5	813.8							
[C <sub>2</sub> H <sub>12</sub> O]	625-54-7	C <sub>2</sub> H <sub>5</sub> O(i-C <sub>3</sub> H <sub>7</sub> )				813.5			842.7			11	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-4.1	814.0							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	30.5	812.6							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-4.1	814.0							
[C <sub>7</sub> H <sub>6</sub> O]	694-98-4	Bicyclo[2.2.1]hept-2-ene-5-one				813.4			845.3			2	
86HOU/SCH	7664-41-7	NH <sub>3</sub>	323	819	-5.4	813.4							
[C <sub>18</sub> H <sub>15</sub> Sb]	603-36-1	(C <sub>6</sub> H <sub>5</sub> ) <sub>3</sub> Sb				813.1			845.5			0	
86TRA/MUN	100-66-3; 7664-41-7	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub> ; NH <sub>3</sub>				807-819							
[C <sub>7</sub> H <sub>12</sub> O]	589-92-4	4-methylcyclohexanone				813.0			844.9			2	
84BOU/HOU	589-38-8	3-hexanone	300	811.3	1.7	813.0							
[C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> ]	541-42-4	i-C <sub>3</sub> H <sub>7</sub> ONO				813			845.5			0	
78FAR/MCM	96-22-0; 7664-41-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; NH <sub>3</sub>				807-819							
[C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> N]	753-90-2	CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>				812.9			846.8			-5	
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600				853.6	-4.2	849.4				
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	31.8	814.9	802.1	42.7	844.8	20	-18.0	2.0	
91MAU/SIE	75-18-3	(CH <sub>3</sub> ) <sub>2</sub> S	600	801.2	9.2	814.6	830.9	18.0	848.9	9.1	-14.6	-5.5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-8.7	810.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0(R)$	$\Delta \Delta S_p^0(M,R)$	$\Delta S_p^0(M)$
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-8.7	810.2						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-7.3	811.7						
77STA/TAA	7664-41-7	NH <sub>3</sub>	320	819	-7.9	811.0						
75TAF	7664-41-7	NH <sub>3</sub>	350	819	-6.9	812.1						
75ARN	7664-41-7	NH <sub>3</sub>	350	819	-6.9	812.1						
[C <sub>8</sub> H <sub>7</sub> Cl]	2039-85-2	3-ClC <sub>8</sub> H <sub>7</sub> CH=CH <sub>2</sub>				812.6			841.5			12
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-5.5	812.6						
[C <sub>8</sub> H <sub>12</sub> ]	694-92-8	2-Methylbicyclo[2.2.1]hept-2-ene				812.5			846			0
76SOL/FIE	See Refs.		300						845±6			
[CH <sub>3</sub> N <sub>2</sub> ]	26981-93-1:a	CH <sub>3</sub> N=NH at terminal N				812.5			845			0
92GAR/RUT	theory								845			
[C <sub>3</sub> H <sub>12</sub> O]	1634-04-4	t-C <sub>3</sub> H <sub>7</sub> OCH <sub>3</sub>				812.4			841.6			11
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-9.6	808.5						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-10.1	808.1						
82MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	810.5	0.8	811.5						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-2.0	817.1						
75PIT/BUR	60-29-7; 108-20-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O, (t-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				801-828						
[CH <sub>2</sub> NO]	67-62-9	CH <sub>3</sub> ONH <sub>2</sub>				812.3			844.8			0
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-6.4	812.3						
[C <sub>10</sub> H <sub>10</sub> O <sub>2</sub> ]	120-61-6	4-CH <sub>3</sub> COO-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				812.3			843.2			5
94DEC/EXN2	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	338	801	11.1	812.6						
94DEC/EXN2	2868-37-3	c-C <sub>3</sub> H <sub>5</sub> COOCH <sub>3</sub>	338	811.2	0.5	811.7						
94DEC/EXN2	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	338	810.5	1.6	812.5						
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-7.1	812.4						
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ]	591-31-1	3-CH <sub>3</sub> OC <sub>6</sub> H <sub>4</sub> CHO				812.2			844.1			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-6.4	812.2						
[C <sub>5</sub> H <sub>8</sub> O]	6038-09-1	2-methyl-2-butenal(Z)				812.1			843.9			2
88BOU/DIA	589-38-8	3-hexanone	313	811.3	0.8	812.1						
88BOU/DIA	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	313	810.5	2.1	812.8						
88BOU/DIA	589-92-4	4-methylcyclohexanone	313	813.0	-1.7	811.3						
[C <sub>5</sub> H <sub>10</sub> O]	96-47-9	c-C <sub>4</sub> H <sub>7</sub> O(2-CH <sub>3</sub> )				811.6			840.8			11
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-5.9	812.2						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	28.9	811.0						
[C <sub>6</sub> H <sub>12</sub> O]	589-38-8	3-hexanone				811.3			843.2			2
84BOU/HOU	108-94-1	cyclohexanone	300	811.2	0	811.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>7</sub> H <sub>14</sub> O] 87TAF	931-56-6 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-6.9	811.3 811.3			840.5			11
[C <sub>3</sub> H <sub>8</sub> O] 84BOU/HOP	814-78-8 111-43-3	CH <sub>3</sub> C(=O)C(=CH <sub>2</sub> )CH <sub>3</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	0.4	811.3 811.3			843.1			2
[C <sub>6</sub> H <sub>10</sub> O] 87TAF	108-94-1 7664-41-7	cyclohexanone NH <sub>3</sub>	350	819	-7.3	811.2 810.9			841.0			9
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	-7.3	810.9						
84BOU/HOU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	300	810.5	0.4	810.9						
84BOU/HOU	502-42-1	cycloheptanone	300	815.9	-3.8	812.1						
83MAU	624-89-5	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub>	600	815.3	4.2	817.9						
83MAU	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	10.5	817.5						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1		810.4						
79SAL/KEB	100-66-3	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub>	560	807.2	7.9	812.8						
[C <sub>3</sub> H <sub>8</sub> O] 87TAF	2868-37-3 7664-41-7	c-C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub> NH <sub>3</sub>	350	819	-6.9	811.2 811.6			842.1			5
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	1.7	813.7						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-6.9	811.6						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	25.9	808.2						
[C <sub>8</sub> H <sub>8</sub> O] 86MIS/FUJ2	1126-46-1 93-58-3	4-Cl-C <sub>6</sub> H <sub>4</sub> COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-8.4	811.1 811.1			842.1			5
[C <sub>12</sub> H <sub>15</sub> O] 92NAK/NOM	146558-43-2 141-78-6	α-t-butylstyrene,3-Cl CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	343	804.7	7.5	811.0 811.9			839.8			12
92NAK/NOM	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	343	810.5	0	810.7						
92NAK/NOM	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	343	807	3.8	810.6						
[C <sub>4</sub> H <sub>8</sub> O] 87TAF	623-53-0 7664-41-7	C <sub>2</sub> H <sub>5</sub> OCCOCH <sub>3</sub> NH <sub>3</sub>	350	819	-7.8	810.8 810.8			842.7			2
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-7.8	810.8						
[C <sub>9</sub> H <sub>9</sub> F] 87TAF	3825-81-8 7664-41-7	3-FC <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	-7.3	810.8 810.8			839.7			12
[C <sub>9</sub> H <sub>10</sub> O] 93SZU/MCM	103-79-7 96-22-0	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> COCH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	1.7	810.8 810.8			842.6			2
[C <sub>9</sub> H <sub>8</sub> ] 92MIS/ARI	766-82-5 536-74-3	3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	9.2	810.6 810.6			843.0			0
[C <sub>6</sub> H <sub>10</sub> O] 87TAF	111-43-3 7664-41-7	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O NH <sub>3</sub>	350	819	-7.8	810.5 810.1			837.9			17

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>i</sub>, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (R)
86SAN/BAL	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	428	810.5	0	810.5							
83CAS/KIM	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	323	810.5	0	810.5							
82MAU	111-43-3	(n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O	335	810.5	0	810.5							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	23.0	805.0							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	29.3	805.0							
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-3.9	815.1							
[C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> ]	2237-30-1	3-NH <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CN				810.4			842.3				2
81LAU/NIS	62-53-3	C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-40.2	810.4							
[C <sub>8</sub> H <sub>7</sub> FO <sub>2</sub> ]	403-33-8	4-F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				810.3			841.3				5
86MIS/FUJ2	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-9.2	810.3							
[C <sub>18</sub> H <sub>12</sub> ]	218-01-9	Chrysene				810.1			840.9				5.8
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-5.9	810.1							
[C <sub>13</sub> H <sub>16</sub> F]	14658-44-3	α-4-butylstyrene,3-F				809.9			838.8				12
92NAK/NOM	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	343	807	2.9	809.8							
92NAK/NOM	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	343	804.7	5.9	810.3							
[C <sub>8</sub> H <sub>7</sub> Br]	2039-82-9	4-Br-C <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>				809.8			838.7				12
84HAR/HOU	7664-41-7	NH <sub>3</sub>	323	819	-8.8	809.8							
[C <sub>9</sub> H <sub>11</sub> ]	19019-92-2	C <sub>6</sub> H <sub>5</sub> (CHC <sub>2</sub> H <sub>5</sub> ) radical				809.7			842.2				0
82MAU	96-22-0;	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO;(t-C <sub>4</sub> H <sub>9</sub> )OCH <sub>3</sub>				807-812							
	1634-04-4												
[C <sub>9</sub> H <sub>11</sub> ]	16804-70-9	C <sub>6</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub> radical				809.7			842.2				0
82MAU	96-22-0;	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO;(t-C <sub>4</sub> H <sub>9</sub> )OCH <sub>3</sub>				807-812							
	1634-04-4												
[C <sub>8</sub> H <sub>14</sub> O]	823-76-7	e-C <sub>6</sub> H <sub>11</sub> COCH <sub>3</sub>				809.5			841.4				2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-9.2	809.4							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-9.2	809.4							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	26.8	809.1							
[C <sub>8</sub> H <sub>8</sub> ]	100-42-5	C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>				809.2			839.5				7.4
91MAU/SIE	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	26.4	808.9			835.8				12.9
91MAU/SIE	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	3.8	811.2			838.4				12.3
89KAF/MAU	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	570	782.1	26.2	808.7			835.8				12.9
89KAF/MAU	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	570	807	3.6	811.0			838.5				12.3
89KAF/MAU	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	570	829.3	-20.6	807.2			838.1				6.2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-10.5	807.8			838.1				
84HAR/HOU	7664-41-7	NH <sub>3</sub>	323	819	-5.0	813.7							
75WOL/HAR	7664-41-7	NH <sub>3</sub>	350	819	-11.0	807.3							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y+Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>9</sub> H <sub>12</sub> ]	108-67-8	1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>				808.6			836.2			16.2
86STO/LI	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	300	804.7	4.8	809.5	835.7	1.5	837.1	5	11.2	16.2
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-5.9	807.5						
76DEV/WOL	71-43-2	C <sub>6</sub> H <sub>6</sub>	350	725.4	82.4	808.2						
[H <sub>2</sub> OSi]	22755-01-7:a	H <sub>2</sub> SiO at O theory	298			808.5			841			0
93LUC/CUR									841			
[C <sub>6</sub> H <sub>4</sub> ]	462-80-6	ortho-benzynes				808.5			841			0
91GUO/GRA		See Refs.	300						841			
80POL/HEH	107-47-1; 687-48-9	(t-C <sub>4</sub> H <sub>9</sub> ) <sub>2</sub> S; (CH <sub>3</sub> ) <sub>2</sub> NCOOC <sub>2</sub> H <sub>5</sub>				864-866						
[CH <sub>4</sub> N <sub>2</sub> ]	26981-93-1:b	CH <sub>3</sub> N=NH at interior N theory				808.5			841			0
92GAR/RUT									841			
[C <sub>6</sub> H <sub>2</sub> O]	75-97-8	t-C <sub>4</sub> H <sub>9</sub> COCH <sub>3</sub>				808.2			840.1			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-9.2	809.4						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-9.6	809.0						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	24.3	806.5						
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	96-48-0	$\gamma$ -Butyrolactone				808.1			840.0			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-10.5	808.1						
[C <sub>8</sub> H <sub>8</sub> O]	620-23-5	3-CH <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO				808.1			840.0			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-10.5	808.1						
[C <sub>6</sub> H <sub>6</sub> ]	628-41-1	1,4-c-C <sub>6</sub> H <sub>8</sub>				808.0			837			11.5
83GAU/HOU		See Refs.							837			
[C <sub>10</sub> H <sub>12</sub> ]	27546-46-9	Benzene, 1-cyclopropyl-2-methyl- See Refs.				807.9			840.4			0
89GAL/SPE						807.9						
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ]	118-90-1	Benzoic acid, 2-methyl				807.8			838.8			5
91NOU/COO	563-80-4; 108-94-1	3-methyl-2-butanone; c-hexanone				804-811						
[C <sub>6</sub> H <sub>10</sub> ]	513-81-5	CH <sub>2</sub> =C(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub>				807.8			835.0			17.8
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-11.2	807.8						
[H <sub>2</sub> OSi]	83892-34-6	HSiOH at Si theory	298			807.5			840			0
93LUC/CUR									840			
[C <sub>9</sub> H <sub>10</sub> ]	766-90-5	Benzene, cis-(2-methylethenyl)				807.5			836.4			12
89GAL/SPE						807.5						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>3</sub> H <sub>8</sub> ] 76AUE/DAV	1489-60-7 7664-41-7	1-Methylcyclobutene NH <sub>3</sub>	298	819	-11.7	807.3			841.5			-5.8
[C <sub>6</sub> H <sub>10</sub> ] 76AUE/DAV	1501-58-2 7664-41-7	1,2-Dimethylcyclobutene NH <sub>3</sub>	298	819	-11.7	807.3			838.0			5.8
[C <sub>5</sub> H <sub>8</sub> O] 88BOU/DJA	1576-87-0 109-60-4	2-pentenal(E) CH <sub>3</sub> COOC <sub>3</sub> H <sub>7</sub>	313	805.6	1.3	807.2			839.0			2
88BOU/DJA	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	313	807	-0.4	806.7						
88BOU/DJA	557-31-3	C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CH=CH <sub>2</sub>	313	804.5	3.3	807.9						
[C <sub>7</sub> H <sub>8</sub> O] 81LAU/NIS	100-66-3 62-53-3	C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-41.0	807.2			839.6			0
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-11.3	810.2						
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	650	725.4	71.2	805.5						
[C <sub>5</sub> H <sub>10</sub> O] 93SZU/MCM	96-22-0 115-11-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	25.1	807			836.8			9
93SZU/MCM	7664-41-7	NH <sub>3</sub>	600	819	-5.9	804.0	802.1	32.2	834.3	20	-12.1	7.9
93SZU/MCM	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600	823	-15.1	808.5	853.6	-18.0	835.6	-6.4	20.5	14.1
91SZU/MCM	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	300	775.6	28.5	805.8	854.9	-20.5	834.4	2	9.6	11.6
91SZU/MCM	7664-41-7	NH <sub>3</sub>	300	819	-11.7	804.1	802.1	32.2	834.3	20	-12.1	7.9
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600	819	-8.8	807.3	853.6	-18.0	835.6	-6.4	20.5	14.1
91MAU/SIE	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	600	790.7	16.3	805.6	853.6	-21.8	831.8	-6.4	21.8	15.4
91MAU/SIE	90-12-0	1-methylnaphthalene	600	805.3		805.8	821.6	18.8	840.5	5	-4.2	0.8
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	26.4	805.3	834.8	11.7	846.5			
91MAU/SIE	75-18-3	(CH <sub>3</sub> ) <sub>2</sub> S	600	801.2	4.6	805.8	802.1	31.0	833.1	20	-7.5	12.5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-11.9	806.3	830.9	7.5	838.4	9.1	-5.0	4.1
84BOU/HOU	108-94-1	cyclohexanone	300	811.2	-3.8	807.5						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-12.8	805.4						
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	25.1	801.2						
[C <sub>6</sub> H <sub>12</sub> O] 87TAF	592-90-5 7664-41-7	c-C <sub>6</sub> H <sub>12</sub> O(Oxepane) NH <sub>3</sub>	350	819	-12.4	806.8			834.2			17
83MAU	624-89-5	CH <sub>3</sub> SC <sub>2</sub> H <sub>5</sub>	600	815.3	1.3	805.5						
83MAU	142-68-7	c-C <sub>5</sub> H <sub>10</sub> O	600	795.4	7.9	812.6						
83MAU	109-99-9	Tetrahydrofuran	600	794.7	11.3	803.3						
[C <sub>2</sub> H <sub>3</sub> N] 86MAU/KAR	593-75-9 96-22-0	CH <sub>3</sub> NC (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	335	807	-7.5	806.6			839.1			0.1
86MAU/KAR	109-99-9	Tetrahydrofuran	335	794.7	-0.4	799.8						
86KNI/FRE	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	303	801	5.0	794.9						
81AUE/PED	753-90-2	CF <sub>3</sub> CH <sub>2</sub> NH <sub>2</sub>	298	812.9	-5.4	806.1						
81AUE/PED	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	298	804.7	1.7	807.5						
[C <sub>3</sub> H <sub>5</sub> O] #1169	#1169	•CH <sub>2</sub> CH <sub>2</sub> CH=CO				806.2			838.6			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
94SMJ/CHY	75-18-3; 108-94-1	(CH <sub>3</sub> ) <sub>2</sub> S; c-C <sub>6</sub> H <sub>10</sub> (=O)	300			801-811							
[C <sub>9</sub> H <sub>8</sub> O <sub>2</sub> ] 91NOU/COO	99-94-5 563-80-4; 96-22-0	Benzoic acid, 4-methyl (i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub> ; C <sub>2</sub> H <sub>5</sub> COC <sub>2</sub> H <sub>5</sub>				805.7 804-807			836.7			5	
[C <sub>3</sub> H <sub>10</sub> O <sub>2</sub> ] 87TAF 83TAF	547-63-7 7664-41-7 7664-41-7	i-C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-12.8 -12.8	805.7 805.6 805.6			836.6			5	
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ] 86KAM/YOU	108-21-4 563-80-4	isopropyl acetate (i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub>	333	804.4	1.3	805.6 805.6			836.6			5	
[C <sub>3</sub> H <sub>10</sub> O <sub>2</sub> ] 80MAU 79LAU	109-60-4 7664-41-7 7664-41-7	CH <sub>3</sub> COOC <sub>3</sub> H <sub>7</sub> NH <sub>3</sub> NH <sub>3</sub>	550 650	819 819	-9.6 -10.4	805.6 806.5 804.6			836.6			5	
[C <sub>3</sub> H <sub>10</sub> O <sub>2</sub> ] 87TAF 80MAU 79MAU	623-42-7 7664-41-7 7664-41-7 75-04-7	C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350 550 550	819 819 878	-14.2 -9.6 -64.0	805.4 804.2 806.5 811.5			836.4			5	
[C <sub>11</sub> H <sub>10</sub> ] 91MAU/SIE 91MAU/SIE 80MAU	90-12-0 67-64-1 96-22-0 7664-41-7	1-methylnaphthalene (CH <sub>3</sub> ) <sub>2</sub> CO (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO NH <sub>3</sub>	600 600 550			805.3	812 836.8	15.1 -11.7	834.8 827.1 825.1			10	
[C <sub>9</sub> H <sub>10</sub> ] 89GAL/SPE 89KAF/MAU 89KAF/MAU	873-66-5 96-22-0 100-42-5	Benzene, trans-(2-methylethenyl) See Refs. (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO C <sub>6</sub> H <sub>5</sub> CHCH <sub>2</sub>	570 500	807 809.2	-2.3 -2.1	803.9 806.2	836.8	-1.3	835.5	9	6.3	15.3	
[C <sub>4</sub> H <sub>7</sub> F <sub>2</sub> N] 87TAF	407-01-2 7664-41-7	(CF <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> NH NH <sub>3</sub>	350	819	-13.7	805.1 805.1			838.1			-2	
[C <sub>3</sub> H <sub>6</sub> S] 87TAF 79AUE/BOW	287-27-4 7664-41-7 7664-41-7	Thietane NH <sub>3</sub> NH <sub>3</sub>	350 298	819 819	-15.6 -11.7	805.0 802.7 807.3			834.8			9	
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O] 86MIS/FUJ	709-63-7 98-86-2	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-24.3	805.0 805.0			836.9			2	
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 93SZUM/MCM	141-78-6 115-11-7	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	23.4	804.7 803.5	802.1	27.6	835.7 829.7	20	-7.1	5	12.9

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M) $\Delta S_p^0$ (M)
93SZU/MCM	765-43-5	c-C <sub>3</sub> H <sub>5</sub> COCH <sub>3</sub>	600	823	-17.6	804.5	854.9	-26.4	828.5	2	14.6	16.6
91SZU/MCM	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	300	775.6	25.5	801.1	802.1	27.6	829.7	20	-7.1	12.9
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600	819	-13.4	802.2	853.6	-23.0	830.6	-6.4	15.9	9.5
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	27.2	807.3	802.1	32.2	834.3	20	-9.2	10.8
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-16.5	802.0						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	18.0	800.2						
80LJA/SO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	22.2	798.4						
79VAJ/HAR	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	373	804.7	0	804.7						
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-14.2	804.8						
77WOLSTA	7664-41-7	NH <sub>3</sub>	350	819	-16.9	801.5						
76YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	-11.3	804.3						
76KEB/YAM	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	804.7	0	804.7						
76HAR/LIN	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	370	782.1	8.4	790.8						
[C <sub>6</sub> H <sub>6</sub> O] 86HOU/SCH	6705-50-6 7664-41-7	Bicyclo[2.2.1]hept-2-ene,7-oxa- NH <sub>3</sub>	323	819	-14.2	804.7 804.6			837.1			0
[C <sub>6</sub> H <sub>6</sub> ] 83GAU/HOU	592-57-4	1,3-c-C <sub>6</sub> H <sub>8</sub> See Refs.				804.5			837 837			0
[C <sub>5</sub> H <sub>10</sub> O] 86BOU/DJA	557-31-3 109-60-4	C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CH=CH <sub>2</sub> CH <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>	313	805.6	-1	804.5 804.5			833.7			11
[C <sub>8</sub> H <sub>7</sub> ClO] 86MIS/FUJ2	2905-65-9 93-58-3	3-Cl-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-15.1	804.4 804.4			835.4			5
[C <sub>5</sub> H <sub>10</sub> O] 87TAF 83TAF	563-80-4 7664-41-7 7664-41-7	(i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-14.2 -14.2	804.4 804.4 804.4			836.3			2
[C <sub>6</sub> H <sub>6</sub> ] 79AUE/BOW	2004-70-8 7664-41-7	(E)CH <sub>3</sub> CH=CHCH=CH <sub>2</sub> NH <sub>3</sub>	298	819	-14.6	804.4 804.4			834.1			9.1
[C <sub>6</sub> H <sub>12</sub> Si] 88HAJ/SQU	754-05-2	(CH <sub>3</sub> ) <sub>3</sub> SiCH=CH <sub>2</sub> See Refs.				804.1			833 833±8			12
[H <sub>2</sub> Si] 86SHI/BEA	13825-90-6 75-18-3; 96- 22-0	SiH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> S; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO				804.1 801-807			839.2			-9.1
[C <sub>7</sub> H <sub>10</sub> ] 86HOU/SCH 79SAL/KEB 79AUE/BOW 77STA/WIE 76SOL/FIE	498-66-8 7664-41-7 100-66-3 7664-41-7 77STA/WIE 76SOL/FIE	Bicyclo[2.2.1]hept-2-ene NH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> OCH <sub>3</sub> NH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O See Refs.	323 560 298 320 300	819 807.2 819 801	-13.4 -6.3 -12.7 2.1	804.0 805.5 800.9 806.3 803.4	839.6 0.4	840.0	836.5	0	-11.7	0 -11.7

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[C <sub>7</sub> H <sub>6</sub> F] 82MAU	2599-73-7 60-29-7; 96- 22-0	3-FC <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> radical (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO				804 801-807			836.5			0
[C <sub>8</sub> H <sub>9</sub> ] 82MAU	2348-51-8 60-29-7; 96- 22-0	C <sub>6</sub> H <sub>5</sub> CHCH <sub>3</sub> radical (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO				804 801-807			836.5			0
[C <sub>13</sub> H <sub>10</sub> ] 80MAU	86-73-7 7664-41-7	Fluorene NH <sub>3</sub>	550	819	-9.6	803.8 803.8			831.5			16
[C <sub>11</sub> H <sub>15</sub> N] 87TAF	23074-42-2 7664-41-7	Tricyclo[3.3.1.1 <sup>3,7</sup> ]decane-1-carbonitrile NH <sub>3</sub>	350	819	-15.1	803.8 803.3			834.4			6
87MAR/GAL 87MAR/GAL	96-22-0 563-80-4	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO (i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub>	350 350	807 804.4	-2.2 -1.2	805.0 803.0						
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O] 87TAF	349-76-8 7664-41-7	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> NH <sub>3</sub>	350	819	-18.3	803.7 800.3			835.6			2
86MIS/FUJ 77POL/WOL	98-86-2 1528-30-9 7664-41-7	C <sub>8</sub> H <sub>5</sub> COCH <sub>3</sub> c-C <sub>3</sub> H <sub>8</sub> =CH <sub>2</sub> NH <sub>3</sub>	343 350	829.3 819	-22.2 -14.6	807.1 803.5 803.4			832.4			12
[C <sub>3</sub> H <sub>4</sub> O] 96BOU/SAL2	6004-44-0 96-22-0; 565-80-0	CH <sub>3</sub> CH=CO (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO; (i-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> CO				803.4 807-821			834.1			6
85TRA 80ARM/HIG	79-20-9	threshold value CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	320	790.7	6.7	797.3			834.1			
[C <sub>10</sub> H <sub>12</sub> ] 89GAL/SPE	19714-73-9	Benzene, 1-cyclopropyl-3-methyl-				803.3 803.3			835.8			0
[C <sub>5</sub> HMnO <sub>5</sub> ] 81STE/BEA	16972-33-1 7664-41-7	(CO) <sub>2</sub> MnH NH <sub>3</sub>	320	819	-15.9	803.0 803.0			835.5			0
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S] 87TAF	38103-96-7 7664-41-7	C <sub>2</sub> H <sub>5</sub> S(OCH <sub>3</sub> )CO NH <sub>3</sub>	350	819	-15.6	802.9 802.9			833.9			5
83TAF2 [C <sub>4</sub> H <sub>6</sub> O] 79VAJ/HAR	7664-41-7 78-94-4 141-78-6	NH <sub>3</sub> CH <sub>2</sub> =CHCOCH <sub>3</sub> CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	350 373	819 804.7	-15.6 -2.1	802.9 802.8 802.8			834.7			2
[C <sub>9</sub> H <sub>10</sub> ] 89GAL/SPE	873-49-4	c-C <sub>3</sub> H <sub>5</sub> -C <sub>6</sub> H <sub>5</sub> See Refs.				802.4 802.4			834.9			0

TABLE 2. Summary of proton transfer thermochemical data for each base  $M_i$ , sorted by gas basicity of  $M_i$ —Continued

[Formula] Y: Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)	$\Delta\Delta$ S <sub>p</sub> (M)
[C <sub>11</sub> H <sub>10</sub> ] 80MAU	91-57-6 7664-41-7	2-Methylnaphthalene NH <sub>3</sub>	550	819	-12.6	802.4 802.3			831.9			10	
[C <sub>7</sub> H <sub>10</sub> O] 86HOU/SCH	10218-02-7 7664-41-7	Bicyclo[2.2.1]heptan-7-one NH <sub>3</sub>	323	819	-16.3	802.4 802.3			832.1			9	
[CH <sub>3</sub> NO] 87TAF	4312-87-2 7664-41-7	HCOONH <sub>2</sub> NH <sub>3</sub>	350	819	-16.5	802.2 802.2			834.7			0	
[C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> ] 92NAK/NOM 92NAK/NOM	146558-45-4 111-43-3 60-29-7	$\alpha$ -t-butylstyrene,3-CF <sub>3</sub> (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	343 343	810.5 801	-9.2 1.7	802.2 801.5 802.9			831.1			12	
[C <sub>2</sub> H <sub>6</sub> O] 87TAF 83TAF 81BRO/ABB 80MAU 79LAU 76LAU/KEB	100-52-7 7664-41-7 7664-41-7 67-64-1 7664-41-7 7664-41-7 71-43-2	C <sub>2</sub> H <sub>5</sub> CHO NH <sub>3</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> CO NH <sub>3</sub> NH <sub>3</sub> C <sub>2</sub> H <sub>6</sub>	350 350 320 550 650 600	819 819 782.1 819 819 725.4	-16.0 -16.0 17.6 -13.4 -13.6 64.4	802.1 802.6 802.6 799.8 803.5 802.5 796.7			834.0			2	
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ] 86MIS/FUJ2	1571-08-0 93-58-3	4-HC(O)-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-17.6	801.9 801.9			832.9			5	
[C <sub>8</sub> H <sub>7</sub> FO] 86MIS/FUJ2	455-68-6 93-58-3	3-F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-17.6	801.9 801.9			832.9			5	
[C <sub>8</sub> H <sub>5</sub> Cl] 92MIS/ARI 85MAR/MOD	873-73-4 536-74-3 109-99-9	4-Cl-C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH Tetrahydrofuran	323 ~300	801.3 794.7	0.4 1.3	801.7 801.7 796.0			832.4			5.8	
[C <sub>9</sub> H <sub>16</sub> O] 87TAF	19752-94-4 7664-41-7	C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-16.9	801.6 801.6			833.5			2	
[CH <sub>4</sub> N] 96AUD/FOS 89HOL/LOS 81MCA/NIC	10507-29-6 60-29-7; 100- 67-64-1; 60-	•CH <sub>2</sub> NH <sub>2</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O; C <sub>6</sub> H <sub>5</sub> CHO See Refs. (CH <sub>3</sub> ) <sub>2</sub> CO; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	298			801.6 801-802 782-801			832.8			4	
[C <sub>3</sub> H <sub>6</sub> S] 79AUE/BOW	1072-43-1 7664-41-7	2-Methylthiirane NH <sub>3</sub>	298	819	-17.6	801.5 801.4			833.3			2	
[C <sub>9</sub> H <sub>7</sub> MnO <sub>3</sub> ] 81STE/BEA	12108-13-3 7664-41-7	(CH <sub>3</sub> C <sub>2</sub> H <sub>4</sub> )Mn(CO) <sub>3</sub> NH <sub>3</sub>	320	819	-17.6	801.3 801.3			833.8			0	
[C <sub>8</sub> H <sub>6</sub> ] 87TAF	536-74-3	C <sub>6</sub> H <sub>5</sub> -CCH				801.3			832.0			5.8	

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>i</sub> sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)		PA(R)		ΔPA(M,R)		PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
	79-20-9	7664-41-7					GB(M)	PA(M)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (M)					
96ZHA/STO	79-20-9	7664-41-7	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	588	790.7	9.2	799.6									
92MIS/ARI	7664-41-7		NH <sub>3</sub>	323	819	-16.7	802.0									
85MAR/MOD	100-52-7		C <sub>6</sub> H <sub>5</sub> CHO	300	802.1	0	802.1									
[C <sub>2</sub> H <sub>6</sub> S]	75-18-3		(CH <sub>3</sub> ) <sub>2</sub> S				801.2						830.9			9.1
97EAS/SMI			theory	298												9.1
93SMI/RAD			theory	600									834.2			
93SMI/RAD			theory	0									825.3			
93SMI/RAD			theory	298									830.9			9.1
91MAU/SIE	7664-41-7		NH <sub>3</sub>	600	819	-16.3	798.0		853.6		-23.0		830.6	-6.4	10.9	4.5
91MAU/SIE	79-20-9		CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	600	790.7	11.7	801.1		821.6		12.1		833.8	5	-0.4	4.6
91MAU/SIE	115-11-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	23.8	802.7		802.1		28.5		830.6	20	-8.8	11.2
87TAF	7664-41-7		NH <sub>3</sub>	350	819	-16.9	801.3									
83TAF	7664-41-7		NH <sub>3</sub>	350	819	-16.9	801.3									
79AUE/BOW	7664-41-7		NH <sub>3</sub>	298	819	-14.6	804.4									
77WOL/STA	7664-41-7		NH <sub>3</sub>	350	819	-16.9	801.3									
[C <sub>4</sub> H <sub>10</sub> ]	34403-06-0		3-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> (CH <sub>2</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>5</sub>				801.0						833.5			0
95CRE/FOR	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO	300	782.1	15.9	798.1									
95CRE/FOR	79-20-9		CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	300	790.7	10.5	801.1									
95CRE/FOR	141-78-6		CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	300	804.7	-0.8	803.9									
[C <sub>4</sub> H <sub>10</sub> O]	60-29-7		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O				801						828.4			17
93SZU/MCM	96-22-0		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	-17	802.9		836.8		-7.1		829.7	9	8.8	17.8
91SZU/MCM	96-22-0		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	300	807	-4.6	802.4		836.8		-7.1		829.7	9	8.8	17.8
87TAF	7664-41-7		NH <sub>3</sub>	350	819	-19.7	798.2									
86MAU/LIE	60-29-7		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	0	801									
86KNI/FRE	7664-41-7		NH <sub>3</sub>	303	819	-10.9	808.1									
86KNI/FRE	60-29-7		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	303	801	0	801									
83TAF	7664-41-7		NH <sub>3</sub>	350	819	-17.8	800.0									
81LAU/NIS	62-53-3		C <sub>6</sub> H <sub>5</sub> NH <sub>2</sub>	600	850.6	-42.3	803.8									
81BRO/ABB	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	14.6	796.6									
80LA/SHO	115-11-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	20.5	796.2									
79AUE/BOW	7664-41-7		NH <sub>3</sub>	298	819	-16.1	802.9									
78DAV/LAU	7664-41-7		NH <sub>3</sub>	600	819	-11.7	800.3									
77WOL/STA	7664-41-7		NH <sub>3</sub>	350	819	-17.8	800.0									
77STA/WIE	60-29-7		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	320	801	0	801									
76HAR/LIN	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO	370	782.1	9.2	790.8									
[C <sub>10</sub> H <sub>10</sub> O]	206-44-0		Fluoranthene				800.9						828.6			16
80MAU	7664-41-7		NH <sub>3</sub>	550	819	-12.6	800.8									
[C <sub>5</sub> H <sub>10</sub> O]	107-87-9		n-C <sub>3</sub> H <sub>7</sub> COCH <sub>3</sub>				800.9						832.7			2
97HOM/HER	78-93-3		CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>	333	795.5	4.8	800.2									
97HOM/HER	60-29-7		(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	333	801	2.8	804.4									
97HOM/HER	547-63-7		1-C <sub>3</sub> H <sub>7</sub> COOCH <sub>3</sub>	333	805.7	-6.2	799.6									

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,7)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
9THOM/HER	75-97-8	t-C <sub>4</sub> H <sub>9</sub> COCH <sub>3</sub>	333	808.2	-9.2	799.0						
[C <sub>2</sub> H <sub>7</sub> ]	2154-56-5	C <sub>2</sub> H <sub>5</sub> CH <sub>2</sub>				800.7			831.4			6
82MAU	60-29-7; 111-43-3	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O, (n-C <sub>3</sub> H <sub>7</sub> ) <sub>2</sub> O				801-810						
80DEF/MCI	79-20-9; 109-99-9	CH <sub>3</sub> COOCH <sub>3</sub> ; c-C <sub>4</sub> H <sub>8</sub> O				791-795						
78HOU/BEA		threshold value							831.4			
[CH <sub>3</sub> N <sub>3</sub> ]	624-90-8	CH <sub>3</sub> NNN	358			800.5			833			0
89ATT/CAC		See Refs.; bracketed							833±12			
[Cil <sub>i</sub> ]	7447-41-8	LiCl				800.5			827			20
87CRE/FAR		See Refs.							827±54			
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ]	80-62-6	CH <sub>2</sub> =C(CH <sub>3</sub> )COOCH <sub>3</sub>				800.5			831.4			5
90WOL/GRU	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	320	790.7	4	794.7						
90WOL/GRU	563-80-4	(i-C <sub>3</sub> H <sub>7</sub> )COCH <sub>3</sub>	320	804.4	1.9	806.3						
[CSe]	16674-18-3	CSe at C theory				800.2			831.8			3
85JAS/STE									831.8			
[C <sub>6</sub> H <sub>10</sub> O]	557-40-4	(CH <sub>2</sub> =CHCH <sub>2</sub> ) <sub>2</sub> O				800.0			827.4			17
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-17.8	800.0						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-18.3	799.5						
[C <sub>7</sub> H <sub>7</sub> ]	3551-27-7	c-C <sub>7</sub> H <sub>7</sub> radical				800.0			832.4			0
80DEF/MCI	78-93-3; 563-80-4	CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub> ; i-C <sub>3</sub> H <sub>7</sub> COCH <sub>3</sub>				795-804						
[C <sub>3</sub> H <sub>10</sub> O <sub>4</sub> S]	22821-69-8	3-CH <sub>3</sub> SO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				799.5			830.5			5
94DEC/EXN2	120-92-3	Cyclopentanone	338	794.0	3.2	797.3						
94DEC/EXN2	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	338	790.7	9.1	799.8						
94DEC/EXN2	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	338	801	0	801.5						
[C <sub>7</sub> H <sub>5</sub> ClO]	104-88-1	4-ClC <sub>6</sub> H <sub>4</sub> CHO				799.4			831.3			2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.4						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.4						
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	564-12-1	C <sub>2</sub> H <sub>5</sub> COOCH <sub>3</sub>				799.2			830.2			5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.2						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.2						
[C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> ]	616-38-6	(CH <sub>3</sub> O) <sub>2</sub> CO				799.2			830.2			5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.2						
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-19.2	799.2						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>2</sub> H <sub>5</sub> ] 80DEF/MCI	2143-63-5	c-C <sub>2</sub> H <sub>5</sub> radical				799.1			831.5				0
	598-53-8; 60-29-7	(t-C <sub>3</sub> H <sub>7</sub> )OCH <sub>3</sub> ; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O				797-801							
[C <sub>4</sub> H <sub>6</sub> O] 79VAJ/HAR	4170-30-3	CH <sub>3</sub> CH=CHCHO				799.0			830.8				2
	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	373	804.7	-2.2	802.7							
	79VAJ/HAR 67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	373	782.1	12.8	795.4							
	79VAJ/HAR 79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	373	790.7	7.9	798.8							
[C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> ] 91NOU/COO	99-04-7	Benzoic acid, 3-methyl				798.8			829.8				5
	78-93-3; 100-52-7	C <sub>2</sub> H <sub>5</sub> COCH <sub>3</sub> ; C <sub>6</sub> H <sub>5</sub> CHO				795-802							
[C <sub>5</sub> H <sub>5</sub> NNiO] 81STE/BEA	12071-73-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> NiNO	320	819	-20.1	798.6			827.0				13.4
	7664-41-7	NH <sub>3</sub>				798.5							
[C <sub>8</sub> H <sub>6</sub> NO <sub>2</sub> ] 84ROL/HOU	89-87-2	2,4-Dimethylnitrobenzene				798.5			831.0				0
	1089-99-9	Tetrahydrofuran	320	794.7	2.1	797.1							
	84ROL/HOU 60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	320	801	-1.3	800.1							
	13463-40-6	(CO) <sub>2</sub> Fe				798.5			833.0				-7
	7664-41-7	NH <sub>3</sub>	300	819				5±5					
[C <sub>5</sub> FeO <sub>5</sub> ] 93EKE/HAG	108-67-8	1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	300	808.6	-10.0	798.5			833.3				-35±30
	616-38-6; 7664-41-7	(CH <sub>3</sub> O) <sub>2</sub> CO, NH <sub>3</sub>	300			799-819				16.2			-6.8
	7664-41-7	NH <sub>3</sub>	320	819	-12.6	806.5							
	542-92-7	1,3-c-C <sub>3</sub> H <sub>6</sub>				798.4			821.6				31
	71-23-8; 115-10-6	n-C <sub>3</sub> H <sub>7</sub> OH; (CH <sub>3</sub> ) <sub>2</sub> O				756-764							
	7664-41-7	NH <sub>3</sub>	550	819	-11.3	798.4							
[C <sub>7</sub> H <sub>8</sub> O] 86HOU/SCH	7664-41-7	NH <sub>3</sub>	298	819	-20.5	798.5							
	75LOS/TRA	threshold value							827.6				
	694-71-3	Bicyclo[2.2.1]hept-2-ene-7-one	323	819	-20.5	798.3			830.2				2
[C <sub>3</sub> H <sub>6</sub> OS] 87TAF	7664-41-7	NH <sub>3</sub>				798.3							
	1534-08-3	CH <sub>3</sub> C(=O)SCH <sub>3</sub>				798.0			829.0				5
	7664-41-7 79-20-9	NH <sub>3</sub> CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	350 323	819 790.7	-21.1 7.9	797.4 798.6							
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ] 85GUE/HOU	5515-64-0	trans-1,3-cyclohexanol				797.9			828.6				5.8
	109-99-9; 60-29-7	tetrahydrofuran; (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	323			795-801							



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[C <sub>2</sub> H <sub>4</sub> ] 79AUE/BOW	78-79-5 7664-41-7	CH <sub>2</sub> =CHC(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	298	819	-21.5	797.6 797.5			826.4			12
[C <sub>4</sub> H <sub>12</sub> Sn] 84STO/SPL	594-27-4 108-38-3; 108-67-8	(CH <sub>3</sub> ) <sub>4</sub> Sn 1,3-C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub> ; 1,3,5-C <sub>6</sub> H <sub>3</sub> (CH <sub>3</sub> ) <sub>3</sub>				797.4 786-809			823.7			20.6
[Mg] 77PO/POR	7439-95-4 115-11-7; 7664-41-7	Mg 1-C <sub>4</sub> H <sub>8</sub> ; NH <sub>3</sub>				797.3 776-819			819.6			34
[C <sub>4</sub> H <sub>10</sub> O] 87TAF	598-53-8 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> CHOCH <sub>3</sub> NH <sub>3</sub>	350	819	-21.1	797.1 797.1			826.3			11
[C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O] 87TAF	16703-51-8 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> NCOCN NH <sub>3</sub>	350	819	-21.5	797.1 797.1			829.0			2
[C <sub>3</sub> H <sub>10</sub> O <sub>4</sub> S] 94DEC/EXN2	22821-70-1 60-29-7	4-CH <sub>3</sub> SO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	338	801	-2.6	796.7 798.9			827.7			5
94DEC/EXN2	120-92-3	Cyclopentanone	338	794.0	0.4	794.5						
94DEC/EXN2	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	338	790.7	6.1	796.8						
[C <sub>8</sub> H <sub>8</sub> F] 85MAR/MOD	766-98-3 598-53-8	4-FC <sub>6</sub> H <sub>4</sub> CCH (CH <sub>3</sub> ) <sub>2</sub> CHOCH <sub>3</sub>	~300	797.1	-0.4	796.7 796.7			827.4			5.8
[C <sub>8</sub> H <sub>14</sub> O] 87TAF	118-00-9 7664-41-7	neo-C <sub>5</sub> H <sub>11</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-21.5	796.7 796.6			825.8			11
[C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> ] 87TAF	55186-75-9 7665-41-7	4-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )CH <sub>2</sub> NH <sub>3</sub>	350	819	-21.5	796.6 796.6			825.5			12
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-22.0	796.1						
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ] 86MIS/FUJ2	2967-66-0 93-58-3	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-23.0	796.5 796.5			827.5			5
[C <sub>13</sub> H <sub>15</sub> F <sub>3</sub> ] 92NAK/NOM	22666-67-7 616-38-6	α-t-butylstyrene,4-CF <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	343	799.2	-2.9	796.5 796.0			825.3			12
92NAK/NOM	109-99-9	Tetrahydrofuran	343	794.7	2.1	797.0						
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 83MAU	505-22-6 60-29-7	1,3-Dioxane (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	-5.9	796.2 797.0			825.4			11
83MAU	109-99-9	Tetrahydrofuran	600	794.7	-0.8	795.7						
[C <sub>4</sub> H <sub>6</sub> O] 86BOU/DIA	1708-29-8 60-29-7	2,5-Dihydrofuran (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	313	801	-5	796 796			823.4			17

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: Squire	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> ] 87TAF	4164-28-7	(CH <sub>3</sub> ) <sub>2</sub> NNO <sub>2</sub>	350	819	-22.9	795.8			828.3			0	
	7664-41-7	NH <sub>3</sub>				795.8							
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ] 86MIS/FUJ2	2557-13-3	4-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>	343	819.5	-23.8	795.7			826.6			5	
	93-58-3	C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>				795.7							
[C <sub>13</sub> H <sub>12</sub> ] 89GAL/SPE	643-93-6	3-Methylbiphenyl				795.5			828.0			0	
		See Refs.				795.5							
[C <sub>4</sub> H <sub>8</sub> O] 87TAF 84BOU/HOU 83TAF 80LLA/SHO 76KEBYAM	78-93-3	CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>	350	819	-22.0	795.5			827.3			2	
	7664-41-7	NH <sub>3</sub>				796.6							
	120-92-3	Cyclopentanone	300	794.0	0.8	794.8							
	7664-41-7	NH <sub>3</sub>	350	819	-21.5	797.1							
	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	18.4	794.7							
	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	804.7	-0.4	805.2							
[C <sub>2</sub> H <sub>2</sub> S] 83CAS/KIM 83CAS/KIM	18282-77-4	CH <sub>2</sub> =C=S	323	793.6	12.6	795.4			826.2			5.8	
	463-51-4	CH <sub>2</sub> =C=O				806.0							
	79-20-9;	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> ; CH <sub>3</sub> C(=O)SCH <sub>3</sub>	323			791-798							
	1534-08-3												
[C <sub>9</sub> H <sub>7</sub> NO] 86MIS/FUJ	6136-68-1	3-CN-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	343	829.3	-33.9	795.4			827.2			2	
	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>				795.4							
[C <sub>2</sub> H <sub>10</sub> O] 87TAF 83MAU 81BRO/ABB 77WOL/STA	142-68-7	c-C <sub>3</sub> H <sub>10</sub> O	350	819	-19.7	795.4			822.8			17	
	7664-41-7	NH <sub>3</sub>				798.2							
	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	11.7	791.4							
	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	14.2	796.2							
	7664-41-7	NH <sub>3</sub>	350	819	-19.7	798.2							
[C <sub>7</sub> H <sub>6</sub> FO] 87TAF 83TAF2	459-57-4	4-FC <sub>6</sub> H <sub>4</sub> CHO	350	819	-23.3	795.3			827.1			2	
	7664-41-7	NH <sub>3</sub>				795.2							
	7664-41-7	NH <sub>3</sub>	350	819	-23.3	795.2							
[C <sub>14</sub> H <sub>10</sub> ] 85VAN/LEA 80MAU	85-01-8	Phenanthrene				795.0			825.7			5.8	
	67-64-1	See Refs. (CH <sub>3</sub> ) <sub>2</sub> CO	547	782.1	12.1	795.0							
[C <sub>9</sub> H <sub>7</sub> NO] 86MIS/FUJ	1443-80-7	4-CN-C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>	343	829.3	-34.3	795.0			826.8			2	
	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>				795.0							
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ] 90WOL/GRU 90WOL/GRU	96-33-3	CH <sub>2</sub> =CHCOOCH <sub>3</sub>	320	794.7	0.3	794.8			825.8			5	
	109-99-9	Tetrahydrofuran				795.2							
	120-92-3	Cyclopentanone	320	794.0	0.3	794.4							
[C <sub>10</sub> H <sub>9</sub> F <sub>3</sub> ]	368-79-6	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>				794.8			823.7			12	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-23.3	794.7							
[C <sub>6</sub> H <sub>16</sub> O <sub>5</sub> I]	597-52-4	(C <sub>2</sub> H <sub>5</sub> ) <sub>3</sub> SiOH				794.8			822.1			17	
88LI/STO	108-38-3	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	300	786.2	10.5	796.7	812.1	12.6	824.7	22	-7.1	14.9	
88LI/STO	91-20-3	Naphthalene	300	779.4	13.4	792.8	802.9	16.7	819.7	30	-10.8	19.2	
[C <sub>4</sub> H <sub>8</sub> O]	109-99-9	Tetrahydrofuran				794.7			822.1			17	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-23.8	794.0							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-22.9	794.9							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	11.3	793.3							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	16.7	792.5							
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-20.0	799.0							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-22.9	794.9							
[C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> ]	121-89-1	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub>				794.1			826.0			2	
86MIS/FUJ	98-86-2	C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-35.1	794.1							
[C <sub>2</sub> H <sub>6</sub> O]	120-92-3	Cyclopentanone				794.0			823.7			9	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-23.3	794.9							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	10.9	793.0							
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-19.0	800.0							
[C <sub>2</sub> H <sub>2</sub> O]	463-51-4	CH <sub>2</sub> =C=O				793.6			825.3			2.4	
97EAS/SMI	67-64-1;	theory	298									2.4	
96BOU/SAL2	141-78-6	(CH <sub>3</sub> ) <sub>2</sub> CO; CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>				782-805							
93SMI/RAD		theory	298						825				
93SMI/RAD		theory	600						829.8				
93SMI/RAD		theory	0						819.1				
84BEA/EYE		See Refs.							807.5				
82TRA/MCL		threshold value							825.3				
79LIA	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	298	782.1	3.8	786.0							
79LIA	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	300	790.7	0	790.7							
78DAV/LAU	7664-41-7	NH <sub>3</sub>	600	819	-26.4	790.0							
[C <sub>8</sub> H <sub>7</sub> Br]	2039-86-3	3-Br-C <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub>				793.5			822.4			12	
84HAR/HOU	7664-41-7	NH <sub>3</sub>	323	819	-25.1	793.5							
[C <sub>9</sub> H <sub>11</sub> NO <sub>2</sub> ]	603-71-4	2,4,6-Trimethylnitrobenzene				793.1			823.8			5.8	
84ROL/HOU	89-87-2	2,4-Dimethylnitrobenzene	320	798.5	-5.4	793.0							
84ROL/HOU	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	320	790.7	2.5	793.2							
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ]	107-93-7	(E)-CH <sub>3</sub> CH=CHCOOH				793			824.0			5	
84BOU/HOP	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	323	801	-6.3	795							
84BOU/HOP	109-99-9	Tetrahydrofuran	323	794.7	-3.8	791.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M) ΔS <sub>p</sub> (M)
[C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> ] 91NOU/COO	98-89-5 65-85-0; 78- 93-3	Cyclohexane carboxylic acid C <sub>6</sub> H <sub>5</sub> COOH; CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>				792.8 790-795			823.8			5
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ] 86BOU/HAN 86BOU/HAN	543-75-9 99-99-0 79-20-9	Dihydro-1,4-dioxin 4-Nitrotoluene CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	313 313	782.7 790.7	3.3 2.1	792.8 786.0 792.8			823.5			5.8
[C <sub>7</sub> H <sub>12</sub> ] 87TAF 77POL/WOL	591-49-1 7664-41-7 7664-41-7	1-Methylcyclohexene NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-26.1 -25.6	792.6 792.6 793.1			825.1			0
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ] 88BOU/DJA 88BOU/DJA 88BOU/DJA	13991-37-2 79-20-9 109-99-9 60-29-7	(E)CH <sub>3</sub> CH <sub>2</sub> CH=CHCOOH CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> Tetrahydrofuran (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	313 313 313	790.7 794.7 801	2.5 -3.8 -7.5	792.6 793.2 791.1 793.7			823.6			5
[BrLi] 87CRE/FAR	7550-35-8	LiBr See Refs.				792.5			819 819±54			20
[C <sub>8</sub> H <sub>7</sub> NO <sub>3</sub> ] 86MIS/FUJ	100-19-6 98-86-2	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> COCH <sub>3</sub>	343	829.3	-36.8	792.5 792.5			824.3			2
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ] 88BOU/DJA 88BOU/DJA 88BOU/DJA 88BOU/DJA	541-47-9 120-92-3 78-93-3 142-68-7 60-29-7	(CH <sub>3</sub> ) <sub>2</sub> C=CHCOOH Cyclopentanone CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub> c-C <sub>3</sub> H <sub>10</sub> O (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	313 313 313 313	794.0 795.5 795.4 801	-2.9 -3.8 -2.5 -2.1	791.9 791.1 791.6 793.0 799.1			822.9			5
[C <sub>7</sub> H <sub>12</sub> ] 77POL/WOL	765-47-9 7664-41-7	c-C <sub>3</sub> H <sub>6</sub> -1,2-(CH <sub>3</sub> ) <sub>2</sub> NH <sub>3</sub>	350	819	-26.5	791.9 791.8			822.6			5.8
[C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> ] 88BOU/DJA 88BOU/DJA	565-63-9 109-99-9 120-92-3	(Z)CH <sub>3</sub> CH=C(CH <sub>3</sub> )COOH Tetrahydrofuran Cyclopentanone	313 313	794.7 794.0	-3.3 -2.5	791.5 791.6 791.5			822.5			5
[C <sub>4</sub> H <sub>7</sub> O <sub>3</sub> P] 80HOD/HOU 80HOD/HOU	61580-09-4 79-20-9 109-99-9	4-Methyl-2,6,7-trioxo-1- phosphabicyclo[2.2.1]heptane CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> Tetrahydrofuran	325 325	790.7 794.7	0.8 -3.8	791.6 791.4			823.9			0
[CH <sub>3</sub> NO] 83MAU	75-12-7 67-64-1	HCONH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	7.9	791.2 791.2			822.2			5
[C <sub>18</sub> H <sub>12</sub> ] 819.2	217-59-4	Triphenylene				791.2			819.2			14.9

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
80MAU	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	530	782.1	10.5	791.2						
[C <sub>5</sub> H <sub>12</sub> O] 87TAF	628-28-4 7664-41-7	n-C <sub>4</sub> H <sub>9</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-27.0	791.2 791.1			820.3			11
[C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ] 86KAM/YOU	123-42-2 78-93-3	(CH <sub>3</sub> ) <sub>2</sub> C(OH)CH <sub>2</sub> (C=O)CH <sub>3</sub> CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>	330	795.5	-4.4	791.1 791.1			822.9			2
[C <sub>2</sub> H <sub>4</sub> N <sub>2</sub> ] 87TAF 83TAF	540-61-4 7664-41-7 75-04-7	NCCH <sub>2</sub> NH <sub>2</sub> NH <sub>3</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>2</sub>	350 350	819 878	-28.4 -86.5	791.0 790.6 791.5			824.9			-5
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ] 93SZU/MCM 93SZU/MCM 91SZU/MCM 91MAU/SIE 91MAU/SIE 87TAF 83TAF 83CAS/KIM 81BRO/ABB 80LIA/SHO 80ARM/HIG 79LAU 79AUE/BOW 78AUS/LIA 77WOL/STA 76KEB/YAM 76HAR/LIN	79-20-9 115-11-7 109-86-4 115-11-7 115-11-7 67-64-1 7664-41-7 7664-41-7 79-20-9 67-64-1 115-11-7 79-20-9 7664-41-7 115-11-7 7664-41-7 141-78-6 67-64-1	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OH (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> CO NH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> CO (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> NH <sub>3</sub> CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	600 600 300 600 600 350 350 320 320 340 320 650 298 340 350 600 370	775.6 729.8 775.6 775.6 782.1 819 819 790.7 782.1 775.6 790.7 819 819 775.6 819 804.7 782.1	10.9 -2.9 12.6 15.1 7.9 -29.7 -29.7 0 5.0 11.3 0 -25.8 -28.8 11.3 -29.7 -12.1 0.8	790.7 791.0 718.7 788.2 795.2 791.2 788.7 788.7 790.7 787.2 787.5 790.7 789.2 790.2 787.5 788.7 792.6 783.2	802.1 768.8 802.1 802.1 812	14.2 -20.1 14.2 13.0 2.9	821.6 816.3 748.7 816.3 815.1 814.9	20 -22 20 20 8.7	-5.4 28.5 -5.4 3.8 8.4	5 14.6 6.5 14.6 23.8 17.1
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ] 91NOU/COO	1759-53-1 65-85-0, 79- 20-9	Cyclopropane carboxylic acid C <sub>6</sub> H <sub>5</sub> COOH; CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>				790.4 790-791			821.4			5
[C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> ] 79LAU	65-85-0 7664-41-7	C <sub>6</sub> H <sub>5</sub> COOH NH <sub>3</sub>	650	819	-24.9	790.1 790.1			821.1			5
[C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub> ] 92ABB/CAB 92ABB/CAB	26621-44-3 109-99-9 67-64-1	3(5)-nitropyrzazole Tetrahydrofuran (CH <sub>3</sub> ) <sub>2</sub> CO	333 333	794.7 782.1	-5.1 5.8	789.0 790.1 788.1			820.8			2
[H <sub>3</sub> O <sub>3</sub> P] 94DEP/OCC	10294-56-1 67-64-1; 78- 93-3	H <sub>3</sub> PO <sub>3</sub> CH <sub>3</sub> COCH <sub>3</sub> ; CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub>				788.8 782-795			821.3			0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta GB(M,R,T)$	GB(M) GB(M)	PA(R)	$\Delta PA(M,R)$	PA(M) PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$ $\Delta S_p(M)$
[C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O] 93NOT/HER 94NOT/HER	2075-46-9 109-99-9 67-64-1	4-NO <sub>2</sub> -pyrazole Tetrahydrofuran (CH <sub>2</sub> ) <sub>2</sub> CO	333 333	794.7 782.1	-5.4 4.8	788.7 790.0 787.4			822.2			-3.8
[C <sub>3</sub> H <sub>6</sub> ] 79AUE/BOW	698-23-2 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> CHCCH NH <sub>3</sub>	298	819	-31.2	787.8 787.8			814.9			18
[C <sub>3</sub> H <sub>4</sub> ] 76AUE/DAV	2781-85-3 7664-41-7	Cyclopropene NH <sub>3</sub>	298	819	-31.2	787.8 787.8			818.5			5.8
[C <sub>13</sub> H <sub>16</sub> ] 95CRE/FOR 95CRE/FOR 95CRE/FOR	1081-75-0 78-82-0 67-64-1 79-20-9	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>3</sub> C <sub>6</sub> H <sub>5</sub> i-C <sub>3</sub> H <sub>7</sub> CN (CH <sub>3</sub> ) <sub>2</sub> CO CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	300 300 300	772.8 782.1 790.7	12.6 6.3 -1.7	787.6 785.4 788.4 789.0			820.1			0
[C <sub>3</sub> H <sub>5</sub> O] 89HOL/LOS	3122-07-4	•CH <sub>2</sub> COCH <sub>3</sub>	298			787.5			820 820			0
[C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> ] 89ATT/CAC	622-37-7	phenyl azide See Refs.; bracketed	358			787.5			820 820±12			0
[C <sub>8</sub> H <sub>10</sub> O] 87TAF	638-86-3 7664-41-7	C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-30.7	787.5 787.5			816.7			11
[C <sub>5</sub> H <sub>8</sub> ] 87TAF 77WOL/STA	693-86-7 7664-41-7 7664-41-7	c-C <sub>3</sub> H <sub>5</sub> CH=CH <sub>2</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-30.7 -30.7	787.5 787.4 787.4			816.3			12
[C <sub>6</sub> H <sub>10</sub> ] 87TAF 79AUE/BOW 77POL/WOL 76SOL/FIE	693-89-0 7664-41-7 7664-41-7 7664-41-7	1-Methylcyclopentene NH <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub> See Refs.	350 298 350 300	819 819 819	-33.9 -29.3 -34.8	787.1 784.3 789.7 783.4			816.5			10
[C <sub>8</sub> H <sub>5</sub> Cl <sub>3</sub> O] 87TAF	2902-69-4 7664-41-7	C <sub>6</sub> H <sub>5</sub> COCCl <sub>3</sub> NH <sub>3</sub>	350	819	-31.6	787.0 787.0			818.9			2
[C <sub>7</sub> H <sub>5</sub> CrNO <sub>3</sub> ] 81STE/BEA	36312-04-6 7664-41-7	(C <sub>5</sub> H <sub>5</sub> )Cr(CO) <sub>2</sub> NO NH <sub>3</sub>	320	819	-32.2	786.7 786.7			819.1			0
[C <sub>6</sub> H <sub>5</sub> ] 87KIN/BUR 87KIN/BUR	116138-99-9 67-56-1 7732-18-5	CH <sub>3</sub> -CC-CC-CH <sub>2</sub> - CH <sub>3</sub> OH H <sub>2</sub> O		724.5 660.0		786.6			819.1 812.2 826	754.3 691	57.9 135	0
[C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> ] 87KIN/BUR	1830-68-8	4-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub>				786.5			815.4			12

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T (K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-31.6	786.5			817.4			5
[C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub> ] 86MIS/FUI2	13531-48-1 93-58-3	3-CN-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-33.1	786.5 786.5			817.4			5
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ] 78FAR/MCM	109-95-5 67-64-1; 79- 20-9	C <sub>2</sub> H <sub>5</sub> ONO (CH <sub>3</sub> ) <sub>2</sub> CO; CH <sub>3</sub> COOCH <sub>3</sub>				786.4 782-791			818.9			0
[C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O] 84BOL/YVE	1656-48-0 67-64-1; 79- 20-9	O(CH <sub>2</sub> CH <sub>2</sub> CN) <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> CO; CH <sub>3</sub> COOCH <sub>3</sub>	298			786.4 782-791			813.8			17
[C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ] 91NOU/COO	3400-45-1 67-64-1; 79- 20-9	cyclopentane carboxylic acid (CH <sub>3</sub> ) <sub>2</sub> CO; CH <sub>3</sub> COOCH <sub>3</sub>				786.4 782-791			817.4			5
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ] 91NOU/COO	3721-95-7 67-64-1; 79- 20-9	Cyclobutane carboxylic acid (CH <sub>3</sub> ) <sub>2</sub> CO; CH <sub>3</sub> COOCH <sub>3</sub>				786.4 782-791			817.4			5
[C <sub>6</sub> H <sub>6</sub> O] 80MAU 79LAU 77DEF/MCI	108-95-2 7664-41-7 7664-41-7 74-90-81; 115-07-1 71-43-2	C <sub>6</sub> H <sub>5</sub> OH NH <sub>3</sub> NH <sub>3</sub> HCN; C <sub>3</sub> H <sub>6</sub>	550 650	819 819	-26.4 -32.2	786.3 789.8 782.8 682-723			817.3			5
76LAU/KEB		C <sub>6</sub> H <sub>6</sub>	600	725.4	47.3	778.7						
[C <sub>8</sub> H <sub>10</sub> ] 87LJ/STO	108-38-3 108-67-8	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> 1,3,5-(CH <sub>3</sub> ) <sub>3</sub> -C <sub>6</sub> H <sub>3</sub>	300	808.6	-23.4	786.2 785.1			812.1 810.7			22 22.2
76DEV/WOL 72CHO/FRA2 72CHO/FRA2	71-43-2 115-10-6 74-93-1	C <sub>6</sub> H <sub>6</sub> (CH <sub>3</sub> ) <sub>2</sub> O CH <sub>3</sub> SH	350 340 340	725.4 764.5 742	61.8 3.3 10.8	787.3 767.6 752.1				16.2	6	
[C <sub>6</sub> H <sub>12</sub> ] 75SOL/FIE	563-79-1	(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> hydride transfer	300			785.9						15
[C <sub>4</sub> H <sub>6</sub> O] 84BOU/HOP 84BOU/HOP	79-41-4 109-99-9 79-20-9	CH <sub>3</sub> C(=CH <sub>2</sub> )COOH Tetrahydrofuran CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	323 323	794.7 790.7	-8.4 -5.9	785.7 786.6 784.8			816.7			5
[C <sub>4</sub> H <sub>10</sub> O] 87TAF	557-17-5 7664-41-7	n-C <sub>3</sub> H <sub>7</sub> OCH <sub>3</sub> NH <sub>3</sub>	350	819	-32.5	785.7 785.6			814.9			11
[C <sub>9</sub> H <sub>7</sub> NO <sub>2</sub> ] 86MIS/FUI2	1129-35-7 93-58-3	4-CN-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-33.9	785.6 785.6			816.6			5

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>13</sub> H <sub>12</sub> ] 89GAL/SPE	644-08-6	4-Methylbiphenyl See Refs.				785.4 785.4			817.9				0
[C <sub>3</sub> H <sub>3</sub> P] 85HOD/BEA 85HOD/BEA	289-68-9 79-20-9 67-64-1	Phosphabenzene CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	320 320	790.7 782.1	-3.3 0.8	785.3 787.4 783.2			817.7				0
[C <sub>4</sub> H <sub>10</sub> S] 87TAF 83TAF2	75-66-1 7664-41-7 7664-41-7	t-C <sub>4</sub> H <sub>9</sub> SH NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-33.4 -34.8	785.1 785.1 783.7			816.4				4
[C <sub>8</sub> H <sub>7</sub> NO <sub>4</sub> ] 86MIS/FUJ2	618-95-1 93-58-3	3-O <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-35.1	784.7 784.4			815.7				5
[C <sub>4</sub> H <sub>10</sub> O] 78PAU/KIM	78-92-2	CH <sub>3</sub> CH <sub>2</sub> CH(OH)CH <sub>3</sub> See Refs.				784.6			815 815				7
[C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> ] 87TAF	96-49-1 7664-41-7	1,3-Dioxolane-2-one NH <sub>3</sub>	350	819	-33.9	784.4 784.4			814.2				9
[C <sub>7</sub> H <sub>11</sub> N] 87TAF 87MAR/GAL 87MAR/GAL 87MAR/GAL	766-05-2 7664-41-7 78-82-0 5500-21-0 100-47-0	c-C <sub>6</sub> H <sub>11</sub> CN NH <sub>3</sub> i-C <sub>3</sub> H <sub>7</sub> CN c-C <sub>3</sub> H <sub>5</sub> CN C <sub>6</sub> H <sub>5</sub> CN	350 320 320 320	819 772.8 777.5 780.9	-33.4 12 6.5 2.7	784.4 785.0 784.8 784 783.6			815.0				6
[C <sub>4</sub> H <sub>4</sub> S] 86MAU 83TAF2 83MAU 83MAU 81HOU/SCH	110-02-1 67-64-1 7664-41-7 123-91-1 78-93-3 71-23-8; 115-10-6	Thiophene (CH <sub>3</sub> ) <sub>2</sub> CO NH <sub>3</sub> 1,4-Dioxane CH <sub>3</sub> COC <sub>2</sub> H <sub>5</sub> n-C <sub>3</sub> H <sub>7</sub> OH; (CH <sub>3</sub> ) <sub>2</sub> O	600 350 600 600	782.1 819 770.0 795.5	-0.4 -27.9 6.3 -10.5	784.3 782.6 790.5 779.7 783.9 756-764			815.0				5.8
[C <sub>6</sub> H <sub>12</sub> ] 76GORMUN 75SOL/FIE	922-61-2	CH <sub>3</sub> CH=C(CH <sub>3</sub> )C <sub>2</sub> H <sub>5</sub> hydride transfer hydride transfer	300 300			784.0			812.9 809.6 816.1				12
[C <sub>18</sub> H <sub>22</sub> ] 95CRE/FOR 95CRE/FOR	1087-49-6 78-82-0 67-64-1	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>6</sub> C <sub>6</sub> H <sub>5</sub> i-C <sub>3</sub> H <sub>7</sub> CN (CH <sub>3</sub> ) <sub>2</sub> CO	300 300	772.8 782.1	12.6 0	783.8 785.5 782.2			826.1				-33
[C <sub>3</sub> H <sub>5</sub> O <sub>2</sub> ] 89HOL/LOS	#1324	•CH <sub>2</sub> COOCH <sub>3</sub>	298			783.5			816 816				0



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y:Subst	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (M)
[C <sub>13</sub> H <sub>12</sub> ] 89GAL/SPE	643-58-3	2-Methylbiphenyl See Refs.				783.4 783.4			815.9			0	0
[C <sub>3</sub> H <sub>6</sub> B <sub>3</sub> O] 93RAN/POU	121-43-7 78-92-2; 67- 64-1	B(OCH <sub>3</sub> ) <sub>3</sub> 2-butanol, CH <sub>3</sub> COCH <sub>3</sub>				783.4 785-782			815.8			0	0
[C <sub>9</sub> H <sub>9</sub> NO <sub>2</sub> ] 87TAF	64416-49-5 7664-41-7	3-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> NH <sub>3</sub>	350	819	-34.8	783.3 783.3			812.2			12	12
[C <sub>6</sub> H <sub>12</sub> ] 78AUS/LIA 76GORMUN 75SOL/FIE	625-27-4 115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>2</sub> CH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> hydride transfer hydride transfer	340 300 300	775.6	11.7	783.1 787.6			812 811.1 807.8			12	12
[C <sub>7</sub> H <sub>14</sub> ] 76MAU/SOL	625-65-0	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH(CH <sub>3</sub> ) <sub>2</sub> See Refs.				783.1			812 812			12	12
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ] 86MAU 86MAU	108-05-4 67-64-1 109-94-4	CH <sub>3</sub> COOCH=CH <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> CO HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600 600	782.1 768.4	-1.7 15.9	782.9 781.6 784.3			813.9			5	5
[C <sub>12</sub> H <sub>10</sub> ] 80MAU	92-52-4 67-64-1	Biphenyl (CH <sub>3</sub> ) <sub>2</sub> CO	550	782.1	0	782.9 782.9			813.6			5.8	5.8
[C <sub>2</sub> H <sub>6</sub> S <sub>2</sub> ] 81KIM/BON	624-92-0 115-10-6; 75-18-3	CH <sub>3</sub> SSCH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> O; (CH <sub>3</sub> ) <sub>2</sub> S				782.8 764-801			815.3			0	0
[C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> ] 84ROL/HOU	99-99-0 67-64-1	4-Nitrotoluene (CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	0.4	782.7 782.7			815.2			0	0
[C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> ] 87BOU/HOP	637-88-7 79-41-4	c-hexane-1,4-dione CH <sub>3</sub> C(=CH <sub>2</sub> )COOH	313	785.7	-2.9	782.7 782.7			812.5			9	9
[C <sub>7</sub> H <sub>5</sub> FO] 87TAF 83TAF2	456-48-4 7664-41-7 7664-41-7	3-FC <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-36.2 -37.1	782.5 782.4 781.5			814.3			2	2
[C <sub>7</sub> H <sub>11</sub> S] 87TAF	2550-37-0 7664-41-7	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> SH NH <sub>3</sub>	350	819	-36.2	782.4 782.3			813.6			4	4
[C <sub>17</sub> H <sub>20</sub> ] 95CRE/FOR 95CRE/FOR	1718-50-9 78-82-0 67-64-1	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>5</sub> C <sub>6</sub> H <sub>5</sub> i-C <sub>3</sub> H <sub>7</sub> CN (CH <sub>3</sub> ) <sub>2</sub> CO	300 300	772.8 782.1	11.7 -2.1	782.4 784.6 780.1			824.7			-33	-33

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	7(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>3</sub> H <sub>7</sub> NO <sub>4</sub> ] 86MIS/FUJ2	619-50-1 93-58-3	4-O <sub>2</sub> N-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub> C <sub>6</sub> H <sub>5</sub> CO <sub>2</sub> CH <sub>3</sub>	343	819.5	-37.2	782.3 782.3			813.2			5	
[C <sub>3</sub> H <sub>6</sub> O] 97EAS/SMI	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO theory	298			782.1			812			8.7	8.7
95SMI/RAD		theory	298						811.9				
93SZU/MCM	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	7.5	786.5	802.1	8.8	810.9	20	-2.1	17.9	17.9
93SZU/MCM	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	600	801	-16.3	787.2	828.4	-21.3	807.0	17	8.4	25.4	25.4
93SZU/MCM	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	600	807	-18.0	789.1	836.8	-22.6	814.2	9	7.5	16.5	16.5
91SZU/MCM	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	300	775.6	8.4	784.0	802.1	8.8	810.9	20	-2.1	17.9	17.9
91SZU/MCM	96-22-0	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> CO	300	807	-20.5	786.5	836.8	-22.6	814.2	9	7.5	16.5	16.5
91SZU/MCM	60-29-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> O	300	801	-18.8	782.2	828.4	-21.3	807.0	17	8.4	25.4	25.4
91MAU/SIE	91-20-3	Naphthalene	600	779.4	4.2	790.0	802.9	16.7	819.7	30	-20.9	9.1	9.1
91MAU/SIE	78-82-0	1-C <sub>3</sub> H <sub>7</sub> CN	600	772.8	12.1	784.1	803.6	14.6	818.2	5.7	-3.8	1.9	1.9
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	7.1	786.1	802.1	9.2	811.3	20	-2.9	17.1	17.1
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-35.2	783.0							
83MAU	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	0	782.1							
81BRO/ABB	64-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	0	782.1							
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-28.9	786.4							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	6.7	782.8							
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-31.7	787.3							
78DAV/LAU	7664-41-7	NH <sub>3</sub>	600	819	-27.2	787.3							
78AUS/LIA	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	6.3	782.3							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-36.2	782.1							
76KEB/YAM	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	804.7	-14.6	788.9							
76HAR/LIN	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	370	782.1	0	782.1							
[C <sub>3</sub> H <sub>6</sub> CIN] 94DEC/EXN2	874-86-2 100-47-0	4-(CH <sub>2</sub> Cl)-C <sub>6</sub> H <sub>4</sub> -CN C <sub>6</sub> H <sub>5</sub> CN	338	780.9	0.8	782.1			812.8			6	
94DEC/EXN2	5500-21-0	c-C <sub>3</sub> H <sub>3</sub> CN	338	777.5	5.1	781.7 782.6							
[C <sub>10</sub> H <sub>12</sub> ] 80MAU	119-64-2 7664-41-7	1,2,3,4-Tetrahydronaphthalene NH <sub>3</sub>	550	819	-31.4	782.1 782.0			809.7			16	
[C <sub>9</sub> H <sub>7</sub> F <sub>3</sub> ] 84HAR/HOU	402-24-4 7664-41-7	3-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CH=CH <sub>2</sub> NH <sub>3</sub>	323	819	-36.8	781.8 781.8			810.7			12	
[C <sub>4</sub> H <sub>10</sub> S] 78PAU/KIM	513-53-1	CH <sub>3</sub> CH <sub>2</sub> CH(SH)CH <sub>3</sub> See Refs.				781.7			813 813			4	
[C <sub>3</sub> H <sub>10</sub> OSi] 89ORL/ALL	1066-40-6 95-47-6; 108-38-3	Silanol, trimethyl o-xylene; m-xylene				781.5 768-786			814.0			0	
85CLE/MUN	100-47-0; 109-99-9	C <sub>6</sub> H <sub>5</sub> CN; tetrahydrofuran	470			781-795							
75PIT/BUR		See Refs.											

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>3</sub> H <sub>6</sub> O] 87TAF	540-67-0 7664-41-7	CH <sub>3</sub> OC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	-36.6	781.2			808.6			17
79AUE/BOW 77WOL/STA	115-10-6 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> O NH <sub>3</sub>	298 350	764.5 819	17.6 -37.5	782.0 780.3						
[C <sub>6</sub> H <sub>10</sub> ] 96ZHA/STO	764-35-2 108-38-3	2-hexyne 1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	603	786.2	-4.2	781.1 781.1			806.1			25
[C <sub>7</sub> H <sub>5</sub> ClO] 87TAF	587-04-2 7664-41-7	3-ClC <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub>	350	819	-37.5	781.1 781.1			813.0			2
[C <sub>7</sub> H <sub>5</sub> N] 87TAF	100-47-0 7664-41-7	C <sub>6</sub> H <sub>5</sub> CN NH <sub>3</sub>	350	819	-36.6	780.9 781.8			811.5			6
86MAR/TOP 86MAR/TOP	78-82-0 74-90-8	i-C <sub>3</sub> H <sub>7</sub> CN HCN	300 300	772.8 681.6	7.9 96.2	780.8 777.9						
79LAU 76LAU/KEB	7664-41-7 71-43-2	NH <sub>3</sub> C <sub>6</sub> H <sub>6</sub>	650 600	819 725.4	-31.7 47.7	782.9 778.8						
[C <sub>8</sub> H <sub>6</sub> CIN] 94DEC/EXN2	64407-07-4 100-47-0	3-(CH <sub>2</sub> Cl)-C <sub>6</sub> H <sub>4</sub> -CN C <sub>6</sub> H <sub>5</sub> CN	338	780.9	-0.9	780.6 780.0			811.2			6
94DEC/EXN2	5500-21-0	c-C <sub>3</sub> H <sub>5</sub> CN	338	777.5	3.7	781.2						
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 76HAR/LIN	625-55-8 67-64-1	HCOOCH(CH <sub>3</sub> ) <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	370	782.1	-2.1	780.3 780.3			811.3			5
[C <sub>7</sub> H <sub>8</sub> O <sub>2</sub> S] 87TAF	3112-85-4 7664-41-7	C <sub>6</sub> H <sub>5</sub> SO <sub>2</sub> CH <sub>3</sub> NH <sub>3</sub>	350	819	-38.4	780.3 780.2			812.7			0
[C <sub>5</sub> H <sub>9</sub> N] 87TAF	630-18-2 7664-41-7	t-C <sub>4</sub> H <sub>9</sub> CN NH <sub>3</sub>	350	819	-37.1	780.2 781.3			810.9			6
86MAU/KAR 86MAU/KAR	108-38-3 67-64-1	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> (CH <sub>3</sub> ) <sub>2</sub> CO	335 335	786.2 782.1	-2.9 -4.2	783.9 778.1						
86MAR/TOP 86MAR/TOP	78-82-0 74-90-8	i-C <sub>3</sub> H <sub>7</sub> CN HCN	300 300	772.8 681.6	7.5 95.8	780.4 777.5						
[C <sub>5</sub> H <sub>10</sub> ] 79AUE/BOW	513-35-9 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> NH <sub>3</sub>	298	819	-33.7	779.9 785.3			808.8			12
78AUS/LIA 76GORMUN	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> hydride transfer	340 300	775.6	5.4	781.4						
75SOL/FIE	300	hydride transfer	300						807.7 809.8			
[C <sub>8</sub> H <sub>5</sub> Cl] 92MIS/ARI	766-83-6 536-74-3	3-ClC <sub>6</sub> H <sub>4</sub> CCH C <sub>6</sub> H <sub>5</sub> -CCH	323	801.3	-21.3	779.8 780.1			812.3			0
85MAR/MOD	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	~300	782.1	-2.5	779.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>6</sub> H <sub>6</sub> ] 95CRE/FOR	1083-56-3 78-82-0	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>4</sub> C <sub>6</sub> H <sub>5</sub> 1-C <sub>3</sub> H <sub>7</sub> CN	300	772.8	7.9	779.8			822.0			-33
95CRE/FOR	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	300	782.1	-2.5	779.7						
80MAU/HUN	95-47-6	o-Xylene	350	768.3	7.5	778.3	796.0	24.7	820.7	16	-49	-33
[C <sub>10</sub> H <sub>8</sub> ] 88LI/STO	91-20-3 108-38-3	Naphthalene 1,3-(CH <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub>	300	786.2	-3.8	779.4			802.9			30
85VAN/LEA	See Refs.					782.5	812.1	-6.3	805.9	22	8	30
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-31.8	778.1						
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	-30.1	778.0						
[C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ] 96IEB/ZHA	26655-34-5 115-11-7; 67-64-1	alpha-D-glucose (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> , (CH <sub>3</sub> ) <sub>2</sub> CO				778.9 776-782			NE			NE
[C <sub>6</sub> H <sub>12</sub> O <sub>6</sub> ] 96IEB/ZHA	28905-12-6 115-11-7; 67- 64-1	beta-D-glucose (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> ; (CH <sub>3</sub> ) <sub>2</sub> CO				778.9 776-782			NE			NE
[C <sub>3</sub> H <sub>7</sub> S] 87TAF	1679-08-9 7664-41-7	neo-C <sub>3</sub> H <sub>7</sub> SH NH <sub>3</sub>	350	819	-40.3	778.2 778.2			809.5			4
[C <sub>7</sub> H <sub>7</sub> NO <sub>3</sub> ] 86SUN/KUL	619-73-8	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CH <sub>2</sub> OH See Refs.	300			778.0 778			810.5 812			0
[C <sub>5</sub> H <sub>8</sub> ] 79AUE/BOW 74MCA	627-21-4 7664-41-7 115-11-7; 67-64-1	C <sub>2</sub> H <sub>5</sub> CCCH <sub>3</sub> NH <sub>3</sub> 1-C <sub>4</sub> H <sub>8</sub> ; (CH <sub>3</sub> ) <sub>2</sub> CO	298	819	-41	778.0 778 776-782			810.2			1
[C <sub>2</sub> H <sub>6</sub> S] 80AUE/WEB	420-12-2	c-C <sub>2</sub> H <sub>5</sub> S(Thiirane)				777.6			807.4			9
80AUE/WEB	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	298	790.7	-8.8	781.9						
80AUE/WEB	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	298	775.6	1.0	776.6						
80AUE/WEB	592-84-7	HCO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )	298	775	2.4	777.4						
80AUE/WEB	513-35-9	(CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub>	298	779.9	-5.4	774.6						
[HOSi] 93LUC/CUR	97402-81-8;a	HSiO at O theory	298			777.5			810 810			0
[C <sub>4</sub> H <sub>5</sub> N] 87TAF	5500-21-0 7664-41-7	c-C <sub>3</sub> H <sub>5</sub> CN NH <sub>3</sub>	350	819	-40.7	777.5 777.7			808.2			6
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-5.0	777.2						
76STA/KLE	7664-41-7	NH <sub>3</sub>	320	819	-37.2	781.5						
[C <sub>4</sub> H <sub>6</sub> O] 79VAJ/HAR	78-85-3 123-91-1	CH <sub>2</sub> =C(CH <sub>3</sub> )CHO 1,4-Dioxane	373	770.0	4.6	776.8 775.7			808.7			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
79VAJ/HAR	592-84-7	HCO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )	373	775	2.5	777.7							
79VAJ/HAR	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	373	782.1	-5.4	777.2							
[C <sub>5</sub> H <sub>9</sub> NO]	2141-62-0	C <sub>2</sub> H <sub>5</sub> CH(OC <sub>2</sub> H <sub>5</sub> )CH <sub>2</sub> CN				776.5			807.2				6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-42.1	776.3							
87MAR/GAL	100-47-0	C <sub>6</sub> H <sub>5</sub> CN	320	780.9	-3.3	777.6							
87MAR/GAL	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	320	772.8	3	775.8							
87MAR/GAL	110-74-7	HCO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )	320	773.9	2.5	776.4							
[C <sub>6</sub> H <sub>12</sub> ]	592-41-6	1-hexene				776.3			805.2				12
96ZHA/STO	108-38-3	1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>	580	786.2	-9.6	779.4							
96ZHA/STO	79-20-9	CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>	573	790.7	-15.5	773.3							
[C <sub>8</sub> H <sub>5</sub> F]	2561-17-3	3-FC <sub>6</sub> H <sub>4</sub> CCH				776.3			808.7				0
85MAR/MOD	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	~300	782.1	-5.9	776.3							
[C <sub>4</sub> H <sub>8</sub> ]	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>				775.6			802.1				20
97EAS/SMI		theory	298										15.7
96TRA		threshold value	298						801.7				
93SZU/MCM	7664-41-7	NH <sub>3</sub>	600	819	-32.2	778.9		853.6	803.4	-6.4	30.5		24.1
93SMI/RAD		theory	0						798.7				
93SMI/RAD		theory	600						804.7				
93SMI/RAD		theory	298						802.1				
93KEI/RIL		appearance	298						802				
91SZU/MCM	7664-41-7	NH <sub>3</sub>	300	819	-41.4	777.6			803.4	-6.4	30.5		24.1
91MAU/SIE	7664-41-7	NH <sub>3</sub>	600	819	-37.7	773.4			800.0	-6.4	25.9		19.5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-42.1	775.6							
80LIA/SHO	75-07-0	CH <sub>3</sub> CHO	340	736.5	36.8	772.6							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	0	775.6			853.6	-53.6			
79HOU/BEA		threshold value											
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-39.5	779.5							
78DAV/LAU	7664-41-7	NH <sub>3</sub>	600	819	-33.9	777.2							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-42.1	775.6							
76KEB/YAM	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	804.7	-21.3	778.9							
[C <sub>6</sub> O <sub>8</sub> V]	20644-87-5	(CO) <sub>8</sub> V				775.3			799.9				26.4
81STE/BEA	7664-41-7	NH <sub>3</sub>	320	819	-43.1	775.2							
[C <sub>8</sub> H <sub>7</sub> FO <sub>4</sub> S]	124397-36-0	3-SO <sub>2</sub> F-C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				775.1			806.1				5
94DEC/EXN2	630-18-2	t-C <sub>4</sub> H <sub>9</sub> CN	338	780.2	-4.9	775.4							
94DEC/EXN2	5500-21-0	c-C <sub>3</sub> H <sub>5</sub> CN	338	777.5	-2.1	775.4							
94DEC/EXN2	109-94-4	CHO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	338	768.4	6	774.4							
[C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ]	592-84-7	HCO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> )				775			806.0				5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-43.9	774.5							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-1.7	774.5							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		PA(M)		$\Delta S_p(M)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
		Base(R)	Base(M)				GB(M)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	PA(M)			
79AUE/BOW 77WOL/STA	115-10-6 7664-41-7	(CH <sub>3</sub> ) <sub>2</sub> O NH <sub>3</sub>		298 350	764.5 819	11.7 -43.9	776.2 774.5								
[CH <sub>2</sub> N <sub>2</sub> ] 93CAC/DEP 84BEA/EYE	420-04-2 78-82-0	NH <sub>2</sub> -CN i-C <sub>3</sub> H <sub>7</sub> CN See Refs.		298	772.8	2.1	774.9 774.9					805.6 686			6
[C <sub>8</sub> H <sub>7</sub> N] 87TAF 87MAR/GAL 87MAR/GAL 87MAR/GAL	140-29-4 7664-41-7 5500-21-0 78-82-0 107-12-0	Benzyl cyanide NH <sub>3</sub> c-C <sub>3</sub> H <sub>5</sub> CN i-C <sub>3</sub> H <sub>7</sub> CN C <sub>2</sub> H <sub>5</sub> CN		350 350 350 350	819 777.5 772.8 763.0	-43.5 -1.7 1.7 11	774.8 774.9 775.8 774.5 774.0					805.5			6
[C <sub>8</sub> H <sub>10</sub> ] 96ZHA/STO 96ZHA/STO	693-02-7 108-38-3 79-20-9	1-hexyne 1,3-(CH <sub>3</sub> ) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CH <sub>3</sub> CO <sub>2</sub> CH <sub>3</sub>		610 574	786.2 790.7	-8.8 -12.1	774.8 776.5 773.0					799.8			25
[Mn] 86ELK/ARM2	7439-96-5	Mn See Refs.		298			774.4					797.3 797±13			32
[C <sub>14</sub> H <sub>14</sub> ] 95CRE/FOR 95CRE/FOR 80MAU/HUN	103-29-7 115-10-6 78-82-0 95-47-6	C <sub>6</sub> H <sub>5</sub> (CH <sub>2</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub> O i-C <sub>3</sub> H <sub>7</sub> CN o-Xylene		300 300 350	764.5 772.8 768.3	11.3 1.3 3.8	774.1 775.8 774.1 772.1					801.8			16
[C <sub>3</sub> H <sub>6</sub> O] 87TAF 79AUE/BOW	503-30-0 7664-41-7 115-10-6	c-C <sub>3</sub> H <sub>6</sub> O(Oxetane) NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> O		350 298	819 764.5	-43.9 19.5	773.9 773.9 784.0					801.3			17
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 87TAF 80LIA/SHO 79LAU 79AUE/BOW 77WOL/STA 76KEB/YAM 76HAR/LIN	110-74-7 7664-41-7 115-11-7 7664-41-7 115-10-6 7664-41-7 141-78-6 67-64-1	HCO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> ) NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> O NH <sub>3</sub> CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> (CH <sub>3</sub> ) <sub>2</sub> CO		350 340 650 298 350 600 370	819 775.6 819 764.5 819 804.7 782.1	-44.8 -2.5 -43.1 8.8 -44.8 -27.6 -8.4	773.9 773.6 773.7 771.9 773.2 773.6 777.1 774.0					804.9			5
[C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> ] 92MIS/ARI 85MAR/MOD	705-28-2 536-74-3 115-10-6	3-CF <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> -CCH C <sub>6</sub> H <sub>5</sub> -CCH (CH <sub>3</sub> ) <sub>2</sub> O		323 ~300	801.3 764.5	-27.6 2.5	773.8 773.8 767.0					806.2			0
[C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> O] 87TAF 87TAF 83TAF2	455-19-6 7664-41-7 115-11-7 7664-41-7	p-CF <sub>3</sub> C <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> NH <sub>3</sub>		350 350 350	819 775.6 819	-44.8 -2.7 -60.4	773.8 773.7 773.8 758.2					805.6			2

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T (K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	PA(M)	$\Delta S_p$ (M)
[C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ]	107-21-1	HOCH <sub>2</sub> CH <sub>2</sub> OH				773.6					815.9	-33
95CHE/STO	108-88-3	C <sub>8</sub> H <sub>5</sub> CH <sub>3</sub>	600	756.3	2.7	773.6	784.0	33.1	16	-50.6	817.0	-34.6
93BOU/JEZ	78-85-3; 67-64-1	CH <sub>2</sub> =C(CH <sub>3</sub> )CHO; (CH <sub>3</sub> ) <sub>2</sub> CO	300			777-782					820	
[C <sub>20</sub> H <sub>24</sub> ]	128-484-66-2	<i>trans</i> -1,4-dibenzylcyclohexane				773.3					805.7	0
95CRE/FOR	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	300	764.5	7.5	772.0						
95CRE/FOR	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	300	772.8	1.7	774.5						
[C <sub>4</sub> H <sub>7</sub> N]	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN				772.8					803.6	5.7
93SZU/MCM	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	-13.0	770.1	812	-1.7	8.7	-19.2	810.3	-10.5
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	-5.0	774.9	802.1	-3.8	20	-2.1	798.3	17.9
91MAU/SIE	107-12-0	C <sub>3</sub> H <sub>5</sub> CN	600	763.0	9.6	772.4	794.1	10.0	4.7	0.8	804.1	5.5
91MAU/SIE	91-20-3	Naphthalene	600	779.4	-9.6	777.1	802.9	2.1	30	-19.2	805.0	10.8
91MAU/SIE	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	600	756.3	17.2	776.5	784.0	21.3	16	-7.1	805.3	8.9
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-45.3	773.1						
86MAT/OTOP	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	300	772.8	0	772.8						
77WOL/STA	7764-41-7	NH <sub>3</sub>	350	819	-44.8	773.5						
76STA/KLE	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	320	768.4	4.2	772.6						
[B <sub>3</sub> H <sub>6</sub> N <sub>3</sub> ]	6569-51-3	Borazine				772.8					802.5	9.1
79DOI/GRE	123-91-1	1,4-Dioxane	298	770.0	2.9	773.0						
79DOI/GRE	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	298	768.4	4.2	772.6						
[C <sub>4</sub> H <sub>6</sub> O]	1191-95-3	cyclobutanone				772.7					802.5	9
92ABB/CAN	110-74-7	HCO <sub>2</sub> ( <i>n</i> -C <sub>3</sub> H <sub>7</sub> )	333	773.9	0.3	774.0						
92ABB/CAN	109-74-0	333	767.7	4.9	772.5							
92ABB/CAN	100-47-0	C <sub>6</sub> H <sub>5</sub> CN	333	780.9	-7.6	773.2						
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-46.7	771.6						
84BOU/HOU	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	300	764.5	5.0	769.5						
84BOU/HOU	79-09-4	C <sub>2</sub> H <sub>5</sub> COOH	300	766.2	0.4	766.7						
84BOU/HOU	75-65-0	i-C <sub>4</sub> H <sub>9</sub> OH	300	772.2	-1.7	770.5						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-10.5	771.7						
[C <sub>3</sub> H <sub>6</sub> O]	75-56-9	2-Methylloxirane				772.7					803.3	6
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-46.4	772.6						
[C <sub>3</sub> H <sub>6</sub> S]	75-33-2	i-C <sub>3</sub> H <sub>7</sub> SH				772.3					803.6	4
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-46.2	772.3						
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-46.2	772.3						
[H <sub>2</sub> N <sub>2</sub> ]	3618-05-1	HN=NH theory				772.3					803	5.8
92GAR/RUT											803	
[C <sub>3</sub> H <sub>6</sub> F <sub>3</sub> N]	677-41-8	CF <sub>3</sub> N(CH <sub>3</sub> ) <sub>2</sub>				772.2					803.0	5.6

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T (K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-45.3	773.1						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	6.8	771.3						
77STA/TAA	7664-41-7	NH <sub>3</sub>	350	819	-47.6	770.8						
[C <sub>4</sub> H <sub>10</sub> O]	75-65-0	t-C <sub>4</sub> H <sub>9</sub> OH				772.2			802.6			7
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-41.7	772.6						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	6.8	771.3						
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	320	724.5	48.1	772.7						
77HIR/KEB		See Refs.							795			84
[C <sub>5</sub> H <sub>9</sub> N]	110-59-8	n-C <sub>4</sub> H <sub>9</sub> CN				771.7			802.4			6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-46.7	771.7						
76STA/KLE	7664-41-7	NH <sub>3</sub>	320	819	-42.7	776.1						
[C <sub>18</sub> H <sub>26</sub> ]	21072-42-4	<i>trans</i> -1,4-diphenylcyclohexane				771.7			804.1			0
95CRE/FOR	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	300	772.8	-1.3	771.6						
[C <sub>7</sub> H <sub>13</sub> O]	100-49-2	c-C <sub>6</sub> H <sub>11</sub> CH <sub>2</sub> OH				771.7			802.1			7
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-46.7	771.7						
[C <sub>8</sub> H <sub>7</sub> FO <sub>2</sub> S]	124397-38-2	4-SO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -COOCH <sub>3</sub>				771.6			802.6			5
94DEC/EXN2	630-18-2	i-C <sub>4</sub> H <sub>9</sub> CN	338	780.2	-8.4	771.9						
94DEC/EXN2	5500-21-0	c-C <sub>3</sub> H <sub>5</sub> CN	338	777.5	-5.5	772.0						
94DEC/EXN2	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	338	768.4	2.4	770.8						
[C <sub>4</sub> H <sub>10</sub> S]	513-44-0	i-C <sub>4</sub> H <sub>9</sub> SH				771.4			802.6			4
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-47.1	771.3						
[C <sub>4</sub> H <sub>4</sub> O]	110-00-9	Furan				770.9			803.4			0
83MAU	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	600	756.3	13.4	774.5						
83MAU	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	768.4	-2.5	767.4						
81HOU/SCH	71-23-8;	n-C <sub>3</sub> H <sub>7</sub> OH; (CH <sub>3</sub> ) <sub>2</sub> O				756-764						
	115-10-6											
80HOU/SCH	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	323	782.1	-2.5	779.8						
[C <sub>4</sub> H <sub>7</sub> O <sub>2</sub> ]	4598-47-4	1,4-Dioxyl radical				770.7			803.2			0
83AUS/LUT	123-91-1	1,4-Dioxane	340	770.0	~0	770.7						
[C <sub>3</sub> H <sub>5</sub> O <sub>3</sub> P]	279-53-8	2,6,7-Trioxa-1-phosphabicyclo[2.2.1]heptane				770.6			803.1			0
80HOD/HOU	109-74-0	n-C <sub>3</sub> H <sub>7</sub> CN	320	767.7	1.7	769.5						
80HOD/HOU	5500-21-0	c-C <sub>3</sub> H <sub>5</sub> CN	320	777.5	-5.9	771.8						
[B <sub>3</sub> H <sub>8</sub> N <sub>3</sub> ]	61110-11-0	B-Borazanyl radical				770.6			803.0			0
76DES/POR	109-94-4;	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ; H <sub>3</sub> B <sub>3</sub> N <sub>3</sub> H <sub>3</sub>				770.6						
	6569-51-3					768-773						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
	109-79-5 7664-41-7	Reg No(R)	Base(R)	Base(M)										
[C <sub>4</sub> H <sub>10</sub> S] 87TAF	109-79-5 7664-41-7		n-C <sub>4</sub> H <sub>9</sub> SH NH <sub>3</sub>		350	819	-48.1	770.5 770.4			801.7			4
[C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> ] 87BOU/HOP	431-03-8		CH <sub>3</sub> COCOCCH <sub>3</sub>		313	768.4	2.5	770.1			801.9			2
87BOU/HOP	109-94-4		HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>		313	772.7	-3.3	769.5						
87BOU/HOP	1191-95-3		cyclobutanone		313	764.5	5.0	769.7						
83MAU	115-10-6		(CH <sub>3</sub> ) <sub>2</sub> O		600	782.1	-14.1	770.1	812	-7.5	804.5	8.7	-10.9	-2.2
	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO											
[C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ] 87TAF	123-91-1		1,4-Dioxane		350	819	-48.1	770.0			797.4			17
81BRO/ABB	7664-41-7		NH <sub>3</sub>		320	782.1	-11.7	770.3						
77WOL/STA	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO		350	819	-47.6	770.2						
[C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> ] 87TAF	98-95-3		C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub>		350	819	-49.4	769.5			800.3			5.8
84ROL/HOU	7664-41-7		NH <sub>3</sub>		320	770.0	-1.3	769.0						
79LAU	123-91-1		1,4-Dioxane		650	819	-43.1	771.7						
76LAU/KEB	7664-41-7		NH <sub>3</sub>		600	725.4	37.2	768.4						
	71-43-2		C <sub>6</sub> H <sub>6</sub>											
[C <sub>13</sub> H <sub>12</sub> ] 95CRE/FOR	101-81-5		C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> C <sub>6</sub> H <sub>5</sub>		300	764.5	6.7	769.5			802.0			0
95CRE/FOR	115-10-6		(CH <sub>3</sub> ) <sub>2</sub> O		300	772.8	-5.0	767.8						
	78-82-0		i-C <sub>3</sub> H <sub>7</sub> CN											
[C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> ] 96IRI/MAU	106-51-4		p-benzoquinone					769.3			799.1			9
	107-12-0;		C <sub>2</sub> H <sub>5</sub> CN; i-C <sub>3</sub> H <sub>8</sub>					763-776						
	115-11-7													
[C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub> S] 94DEC/EXN2	22821-75-6		3-(CH <sub>3</sub> SO <sub>2</sub> )-C <sub>6</sub> H <sub>4</sub> -CN		338	767.7	0.5	768.8			799.5			6
94DEC/EXN2	109-74-0		n-C <sub>3</sub> H <sub>7</sub> CN		338	768.4	1.1	768.2						
	109-94-4		HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>					769.5						
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ] 87TAF	109-94-4		HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>		350	819	-50.3	768.4			799.4			5
81BRO/ABB	7664-41-7		NH <sub>3</sub>		320	782.1	-13.8	768.4						
80LIA/SHO	67-64-1		(CH <sub>3</sub> ) <sub>2</sub> CO		340	775.6	-10.0	766.2						
79AUJ/BOW	115-11-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>		298	764.5	3.9	768.4						
78DAV/LAU	115-10-6		(CH <sub>3</sub> ) <sub>2</sub> O		600	819	-41.8	773.7						
77WOL/STA	7664-41-7		NH <sub>3</sub>		350	819	-50.3	768.1						
76STA/KLE	7664-41-7		HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>		320	768.4	0	768.4						
76HAR/LIN	109-94-4		(CH <sub>3</sub> ) <sub>2</sub> CO		370	782.1	-8.4	774.0						
	67-64-1													
[Cr] 87ELK/ARM	7440-47-3		Cr					768.4			791.3			32
			See Refs.								791±9			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)	ΔS <sub>p</sub> (M)
[C <sub>8</sub> H <sub>10</sub> ]	95-47-6	o-Xylene				768.3			796.0				16
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-49.0	768.9							
80MAU/HUN	95-47-6	o-Xylene	350	768.3	0	768.3							
80MAU	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	492	756.3	9.2	765.5							
76DEV/WOL	71-43-2	C <sub>6</sub> H <sub>6</sub>	350	725.4	43.9	769.8							
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-48.5	769.4							
72CHO/FRA2	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	340	764.5	3.3	767.7							
72CHO/FRA2	74-93-1	CH <sub>3</sub> SH	340	742	10.4	751.9							
[C <sub>2</sub> H <sub>5</sub> P]	6569-82-0	e-C <sub>2</sub> H <sub>4</sub> PH				768.3			802.5				-5.8
80AUE/WEB	123-91-1	1,4-Dioxane	298	770.0	-2.4	767.6							
80AUE/WEB	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	2.4	766.9							
80AUE/WEB	110-74-7	HCO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )	298	773.9	-3.4	770.5							
[C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub> S]	22821-76-7	4-(CH <sub>3</sub> SO <sub>2</sub> )-C <sub>8</sub> H <sub>7</sub> -CN				768.0			798.7				6
94DEC/EXN2	109-74-0	n-C <sub>3</sub> H <sub>7</sub> CN	338	767.7	-0.3	767.4							
94DEC/EXN2	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	338	768.4	0.3	768.7							
[C <sub>4</sub> H <sub>7</sub> N]	109-74-0	n-C <sub>3</sub> H <sub>7</sub> CN				767.7			798.4				6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-49.4	769.0							
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	2.0	766.4							
76STA/KLE	7664-41-7	NH <sub>3</sub>	320	819	-44.8	774.0							
[C <sub>8</sub> H <sub>5</sub> F <sub>3</sub> O]	434-45-7	C <sub>8</sub> H <sub>5</sub> COCF <sub>3</sub>				767.4			799.2				2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-51.3	767.3							
[CH <sub>2</sub> Te]	43309-26-8	H <sub>2</sub> C=Te				766.8			796				11
85JAS/STE		theory							796				
[C <sub>8</sub> H <sub>10</sub> ]	106-42-3	p-Xylene				766.8			794.4				16
76DEV/WOL	71-43-2	C <sub>6</sub> H <sub>6</sub>	350	725.4	40.7	766.6							
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-51.7	766.2							
72CHO/FRA2	74-93-1	CH <sub>3</sub> SH	340	742	10.2	751.7							
72CHO/FRA2	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	340	764.5	3.0	767.5							
[C <sub>2</sub> H <sub>3</sub> NS]	556-61-6	CH <sub>3</sub> NCS				766.7			799.2				0
85KAR/STE	109-74-0	n-C <sub>3</sub> H <sub>7</sub> CN	300	767.7	-1.3	766.5							
85KAR/STE	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	300	764.5	2.5	767.0							
74MCA	115-11-7; 67-64-1	1-C <sub>4</sub> H <sub>8</sub> ; (CH <sub>3</sub> ) <sub>2</sub> CO				776-782							
[CH <sub>3</sub> OS]	40100-16-1	CH <sub>2</sub> =S=O				766.4			798.9				0
96BOU/SAL	115-10-6; 109-94-4	(CH <sub>3</sub> ) <sub>2</sub> O; HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>				764-768							
[CH <sub>3</sub> NO <sub>2</sub> ]	624-91-9	CH <sub>3</sub> ONO				766.4			798.9				0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
78FAR/MCM	115-10-6; 109-94-4 64-17-5; 67- 64-1	(CH <sub>3</sub> ) <sub>2</sub> O; HCOOC <sub>2</sub> H <sub>5</sub> C <sub>2</sub> H <sub>5</sub> OH; CH <sub>3</sub> COCH <sub>3</sub>				764-768 746-782							
[C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> S] 87TAF	5187-62-2 7664-41-7	CF <sub>3</sub> CH <sub>2</sub> SC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	-52.2	766.4 766.3			797.6			4	
[C <sub>5</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ] 87TAF	352-23-8 7664-41-7	CF <sub>3</sub> CH <sub>2</sub> COOC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	-52.2	766.3 766.3			797.3			5	
[C <sub>6</sub> H <sub>5</sub> NO] 87TAF 83TAF2	105-07-7 7664-41-7 7664-41-7	4-CNC <sub>6</sub> H <sub>4</sub> CHO NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-52.2 -78.3	766.3 766.2 740.1			796.9			6	
[C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> ] 76YAM/KEB	79-09-4 7664-41-7	C <sub>2</sub> H <sub>5</sub> COOH NH <sub>3</sub>	600	819	-49.4	766.2 766.2			797.2			5	
[C <sub>2</sub> H <sub>3</sub> NS] 83KAR/STE	556-64-9 115-10-6; 109-74-0	CH <sub>3</sub> SCN (CH <sub>3</sub> ) <sub>2</sub> O; n-C <sub>3</sub> H <sub>7</sub> CN				766.1 764-768			796.7			6	
74MCA	115-11-7; 67-64-1	1-C <sub>4</sub> H <sub>8</sub> ; (CH <sub>3</sub> ) <sub>2</sub> CO				776-782							
[C <sub>4</sub> H <sub>3</sub> NO] 94FLA/HAV	57681-10-4	NCC(CH <sub>3</sub> )CO theory				765.5			798 798			0	
[C <sub>4</sub> H <sub>8</sub> O] 87TAF 79AUE/BOW 77WOL/STA	78-84-2 7664-41-7 115-10-6 7664-41-7	i-C <sub>3</sub> H <sub>7</sub> CHO NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> O NH <sub>3</sub>	350 298 350	819 764.5 819	-53.1 1.0 -53.1	765.5 765.5 765.4 765.5			797.3			2	
[C <sub>5</sub> H <sub>12</sub> O] 78TAF/TAA	75-84-3 67-56-1	neo-C <sub>3</sub> H <sub>11</sub> OH CH <sub>3</sub> OH	320	724.5	40.6	765.2 765.2			795.5			7	
[C <sub>3</sub> H <sub>4</sub> O] 79VAJ/HAR	107-02-8 109-94-4	CH <sub>2</sub> =CHCHO HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	373	768.4	-3.3	765.1 765.3			797.0			2	
[C <sub>5</sub> H <sub>10</sub> O] 87TAF 79AUE/BOW 77WOL/STA	110-62-3 7664-41-7 115-10-6 7664-41-7	n-C <sub>4</sub> H <sub>9</sub> CHO NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> O NH <sub>3</sub>	350 298 350	819 764.5 819	-53.1 -0.5 -53.1	764.8 765.5 764.0 765.5			796.6			2	
[C <sub>2</sub> H <sub>6</sub> O] 97EAS/SMI 93SZU/MCM	115-10-6 115-11-7	(CH <sub>3</sub> ) <sub>2</sub> O theory (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	298 600	775.6	-11.7	764.5 764.9			792 793.3			16.5 17.1 15.0	
										802.1	-8.8		20

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Ysquire	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
93SMI/RAD		theory	298						792				
93SMI/RAD		theory	600						794.6				
93SMI/RAD		theory	0						787.3				
91MAU/SIE	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	-12.6	764.1	802.1	-13.4	788.7	20	1.7	21.7	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-53.5	764.3							
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	-53.0	764.8							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-53.5	764.3							
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-16.7	765.2							
80LJA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-13.4	762.4							
79AUJ/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	0	764.5							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-53.5	764.3							
76YAM/KEB	7664-41-7	NH <sub>3</sub>	600	819	-46.4	765.7							
76KEB/YAM	141-78-6	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	600	804.7	-32.2	769.0							
76HAR/LIN	75-07-0	CH <sub>3</sub> CHO	370	736.5	18.4	753.9							
75SOL/HAR	75-07-0	CH <sub>3</sub> CHO	373	736.5	18.8	754.2							
[C <sub>10</sub> H <sub>14</sub> ]	104-51-8	n-C <sub>4</sub> H <sub>9</sub> C <sub>6</sub> H <sub>5</sub>				764.2			791.9				16
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-52.2	765.7							
76YAM/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	33.1	761.2							
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-52.2	765.7							
[C <sub>9</sub> H <sub>12</sub> ]	98-82-8	i-C <sub>3</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>				763.9			791.6				16
76YAM/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	33.1	761.2							
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-51.7	766.2							
[CHF]	13453-52-6	CFH				763.8			797.9				-5.8
85LIA/KAR	115-10-6; 107-12-0	(CH <sub>3</sub> ) <sub>2</sub> O; C <sub>2</sub> H <sub>5</sub> CN				764-763							
[C <sub>3</sub> H <sub>8</sub> S]	107-03-9	n-C <sub>3</sub> H <sub>7</sub> SH				763.6			794.9				4
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-54.9	763.6							
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-57.7	760.8							
[C <sub>3</sub> H <sub>5</sub> FO]	430-61-3	CH <sub>3</sub> COCH <sub>2</sub> F				763.5			795.4				2
81DRUM/MCM	109-94-4	HCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	298	768.4	-5.4	763.0							
81DRUM/MCM	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-0.4	764.0							
[C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub> ]	555-16-8	4-(NO <sub>2</sub> )C <sub>6</sub> H <sub>4</sub> CHO				763.2			795.1				2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-55.4	763.2							
[C <sub>3</sub> H <sub>5</sub> N]	107-12-0	C <sub>2</sub> H <sub>5</sub> CN				763.0			794.1				4.7
97EAS/SMI		theory	298										5.6
95SMI/RAD		theory	298										
91MAU/SIE	75-05-8	CH <sub>3</sub> CN	600	748	17.6	765.5	779.2	15.9	794.3	4.3	2.5	6.8	
91MAU/SIE	107-31-3	HCOOCH <sub>3</sub>	600	751.5	10.5	762.1	782.5	13.0	795.5	5	-4.2	0.8	
91MAU/SIE	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	600	756.3	3.3	763.0	784.0	11.7	795.7	16	-14.2	1.8	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)	$\Delta$ S <sub>p</sub> (M)
91MAU/SIE	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	600				792	2.9	794.9				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-55.4	763.1							
80LIA/SO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-14.2	762.0							
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-2.9	761.5							
76STA/KLE	7664-41-7	NH <sub>3</sub>	320	819	-50.2	768.6							
[C <sub>3</sub> H <sub>8</sub> O]	67-63-0	i-C <sub>3</sub> H <sub>7</sub> OH				762.6			793.0				7
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-53.0	761.3							
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	350	724.5	38.9	763.5							
[C <sub>9</sub> H <sub>12</sub> ]	103-65-1	n-C <sub>3</sub> H <sub>7</sub> C <sub>6</sub> H <sub>5</sub>				762.4			790.1				16
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-54.0	763.9							
76YAM/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	31.4	759.5							
74HEH/MCI	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	350	775.6	-12.4	763.5							
[C <sub>4</sub> H <sub>10</sub> O]	78-83-1	i-C <sub>4</sub> H <sub>9</sub> OH				762.2			793.7				3
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	320	724.5	35.6	760.2							
78TAF/TAA	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-18.0	764.3							
[C <sub>7</sub> H <sub>5</sub> O <sub>3</sub> ]	1124-18-1	C <sub>6</sub> H <sub>5</sub> CD <sub>3</sub>				762			789.7				16
77AUS/LIA		See Refs.	340			762							
[C <sub>7</sub> H <sub>7</sub> Cl]	95-49-8	2-Cl-toluene				761.1			790.5				10
87FER/JEN	352-70-5	3-F-toluene	478	756.0	5.1	761.1		23	808.4				
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-15.5	741.2							
[C <sub>4</sub> H <sub>8</sub> O]	123-72-8	n-C <sub>3</sub> H <sub>7</sub> CHO				760.8			792.7				2
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-57.7	760.9							
80LIA/SO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-15.5	760.8							
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	1.0	765.4							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-57.7	760.9							
[C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> N]	368-77-4	3-(CF <sub>3</sub> ) <sub>2</sub> C <sub>6</sub> H <sub>4</sub> CN				760.8			791.4				6
94DEC/EXN2	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	6.4	760.2							
94DEC/EXN2	123-72-8	n-C <sub>3</sub> H <sub>7</sub> CHO	338	760.8	0.7	761.3							
[C <sub>8</sub> H <sub>10</sub> ]	100-41-4	C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub>				760.3			788.0				16
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-58.1	759.8							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-50.3	760.8							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-58.1	759.8							
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	30.5	758.7							
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-58.1	759.6							
[CS]	2944-05-0	CS				760			791.5				3.3
97EAS/SMI		theory	298										3.3
93SMI/RAD		theory	0						789.9				

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y+Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
						GB(M)	GB(M)	PA(M)	PA(M)				
93SMI/RAD		theory	298										
93SMI/RAD		theory	600										
92CUR/NOB		theory	298										
85SMI/ADA		See Refs.	300				756.0						
85JAS/STE		theory											
85BOT/SEB		theory	0										
78MCA	74-96-4; 115-07-1	C <sub>2</sub> H <sub>3</sub> Br; C <sub>3</sub> H <sub>6</sub>				670-723							
[C <sub>8</sub> H <sub>8</sub> FeO]	12080-06-7	(C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> Fe(CO) <sub>2</sub> CH <sub>3</sub>											
81STE/BEA	7664-41-7	NH <sub>3</sub>	320	819	-59.4	759.5	759.5	792.0					0
[C <sub>4</sub> H <sub>5</sub> Cl <sub>2</sub> O <sub>2</sub> ]	515-84-4	CCl <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub>											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-59.0	759.4	759.4	790.4					5
[C <sub>4</sub> H <sub>10</sub> O]	71-36-3	n-C <sub>4</sub> H <sub>9</sub> OH											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-59.5	758.9	758.8	789.2					7
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-59.9	758.4	758.4						
78PAU/KIM	7664-41-7	NH <sub>3</sub>	320	819	-54.8	763.9	763.9						
[C <sub>2</sub> H <sub>6</sub> S]	75-08-1	C <sub>2</sub> H <sub>5</sub> SH											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-61.3	758.4	757.2	789.6					4
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-63.2	755.3	755.3						
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-16.7	759.5	759.5						
[C <sub>8</sub> H <sub>4</sub> F <sub>3</sub> N]	455-18-5	4-(CF <sub>3</sub> )-C <sub>6</sub> H <sub>4</sub> -CN											
94DEC/EXN2	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	5	758.6	758.6	787.2					11.8
94DEC/EXN2	123-72-8	n-C <sub>3</sub> H <sub>7</sub> CHO	338	760.8	-2.5	757.9	757.9						
[C <sub>4</sub> H <sub>6</sub> ]	106-99-0	CH <sub>2</sub> =CHCH=CH <sub>2</sub>											
87LIA/AUS	75-05-08	CH <sub>3</sub> CN	340	748	9.2	757.6	756.5	783.4					22
87LIA/AUS	107-31-3	HCOOCH <sub>3</sub>	340	751.5	3.8	754.6	754.6						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-2.9	761.5	761.5						
[C <sub>4</sub> H <sub>4</sub> N <sub>4</sub> O <sub>4</sub> ]	32683-48-0	1-methyl-3,5-dinitroproazole											
92ABB/CAB	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	333	754.0	3.4	757.0	757.4	788.8					2
92ABB/CAB	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	333	756.3	-0.5	756.2	756.2						
92ABB/CAB	100-41-4	C <sub>2</sub> H <sub>5</sub> C <sub>6</sub> H <sub>5</sub>	333	760.3	-3.5	757.3	757.3						
[NP]	17739-47-8	PN											
90ADA/MIC	7803-51; 2 107-12-0	PH <sub>3</sub> ; C <sub>2</sub> H <sub>5</sub> CN	300			757.0	751-763	789.4					0
[C <sub>6</sub> H <sub>6</sub> O]	6921-27-3	(HCCCH <sub>2</sub> ) <sub>2</sub> O											
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-61.3	756.5	756.5	783.9					17
83TAF2	7664-41-7	NH <sub>3</sub>	350	819	-61.3	756.5	756.5						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>7</sub> H <sub>9</sub> ]	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>				756.3			784.0			16
97EAS/SMI		theory	298									11.5
93SZUM/MCM	462-06-6	C <sub>6</sub> H <sub>5</sub> F	600	726.6	30.1	755.0	755.9	25.5	781.4	10.5	7.5	18.0
93SZUM/MCM	78-82-0	i-C <sub>3</sub> H <sub>7</sub> CN	600	772.8	-15.1	754.7	803.6	-25.6	777.7	5.7	18.0	23.7
91MAU/SIE	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	29.7	757.8	750.4	34.7	785.1	2.5	-8.4	16.6
91MAU/SIE	75-05-8	CH <sub>3</sub> CN	600	748	12.1	756.6	779.2	6.7	785.9	4.3	9.2	13.5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-62.2	755.6						
82STO/SPL	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	478	756.3	0	756.3						
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	0	756.3						
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-46.0	767.4						
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-54.8	756.3						
77AUS/LIA		See Refs.	340			762						
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	26.4	754.5						
76DEV/WOL	71-43-2	C <sub>6</sub> H <sub>6</sub>	350	725.4	30.2	756.1						
74HEH/MCI	7664-41-7	NH <sub>3</sub>	350	819	-62.7	755.2						
72CHO/FRA2	74-93-1	CH <sub>3</sub> SH	340	742	6.6	748.1						
[C <sub>3</sub> H <sub>8</sub> O]	71-23-8	n-C <sub>3</sub> H <sub>7</sub> OH				756.1			786.5			7
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-62.2	756.1						
81BRO/ABB	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-24.7	757.5						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-9.8	754.7						
78TAF/TAA	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	320	782.1	-24.7	757.5						
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	320	724.5	28.9	753.4						
[C <sub>7</sub> H <sub>7</sub> F]	352-70-5	3-F-toluene				756.0			785.4			10
87FER/JEN	352-70-5	3-F-toluene	478	756.0	0	756.0		0	785.4			
82STO/SPL	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	478	756.3	-0.8	756.5						
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-1.3	755.4						
[C <sub>7</sub> H <sub>7</sub> Cl]	108-41-8	3-Cl-toluene				754.5			783.9			10
87FER/JEN	352-70-5	3-F-toluene	478	756.0	-0.4	755.6		3	788.4			
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-3.3	753.3						
[C <sub>4</sub> H <sub>7</sub> ]	#1452	CH <sub>3</sub> CH=CHCH <sub>2</sub> •				754.4			785.1			6
87LIA/AUS	64-19-7; 71-23-8	CH <sub>3</sub> COOH; n-C <sub>3</sub> H <sub>7</sub> OH	340			753-756						
[C <sub>3</sub> H <sub>5</sub> NS]	35120-10-6	CH <sub>3</sub> SCH <sub>2</sub> CN				754.1			784.8			6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-65.0	753.4						
87MAR/GAL	75-05-8	CH <sub>3</sub> CN	320	748	5.8	753.8						
87MAR/GAL	75-08-1	C <sub>2</sub> H <sub>5</sub> SH	320	758.4	-3.8	754.5						
87MAR/GAL	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	320	754.0	1	754.9						
[C <sub>3</sub> H <sub>6</sub> O]	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO				754.0			786.0			1.5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-65.9	752.7						

TABLE 2 Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta$ S <sub>p</sub> (R)	$\Delta\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M)	$\Delta$ S <sub>p</sub> (R)
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-23.4	752.9							
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-9.8	754.7							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-65.9	752.7							
76YAM/KEB	7664-41-7	NH <sub>3</sub>	650	819	-60.8	755.5							
75SOL/HAR	75-07-0	CH <sub>3</sub> CHO	370	736.5	10.5	747.0			792				
68REF/CHU		threshold value	298										
[C <sub>3</sub> H <sub>3</sub> N]	107-13-1	CH <sub>2</sub> =CHCN				753.7			784.7				4.9
97EAS/SMI		theory	298										4.9
93SMI/RAD		theory	600						787.3				
93SMI/RAD		theory	298						784.7				
93SMI/RAD		theory	0						779.4				
91MAU/SIE	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	600	764.5	-17.2	750.8	792	-14.2	777.8	16.5	-5.0		11.5
91MAU/SIE	107-31-3	HCOOCH <sub>3</sub>	600	751.5	0.8	752.4	782.5	0.4	782.9	5	0.4		5.4
91MAU/SIE	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	600	756.3	-8.4	751.2	784.0	0.4	784.4	16	-14.6		1.4
91MAU/SIE	75-05-8	CH <sub>3</sub> CN	600	748	4.6	752.4	779.2	2.5	781.7	4.3	3.3		7.6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-66.4	752.1							
76STA/KLE	7664-41-7	NH <sub>3</sub>	320	819	-60.7	758.1							
[C <sub>4</sub> H <sub>6</sub> ]	822-35-5	Cyclobutene				753.6			784.4				5.8
79AUE/BOW	7664-41-7	NH <sub>3</sub>	298	819	-65.4	753.6							
[C <sub>2</sub> D <sub>6</sub> O]	17222-37-6	(CD <sub>3</sub> ) <sub>2</sub> O				753.0			780.4				17
76HAR/LIn	75-07-0	CH <sub>3</sub> CHO	370	736.5	17.6	753.0							
[C <sub>4</sub> H <sub>2</sub> F <sub>9</sub> N]	2809-92-9	(CF <sub>3</sub> ) <sub>3</sub> CNH <sub>2</sub>				752.9			783.7				5.6
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-62.7	755.7							
80AUE/WEB	75-21-8	c-C <sub>2</sub> H <sub>4</sub> O	298	745.3	5.9	751.1							
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-12.2	752.3							
[C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ]	64-19-7	CH <sub>3</sub> COOH				752.8			783.7				5
90FEL/KIM		theory	300						823				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-67.7	750.7							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-67.7	750.7							
76YAM/KEB	7664-41-7	NH <sub>3</sub>	650	819	-60.3	754.7							
[C <sub>7</sub> H <sub>7</sub> Br]	591-17-3	3-Br-toluene				752.5			782.0				10
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-4.2	752.5							
[B <sub>4</sub> H <sub>6</sub> ]	12007-71-5	B <sub>4</sub> H <sub>6</sub>				752.4			784.9				0
72SOL/POR	115-07-1; 67-64-1	C <sub>3</sub> H <sub>6</sub> ; (CH <sub>3</sub> ) <sub>2</sub> CO	~373			723-782							
[C <sub>5</sub> H <sub>5</sub> As]	289-31-6	Arsabenzene				752.4			784.8				0
85HOD/BEA	75-05-8	CH <sub>3</sub> CN	320	748	3.8	751.9							
85HOD/BEA	107-31-3	HCOOCH <sub>3</sub>	320	751.5	1.3	752.9							



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)	
[C <sub>6</sub> H <sub>10</sub> ] 80LIA/SHO	110-83-8	c-C <sub>6</sub> H <sub>10</sub>	340	775.6	-24.3	752.0			784.5			0		
	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>				752.1								
[C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> ] 94DEC/EXN2 94DEC/EXN2	623-26-7	1,4-(CH) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				751.8			779.0			17.5		
	75-05-8	CH <sub>3</sub> CN	338	748	2.4	749.9								
	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	0.4	753.8								
[C <sub>3</sub> HNO] 94FLA/HAV	4452-08-8	NCCHCO theory				751.5			784 784			0		
	107-31-3	HCOOCH <sub>3</sub> theory	298			751.5			782.5			5	5.1	
[C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> ] 97EAS/SMI 95SMI/RAD 93SZU/MCM 91MAU/SIE 87TAF 86KNI/FRE 82STO/SPL 80LIA/SHO 79LAU 77WOL/STA 76HAR/LIN	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	782.1	-32.6	750.6	812	-23.4	788.6	8.7	-15.1	-6.4		
	75-05-8	CH <sub>3</sub> CN	600	748	5.9	753.6	779.2	2.5	781.7	4.3	5.4	9.7		
	7664-41-7	NH <sub>3</sub>	350	819	-67.3	751.2								
	75-07-0	CH <sub>3</sub> CHO	303	736.5	8.4	744.9								
	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	478	756.3	-5.4	752.8								
	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-25.1	751.1								
	7664-41-7	NH <sub>3</sub>	650	819	-61.2	753.8								
	7664-41-7	NH <sub>3</sub>	350	819	-67.3	751.2								
	75-07-0	CH <sub>3</sub> CHO	370	736.5	8.4	744.6								
	7440-18-8	Ru See Refs.				751.4			774 774±12			33		
	[H <sub>3</sub> P] 97EAS/SMI 93SMI/RAD 93SMI/RAD 93SMI/RAD 87TAF 87POP/CUR 83TAF 80LIA/SHO 79AUE/BOW 78COR/BEA	7803-51-2	PH <sub>3</sub> theory	298			750.9			785			-5.6	-6.7
			theory	600						788.9				
		theory	0						778.9					
		theory	298						784.8					
7664-41-7		NH <sub>3</sub>	350	819	-73.2	745.7								
		theory	298						785.3					
7664-41-7		NH <sub>3</sub>	350	819	-72.3	746.7								
115-11-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-31.0	745.7								
115-10-6		(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-15.1	749.3								
7783-54-2; 684-16-2		NF <sub>3</sub> ; (CF <sub>3</sub> ) <sub>2</sub> CO				539-640								
77WOL/STA 77WOL/STA	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	350	775.6	-31.1	745.8								
	7664-41-7	NH <sub>3</sub>	350	819	-72.3	746.7								
[C <sub>7</sub> H <sub>7</sub> ] 82MAS/BOH	615-37-2	2-1-toluene				750.8			780.3			10		
	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-5.9	750.8								
[C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ]	619-24-9	3-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> -CN				750.7			781.4			6		

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/squib	Reg No(M)		Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$
	Reg No(R)	Reg No(M)											
94DEC/EXN2	123-38-6		C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	-2.1	751.7						
94DEC/EXN2	75-05-8		CH <sub>3</sub> CN	338	748	1.8	749.7						
[OSi]	10097-28-6:a		SiO at O				750.4			777.8			17
93LUC/CUR			theory	298						799			
89FOX/WLO	75-05-8; 64-19-7		CH <sub>3</sub> CN; CH <sub>3</sub> COOH	295			748-753						
85BOT/ROS				298						814±5			
[C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> ]	626-17-5		1,3-(CN) <sub>2</sub> -C <sub>6</sub> H <sub>4</sub>				750.4			779.3			11.8
94DEC/EXN2	75-05-8		CH <sub>3</sub> CN	338	748	1.9	749.6						
94DEC/EXN2	123-38-6		C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	-2.4	751.2						
[C <sub>4</sub> H <sub>6</sub> ]	590-19-2		CH <sub>2</sub> =C=CHCH <sub>3</sub>				749.8			778.9			11
87LIA/AUS	75-05-8; 107-31-3		CH <sub>3</sub> CN; HCOOCH <sub>3</sub>	340			748-752						
[C <sub>2</sub> H <sub>3</sub> N]	75-05-8		CH <sub>3</sub> CN				748			779.2			4.3
97EAS/SMI			theory	298									4.3
93SMI/RAD			theory	600						783.3			
93SMI/RAD			theory	0						775.4			
93SMI/RAD			theory	298						780.1			
91MAU/SIE	75-07-0		CH <sub>3</sub> CHO	600	736.5	10.5	746.1			768.5		12.1	1.5
87TAF	7664-41-7		NH <sub>3</sub>	350	819	-70.9	747.5						-1.0
86MAR/TOP	74-90-8		HCN	300	681.6	65.7	747.3						
86KNI/FRE	75-07-0		CH <sub>3</sub> CHO	303	736.5	7.5	744.0						
84BEA/EYE			See Refs.							765			
80LIA/SHO	115-11-7		(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-28.9	747.4						
79LAU	7664-41-7		NH <sub>3</sub>	650	819	-65.7	749.5						
79AUE/BOW	115-10-6		(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-12.2	752.3						
77WOL/STA	7664-41-7		NH <sub>3</sub>	350	819	-70.9	747.5						
[C <sub>7</sub> H <sub>6</sub> O]	100-51-6		C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> OH				748.0			778.3			7
78TAF/TAA	67-56-1		CH <sub>3</sub> OH	350	724.5	23.3	748.0						
[CTe <sub>2</sub> ]	12192-34-6		CTe <sub>2</sub>				747.8			771			31
85JAS/STE			theory							771			
[C <sub>4</sub> H <sub>7</sub> ]	15157-95-6		CH <sub>2</sub> =C(CH <sub>3</sub> )CH <sub>2</sub> •				747.3			778			6
89HOL/LOS	79-24-3;		C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ; 4-FC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>	298						778			
87LIA/AUS	352-32-9			340			733-736						
[C <sub>2</sub> O]	12071-23-7		CCO				747.0			774.7			16
93MAC/SUD			theory	298						774.7			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>2</sub> H <sub>6</sub> O] 92PAR/FER	64-17-5	C <sub>2</sub> H <sub>5</sub> OH	550	725.4	11.4	746	750.4	24	776.4	25	-23	7
92PAR/FER	71-43-2	C <sub>6</sub> H <sub>6</sub>	530	736.5	5.3	741.3	774.4		774.4			2
92DOT/IRA	75-07-0	CH <sub>3</sub> CHO	298	736.5	6.3	740.5						
90FEL/KIM	75-07-0	CH <sub>3</sub> CHO theory	300			742.8			810			
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-72.3	746.0						
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-72.3	746.0						
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-66.6	747.7						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-15.1	749.3						
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	350	724.5	22.0	746.6						
78TAF/TAA	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	350	782.1	-38.9	743.3						
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-72.3	746.0						
76HAR/LIN	75-07-0	CH <sub>3</sub> CHO	370	736.5	5.4	741.5						
[C <sub>6</sub> H <sub>5</sub> O <sub>3</sub> Re] 81STE/BEA	14524-92-6 7664-41-7	(CO) <sub>5</sub> ReCH <sub>3</sub> NH <sub>3</sub>	320	819	-72.8	745.9 745.8			774.9			11.5
[C <sub>3</sub> H <sub>4</sub> ] AUS/LIA	463-49-0 75-07-0; 74- 93-1	H <sub>2</sub> C=C=CH <sub>2</sub> CH <sub>3</sub> CHO; CH <sub>3</sub> SH threshold value				745.8 736-742			775.3			10
77ROS/DRA									775.3			
[C <sub>7</sub> H <sub>7</sub> Br] 82MAS/BOH	106-38-7 108-88-3	4-Br-toluene C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-10.9	745.8 745.8			775.3			10
[C <sub>7</sub> H <sub>7</sub> Br] 82MAS/BOH	95-46-5 108-88-3	2-Br-toluene C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-10.9	745.8 745.8			775.3			10
[Rh] 84MAN/HAL	7440-16-6	Rh See Refs.				745.4			768 768±12			33
[C <sub>2</sub> H <sub>4</sub> O] 87TAF	75-21-8 7664-41-7	c-C <sub>2</sub> H <sub>4</sub> O NH <sub>3</sub>	350	819	-75.1	745.3 743.0			774.2			12
80AUE/WEB	75-05-8	CH <sub>3</sub> CN	298	748	-2.5	747.0						
80AUE/WEB	64-17-5	C <sub>2</sub> H <sub>5</sub> OH	298	746	-1.3	745.8						
[C <sub>4</sub> H <sub>6</sub> ] 87LIA/AUS	503-17-3 107-31-3	CH <sub>2</sub> =CC-CH <sub>3</sub> HCOOCH <sub>3</sub>	340	751.5	-6.7	745.1 744.8			775.8			5.8
87LIA/AUS	75-05-8	CH <sub>3</sub> CN	340	748	-2.5	745.4						
79AUE/BOW	67-56-1	CH <sub>3</sub> OH	298	724.5	9.3	733.8						
[C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> ] 94DEC/EXN2	619-72-7	4-NO <sub>2</sub> -C <sub>6</sub> H <sub>4</sub> CN				745.1			775.7			6
94DEC/EXN2	123-38-6	C <sub>2</sub> H <sub>5</sub> CHO	338	754.0	-6.9	746.9						
94DEC/EXN2	75-07-0	CH <sub>3</sub> CHO	338	736.5	6.3	742.6						
94DEC/EXN2	75-05-8	CH <sub>3</sub> CN	338	748	-2.3	745.6						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>7</sub> H <sub>7</sub> F] 82STO/SPL	95-52-3	2-F-toluene	478	756.3	-13.4	743.8			773.3			10	
[C <sub>8</sub> H <sub>5</sub> CH <sub>3</sub> ] 82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-13.0	743.7							
[HOS] 93LUC/CUR	71132-80-4:a	SiOH at Si theory	298			742.8			775.3			0	
[C <sub>3</sub> H <sub>4</sub> CIN] 87TAF	542-76-7	Cl(CH <sub>2</sub> ) <sub>2</sub> CN	350	819	-76.0	742.4			773.1			6	
[C <sub>2</sub> H <sub>5</sub> FSI] 90ALL/MCM	7664-41-7 7664-41-7	NH <sub>3</sub> NH <sub>3</sub>	320	819	-68.6	750.1							
[H <sub>2</sub> ] 82DER/HEH	125413-85-6 75-07-0; 75- 05-8	F(CH <sub>3</sub> )Si=CH <sub>2</sub> CH <sub>3</sub> CHO; CH <sub>3</sub> CN				742.2 736-748			771.1			12	
[CH <sub>4</sub> ] 97EAS/SMI	15194-15-7	NH <sub>2</sub>	350	742	0	742.0			773.4			3.4	
[C <sub>2</sub> H <sub>6</sub> ] 93SMI/RAD	74-93-1	CH <sub>3</sub> SH	298			742			773.4			3.5	3.6
[C <sub>2</sub> H <sub>4</sub> ] 93SMI/RAD	74-93-1	CH <sub>3</sub> SH theory	600						780.1				
[C <sub>2</sub> H <sub>2</sub> ] 92CUR/NOB	71-43-2	C <sub>6</sub> H <sub>6</sub>	298						770.6				
[C <sub>2</sub> H <sub>2</sub> ] 87TAF	7664-41-7	NH <sub>3</sub>	298						776.4				
[C <sub>2</sub> H <sub>2</sub> ] 80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	725.4	12.1	744.0	750.4	22.2	772.6	25	-16.7	8.3	
[C <sub>2</sub> H <sub>2</sub> ] 76HAR/LIN	7664-41-7	NH <sub>3</sub>	350	819	-77.3	741.2							
[C <sub>2</sub> H <sub>2</sub> ] 75SOL/HAR	75-07-0	CH <sub>3</sub> CHO	340	775.6	-33.1	743.2							
[C <sub>2</sub> H <sub>2</sub> ] 89HOL/LOS	4400-01-5	•CH <sub>2</sub> CHO	350	819	-76.0	742.5							
[C <sub>2</sub> H <sub>2</sub> ] 80STO/CAM	71-43-2; 108-88-3	C <sub>6</sub> H <sub>6</sub> ; C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	370	736.5	1.7	738.0			774			0	
[C <sub>2</sub> H <sub>2</sub> ] 85LIA/KAR	1691-88-9	CFCI	298			741.5			774				
[C <sub>2</sub> H <sub>2</sub> ] 97EAS/SMI	352-32-9; 95-52-3	(CH <sub>3</sub> ) <sub>2</sub> Hg C <sub>6</sub> H <sub>6</sub> ; C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>				740.8 725-756			771.6			5.8	
[C <sub>2</sub> H <sub>2</sub> ] 95SMI/RAD	6914-07-4	HNC theory				740.0 736-744			772.4			0	
[C <sub>2</sub> H <sub>2</sub> ] 95SMI/RAD	6914-07-4	HNC theory	298			739.8			772.3			0	0.1

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
82PAU/HEH	123-38-6; 75-08-1	C <sub>2</sub> H <sub>5</sub> CHO; C <sub>2</sub> H <sub>5</sub> SH				754-758						
[C <sub>2</sub> HCl <sub>3</sub> O <sub>2</sub> ] 76YAM/KEB	76-03-9 7664-41-7	CCl <sub>3</sub> COOH NH <sub>3</sub>	600	819	-76.6	739.1 739.0			770.0			5
[C <sub>6</sub> MoO <sub>6</sub> ] 81STE/BEA	13939-06-5 7664-41-7	(CO) <sub>6</sub> Mo NH <sub>3</sub>	320	819	-80.3	738.1 738.0			762.6			26.4
[C <sub>2</sub> H <sub>3</sub> O <sub>2</sub> ] 89HOL/LOS	#1498	•CH <sub>2</sub> COOH	298			737.5			770 770			0
[C <sub>2</sub> H <sub>4</sub> O] 97EAS/SMI	75-07-0	CH <sub>3</sub> CHO theory	298			736.5			768.5			1.5 1.5
95BOG/NES		appearance	298						767.8			
94RUS/BER		appearance	298						768.5			
93SMI/RAD		theory	0						764.5			
93SMI/RAD		theory	298						770.2			
93SMI/RAD		theory	600						773.9			
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-82.4	736.2						
86TAF/GAL	7664-41-7	NH <sub>3</sub>	350	819	-84.9	733.7						
86KNI/FRE	75-07-0	CH <sub>3</sub> CHO	303	736.5	0	736.5						
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-73.0	743.3						
79AUE/BOW	115-10-6	(CH <sub>3</sub> ) <sub>2</sub> O	298	764.5	-22.0	742.5						
77VOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-80.5	738.1						
76HAR/LIN	75-07-0	CH <sub>3</sub> CHO	370	736.5	0	736.5						
75SOL/HAR	75-07-0	CH <sub>3</sub> CHO	370	736.5	0	736.5						
68REF/CHU		threshold value	298						772.4			
[C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub> O] 87TAF	918-00-3 7664-41-7	CCl <sub>3</sub> COCH <sub>3</sub> NH <sub>3</sub>	350	819	-82.4	736.3 736.2			768.3			1.5
[C <sub>3</sub> ] 83RAK/BOH	12075-35-3 67-56-1; 75- 05-8	C <sub>3</sub> CH <sub>3</sub> OH; CH <sub>3</sub> CN				736.3 725-748			767.0			5.8
[C <sub>1</sub> H <sub>2</sub> F] 92PAR/FER	352-32-9 71-43-2	4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> F C <sub>6</sub> H <sub>6</sub>	390	725.4	6.0	736.1			763.8			16
87FER/JEN	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	478	756.3	-8.4	732.2			770.4			-11
82STO/SPL	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	478	756.3	-16.7	747.9			750.4	20	-36	
82MAS/BOH	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	369	756.3	-19.7	739.5						
[C <sub>2</sub> H <sub>3</sub> BrO] 93HEC/DEK	540-51-2 71-43-2; 64- 17-5	BrCH <sub>2</sub> CH <sub>2</sub> OH C <sub>6</sub> H <sub>6</sub> ; C <sub>2</sub> H <sub>5</sub> OH				735.7 725-746			766.1			7

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squbit	Reg No(M)		Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		PA(M)		$\Delta S_p$ (M)	
	107-07-3	71-43-2; 64-17-5					735.7	725-746	766.1	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)	
[C <sub>2</sub> H <sub>5</sub> ClO] 93HEC/DEK	107-07-3	71-43-2; 64-17-5	CICH <sub>2</sub> CH <sub>2</sub> OH C <sub>6</sub> H <sub>6</sub> ; C <sub>2</sub> H <sub>5</sub> OH				735.7	725-746			766.1			7
[C <sub>6</sub> H <sub>3</sub> MnO <sub>5</sub> ] 81STE/BEA 79STE/BEA	13601-24-6 7664-41-7 115-07-1; 75-07-0		(CO) <sub>5</sub> MnCH <sub>3</sub> NH <sub>3</sub> CH <sub>3</sub> CHCH <sub>2</sub> ; CH <sub>3</sub> CHO	320	819	-83.3	735.4	735.4 723-736			764.4			11.5
[C <sub>7</sub> H <sub>7</sub> Cl] 92PAR/FER 92PAR/FER 87FER/JEN 82MAS/BOH	106-43-4 352-32-9 71-43-2 352-70-5 108-88-3		4-Cl-toluene 4-CH <sub>3</sub> -C <sub>6</sub> H <sub>4</sub> F C <sub>6</sub> H <sub>6</sub> 3-F-toluene C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	390 380 369 369	736.1 725.4 756.0 756.3	-0.8 6.3 -13.5 -18.4	735.2	735.3 732.4 742.1 737.9	763.8 750.4	3.9 15	762.9 767.7 765.4	16 25	-12 -23	16 4 2
[C <sub>4</sub> H <sub>7</sub> F <sub>3</sub> O] 87TAF 83TAF2	461-24-5 7664-41-7 7664-41-7		C <sub>2</sub> H <sub>5</sub> OCH <sub>2</sub> CF <sub>3</sub> NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-82.8 -81.0	735.0	735.0 736.8			764.0			17
[CH <sub>2</sub> Se] 85KAR 85JAS/STE	6596-50-5 79-24-3; 75-07-0		H <sub>2</sub> C=Se C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ; CH <sub>3</sub> CHO theory				734.9	733-736			764.0			11
[CH <sub>3</sub> FO] 76YAM/KEB	144-49-0 7664-41-7		CH <sub>2</sub> FCOOH NH <sub>3</sub>	600	819	-81.2	734.5	734.4			765.4			5
[C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub> ] 76YAM/KEB	79-11-8 7664-41-7		CH <sub>2</sub> ClCOOH NH <sub>3</sub>	600	819	-81.2	734.5	734.4			765.4			5
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> OS] 87TAF	41879-94-1 7664-41-7		CF <sub>3</sub> COSCH <sub>3</sub> NH <sub>3</sub>	350	819	-84.2	734.3	734.2			765.2			5
[C <sub>5</sub> H <sub>8</sub> ] HOU/BEA 80LIA/SHO 80LIA/SHO 76SOL/FIE	142-29-0 75-07-0 79-24-3		c-C <sub>5</sub> H <sub>8</sub> threshold value CH <sub>3</sub> CHO C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> See Refs.	350 350 300	736.5 733.2	-3.8 1.7	733.8	732.8 734.9			766.3 768.2			0
[C <sub>3</sub> H <sub>2</sub> ClO <sub>2</sub> ] 87TAF	541-41-3 7664-41-7		ClCOOC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	-84.7	733.8	733.8			764.8			5
[C <sub>6</sub> H <sub>9</sub> F <sub>3</sub> O <sub>2</sub> ] 87TAF 77WOL/STA	367-64-6 7664-41-7 7664-41-7		CF <sub>3</sub> CO <sub>2</sub> (n-C <sub>4</sub> H <sub>9</sub> ) NH <sub>3</sub> NH <sub>3</sub>	350 350	819 819	-84.7 -83.3	733.8	733.8 735.1			764.8			5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula]	Reg No(M)	Base(M)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
[C <sub>2</sub> O <sub>6</sub> W]	14040-11-0	(CO) <sub>6</sub> W	320	819	-84.9	733.4			758.0			26.4
Yr5quib	7664-41-7	NH <sub>3</sub>				733.4						
[C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> ]	79-24-3	C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>	340	775.6	-43.1	733.2			765.7			0
80LIA/SO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>				733.3						
[C <sub>5</sub> F <sub>3</sub> N]	700-16-3	Pentafluoropyridine	350	819	-85.6	733.0			764.9			2
87TAF	7664-41-7	NH <sub>3</sub>				733.0						
[C <sub>3</sub> H <sub>4</sub> F <sub>2</sub> O]	453-14-5	CFH <sub>2</sub> COCFH <sub>2</sub>	298	736.5	-4.2	733.0			762.8			9
8IDRU/MCM	75-07-0	CH <sub>3</sub> CHO	298	742	-8.4	732.3						
8IDRU/MCM	74-93-1	CH <sub>3</sub> SH				733.6						
[C <sub>3</sub> H <sub>7</sub> F <sub>3</sub> O <sub>2</sub> ]	383-66-4	CF <sub>3</sub> CO <sub>2</sub> (n-C <sub>3</sub> H <sub>7</sub> )	350	819	-85.6	732.9			763.9			5
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-84.2	732.9			765			0
77WOL/STA	7664-41-7	NH <sub>3</sub>				734.2			765			
[CF <sub>2</sub> ]	2154-59-8	CF <sub>2</sub>	298			732.5						
91PAU/SQU	7783-07-5;	threshold value										
85LIA/KAR	109-77-3	H <sub>2</sub> Se; CH <sub>2</sub> (CN) <sub>2</sub>				676-694						
77LIA/AUS	74-90-8; 50-	Bracketing				686						
75VOG/BEA	00-0	HCN; CH <sub>2</sub> O				682-683						
[C <sub>2</sub> H <sub>3</sub> NO]	624-83-9	CH <sub>3</sub> NCO				732.0			764.4			0
85KAR/STE	383-63-1;	CF <sub>3</sub> COOC <sub>2</sub> H <sub>5</sub> ; 4-FC <sub>6</sub> H <sub>4</sub> CH <sub>3</sub>				728-736						
	352-32-9											
[HNO <sub>3</sub> ]	7697-37-2	HNO <sub>3</sub>	298	714.8		731.5			751.4			42
94CAC/ATT	598-58-3	CH <sub>3</sub> ONO <sub>2</sub>	298						750.3			
93SUN/SQU		See Refs.	298						744±10			
92LEERIC		theory	298						764±17			
90CAC/ATT	7732-18-5;	H <sub>2</sub> O; CF <sub>3</sub> CH <sub>2</sub> OH	303			660-670						
	75-89-8											
[Fe]	7439-89-6	Fe				731.1			754			32
86ELK/ARM3		See Refs.							754±8			
84HAL/KLE		See Refs.							796±21			
[B <sub>2</sub> H <sub>6</sub> ]	65930-58-7	B <sub>2</sub> H <sub>6</sub>				731.0			763.4			0
78WAN/DES	71-43-2; 75-	C <sub>6</sub> H <sub>6</sub> ; CH <sub>3</sub> CHO				725-736						
	07-0											
[CH <sub>2</sub> S]	865-36-1	H <sub>2</sub> C=S	298			730.5			759.7			11
97EAS/SMI		theory										10.8

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
93SMI/RAD		theory	600						772.2				
93SMI/RAD		theory	0						762.8				
93SMI/RAD		theory	298						768.7				
85KAR	383-63-1; 79-24-3	CH <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ; C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>				728-733							
85JAS/STE		theory							776.6				
82ROY/MCM	383-63-1; 75-07-0	CF <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> ; CH <sub>3</sub> CHO				728-736							
[CH <sub>3</sub> BO <sub>2</sub> ]	#1524	CH <sub>3</sub> O-B=O				730.6			763.0			0	
87HET/COL	67-56-1; 75- 07-0	CH <sub>3</sub> OH; CH <sub>3</sub> CHO				725-736							
[BHO <sub>2</sub> ]	13460-50-9	HO-B=O				730.5			763.0			0	
92AIT/CAC	67-56-1; 75- 07-0	CH <sub>3</sub> OH; CH <sub>3</sub> CHO	298			725-736							
[C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ]	109-86-4	CH <sub>3</sub> OCH <sub>2</sub> CH <sub>2</sub> OH				729.8			768.8			-22	
93SZU/MCM	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	600	775.6	14.2	802.4	802.1	33.9	836.0	20	-33.5	-13.5	
78TAE/TAA	67-56-1	CH <sub>3</sub> OH	320	724.5	4.6	729.8							
[CH <sub>4</sub> O <sub>3</sub> S]	75-75-2	CH <sub>3</sub> SO <sub>3</sub> H				728.9			761.3			0	
92PET/FOR	67-56-1; 79- 24-3	CH <sub>3</sub> OH; C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub>				725-733							
[C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O <sub>2</sub> ]	383-63-1	CF <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>				727.9			758.8			5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-90.6	727.8							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-89.2	729.2							
[C <sub>3</sub> H <sub>5</sub> N <sub>4</sub> O <sub>4</sub> ]	38858-89-8	3,5-dinitropyrazole				727.5			759.4			2	
92ABB/CAB	71-43-2	C <sub>6</sub> H <sub>6</sub>	333	725.4	0.4	726.6							
92ABB/CAB	67-56-1	CH <sub>3</sub> OH	333	724.5	3.7	728.5							
[C <sub>3</sub> H <sub>5</sub> NO]	1738-36-9	CH <sub>3</sub> OCH <sub>2</sub> CN				727.4			758.1			6	
87MAR/GAL	383-63-1	CF <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub>	320	727.9	-0.4	727.4							
[C <sub>6</sub> H <sub>5</sub> F]	462-06-6	C <sub>6</sub> H <sub>5</sub> F				726.6			755.9			10.5	
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-2.9	726.8	750.4	5.4	755.9	25	-14.2	10.8	
92PAR/FER	71-43-2	C <sub>6</sub> H <sub>6</sub>	550	725.4	-2.4	726.6	750.4	5.8	756.2	25	-14.9	10.1	
91MAU/SIE	67-56-1	CH <sub>3</sub> OH	600	724.5	2.9	727.0	754.3	0.8	755.1	9	3.3	12.3	
91MAU/SIE	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-4.2	725.6	750.4	5.0	755.4	25	-15.5	9.5	
81BOH/STO	71-43-2	C <sub>6</sub> H <sub>6</sub>	334	725.4	0.8	726.7	750.4	5.9	756.3	25	-15	10	
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-87.0	726.1							
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-0.8	726.0							
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-3.3	726.4							



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
[C <sub>3</sub> H <sub>5</sub> FO <sub>2</sub> ] 87TAF	461-64-3 7664-41-7	FCO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> NH <sub>3</sub>	350	819	-92.4	726.0			757.0			5
[C <sub>6</sub> H <sub>5</sub> Br] 81BOH/STO	108-86-1 71-43-2	C <sub>6</sub> H <sub>5</sub> Br C <sub>6</sub> H <sub>6</sub>	334	725.4	0	725.8			754.1			14
[CHNO] 89HOP/HOL	506-85-4	HCNO Appearance				725.5			758 758			0
[C <sub>8</sub> H <sub>6</sub> ] 93SZU/MCM	71-43-2	C <sub>8</sub> H <sub>6</sub>	600	722.7	14.6	725.4			750.4			25
93SZU/MCM	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>	600	756.3	-28.0	733.5	751.6	6.7	758.3	12	13.4	25.4
93SZU/MCM	108-88-3	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	600	724.5	6.7	725.5	784.0	-33.5	750.5	16	8.8	24.8
93SZU/MCM	67-56-1	CH <sub>3</sub> OH	600	751.5	-22.6	726.4	754.3	-7.5	746.8	9	23.0	32.0
93SZU/MCM	107-31-3	HCOOCH <sub>3</sub>	600	782.1	-53.6	722.9	782.5	-33.9	748.6	5	18.8	23.8
93SZU/MCM	67-64-1	(CH <sub>3</sub> ) <sub>2</sub> CO	600	736.5	-7.5	723.2	812	-55.2	756.8	8.7	2.5	11.2
92PAR/FER	75-07-0	CH <sub>3</sub> CHO	550	724.5	6.9	727.4	768.5	-19	749.5	1.5	21	22.5
92PAR/FER	67-56-1	CH <sub>3</sub> OH	550	736.5	-10.9	718.6	754.3	-3	751.3	9	18	27
91MAU/SIE	75-07-0	CH <sub>3</sub> CHO	600	748	-15.9	725.9	768.5	-16.7	751.8	1.5	9.6	11.1
91MAU/SIE	75-05-8	CH <sub>3</sub> CN	600	724.5	5.4	725.2	779.2	-27.6	751.6	4.3	19.2	23.5
91MAU/SIE	67-56-1	CH <sub>3</sub> OH	600	724.5	5.4	725.2	754.3	1.3	755.6	9	6.7	15.7
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-92.9	724.5						
85VAN/LEA		See Refs.										
81BOH/STO	71-43-2	C <sub>6</sub> H <sub>6</sub>	334	725.4	0	725.4						
80MAU	7664-41-7	NH <sub>3</sub>	550	819	-79.1	732.1						
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-50.6	724.8						
78LAU/SAL	7664-41-7	NH <sub>3</sub>	600	819	-77.0	732.6						
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	0	725.4						
77WOL/STA	7664-41-7	NH <sub>3</sub>	320	819	-84.9	733.4						
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	0	725.4						
76DEV/WOL	71-43-2	C <sub>6</sub> H <sub>6</sub>	320	725.4	0	725.4						
[H <sub>2</sub> N <sub>2</sub> O] 93ATU/CAC	7782-94-7 67-56-1; 71- 43-2	H <sub>2</sub> N-NO <sub>2</sub> CH <sub>3</sub> OH; C <sub>6</sub> H <sub>6</sub>	300			725.0 725-725			757.4			0
[C <sub>6</sub> H <sub>5</sub> Cl] 81BOH/STO	108-90-7	C <sub>6</sub> H <sub>5</sub> Cl	334	726.6	-1.6	724.6			753.1			13.5
81BOH/STO	462-06-6	C <sub>6</sub> H <sub>5</sub> F	334	725.4	-0.8	725.0	755.9	-2.5	753.4	10.5	2.8	13.3
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-87.9	724.1	750.4	3	753.4	25	-11	14
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-2.1	724.5						
76LAU/KEB	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-4.2	724.7						
[CH <sub>3</sub> O] 97EAS/SMI	67-66-1	CH <sub>3</sub> OH theory	298			724.5			754.3			9
93SZU/MCM	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub> theory	600	722.7	6.7	730.3	751.6	14.2	765.8	12	-12.6	7.3
93SMI/RAD			0						749.1			-0.6

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
93SMI/RAD		theory	298						754.3				
93SMI/RAD		theory	600						757.3				
92PAR/FER	75-07-0	CH <sub>3</sub> CHO	550	736.5	-13.3	721.4	768.5	-16	752.5	1.5	5	6.5	
91MAU/SIE	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>	600	722.7	8.4	732.0	751.6	11.3	762.9	12	-5.0	7.0	
90FEL/KIM		theory	300						791.2				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-94.7	723.5							
83TAF	7664-41-7	NH <sub>3</sub>	350	819	-94.3	724.0							
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-54.0	722.1							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-89.3	724.3							
77WOL/STA	7664-41-7	NH <sub>3</sub>	350	819	-94.3	723.9							
[C <sub>2</sub> H <sub>5</sub> O]	16520-04-0	•CH <sub>2</sub> OCH <sub>3</sub>	298			723.6			756.1				0
96AUD/FOS	115-07-1; 67-56-1	CH <sub>3</sub> CH=CH <sub>2</sub> ; CH <sub>3</sub> OH				723-725							
[HN <sub>3</sub> ]	7782-79-8	HNNN				723.5			756.0				0
93CAC/ATT	75-52-5; 71- 43-2	CH <sub>3</sub> NO <sub>2</sub> ; C <sub>6</sub> H <sub>6</sub>	298			722-725							
90CAC/ATT2	598-58-3	CH <sub>3</sub> ONO <sub>2</sub>		714.8									
84BEA/EYE		See Refs.											
[C <sub>3</sub> H <sub>4</sub> ]	74-99-7	CH <sub>3</sub> CCH	300			723.0			748				25
83BUR/HOL		Appearance							748				
76AUE/DAV	7783-06-4	H <sub>2</sub> S	298	673.8	8.8	682.6							
[C <sub>3</sub> H <sub>6</sub> ]	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>				722.7			751.6				12
97EAS/SMI		theory	298										11.7
93SMI/RAD		theory	600						747				
93SMI/RAD		theory	0						740.3				
93SMI/RAD		theory	298						744.3				
82ROS/BUF		threshold value	298						751				
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-58.6	717.4							
80LIA/SHO	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>	340	722.7	0	722.7							
80BAE		threshold value	298										
76YAM/KEB	7664-41-7	NH <sub>3</sub>	650	819	-93.8	718.7			751.8				
72CHO/FRA	67-56-1	CH <sub>3</sub> OH	340	724.5	-3.1	721.3							
[C <sub>3</sub> H <sub>6</sub> ]	75-19-4	c-C <sub>3</sub> H <sub>6</sub>				722.2			750.3				14.9
72CHO/FRA	67-56-1	CH <sub>3</sub> OH	340	724.5	-2.1	722.2							
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	372-18-9	1,3-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>				722			749.7				16
93SZU/MCM	107-31-3	HCOOCH <sub>3</sub>	600	751.5	-27.2	721.0	782.5	-34.3	748.2	5	12.1	17.1	
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-5.9	722.3	750.4	0	750.4	25	-9.6	15.4	
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-1.3	725.1							
76YAM/KEB	7664-41-7	NH <sub>3</sub>	650	819	-92.0	719.1							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>1</sub> S] 93ABB/MO 93ABB/MO	463-71-8 108-90-7 75-19-4	Cl <sub>3</sub> S C <sub>6</sub> H <sub>5</sub> Cl c-C <sub>3</sub> H <sub>6</sub>	333 333	724.6 722.2	-3.2 -0.6	721.8 721.7 721.9			752.5			5.8	
[CH <sub>3</sub> NO <sub>2</sub> ] 80LIA/SHO 80LIA/SHO 78MAC/BOH 78MAC/BOH 76MCA/PIT	75-52-5 115-11-7 115-07-1 115-07-1 67-56-1 67-56-1	CH <sub>3</sub> NO <sub>2</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> CH=CH <sub>2</sub> CH <sub>3</sub> CH=CH <sub>2</sub> CH <sub>3</sub> OH CH <sub>3</sub> OH	340 340 297 297 300	775.6 722.7 722.7 724.5 724.5	-59.0 2.5 -0.7 ~0	721.6 717.5 717.1 725.2 723.8 724.5			754.6			-1.6	
[C <sub>2</sub> H] 93DOT/IRA 93DOT/IRA 88LIA/BAR	2122-48-7 383-63-1 107-14-2	HCC• CF <sub>3</sub> CO <sub>2</sub> C <sub>2</sub> H <sub>5</sub> CCl <sub>2</sub> CN	298 298	727.9 715.1	-5.9 4.6	720.8 722.0 719.6			753.3			0	
[C <sub>3</sub> HN] 87DEA/MAU 87DEA/MAU 87DEA/MAU 87DEA/MAU 87DEA/MAU 85KNI/FRE 85KNI/FRE 84RAK/BOH	1070-71-9 108-90-7 75-07-0 75-52-5 67-56-1 431-47-0 75-52-5 506-68-3 75-52-5, 75-05-8	HCC-CN C <sub>6</sub> H <sub>5</sub> Cl CH <sub>3</sub> CHO CH <sub>3</sub> NO <sub>2</sub> CH <sub>3</sub> OH CF <sub>3</sub> COOCH <sub>3</sub> CH <sub>3</sub> NO <sub>2</sub> BrCN CH <sub>3</sub> NO <sub>2</sub> ; CH <sub>2</sub> CN	500 500 500 500 500 300 300	724.6 736.5 721.6 724.5 709.6 721.6 719.2	-6.3 -16.7 -0.4 -5.0 2.9 0.8 3.9	720.5 719.9 718.9 719.7 720.1 712.3 722.4 723.1 722-748			767 751.2			6	
[C <sub>4</sub> H <sub>6</sub> ] 81TRA 80LIA/SHO 80LIA/SHO	624-64-6 115-11-7 115-07-1	E-CH <sub>3</sub> CH=CHCH <sub>3</sub> threshold value (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> CH=CH <sub>2</sub>	298 340 340	775.6 722.7	-59.0	719.9 716.7 718.0			747 747			18	
[C <sub>2</sub> H <sub>3</sub> ] 92PET/IRA 80DEF/MCI	2669-89-8 107-14-2; 67-56-1 431-47-0; 67-56-1	C <sub>2</sub> H <sub>3</sub> CCl <sub>2</sub> CN; CH <sub>3</sub> OH CF <sub>3</sub> COOCH <sub>3</sub> ; CH <sub>3</sub> OH	298			719.8 715-725 710-725			755.2			-10	
[Co] 86ELK/ARM4	7440-48-4	Co See Refs.				719.8			742.7 742.7±6			32	
[C <sub>8</sub> H <sub>2</sub> F <sub>4</sub> ] 78HAR/LIA	2367-82-0 71-43-2	1,2,3,5-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> C <sub>8</sub> H <sub>6</sub>	400	725.4	-6.7	719.6 719.6			747.3			16	
[CBN] 91PET/KNI	506-68-3 75-52-5	BrCN CH <sub>3</sub> NO <sub>2</sub>	300	721.6	-2.3	719.2 719.3			749.8			6	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yrsquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta GB(M,R,T)$	GB(M)	PA(R)	$\Delta PA(M,R)$	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$
	75-52-5 7664-41-7	75-13-8	Base(R)	Base(M)										
85KNI/FRE	75-52-5		CH <sub>3</sub> NO <sub>2</sub>		300	721.6	-2.6	719.0						
76STA/KLE	7664-41-7		NH <sub>3</sub>		320	819	-96.7	722.1						
[CHNO]	75-13-8		HNCO					718.8			753			-5.8
89HOP/HOL			Appearance								753			
84BEA/EYE			See Refs.								740-753			
80WIG/BEA	50-00-0		H <sub>2</sub> C=O		320	683.3	5.0	688.6						
[C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> ]	327-54-8		1,2,4,6-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>		400	725.4	-7.5	718.8			746.5			16
78HAR/LIA	71-43-2		C <sub>6</sub> H <sub>6</sub>					718.8						
[CNS]	15941-77-2		NCS					718.5			751			0
94RUS/BER2			appearance								751			
[C <sub>3</sub> H <sub>5</sub> F <sub>3</sub> O]	460-43-5		CF <sub>3</sub> CH <sub>2</sub> OCH <sub>3</sub>		350	819	-99.8	718.4			747.6			11
87TAF	7664-41-7		NH <sub>3</sub>					718.4						
[H <sub>2</sub> OSi <sub>2</sub> ]	13597-73-4		H <sub>2</sub> SiOSiH <sub>3</sub>		0			718.3			749			5.8
91CUR/BRA			theory								749			
[C <sub>6</sub> H <sub>5</sub> ]	116139-00-5		HCCCH <sub>2</sub> CH(°)CCH			660.0		716.4			748.9			0
87KIN/BUR	7732-18-5		H <sub>2</sub> O						691	57.9	748.9			
[C <sub>3</sub> H <sub>3</sub> NO]	631-57-2		CH <sub>3</sub> COCN		350	819	-100.7	716.2			746.9			6
87TAF	7664-41-7		NH <sub>3</sub>					717.7						
86MAR/TOP	74-90-8		HCN		300	681.6	33.1	714.7						
[C <sub>4</sub> NiO <sub>4</sub> ]	13463-39-3		(CO) <sub>4</sub> Ni		320	819	-102.5	716.0			742.3			20.6
81STE/BEA	7664-41-7		NH <sub>3</sub>					716.0						
[C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> ]	372-38-3		1,3,5-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>		600	724.5	-5.4	715.4			741.9			20
93SZU/MCM	67-56-1		CH <sub>3</sub> OH					715.8			740.1	9	14.6	23.6
93SZU/MCM	71-43-2		C <sub>6</sub> H <sub>6</sub>		600	725.4	-12.6	714.4			744.1	25	-8.8	16.2
79LAU	7664-41-7		NH <sub>3</sub>		650	819	-93.8	715.9						
78HAR/LIA	71-43-2		C <sub>6</sub> H <sub>6</sub>		400	725.4	-2.9	723.0						
[C <sub>2</sub> H <sub>2</sub> CiN]	107-14-2		CCl <sub>2</sub> CH		298	724.5	-4.8	715.1			745.7			6
92DOT/IRA	67-56-1		CH <sub>3</sub> OH					719.7						
86MAR/TOP	74-90-8		HCN		300	681.6	31.8	713.4						
77WOL/STA	109-77-3		CH <sub>2</sub> (CN) <sub>2</sub>		350	694.1	17.6	712.0						
[CH <sub>3</sub> NO <sub>3</sub> ]	598-58-3		CH <sub>3</sub> ONO <sub>2</sub>		298			714.8			733.6			46
93SUN/SQU			See Refs.		298						732±10			
93RIC	75-38-7; 67-56-1		CF <sub>2</sub> CH <sub>2</sub> ; CH <sub>3</sub> OH		298			705-725						
92LEE/RIC2			theory		298						740±21			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta GB(M,R,T)$	GB(M) GB(M)	PA(R)	$\Delta PA(M,R)$	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
[C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> ] 87TAF 77WOL/STA	623-49-4 7664-41-7 109-77-3	NCCOOC <sub>2</sub> H <sub>5</sub> NH <sub>3</sub> CH <sub>2</sub> (CN) <sub>2</sub>	350 819 350	819 694.1	-101.1 17.6	714.7 717.3 712.1			745.7			5	
[C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> ] 86MAR/TOP	17640-15-2 74-90-8	CH <sub>3</sub> COOCN HCN	300	681.6	33.1	714.7 714.7			745.7			5	
[C <sub>6</sub> CrO <sub>6</sub> ] 81STE/BEA	13007-92-6 7664-41-7	(CO) <sub>6</sub> Cr NH <sub>3</sub>	320	819	-103.8	714.6 714.6			739.2			26.4	
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub> ] 87TAF 77WOL/STA	32042-38-9 7664-41-7 109-77-3	HCOOCH <sub>2</sub> CF <sub>3</sub> NH <sub>3</sub> CH <sub>2</sub> (CN) <sub>2</sub>	350 819 320	819 694.1	-100.7 17.1	714.6 717.8 711.4			745.5			5	
[P <sub>4</sub> ] 96ABB/HER 96ABB/HER 96ABB/HER 96ABB/HER 96ABB/HER	12185-10-8 115-20-8 32042-38-9 463-71-8 75-19-4 108-90-7	P <sub>4</sub> CCl <sub>3</sub> CH <sub>2</sub> OH HCOOCH <sub>2</sub> CF <sub>3</sub> Cl <sub>3</sub> CS c-C <sub>3</sub> H <sub>6</sub> C <sub>6</sub> H <sub>5</sub> Cl	333 333 333 333 333	698.9 714.6 721.8 722.2 724.6	9.4 -0.1 -3.4 -5.8 -10	714.3 708.0 714.1 718.1 716.5 714.6			742.3			14.9	
[Ni] 86ELK/ARM4	7440-02-0	Ni See Refs.				714.1			737 737			32	
[H <sub>4</sub> OSi] 93LUC/CUR 91CUR/BRA	14475-38-8	H <sub>3</sub> SiOH at O theory theory	298 0			713.9			746.4 746.4 742.2			0	
[CH <sub>2</sub> F <sub>2</sub> Si] 90ALL/MCM	51675-50-4 75-38-7; 75-52-5	F <sub>2</sub> Si=CH <sub>2</sub> CF <sub>2</sub> =CH <sub>2</sub> ; CH <sub>3</sub> NO <sub>2</sub>				713.4 705-722			742.3			12	
[C <sub>4</sub> H <sub>2</sub> ] 91PET/KNI 90BOT/KNI 87DEA/MAU	460-12-8 506-68-3 75-52-5; 2367-82-0	HCC-CCH BrCN theory CH <sub>3</sub> NO <sub>2</sub> ; 1,2,3,5-C <sub>6</sub> H <sub>3</sub> F <sub>4</sub>	300 300 ~330	719.2	-6.4	712.8 712.8 722-720			737.2 741			27	
[C <sub>2</sub> H <sub>5</sub> O] 89HOL/LOS	4422-54-2	•CH <sub>2</sub> CH <sub>2</sub> OH	298			712.5			745 745			0	
[AsH <sub>3</sub> ] 87TAF 80LIA/SHO 80LIA/SHO	7784-42-1 7664-41-7 115-11-7 115-07-1	AsH <sub>3</sub> NH <sub>3</sub> (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> CH <sub>3</sub> CH=CH <sub>2</sub>	350 340 340	819 775.6 722.7	-117.2 -63.2 -3.3	712.0 702.1 713.7 720.3			747.9			-11.5	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(M)		$\Delta S_p^0(M,R)$	$\Delta S_p^0(M)$
						GB(M)	$\Delta$ GB(M,R)	PA(R)	$\Delta$ PA(M,R)		
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	13.7	709.0		742.0		2.7	2.7
[CH <sub>2</sub> O <sub>2</sub> ]	64-18-6	HCOOH	298			710.3		746.7			
97EAS/SMI		theory	600					742.9			
93SMI/RAD		theory	298					737.1			
93SMI/RAD		theory	0					781			
90FEL/KIM		theory	300								
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-120.4	698.2					
80LIA/SHO	115-11-7	(CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	340	775.6	-64.4	711.9					
80LIA/SHO	115-07-1	CH <sub>3</sub> CH=CH <sub>2</sub>	340	722.7	-4.2	718.9					
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-115.9	699.9					
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	320	694.1	11.7	706.0					
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O <sub>2</sub> ]	431-47-0	CF <sub>3</sub> COOCH <sub>3</sub>				709.6		740.5		5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-108.9	709.5					
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	13.7	708.2					
[C <sub>3</sub> H <sub>3</sub> ]	2932-78-7	HCCCH <sub>2</sub> <sup>•</sup>	298			708.5		741		0	
89HOL/LLOS								741			
[C <sub>3</sub> H <sub>5</sub> ]	1981-80-2	CH <sub>2</sub> =CHCH <sub>2</sub> <sup>•</sup>				707.4		736		13	
89HOL/LLOS		See Refs.	298					736			
80DEF/MCI	109-77-3, 431-47-0	NCCH <sub>2</sub> CN; CF <sub>3</sub> COOCH <sub>3</sub>				694-710					
[H <sub>3</sub> OSi]	113648-09- 2:a	H <sub>2</sub> SiOH at O				705.5		738		0	
93LUC/CUR		theory	298					738			
[C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ]	75-38-7	CH <sub>2</sub> =CF <sub>2</sub>				705.1		734		12	
76WIL/LEB		threshold value						734			
75RID	75-03-6; 67- 56-1	C <sub>2</sub> H <sub>3</sub> I, CH <sub>3</sub> OH				698-725					
[C <sub>4</sub> H <sub>4</sub> F <sub>4</sub> O <sub>2</sub> ]	1683-88-1	CF <sub>3</sub> COOCH <sub>2</sub> CH <sub>2</sub> F				704.7		735.7		5	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-117.2	701.3					
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	13.7	708.1					
[H <sub>2</sub> Te]	7783-09-7	H <sub>2</sub> Te				704.5		735.9		3.8	
86KAR/JAS	75-38-7	CH <sub>2</sub> =CF <sub>2</sub>	330	705.1	-0.8	704.5					
[C <sub>3</sub> H <sub>7</sub> O]	31594-81-7	•CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> OH				703.5		736		0	
89HOL/LLOS			298					736			
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	367-11-3	1,2-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>				703.5		731.2		16	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-24.7	703.4	750.4	-17.6	732.8	25	-13.0	12.0
93SZU/MCM	67-56-1	CH <sub>3</sub> OH	600	724.5	-18.8	703.6	754.3	-25.5	728.8	9	10.9	19.9
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-1.7	724.6						
[C <sub>3</sub> H <sub>5</sub> ]	2417-82-5	c-C <sub>3</sub> H <sub>5</sub> *				702.0			738.9			-14.9
84LIA/BUC	421-50-1;	CF <sub>3</sub> COCH <sub>3</sub> ; AsH <sub>3</sub>	330			692-712						
	7784-42-1											
80DEF/MCI	75-07-0; 64-17-5	CH <sub>3</sub> CHO; C <sub>2</sub> H <sub>5</sub> OH				736-746						
[C <sub>3</sub> H <sub>3</sub> ]	28933-84-8	c-C <sub>3</sub> H <sub>3</sub> *				701.8			734.3			0
80DEF/MCI	109-77-3;	NCCH <sub>2</sub> CN; CF <sub>3</sub> COOCH <sub>3</sub>				694-710						
	431-47-0											
[CH <sub>3</sub> S]	17032-46-1	•CH <sub>2</sub> SH				701.5			733.9			0
95CHO/SMI	545-06-2;	CCl <sub>3</sub> CN; HCOOH				693-710						
	64-18-6											
[CS <sub>2</sub> ]	506-80-9	CS <sub>2</sub>				700.9			725			28
85JAS/STE		theory							725			
[HOS]	71132-8-4; b	SiOH at O				700.1			732.6			0
93LUC/CUR		theory	298						732.6			
[C <sub>2</sub> H <sub>3</sub> F]	75-02-5	CH <sub>2</sub> =CHF				700.1			729			12
80KOP/COM									703			
76WIL/LEB									729			
75RID	7732-18-5;	See Refs.										
	7783-06-4	H <sub>2</sub> O; H <sub>2</sub> S				660-674						
[C <sub>6</sub> H <sub>3</sub> F <sub>3</sub> ]	367-23-7	1,2,4-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>				699.4			729.5			8
93SZU/MCM	67-56-1	CH <sub>3</sub> OH	600	724.5	-24.7	700.1	754.3	-31.0	723.3	9	10.5	19.5
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-31.8	698.7	750.4	-21.8	728.7	25	-17.2	7.8
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-5.0	722.1						
[C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O]	115-20-8	CCl <sub>3</sub> CH <sub>2</sub> OH				698.9			729.3			7
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-122.6	695.7						
77WOL/STA	109-77-3	CH <sub>2</sub> (CH) <sub>2</sub>	350	694.1	7.8	702.2						
[BH <sub>3</sub> O <sub>3</sub> ]	10043-35-3	B(OH) <sub>3</sub>				698.4			728.1			9.1
92AIT/CAC	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	298	694.1	-2.1	692.0						
92AIT/CAC	75-38-7	CH <sub>2</sub> =CF <sub>2</sub>	298	705.1	-0.4	704.7						
[C <sub>2</sub> H <sub>3</sub> I]	75-03-6	C <sub>2</sub> H <sub>3</sub> I				698.3			724.8			20
72BEA/HOL	7783-06-4;	H <sub>2</sub> S; C <sub>3</sub> H <sub>6</sub>				674-723						
	115-07-1											

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta \Delta S_p(M,R)$	$\Delta S_p(M)$
	359-13-7	7664-41-7	Base(M)	Base(R)										
[C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> O]	359-13-7	CF <sub>2</sub> HCH <sub>2</sub> OH					697.0				727.4			7
87TAF	7664-41-7	NH <sub>3</sub>			350	819	-128.1	690.2						
78TAF/TAA	67-56-1	CH <sub>3</sub> OH			350	724.5	-21.0	703.6						
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			350	694.1	2.7	697.1						
[C <sub>6</sub> H <sub>5</sub> F <sub>3</sub> ]	1489-63-8	1,2,3-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>						696.6			724.3			16
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>			600	725.4	-28.5	699.7	750.4	-29.3	721.1	25	1.3	26.3
93SZU/MCM	7783-06-4	H <sub>2</sub> S			600	673.8	24.3	694.6	705	16.7	721.7	4.3	12.6	16.9
93SZU/MCM	75-15-0	CS <sub>2</sub>			600	657.7	31.4	692.7	681.9	47.7	729.5	28	-27.2	0.8
93SZU/MCM	67-56-1	CH <sub>3</sub> OH			600	724.5	-23.0	699.4	754.3	-35.6	718.7	9	20.9	29.9
[C <sub>3</sub> H <sub>5</sub> N <sub>2</sub> ]	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>						694.1			723.0			12
87TAF	7664-41-7	NH <sub>3</sub>			350	819	-128.6	689.5						
81DRU/MCM	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			298	694.1	0	694.1						
81DOU/MCM	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			298	694.1	0	694.1						
79LAU	7664-41-7	NH <sub>3</sub>			650	819	-118.3	694.3						
78TAF/TAA	67-56-1	CH <sub>3</sub> OH			320	724.5	-26.8	697.7						
77WOL/STA	7664-41-7	NH <sub>3</sub>			350	819	-118.1	700.0						
77WOL/STA	67-56-1	CH <sub>3</sub> OH			350	724.5	-28.8	695.5						
[C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> ]	540-36-3	1,4-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>						692.8			718.7			22
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>			600	725.4	-32.2	694.1	750.4	-36.0	714.4	25	6.3	31.3
93SZU/MCM	67-56-1	CH <sub>3</sub> OH			600	724.5	-25.5	695.1	754.3	-41.8	712.5	9	27.2	36.2
93SZU/MCM	421-50-1	CF <sub>3</sub> COCH <sub>3</sub>			600	692.0	5.4	691.5	723.9	-8.4	715.5	2	23.0	25.0
93SZU/MCM	7783-06-4	H <sub>2</sub>			600	673.8	22.2	690.7	705	11.3	716.3	4.3	18.0	22.3
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>			400	725.4	-4.2	721.5						
[C <sub>2</sub> Cl <sub>3</sub> N]	545-06-2	CCl <sub>3</sub> CN						692.6			723.2			6
87TAF	7664-41-7	NH <sub>3</sub>			350	819	-125.8	692.5						
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			350	694.1	0.9	695.3						
[COTe]	#1602	OCTe at Te theory						692.1			718			22
85IAS/STE											718			
[C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O]	421-50-1	CF <sub>3</sub> COCH <sub>3</sub>						692.0			723.9			2
93SZU/MCM	75-15-0	CS <sub>2</sub>			600	657.7	24.3	689.8	681.9	50.2	732.1	28	-43.1	-15.1
93SZU/MCM	367-23-7	1,2,4-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>			600	699.4	-5.9	695.4	729.5	-4.2	725.3	8	-2.9	5.1
93SZU/MCM	540-36-3	1,4-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>			600	692.8	-5.4	693.4	718.7	8.4	727.1	22	-23.0	-1.0
81DRU/MCM	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			298	694.1	-4.2	689.9						
81DOU/MCM	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>			298	694.1	-2.5	691.6						
[CCIN]	506-77-4	CICN						691.5			722.1			6
87TAF	7664-41-7	NH <sub>3</sub>			350	819	-130.4	688.0						
86MARTOP	74-90-8	HCN			300	681.6	13.4	695.0						
76STAN/KLE	7664-41-7	NH <sub>3</sub>			320	819	-107.5	711.2						



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)
	75-87-6 7664-41-7	421-14-7 7664-41-7	2348-46-1 50-00-0; 421-50-1	7782-65-2 74-85-1; 115-07-1										
[C <sub>2</sub> HCl <sub>3</sub> O] 87TAF			CCl <sub>3</sub> CHO NH <sub>3</sub>		350	819	-128.1	690.5 690.4			722.3			2
[C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O] 87TAF			CF <sub>3</sub> OCH <sub>3</sub> NH <sub>3</sub>		350	819	-128.1	690.0 690.0			719.2			11
[C <sub>2</sub> H <sub>5</sub> O] 96AUD/FOS			CH <sub>3</sub> CH(OH) H <sub>2</sub> C=O; CF <sub>3</sub> COCH <sub>3</sub>					687.7 683-692			720.1			0
[GeH <sub>4</sub> ] 80SEN/ABE			GeH <sub>4</sub> C <sub>2</sub> D <sub>4</sub> ; CD <sub>3</sub> CDCl <sub>2</sub>					687.1 651-723			713.4			20.6
[C <sub>2</sub> H <sub>5</sub> FO] 93HEC/DEK			FCH <sub>2</sub> CH <sub>2</sub> OH C <sub>6</sub> F <sub>6</sub> ; C <sub>2</sub> H <sub>5</sub> OH					685.2 624-746			715.6			7
[CH <sub>2</sub> O] 97EAS/SMI			H <sub>2</sub> C=O theory		298			683.3			712.9			9.5
93TRA/HOL			threshold value		298						712.9			9.5
93SMI/RAD			theory		0						705.8			
93SMI/RAD			theory		600						715.9			
93SMI/RAD			theory		298						711.8			
87TAF			NH <sub>3</sub>		350	819	-140.9	677.3			726.6			
85JAS/STE			theory								730.1			
84DIX/KOM			theory		300									
80WIG/BEA			H <sub>2</sub> C=O		320	683.3	0	683.3						
78TAN/MAC			H <sub>2</sub> O		298	660.0	21.8	681.8						
78FRE/HAR			H <sub>2</sub> S		300	673.8	5.0	678.9						
77VOL/STA			CH <sub>2</sub> (CN) <sub>2</sub>		320	694.1	-11.2	683.0			709.2			
68REF/CHU			threshold value		298									
[CHN] 97EAS/SMI			HCN		298			681.6			712.9			4
93SMI/RAD			theory		298						712			4
93SMI/RAD			theory		0						706.2			
93SMI/RAD			theory		600						715.2			
87TAF			CH <sub>2</sub> =CH <sub>2</sub>		350	651.5	37.7	689.5						
86MAR/TOP			HCN		300	681.6	0	681.6						
78TAN/MAC			H <sub>2</sub> O		298	660.0	20.5	680.5						
78FRE/HAR2			H <sub>2</sub> S		340	673.8	4.2	678.0						
77VOL/STA			CH <sub>2</sub> (CN) <sub>2</sub>		350	694.1	-13.7	680.9						
[C <sub>2</sub> HF <sub>3</sub> O <sub>2</sub> ] 93HEC/DEK			CF <sub>3</sub> COOH					680.7			711.7			5

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	28.0	680.0							
87TAF	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	33.1	684.9							
81DRU/MCM	360-52-1	CF <sub>2</sub> HCOCF <sub>2</sub> H	298	669.0	-1.7	667.3							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-137.7	677.4							
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	-20.1	674.3							
[SSI]	113443-18-8	SIS				677.7			710.2			0	
89FOX/WLO	7783-06-4; 74-90-8	H <sub>2</sub> S; HCN	295			674-682							
[H <sub>2</sub> Se]	7783-07-5	H <sub>2</sub> Se				676.4			707.8			3.8	
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-143.7	674.8							
85KAR	7783-06-4	H <sub>2</sub> S	340	673.8	4.2	678.0							
79AUE/BWO	67-56-1	CH <sub>3</sub> OH	298	724.5	-37.6	686.9							
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	320	694.1	-13.7	680.6							
[H <sub>2</sub> P]	13765-43-0	PH <sub>2</sub>				675.7			709.2			-3.4	
86BER/CUR		thermo cycles	298						709.2				
[C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> O]	333-36-8	(CF <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> O				674.9			702.3			17	
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	23.8	674.9							
87TAF	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	29.7	680.9							
[H <sub>2</sub> S]	7783-06-4	H <sub>2</sub> S				673.8			705			4.3	
97EAS/SMI		theory	298									3.4	
93SZU/MCM	71-43-2	C <sub>6</sub> H <sub>6</sub>	600	725.4	-52.3	679.3			705.6			12.4	
93SZU/MCM	540-36-3	1,4-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	600	692.8	-22.2	676.0			707.4			4.0	
93SZU/MCM	367-23-7	1,2,4-C <sub>6</sub> H <sub>3</sub> F <sub>3</sub>	600	699.4	-23.0	677.5			706.1			8.8	
93SMI/RAD		theory	600						712.2				
93SMI/RAD		theory	298						707.7				
93SMI/RAD		theory	0						701.6				
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-147.8	670.7							
87POP/CUR		theory	298						705				
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	27.2	679.4							
84WAL/BLA		threshold value	298						704.4				
83PRE/TZE		threshold value	298						705.7				
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-144.1	671.1							
78TAN/MAC	7732-18-5	H <sub>2</sub> O	298	660.0	15.9	675.9							
78FRE/HAR2	7783-06-4	H <sub>2</sub> S	340	673.8	0	673.8							
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	-17.6	676.9							
77MAU/FIE	7732-18-5	H <sub>2</sub> O	550	660.0	16.3	676.5							
73HOP/BON	7732-18-5	H <sub>2</sub> O	296	660.0	19.2	679.3							
[Pd]	7440-05-3	Pd				673.4			696			33	
84MAN/HAL		See Refs.							696±12				

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> ]	551-62-2	1,2,3,4-C <sub>6</sub> H <sub>2</sub> F <sub>4</sub>											
93SZU/MCM	7783-06-4	H <sub>2</sub> S	600	673.8	3.3	672.7	705	-11.7	700.4	4.3	25.1	16	16
93SZU/MCM	75-15-0	CS <sub>2</sub>	600	657.7	10.5	673.7	681.9	18.8	693.3	28	-14.2	29.4	29.4
78HAR/LIA	71-43-2	C <sub>6</sub> H <sub>6</sub>	400	725.4	-6.3	720.0			700.7			13.8	13.8
[C <sub>4</sub> H <sub>10</sub> ]	75-28-5	iso-C <sub>4</sub> H <sub>10</sub>											
78HIR	7732-18-5	H <sub>2</sub> O		660.0		671.3	691	-16.3	677.8			87	87
78HIR	7783-06-4	H <sub>2</sub> S		673.8			705	-32.2	674.7				
76HIR/KEB		See Refs.							672.8				
									685.9				
[CF <sub>3</sub> NO]	334-99-6	CF <sub>3</sub> NO				670.8			703.3			0	0
79FRE/HAR	7732-18-5;	H <sub>2</sub> O; HCN				660-682							
	74-90-8												
[C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O]	75-89-8	CF <sub>3</sub> CH <sub>2</sub> OH				669.9			700.2			7	7
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	21.3	673.1							
87TAF	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	29.7	681.4							
85MCM/KEB	7732-18-5	H <sub>2</sub> O	400	660.0	9.6	669.5							
83COL/MCM	7732-18-5	H <sub>2</sub> O	298	660.0	9.2	669.2							
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-147.3	667.0							
78TAF/TAA	67-56-1	CH <sub>3</sub> OH	350	724.5	-48.8	675.8							
77VOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	-24.9	669.5							
[C <sub>2</sub> H <sub>3</sub> Br]	74-96-4	C <sub>2</sub> H <sub>3</sub> Br				669.7			696.2			20	20
72BEA/HOL	77-88-4;	CH <sub>3</sub> I; H <sub>2</sub> S				666-674							
	7783-06-4												
[C <sub>3</sub> H <sub>2</sub> F <sub>4</sub> O]	360-52-1	CF <sub>2</sub> HCOCF <sub>2</sub> H				669.0			698.8			9	9
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	18.4	670.1							
81DRU/MCM	7783-06-4	H <sub>2</sub> S	298	673.8	-5.9	668.0							
[H <sub>3</sub> OSi]	81429-20-1	H <sub>3</sub> SiO at O				667.5			700			0	0
93LUC/CUR		theory	298						700				
[B <sub>5</sub> H <sub>9</sub> ]	19624-22-7	B <sub>5</sub> H <sub>9</sub>				666.9			699.4			0	0
72SOL/POR	7732-18-5;	H <sub>2</sub> O; H <sub>2</sub> S	~373			660-674							
	7783-06-4												
[C <sub>6</sub> H <sub>12</sub> ]	110-82-7	c-C <sub>6</sub> H <sub>12</sub>				666.9			686.9			42	42
82AUS/REB	7732-18-5;	H <sub>2</sub> O; H <sub>2</sub> S				660-674							
	7783-06-4												
[C <sub>2</sub> H <sub>5</sub> Cl]	56-00-3	C <sub>2</sub> H <sub>5</sub> Cl				666.9			693.4			20	20
72BEA/HOL	7732-18-5;	H <sub>2</sub> O; H <sub>2</sub> H				660-674							
	7783-06-4												
[H <sub>2</sub> O <sub>4</sub> S]	7664-93-9	H <sub>2</sub> SO <sub>4</sub>				666.9			699.4			0	0

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
78SMI/MUN	7732-18-5; 7783-06-4	H <sub>2</sub> O; H <sub>2</sub> S				660-674						
[CHF <sub>3</sub> O <sub>3</sub> S] 78MIN/MUN	1493-13-6 7732-18-5; 7783-06-4	CF <sub>3</sub> SO <sub>3</sub> H H <sub>2</sub> O; H <sub>2</sub> S				666.6 660-674			699.4			0
[C <sub>2</sub> HF <sub>3</sub> ] 75RID	359-11-5 7732-18-5; 7783-06-4	C <sub>2</sub> F <sub>3</sub> H H <sub>2</sub> O; H <sub>2</sub> S				666.9 660-674			699.4			0
[CHP] 90ADA/MIC	6829-52-3	HCP Bracketing, See Refs.	300			666.5			699 699±8			0
[CH <sub>3</sub> I] 94GLU/SZU	74-88-4	CH <sub>3</sub> I theory	298			665.5			691.7 691.1			21
94GLU/SZU	75-15-0	CS <sub>2</sub>	600	657.7	5.2	665.0	681.9	8.4	690.3	28	-5.4	22.6
94GLU/SZU	363-72-4	C <sub>6</sub> HF <sub>5</sub>	600	662.7	4.9	666.1	690.4	-4.6	685.8	16	15.9	31.9
72BEA/HOL	7783-06-4	H <sub>2</sub> S	300	673.8	0	673.8						
[PS] 90ADA/MIC	12281-36-6	PS Bracketing, See Refs.	300			665.5			698 698±8			0
[C <sub>2</sub> H <sub>7</sub> B <sub>5</sub> ] 80DIX	20693-69-0 7732-18-5; 75-89-8	2,4-C <sub>2</sub> B <sub>5</sub> H <sub>7</sub> H <sub>2</sub> O; CF <sub>3</sub> CH <sub>2</sub> OH				665.0 660-670			697.4			0
[F <sub>3</sub> OP] 83COL/MCM	13478-20-1 7732-18-5	OPF <sub>3</sub> H <sub>2</sub> O	298	660.0	4.2	664.2 664.2			694.0			9.1
[F <sub>3</sub> P] 87TAF	7783-55-3 74-85-1	PF <sub>3</sub> CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	9.2	662.8 661.2			695.3			0
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	13.0	664.4						
80DOI/MCM	7446-09-5; 74-85-1	SO <sub>2</sub> ; C <sub>2</sub> H <sub>4</sub>				643-651						
78COR/BEA	7783-54-2; 74-87-3	NF <sub>3</sub> ; CH <sub>3</sub> Cl				539-621						
[C <sub>8</sub> HF <sub>5</sub> ] 93SZU/MCM	363-72-4 7783-06-4	C <sub>8</sub> HF <sub>5</sub> H <sub>2</sub> S	600	673.8	-6.3	662.7 664.0	705	17.6	690.4 687.4	4.3	18.8	16 23.1
93SZU/MCM	75-15-0	CS <sub>2</sub>	600	657.7	0	661.3	681.9	11.7	693.6	28	-19.2	8.8
78HAR/LIA	71-43-2	C <sub>8</sub> H <sub>6</sub>	400	725.4	-9.6	716.7						
[C <sub>4</sub> F <sub>7</sub> N] 83COL/MCM	375-00-8 7732-18-5	C <sub>4</sub> F <sub>7</sub> CN H <sub>2</sub> O	298	660.0	2.5	662.6 662.6			693.2			6

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M) $\Delta S_p$ (M)
[CH <sub>3</sub> O] 93MOU/AUD	2597-43-5 363-72-4; 7783-06-4	•CH <sub>3</sub> OH C <sub>6</sub> H <sub>5</sub> F <sub>5</sub> ; H <sub>2</sub> S				662.5 663-674			695			0
89HOL/LOS		See Refs.	298						695			
[C <sub>2</sub> HF] 84BEA/EYE	2713-09-9	HCCF				661.3			686			26
74REI/BAU		See Refs.							674			
73REI/KRA		threshold value							690			
		threshold value							690			
[C <sub>3</sub> F <sub>5</sub> N] 83COL/MCM	422-04-8 7732-18-5	C <sub>3</sub> F <sub>5</sub> CN H <sub>2</sub> O	298	660.0	1.3	661.3 661.3			692.0			6
[C <sub>4</sub> H <sub>4</sub> F <sub>6</sub> O] 83COL/MCM	1515-14-6 7732-18-5	(CF <sub>3</sub> ) <sub>2</sub> C(CH <sub>3</sub> )OH H <sub>2</sub> O	298	660.0	0.8	660.9 650.9			691.2			7
[Si] 92BRU/GRE	12504-41-5:a	SiS at S theory				660.2			683 683			32.5
[H <sub>2</sub> O] 97EAS/SMI	7732-18-5	H <sub>2</sub> O theory	298			660.0			691			5
93SZU/MCM		H <sub>2</sub> S	600	673.8	-14.6	659.0			689.1	4.3	2.1	4.8
93SMI/RAD	7783-06-4	theory	298						688.4			6.4
93SMI/RAD		theory	600						692.8			
93SMI/RAD		theory	0						682.3			
93DEL		theory	298						687			
88MCU/ADA	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	300	651.5	9.2	660.7			691.0	11.5	-4.2	7.3
87TAF	7664-41-7	NH <sub>3</sub>	350	819	-165.2	653.2			691.6			
87POP/CUR		theory	298						691.6			
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	13.8	665.9			691.6			
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	14.2	665.7			691.6			
81BOH/MAC	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	7.5	659.0			691.6			
79LAU	7664-41-7	NH <sub>3</sub>	650	819	-157.3	657.7			691.6			
78TAN/MAC	7732-18-5	H <sub>2</sub> O	298	660.0	0	660.0			691.6			
77WOL/STA	109-77-3	CH <sub>2</sub> (CN) <sub>2</sub>	350	694.1	-35.1	659.3			691.6			
77NG/TRE		threshold value							691.6			
77MAU/FIE	7732-18-5	H <sub>2</sub> O	550	660.0	0	660.0			691.6			
73HOP/BON	7732-18-5	H <sub>2</sub> O	296	660.0	0	660.0			691.6			
69HAN/FRA		threshold value							691.6			
[C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> ] 75RID	1630-78-0 353-36-6; 7732-18-5	(E)-CHFCHF C <sub>2</sub> H <sub>3</sub> F; H <sub>2</sub> O				657.9 656-660			688.6			5.8
[CS <sub>2</sub> ] 97EAS/SMI	75-15-0	CS <sub>2</sub> theory	298			657.7			681.9			28 31.3

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M)		Base(M)		T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)		PA(R)		PA(M)		$\Delta S_p(M)$	$\Delta S_p(M)$								
	540-36-3	7783-06-4	7732-18-5	74-85-1				7732-18-5	7664-41-7	463-58-1;	74-99-7	74-85-1	7732-18-5			353-85-5	74-85-1	75-15-0	74-85-1	74-85-1	353-36-6	74-85-1;	7732-18-5
93SZU/MCM	1,4-C <sub>6</sub> H <sub>4</sub> F <sub>2</sub>	600	692.8	-30.1	660.9	718.7	-43.5	675.2	22	22.6	44.6												
93SZU/MCM	H <sub>2</sub> S	600	673.8	-5.9	660.9	705	-31.0	674.0	4.3	42.7	47.0												
93SZU/MCM	H <sub>2</sub> O	600	660.0	8.4	661.5	691	-15.9	675.1	5	41.0	46.0												
93SMI/RAD	theory	600						685.4															
93SMI/RAD	theory	298						681.9															
93SMI/RAD	theory	0						677.5															
88MCI/ADA	CH <sub>2</sub> =CH <sub>2</sub>	300	651.5	6.9	658.4	680.5	1.9	682.4	11.5	16.7	28.2												
88MCI/ADA	H <sub>2</sub> O	300	660.0	-2.9	657.1	691	-9.6	681.4	5	23	28												
87TAF	NH <sub>3</sub>	350	819	-168.9	648.4																		
85WEI/PLA	COS; CH <sub>3</sub> CCH				603-723																		
85MCM/KEB	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	18.8	668.7																		
85JAS/STE	theory	550	660.0	6.3	660.6			689															
77MAU/FIE	H <sub>2</sub> O																						
[C <sub>2</sub> F <sub>3</sub> N]																							
94KOP/ANV	CF <sub>3</sub> CN	373	651.5	5.9	657.7			688.4			6												
93SZU/MCM	CH <sub>2</sub> =CH <sub>2</sub>	350	557.7	-18.0	646.4	681.9	-8.4	673.5	28	-15.9	12.1												
87TAF	CS <sub>2</sub>	600	651.5	6.7	658.4																		
85MCM/KEB	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	5.0	657.0																		
83COL/MCM	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	11.7	663.2																		
78COR/BEA	NH <sub>3</sub>	320	819	-155.2	663.5																		
[C <sub>3</sub> H <sub>2</sub> F <sub>8</sub> O]																							
94KOP/ANV	(CF <sub>3</sub> ) <sub>2</sub> CHOH	373	651.5	2.5	656.2			686.6			7												
87TAF	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	2.3	654.0																		
83COL/MCM	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	6.7	658.2																		
[C <sub>2</sub> H <sub>3</sub> F]																							
72BEA/HOL	C <sub>2</sub> H <sub>3</sub> F				655.8			683.4			16												
	CH <sub>2</sub> =CH <sub>2</sub> ; H <sub>2</sub> O				651-660																		
[C <sub>2</sub> HF <sub>3</sub> O]																							
94KOP/ANV	CF <sub>3</sub> CHO	373	651.5	0.8	653.6			685.5			2												
87TAF	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	2.3	654.2																		
83COL/MCM	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	6.7	658.2																		
78COR/BEA	NH <sub>3</sub>	320	819	-159.8	659.0																		
[C <sub>2</sub> H <sub>4</sub> ]																							
97EAS/SMI	CH <sub>2</sub> =CH <sub>2</sub>	298			651.5			680.5			11.5												
93SMI/RAD	theory	0						676.5			12.2												
93SMI/RAD	theory	298						681.9															
93SMI/RAD	theory	600						685.6															
89RUS/BER	threshold value	298						680.3															
87TAF	NH <sub>3</sub>	350	819	-184.9	633.2																		
85MCM/KEB	CO at C	400	562.8	72.8	634.9																		

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta \Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	0	651.5							
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	0	651.5			679.2				
82ROS/BUF		threshold value	298						680.3				
81TRAM/CL		threshold value	298										
81DO/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	0	651.5							
81BOH/MAC	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	0	651.5							
80BAE		threshold value	298						682.1				
[O <sub>4</sub> Os]	208-16-12-0	OsO <sub>4</sub>				650.6			676.9				20.6
89IRI/BEA	354-32-5; 74-85-1	CF <sub>3</sub> COCl; C <sub>2</sub> H <sub>4</sub>				650-651							
[C <sub>2</sub> ClF <sub>3</sub> O]	354-32-5	CF <sub>3</sub> COCl				649.8			681.6				2
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	1.7	653.8							
87TAF	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	-6.9	645.1							
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-6.7	645.7							
[OP]	14452-66-5	PO				649.5			682				0
90ADA/MIC		Bracketing. See Refs.	300						682±8				
[C <sub>4</sub> HF <sub>9</sub> O]	2378-02-1	(CF <sub>3</sub> ) <sub>3</sub> COH				646.7			676.8				8
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	-5.0	646.7							
87TAF	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	350	651.5	-27.5	624.2							
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-1.3	650.2							
[C <sub>2</sub> N <sub>2</sub> ]	460-19-5	NC-CN				645.8			674.7				11.8
89PET/FRE	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	300	651.5	-5.7	645.8							
87DEA/MAU	354-34-7; 74-85-1	CF <sub>3</sub> CFO; C <sub>2</sub> H <sub>4</sub>	~330			637-651							
84RAK/BOH	7446-09-5; 74-85-1	SO <sub>2</sub> ; C <sub>2</sub> H <sub>4</sub>				643-651							
[COSe]	1603-84-5	OCSe AT Se				644.1			670				22
85KAR	463-58-1; 74-85-1	COS; C <sub>2</sub> H <sub>4</sub>				603-651							
85JAS/STE		theory							670				
[H <sub>2</sub> O <sub>2</sub> ]	7722-84-1	H <sub>2</sub> O <sub>2</sub>				643.8			674.5				5.8
75LIN/ALB	3170-83-0; 7732-18-5	HO <sub>2</sub> ; H <sub>2</sub> O				628-660							
[O <sub>2</sub> S]	7446-09-5	SO <sub>2</sub>				643.3			672.3				11.5
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	10.5	641.0							
93SZU/MCM	630-08-0:a	CO at C	600	562.8	46.4	607.1	594	36.8	630.8	4.2	15.9	20.1	
93SZU/MCM	75-15-0	CS <sub>2</sub>	600	657.7	-55.6	607.0	681.9	-43.9	637.9	28	-18.8	9.2	
93SZU/MCM	353-85-5	CF <sub>3</sub> CN	600	657.7	-36.4	619.7	688.4	-35.1	653.3	6	-1.7	4.3	

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
8TTAF	7664-41-7	NH <sub>3</sub>	350	819	-218.7	599.4						
85MCM/KEB	630-08-0:a	CO at C	400	562.8	43.1	605.2						
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-29.7	621.8						
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-5.9	645.6						
81DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-2	649.5						
[S]	7704-34-9	S				640.2			664.3			28
81SMII/ADA		threshold value							664.3			
[C <sub>3</sub> F <sub>6</sub> O]	684-16-2	(CF <sub>3</sub> ) <sub>2</sub> CO				639.7			670.4			5.8
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	-13.4	638.5						
93SZU/MCM	7446-09-5	SO <sub>2</sub>	600	643.3	-9.2	635.8	672.3	-2.9	669.4	11.5	-11.3	0.2
85MCM/KEB	630-08-0:a	CO at C	400	562.8	35.1	597.8						
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-37.7	614.4						
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-9.2	642.3						
83COL/MCM	7446-09-5	SO <sub>2</sub>	298	643.00	-2.9	640.4						
81DRU/MCM	353-50-4	F <sub>2</sub> CO	298	637.0	2.1	639.0						
81DRU/MCM	7446-09-5	SO <sub>2</sub>	298	643.3	2.9	646.2						
81DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-11.3	640.2						
78COR/BEA	7664-41-7	NH <sub>3</sub>	350	819	-179.8	638.5						
[HP]	13967-14-1	PH				639.6			670.3			5.8
86BER/CUR		thermo cycles	298						670.3			
[C <sub>3</sub> H <sub>7</sub> ]	2025-55-0	i-C <sub>3</sub> H <sub>7</sub> *				638.9			671.4			0
88LIA/BAR		threshold value	298						671.4			
[CH <sub>3</sub> Br]	74-83-09	CH <sub>3</sub> Br				638.0			664.2			21
94GLU/SZU		theory	298						662.9			
94GLU/SZU	392-56-3	C <sub>6</sub> F <sub>6</sub>	600	624.4	10	637.1	648.0	18.8	666.8	30	-14.6	15.4
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	9.6	661.1						
72BEA/HOL	630-08-0:a; 7732-18-5	CO; H <sub>2</sub> O	298	651.5		563-660						
[CF <sub>2</sub> O]	353-50-4	F <sub>2</sub> CO				637.0			666.7			9
94KOP/ANV	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	373	651.5	-18.8	632.8						
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-11.3	640.2						
83COL/MCM	7446-09-5	SO <sub>2</sub>	298	643.3	-5.9	637.5						
81DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-13.4	638.1						
[C <sub>2</sub> F <sub>4</sub> O]	354-34-7	CF <sub>3</sub> CFO				636.7			668.6			2
83COL/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-13.4	638.1						
83COL/MCM	7446-09-05	SO <sub>2</sub>	298	643.3	-7.5	635.8						
81DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-15.1	636.4						
[Cu]	7440-50-8	Cu				632.4			655.3			32



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr/squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(R)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(R)	$\Delta$ S <sub>p</sub> (R)	$\Delta$ $\Delta$ S <sub>p</sub> (M,R)	$\Delta$ S <sub>p</sub> (M) $\Delta$ S <sub>p</sub> (R)
86ELK/ARM4		See Refs.							655±13			
[HO <sub>2</sub> ] 38LIA/BAR	3170-83-0	HO <sub>2</sub> <sup>•</sup> threshold value				627.5			660 660			0
[C <sub>6</sub> F <sub>6</sub> ] 93SZU/MCM	392-56-3	C <sub>6</sub> F <sub>6</sub>	600	643.3	20.1	624.4			648.0			30
93SZU/MCM	7446-09-5	SO <sub>2</sub>	600	660.0	-28.5	657.8		12.1	684.5	11.5	13.4	24.9
7BHAR/LIA	71-43-2	H <sub>2</sub> O	400	725.4	-14.6	624.1						
		C <sub>6</sub> H <sub>6</sub>				710.3						
[CH <sub>3</sub> Cl] 94GLU/SZU	74-87-3	CH <sub>3</sub> Cl theory				621.1			647.3			21
94GLU/SZU	392-56-3	C <sub>6</sub> F <sub>6</sub>	600	624.4	-6	621.1			649.8			
89PET/FRE	460-19-5	NC-CN	300	645.8	-1.1	644.7		7.1	655.1	30	-21.8	8.2
89PET/FRE	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	300	651.5	-6.5	645.0						
78COR/BEA		See Refs.	320			~659						
72BEA/HOL	74-86-2; 74-85-1	C <sub>2</sub> H <sub>2</sub> ; C <sub>2</sub> H <sub>4</sub>				617-651						
[C <sub>2</sub> H <sub>3</sub> O] 89HOL/LOS	3170-69-2	CH <sub>3</sub> CO <sup>•</sup>	298			620.5			653 653			0
[C <sub>2</sub> H <sub>2</sub> ] 84SMI/ADA	74-86-2	C <sub>2</sub> H <sub>2</sub> thermochemical cycles	300			616.7			641.4 641.4			26
84LIA/LIE		threshold value				611.3						
[H <sub>4</sub> Si] 92HU/SHE	7803-62-5	SiH <sub>4</sub> theory				613.4			639.7			20.6
87POP/CUR	2025-56-1;	theory	298			584-639			659.4			
73CHE/LAM	2025-55-0	C <sub>2</sub> H <sub>5</sub> ; C <sub>3</sub> H <sub>7</sub>							639.7			
[F <sub>3</sub> HOS] 84REEMUJ	91419-78-2	SIF <sub>3</sub> OH				611.5			641.9			7
	593-53-3;	CH <sub>3</sub> F; C <sub>2</sub> H <sub>4</sub>				572-651						
	74-85-1											
[C <sub>3</sub> H <sub>8</sub> ] 75HIR/KEB	74-98-6	C <sub>3</sub> H <sub>8</sub> See Refs.				607.8			625.7 625.7			49 49
[P] 86BER/CUR	7723-14-0	P thermo cycles	298			604.8			626.8 626.8			35
[AsF <sub>3</sub> ] 80DOJ/MCM	7784-35-2	AsF <sub>3</sub>				604.2			636.7			0
	593-53-3;	CH <sub>3</sub> F; CF <sub>2</sub> O				572-637						
	353-50-4											

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y:Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (M)
[COS]	463-58-1	OCS at S theory	298			602.6			628.5			22	
97EAS/SMI		CO at C	600	562.8	45.6	603.1	594	33.9	627.9	4.2	20.1	26.6	
93SZU/MCM	630-08-0:a	SO <sub>2</sub>	600	643.3	-1.3	638.9	672.3	-3.8	668.6	11.5	3.8	24.3	
93SZU/MCM	7446-09-5	C <sub>2</sub> H <sub>4</sub> ; H <sub>2</sub> O				651-660						15.3	
85WEI/PLA	74-85-1; 7732-18-5	CO at C	400	562.8	41.4	602.4							
85MCM/KEB	630-08-0:a	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-31.4	619.0							
85MCM/KEB	74-85-1	SO <sub>2</sub>	400	643.3	-1.7	640.6							
85MCM/KEB	7446-09-5	theory							636.4				
85JAS/STE	630-08-0:a;	CO; S				563-640							
81SMII/ADA	7704-34-9												
[HOSi]	97402-81-8:b	HSiO at Si theory	298			602.5			635			0	
93LUC/CUR									635				
[CHO]	2597-44-6	HCO threshold value				601.8			636			-5.8	
74WAR									636				
[CFN]	1495-50-7	FCN See Refs.				601.3			632			6	
84BEA/EYE									632				
[HI]	10034-85-2	HI				601.3			627.5			21	
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-43.1	607.4							
85MCM/KEB	630-08-0:a	CO at C	400	562.8	29.7	590.8							
78POL/MUN	10035-10-6; 14362-44-8	HBr; I				558-583							
[CF <sub>3</sub> I]	2314-97-8	CF <sub>3</sub> I				598.2			628.0			9.1	
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-45.2	606.5							
85MCM/KEB	630-08-0:a	CO at C	400	562.8	27.6	589.9							
[SSi]	12504-41-5:b	SIS at Si theory				596.6			627			7	
92BRU/GRE									627				
[O <sub>3</sub> ]	10028-15-6	O <sub>3</sub>				595.9			625.5			9.5	
94CAS/SPE	593-53-3; 7446-09-5	CH <sub>3</sub> F; SO <sub>2</sub> theory	298			572-643							
91MER/QUE			298						625.5			9.5	
[CHO <sub>2</sub> ]	2564-86-5	-COOH				590.9			623.4			0	
89HOL/LOS									623.4				
[CH <sub>2</sub> F <sub>2</sub> ]	75-10-5	CH <sub>2</sub> F <sub>2</sub>				589.7			620.5			5.8	
748LJ/MCM	630-08-0:a; 74-86-2	CO; C <sub>2</sub> H <sub>2</sub>	298			563-617							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M) GB(R)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M) ΔS <sub>p</sub> (R)
[CHF <sub>3</sub> ] 748LJ/MCM	75-46-7 630-08-0;a; 74-86-2	CHF <sub>3</sub> CO; C <sub>2</sub> H <sub>2</sub>				589.7 563-617			619.6			9.1
[Zn] 78FO/RAD	7440-66-6 74-82-8; 74- 85-1	Zn CH <sub>4</sub> ; C <sub>2</sub> H <sub>4</sub>				586.0 521-651			608.6			33
[B <sub>2</sub> H <sub>6</sub> ] 73PIE/POR	19287-45-7	B <sub>2</sub> H <sub>6</sub> See Refs.				586.0			615 615±17			11.5
[C <sub>2</sub> H <sub>5</sub> ] 88LIA/BAR	2025-56-1	C <sub>2</sub> H <sub>5</sub> <sup>*</sup> threshold value	298			583.5			616 616			0
[I] 88LIA/BAR	14362-44-8	I threshold value				583.5			608.2 608.2			26
[F <sub>2</sub> O <sub>2</sub> S] 93SZU/MCM	2699-79-8	F <sub>2</sub> SO <sub>2</sub>				580.5			605.5			25
85MCM/KEB2	630-08-0;a	CO at C	600	562.8	24.7	581.2	594	12.1	606.1	4.2	20.9	25.1
85MCM/KEB	630-08-0;a	CO at C	400	562.8	19.7	580.4						
85MCM/KEB	630-08-0;a	CO at C	400	562.8	19.2	580.0						
81DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-53.6	596.6						
80DOI/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-15.9	635.6						
	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-15.1	636.4						
[B <sub>4</sub> H <sub>10</sub> ] 73PIE/POR	18283-93-7	B <sub>4</sub> H <sub>10</sub> See Refs.				572.5			605 605±20			0
[CH <sub>3</sub> F] 94GLU/SZU	593-53-3	CH <sub>3</sub> F theory				571.5			598.9			17
94GLU/SZU	630-08-0;a; 74-84-0	CO; C <sub>2</sub> H <sub>6</sub>	298			563-570			597.2			
85MCM/KEB2	630-08-0;a; 2699-79-8	CO; SO <sub>2</sub> F <sub>2</sub>	400			563-581						
72BEA/HOL	630-08-0;a; 74-86-2	CO; C <sub>2</sub> H <sub>2</sub>				563-617						
[C <sub>2</sub> H <sub>6</sub> ] 94CAR/SCH	74-84-0	C <sub>2</sub> H <sub>6</sub> theory				569.9			596.3			20
93SZU/MCM	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	298	651.5	-80.8	568.2	680.5	-83.3	597.2	11.5	5.0	16.5
93SZU/MCM	630-08-0;a	CO at C	400	562.8	7.5	568.8	594	3.3	597.3	4.2	10.9	15.1
85MCM/KEB	630-08-0;a	CO at C	400	562.8	7.1	568.3						
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-65.7	584.9						
81MAC/SCH	10024-97-2;a	N <sub>2</sub> O at O	298	548.7	18.1	566.8						
81MAC/SCH	630-08-0;a	CO at C	298	562.8	6	568.8						

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(M)$
81BOH/MAC	630-08-0:a	CO at C	298	562.8	5.9	568.7			561.4A				
76HIR/KEB		See Refs.	~200						593.1B				27.4
76HIR/KEB		See Refs.	~400						589.3				
75FRE/KEB		See Refs.											
[HO]	3352-57-6	OH threshold				564.0			593.2				11
88LIA/BAR									593.2				
[CN]	2074-87-5	CN at N thermo cycles				>564			>596				4.2
90PET/FRE									>595				
[CO]	630-08-0:a	CO at C				562.8			594				4.2
97EAS/SMI		theory	298						594				3.8
93SZU/MCM	630-08-0:a	CO at C	600	562.8	0	562.8	594	0	594				
93SMI/RAD		theory	298						593				
93SMI/RAD		theory	0						587.1				
93SMI/RAD		theory	600						596.6				
92KOM/DIX		theory	298						593.3				
85TRA2		Appearance	298						594				
85MCM/KEB	630-08-0:a	CO at C	400	562.8	0	562.8							
85IAS/STE		theory							583.2				
84DIX/KOM		theory	300						591.6				
84BEA/EYE		See Refs.							577.4				
81BOH/MAC	630-08-0:a	CO at C	298	562.8	0	562.8							
80DYK/JON		threshold value							593.7				
76GUY/CHU		threshold value							604.2				
73HEM/RUN	630-08-0:a	CO at C	298	562.8	0	562.8							
69MAT/WAR		threshold value							594.5				
[NO <sub>2</sub> ]	10102-44-0	NO <sub>2</sub>				560.3			591.0				5.8
84POL/MUN	10035-10-6; 630-08-0:a	HBr; CO				558-563							
[O <sub>3</sub> S]	7446-11-9	SO <sub>3</sub>				560.3			588.3				14.9
77MUN/SMI	10035-10-6; 630-08-0:a	HBr; CO				558-563							
[BrH]	10035-10-6	HBr				657.7			584.2				20
97EAS/SMI		theory	298										20.2
93SMI/RAD		theory	0						581				
93SMI/RAD		theory	298						585.9				
93SMI/RAD		theory	600						589.8				
89TIC/JAV	630-08-0:a	CO at C					594	-8.4	585.6				
89ADA/SMI	630-08-0:a	CO at C	298	562.8			594	-10.9	583.1				
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-78.2	572.4							
85MCM/KEB	630-08-0:a	CO at C	400	562.8	-5.0	556.2							

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] YrSquib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)
84POL/MUN	10024-97-2;a; 10102-44-0	N <sub>2</sub> O; NO <sub>2</sub>				549-560			589.9			
79TIE/AND	7647-01-0;	threshold value										
78POL/MUN	630-08-0;a	HCl; CO				530-563						
[H <sub>3</sub> OSi]	113648-09- 2;b	H <sub>2</sub> SiOH at Si				556.5			589			0
93LUC/CUR		theory	298						589			
[F <sub>6</sub> S]	2551-62-4	SF <sub>6</sub>				550.7			576.3			26.4
94LAT/SMI	10024-97-2;a; 630-08-0;a	N <sub>2</sub> O; CO	5			549-563						
92MAC/SCH	630-08-0;a	CO at C	298	562.8	-12.1	550.7						
[CBrF <sub>3</sub> ]	75-63-8	CF <sub>3</sub> Br				550.3			580.0			9.1
95HIR/NAS		See Refs.							>553			
85MCM/KEB2	10024-97-2;a	N <sub>2</sub> O at O	400	548.7	-1.3	548.6						
85MCM/KEB	74-82-8	CH <sub>4</sub>	400	520.6	27.6	550.5						
85MCM/KEB	630-08-0;a	CO at C	400	562.8	-10.5	551.8						
[N <sub>2</sub> O]	10024-97-2;a	N <sub>2</sub> O at O				548.7			575.2			20
93SZU/MCM	124-38-9	CO <sub>2</sub>	600	515.8	32.6	550.2	540.5	35.1	575.6	26	-4.6	21.4
93SZU/MCM	630-08-0;a	CO at C	600	562.8	-6.3	551.8	594	-17.2	576.8	4.2	18.4	22.6
90JAV/GLO	74-82-8	CH <sub>4</sub>					543.5	32.2	575.7			
89ADA/SMI	7647-01-0	HCl	298				556.9	17.2	574.1			
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-82.8	567.8						
84BEA/EYE		See Refs.							531.4			
80BOH/MAC	630-08-0;a	CO at C	296	562.8	-12.2	550.7						
80BOH/MAC	124-38-9	CO <sub>2</sub>	296	515.8	33.9	549.7						
75LIN/MCF	630-08-0;a	CO at C	298	562.8	-13.4	549.4	594	-18.4	575.6	4.2	16.7	20.9
73HEM/RUN	630-08-0;a	CO at C	298	562.8	-12.6	550.3	594	-14.6	579.4	4.2	7.5	11.7
[CClF <sub>3</sub> ]	75-72-9	CF <sub>3</sub> Cl				541.5			571.3			9.1
85MCM/KEB	74-82-8	CH <sub>4</sub>	400	520.6	18.0	540.9						
85MCM/KEB	630-08-0;a	CO at C	400	562.8	-20.1	542.2						
[F <sub>3</sub> N]	7783-54-2	NF <sub>3</sub>				538.6			568.4			9.1
92GRA/HRU		theory							578.2			
85MCM/KEB	74-82-8	CH <sub>4</sub>	400	520.6	15.1	537.9						
85MCM/KEB	630-08-0;a	CO at C	400	562.8	-23.0	539.3						
80DOJ/MCM	630-08-0;a; 593-53-3	CO; CH <sub>3</sub> F				563-572						
[Br]	10097-32-2	Br				531.2			554.4			31
78POL/MUN		threshold value							554.4			

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p$ (R)	$\Delta\Delta S_p$ (M,R)	$\Delta S_p$ (M)	$\Delta S_p$ (R)
[ClH]	7647-01-0	HCl				530.1			556.9			19	
97EAS/SMI		theory	298									19.3	
93SMI/RAD		theory	600						565.7				
93SMI/RAD		theory	298						561.5				
93SMI/RAD		theory	0						556.6				
89TIC/JAV	10035-10-6	HBr		557.7			584.2	-25.1	559.1				
89ADA/SMI	74-82-8	CH <sub>4</sub>	298	520.6			543.5	13.4	556.9				
87POP/CUR		theory	298						556.5				
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-100.4	550.3							
85MCM/KEB	630-08-0:a	CO at C	400	562.8	-27.6	533.7							
79TIE/AND	10097-32-2;	threshold value											
78POL/MUN	10024-97-2:a	Br; N <sub>2</sub> O				531-549			564.8				
74FEH/FER		thermochemical cycle				>519							
[N <sub>2</sub> O]	10024-97-2:b	N <sub>2</sub> O at N				523.3			549.8			20	
90JAV/GLO	74-82-8	CH <sub>4</sub>		520.6			543.5	6.3	549.8				
[CH <sub>4</sub> ]	74-82-8	CH <sub>4</sub>				520.6			543.5			32	
97EAS/SMI		theory	298									26.2	
94CAR/SCH		theory	298						543.9				
93SZU/MCM	10024-97-2:a	N <sub>2</sub> O at O	600	548.7	-25.5	519.6			543.4			30.5	
93SZU/MCM	630-08-0:a	CO at C	600	562.8	-31.4	523.1			545.9	20	10.5	31.8	
93SZU/MCM	74-84-0	C <sub>2</sub> H <sub>6</sub>	600	569.9	-39.3	526.9			546.6	20	17.2	37.2	
93SMI/RAD		theory	600						542.1				
93SMI/RAD		theory	0						535.5				
93SMI/RAD		theory	298						539.8				
92KOM/DIX		theory	298						542.2				
89TIC/JAV	10035-10-6	HBr		557.7			584.2	-38.1	546.1				
89ADA/SMI	124-38-9	CO <sub>2</sub>	298				540.5	6.3	546.8				
87POP/CUR		theory	298						537.2				
85MCM/KEB	630-08-0:a	CO at C	400	562.8	-38.1	521.9							
85MCM/KEB	74-85-1	CH <sub>2</sub> =CH <sub>2</sub>	400	651.5	-110.9	538.5							
80BOH/MAC	124-38-9	CO <sub>2</sub>	296	515.8	7.8	523.6							
77MAU/FIE	124-38-9	CO <sub>2</sub>	550	515.8	5.4	519.7							
75STA/BEA	124-38-9	CO <sub>2</sub>	320	515.8	8.8	524.5							
72KAS/FRA	124-38-9	CO <sub>2</sub>	340	515.8	5.9	521.4							
73HEM/RUN	124-38-9	CO <sub>2</sub>	296	515.8	7.8	523.6			540.5	26	5.8	31.8	
73BOH/HEM	124-38-9	CO <sub>2</sub>	300	515.8	7.9	523.7							
71CHU/BER		threshold value											
[CO <sub>2</sub> ]	124-38-9	CO <sub>2</sub>				515.8			540.5			26	
97EAS/SMI		theory	298									26.4	
93SZU/MCM	74-82-8	CH <sub>4</sub>	600	520.6	-6.3	516.1			540.2	32	-5.0	27.0	
93SMI/RAD		theory	600						542.7				

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p(R)$	$\Delta\Delta S_p(M,R)$	$\Delta S_p(M)$	$\Delta S_p(R)$
93SMI/RAD		theory	298						539.3				
93SMI/RAD		theory							534.8				
92KOM/DIX		theory	298						541				
91TRA/KOM		Appearance	298						536.5		539.6		
89RUS/SCH		Appearance	298						540.5				
89ADA/SMI	10097-32-2	Br	298				554.4	-13.6	540.8				
85JAS/STE		theory							543.5				
85FRU/SCH		theory	298						547.7				
80BOH/MAC	630-08-0:a	CO at C	296	562.8	-46.0	516.9							
77MAU/FIE	124-38-9	CO <sub>2</sub>	550	515.8	0	518.8							
76MEU/MIT	74-82-8	CH <sub>4</sub>	298	520.6	-8.7	511.9							
76FEH/LIN	124-38-9	CO <sub>2</sub>	298	515.8	0	515.8			536.9	32	-7.1		24.9
75STA/BEA	124-38-9	CO <sub>2</sub>	320	515.8	0	515.8							
72KAS/FRA	124-38-9	CO <sub>2</sub>	340	515.8	0	515.8							
74WAR		threshold value											
73HEM/RUN	124-38-9	CO <sub>2</sub>	298	515.8	0	515.8							
73BOH/HEM	124-38-9	CO <sub>2</sub>	298	515.8	0	515.8							
[NO]	10102-43-9	NO				505.3			531.8				20
89TIC/JAV	75-73-0	CF <sub>4</sub>	300	503.7	-2.2	501.6	529.3	2.5	531.8	23.3	-15.5		7.8
80KOP/COM									456				
71ROC/SUT	<74-82-8	CH <sub>4</sub>		520.6	<0	<520							
[CF <sub>4</sub> ]	75-73-0	CF <sub>4</sub>				503.7			529.3				23.3
89TIC/JAV	7647-01-0	HCl	300	530.1	-28.9	501.2	556.9	-29.3	527.6	19	1.3		20.3
89TIC/JAV	74-82-8	CH <sub>4</sub>	300	520.6	-18.7	501.9	543.5	-16.7	526.8	32	-6.7		25.3
89TIC/JAV	124-38-9	CO <sub>2</sub>	300	515.8	-7.6	508.2	540.5	-7.1	533.4	26	-1.7		24.3
71ROC/SUT	>7727-37-9	>N <sub>2</sub>				>464							
[OSi]	10097-28-6:b	SiO at Si				500.5			533				0
93LUC/CUR		theory	298						533				
[Cl]	22537-15-1	Cl				490.1			513.6				30.1
88LIA/BAR		threshold value							513.6				
78POL/MUN		threshold value											
[FO]	12061-70-0	OF				482.2			508.7				20
88LIA/BAR						488.7			508.7				
80KOP/COM									582				
[Xe]	7440-63-3	Xe				478.1			499.6				36.8
80BOH/MAC	124-38-9	CO <sub>2</sub>	800	515.8	-30.3	480.1							
76FEH/LIN	124-38-9	CO <sub>2</sub>	800	515.8	-30.5	479.9							
76FEH/LIN	7727-37-9	N <sub>2</sub>	298	464.5	9.9	474.4	493.8	2.6	496.4	10.5	24.3		34.8
[F <sub>4</sub> Si]	7783-61-1	SiF <sub>4</sub>				476.6			502.9				20.6

TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Yr-Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M)	$\Delta S_p^0$ (R)	$\Delta \Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M)	$\Delta S_p^0$ (M)
84REE/MUJ		See Refs.							502.9				
[N <sub>2</sub> ]													
97EAS/SMI	7727-37-9	N <sub>2</sub> theory	298			464.5			493.8			10.5	10.5
93SZU/MCM	124-38-9	CO <sub>2</sub>	600	515.8	-53.1	467.3	540.5	-44.8	495.7	26	-13.8	12.2	12.2
93SZU/MCM	7400-63-3	Xe	600	478.1	-20.9	465.1	499.6	-6.7	492.9	36.8	-23.8	13.0	13.0
93SMI/RAD		theory	0						488.3				
93SMI/RAD		theory	600						497				
93SMI/RAD		theory	298						493.9				
92KOM/DIX		theory	298						493.3				
91RUS/BER		appearance	298						<510				
80BOH/MAC	17778-80-2	O	296	459.6	1.3	460.8			494				
79WIB/FIS		threshold value							478.2				
78FON/HUD		threshold value							469.4				
76WIL/LOS		threshold value											
76FEH/LIN	17778-80-2	O	298	459.6	1.3	460.8							
76FEH/LIN	124-38-9	CO <sub>2</sub>	298	515.8	-40.2	475.6							
[O]													
88LIA/BAR	17778-80-2	O				459.6			485.2			23	23
81JON/BIR	7727-37-9	N <sub>2</sub> threshold value	300	464.5	0	464.5			485.2				
80BOH/MAC	124-38-9	CO <sub>2</sub>	296	515.8	-41.4	474.4							
80BOH/MAC	630-08-0:a	CO at C	296	562.8	-87.4	475.4							
80BOH/MAC	17778-80-2	O	296	459.6	0	459.6			486.6				
76MCC		threshold value											
[FH]													
97EAS/SMI	7664-39-3	HF	298			456.7			484			17.3	17.3
93SMI/RAD		theory	600						488.4				
98SMI/RAD		theory	298						484				
98SMI/RAD		theory	0						479.1				
93DEL		theory	298						486.2				
87POP/CUR		theory	298						483.2				
79TIE/AND		threshold value							397.5				
75FOS/BEA	7727-37-9	N <sub>2</sub>	320	464.5	-2.9	461.4							
[Kr]													
80BOH/MAC	7439-90-9	Kr	296	394.7	8.3	402.4			424.6			34.4	34.4
80BOH/MAC	1333-74-0	H <sub>2</sub>	296	396.3	6.1	402.4							
79HUB/HER	7782-44-7	O <sub>2</sub> threshold value	296	394.7	7	401.8			419.7				
75PAY/SCH	1333-74-0	H <sub>2</sub>	296	394.7	7	401.8							
[CO]													
87FRE/KN1	630-08-0:b	CO at O	300			402.2			426.3			28	28
84DIX/KOM		See Refs. theory	300						427±8				
									426.3				



TABLE 2. Summary of proton transfer thermochemical data for each base M, sorted by gas basicity of M—Continued

[Formula] Y: Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	ΔGB(M,R,T)	GB(M)	PA(R)	ΔPA(M,R)	PA(M)	ΔS <sub>p</sub> (R)	ΔΔS <sub>p</sub> (M,R)	ΔS <sub>p</sub> (M)
[O <sub>2</sub> ]												
84ADA/SMI	7782-44-7	O <sub>2</sub>				396.3			421			26
81DYK/JON	1333-74-0	H <sub>2</sub>	300	394.7	1.5	396.2	422.3	-1.3	421	16.3	9.2	25.5
80BOH/MAC	1333-74-0	H <sub>2</sub>	296	394.7	1.7	396.4			420.5			
77MCC		threshold value							422.2			
75FEH/LIN	7782-44-7	O <sub>2</sub>	298	396.3	0	396.3						
73FEN/HEM	7782-44-7	O <sub>2</sub>	298	396.3	0	396.3						
73FEN/HEM	17778-80-2	O	298	459.6	-47.7	411.9						
[H <sub>2</sub> ]												
97EAS/SMI	1333-74-0	H <sub>2</sub>	298			394.7			422.3			16.3
98SMI/RAD		theory										16.3
93SMI/RAD		theory	600						424			
93SMI/RAD		theory	298						419.1			
84DIX/KOM		theory	0						414.2			
80BOH/MAC	17778-80-2	O	300						423.8			
78PO/RAD		See Refs.	296	459.6	-49.4	410.2			422.6			
75PAY/SCH	1333-74-0	H <sub>2</sub>	296	394.7	0	394.7						
75FEH/LIN	7782-44-7	O <sub>2</sub>	298	396.3	-1.3	395.0						
73HAR/CRO												
73FEN/HEM	7782-44-7	O <sub>2</sub>	298	396.3	-1.7	394.6			400±14			
73FEN/HEM	17778-80-2	O	298	459.6	-49.4	410.2						
72COT/ROZ		threshold value							417.6			
[Ar]												
82VIL/FUT	7440-37-1	Ar				346.3			369.2			32
79HUB/HER	1333-74-0	H <sub>2</sub>		394.7			422.3	-53.1	369.2			
71ROC/SUT	7722-84-1	H <sub>2</sub> O <sub>2</sub>		643.8		<644			>255			
[N]												
88MAR/REB	17778-88-0	N				318.7			342.2			30
85ADA/SMI		See Refs.							339.7			
		See Refs.	300						344.7			
[F]												
88LIA/BAR	14762-94-8	F				315.1			340.1			25
		threshold value							340.1			
[F <sub>2</sub> ]												
97CIP/CRE	7782-41-4	F <sub>2</sub>				305.5			332			20
		See Refs.							332±20			
[H <sub>2</sub> Osi]												
93LUC/CUR	22755-01-7:b	H <sub>2</sub> SiO at Si theory	298			295.5			328			0
									328			
[Ne]												
91GLO/TWI	7440-01-9	Ne				174.4			198.8			27
79HUB/HER	7440-59-7	He	300	148.5	25.9	174.4			200.8			
68CHU/RUS		threshold value							201.3			
		threshold value										

TABLE 2. Summary of proton transfer thermochemical data for each base M<sub>i</sub> sorted by gas basicity of M—Continued

[Formula] Yr/Squib	Reg No(M) Reg No(R)	Base(M) Base(R)	T(K)	GB(R)	$\Delta$ GB(M,R,T)	GB(M) GB(M)	PA(R)	$\Delta$ PA(M,R)	PA(M) PA(M)	$\Delta S_p^0$ (R)	$\Delta\Delta S_p^0$ (M,R)	$\Delta S_p^0$ (M) $\Delta S_p^0$ (M)
[He] 79HUB/HER	7440-59-7	He threshold value				148.5			177.8 177.8			10.5

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- 82BUR/HAY Burdett, N. A., Hathurst, A. N., J. Chem. Soc., Faraday Trans. 1 **78**, 2997 (1982). Hydration enthalpies and entropies, respectively, for the reaction  $\text{M}^+ + \text{H}_2\text{O} \rightleftharpoons \text{MOH}_2^+$  and referred to 298 K were measured as follows:  $\text{M}=\text{Na}$ ,  $-101 \text{ kJ mol}^{-1}$  and  $-90.0 \text{ J (mol K)}^{-1}$ ;  $\text{M}=\text{K}$ ,  $-71 \text{ kJ mol}^{-1}$  and  $-86 \text{ J (mol K)}^{-1}$ . Using  $\Delta_f H^0(\text{H}_2\text{O}) = -241.8 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{H}^+) = 1530 \text{ kJ mol}^{-1}$ ,  $S^0(\text{H}_2\text{O}) = 188.7 \text{ J (mol K)}^{-1}$ ,  $\Delta_f H^0(\text{NaOH}) = -197.8 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{Na}^+) = 602.9 \text{ kJ mol}^{-1}$ ,  $S^0(\text{Na}^+) = 147.9 \text{ J (mol K)}^{-1}$  and  $S^0(\text{NaOH}) = 228.4$ , yields  $\text{PA}(\text{NaOH}) = 1072.1 \text{ kJ mol}^{-1}$  and  $\Delta S_p(\text{NaOH}) = 18.2 \text{ J (mol K)}^{-1}$ . Using  $\Delta_f H^0(\text{KOH}) = -234.3 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{K}^+) = 507.9 \text{ kJ mol}^{-1}$ ,  $S^0(\text{K}^+) = 154.6 \text{ J (mol K)}^{-1}$  and  $S^0(\text{KOH}) = 236.3$ , yields  $\text{PA}(\text{KOH}) = 1100.6 \text{ kJ mol}^{-1}$  and  $\Delta S_p(\text{KOH}) = 21 \text{ J (mol K)}^{-1}$ .
- 83BUR/HOL Burgers, P. C., Holmes, J. L., Mommers, A. A., Szulejko, J. E., Org. Mass Spectrom. **18**, 596 (1983). Appearance energy measurements gave  $\Delta_f H^0(2\text{-propenyl cation}) = (969 \pm 5) \text{ kJ mol}^{-1}$ . This value combined with  $\Delta_f H^0(\text{CH}_3\text{CCH}) = 187 \text{ kJ mol}^{-1}$  yields  $\text{PA}(\text{CH}_3\text{CCH}) = (748 \pm 5) \text{ kJ mol}^{-1}$ .
- 84BUT/KUD Butman, M. F., Kudin, L. S., Krasnov, K. S., Zh. Neorg. Khim. **29**, 2150 (1984); English translation, Russ. J. Inorg. Chem. **29**, 1228 (1984). Determinations of enthalpies of reactions of the type:  $\text{M}_2\text{OH}^+ \rightleftharpoons \text{M}^+ + \text{MOH}(\text{solid})$ . Using  $\Delta_f H^0(\text{Li}_2\text{O, gas}) = -167.4 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{Li}^+) = 679.6 \text{ kJ mol}^{-1}$  and  $\Delta_f H^0(\text{LiOH, solid}) = -485 \text{ kJ mol}^{-1}$  gives  $\text{PA}(\text{Li}_2\text{O}) = 1206 \text{ kJ mol}^{-1}$ . Using  $\Delta_f H^0(\text{Na}_2\text{O, gas}) = -25.1 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{Na}^+) = 602.9 \text{ kJ mol}^{-1}$  and  $\Delta_f H^0(\text{NaOH, solid}) = -425.9 \text{ kJ mol}^{-1}$  gives  $\text{PA}(\text{Na}_2\text{O}) = 1375.9 \text{ kJ mol}^{-1}$ . Using  $\Delta_f H^0(\text{K}_2\text{O, gas}) = -142.3 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{K}^+) = 507.9 \text{ kJ mol}^{-1}$  and  $\Delta_f H^0(\text{KOH, solid}) = -424.7 \text{ kJ mol}^{-1}$  gives  $\text{PA}(\text{K}_2\text{O}) = 1342.5 \text{ kJ mol}^{-1}$ . Using  $\Delta_f H^0(\text{Cs}_2\text{O, gas}) = -92 \text{ kJ mol}^{-1}$ ,  $\Delta_f H^0(\text{Cs}^+) = 451.8 \text{ kJ mol}^{-1}$  and  $\Delta_f H^0(\text{CsOH, solid}) = -416.7 \text{ kJ mol}^{-1}$  gives  $\text{PA}(\text{Cs}_2\text{O}) = 1442.9 \text{ kJ mol}^{-1}$ .
- 89CAC/ATT Cacace, F., Attina, M., de Petris, G., Speranza, M., J. Am. Chem. Soc. **111**, 5481 (1989). Data from this reference are tabulated under 90CAC/ATT.
- 90CAC/ATT Cacace, F., Attina, M., de Petris, G., Speranza, M., J. Am. Chem. Soc. **112**, 1014 (1990). ICR. A more complete and detailed account of results first reported in 89CAC/ATT.  $\text{PA}(\text{H}_2\text{O}) < \text{PA}(\text{HNO}_3) < \text{PA}(\text{CF}_3\text{CH}_2\text{OH})$ . Also found that  $\text{H}_2\text{NO}_3^+$  dissociates to  $\text{NO}_2^+$  and  $\text{H}_2\text{O}$  under all conditions regardless of the protonating agent. Evidence of two isomeric structures, i.e.,  $(\text{HO})_2\text{NO}^+$  and  $\text{H}_2\text{O} \cdot \text{NO}_2^+$  with the latter structure being more stable.
- 90CAC/ATT2 Cacace, F., Attina, M., De Petris, G., Grandinetti, F., Speranza, M., Gazz. Chim. Ital. **120**, 691(1990). ICR proton-transfer equilibria. Temperature not explicitly stated but is said to be 298 K in a subsequent re-evaluation (93CAC/ATT). *Ab initio* calculations yield  $\text{PA}(\text{HN}_3) = (731.7 \pm 16) \text{ kJ mol}^{-1}$  at 0 K and  $(737 \pm 16) \text{ kJ mol}^{-1}$  at 298 K.
- 93CAC/ATT Cacace, F., Attina, M., Speranza, M., de Petris, G., Grandinetti, F., J. Org. Chem. **58**, 3639 (1993). ICR bracketing and MIKE measurements. *Ab initio* calculations yield  $\text{PA}(\text{HN}_3) = (744.3 \pm 8) \text{ kJ mol}^{-1}$  at 0 K and  $(750.6 \pm 8) \text{ kJ mol}^{-1}$  at 298 K.

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- 93CAC/DEP Cacace, F., de Petris, G., Grandinetti F., Occhiucci, G., J. Phys. Chem. **97**, 4239 (1993). ICR. The paper states that  $\text{GB}(\text{H}_2\text{N}-\text{CN})$  was determined by equilibrium proton transfer using  $i\text{-C}_3\text{H}_7\text{CN}$  and  $o\text{-xylene}$  as reference bases but no data are given. A figure showing the time dependence of ion intensities associated with the equilibrium  $\text{NH}_2-\text{CNH}^+ + i\text{-C}_3\text{H}_7\text{CN} \rightleftharpoons \text{NH}_2-\text{CN} + i\text{-C}_3\text{H}_7\text{CNH}^+$  would suggest that  $\text{GB}(\text{NH}_2-\text{CN}) = \text{GB}(i\text{-C}_3\text{H}_7\text{CN}) + 2 \text{ kJ mol}^{-1}$ . This is the value tabulated here. *Ab initio* calculations suggest that the most stable protonated form has the proton on the N of CN in a linear arrangement, while protonation at the amino N and at C are less stable by  $94 \text{ kJ mol}^{-1}$  ( $22.4 \text{ kcal mol}^{-1}$ ) and  $226 \text{ kJ mol}^{-1}$  ( $54 \text{ kcal mol}^{-1}$ ), respectively.
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- 96CAR/CAS Carr S. R., Cassady, C. J., J. Am. Soc. Mass Spectrom. **7**, 1203 (1996). FT-ICR bracketing.
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- 84CAS/FRE Cassady, C. J., Freiser, B. S., J. Am. Chem. Soc. **106**, 6176 (1984). ICR. Bracketing:  $\text{GB}(\text{Pyridine}) < \text{GB}(\text{FeO}) < \text{GB}(1\text{-Propylamine})$ .
- 83CAS/KIM Caserio, M. C., Kim, J. K., J. Am. Chem. Soc. **105**, 6896 (1983). ICR. Equilibrium. Thioketene determined relative to ketene.
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- 68CHU/RUS Chupka, W. A., Russell, M. E., J. Chem. Phys. **49**, 5426 (1968).
- 95CHY/SQU Chyall, L. J., Squires, R. R., Int. J. Mass Spectrom. Ion Processes **149**, 257 (1995). Determined translational energy thresholds for the endothermic proton transfer reactions;  $\text{C}_3\text{H}_5\text{NH}^+ + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{C}_3\text{H}_5\text{N}$ ,  $\Delta H^0(298 \text{ K}) = (78.7 \pm 5.0) \text{ kJ mol}^{-1}$  [ $(18.8 \pm 1.2) \text{ kcal mol}^{-1}$ ] and  $\text{c-C}_3\text{H}_3^+ + \text{NH}_3 \rightarrow \text{c-C}_3\text{H}_2 + \text{NH}_4^+$ ,  $\Delta H^0(298 \text{ K}) = (97.5 \pm 8) \text{ kJ mol}^{-1}$  [ $(23.3 \pm 1.8) \text{ kcal mol}^{-1}$ ].
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- 78COR/BEA Corderman, R. R., Beauchamp, J. L., Inorg. Chem. **17**, 1585 (1978). ICR. Equilibrium between  $\text{PF}_3$  and  $\text{CH}_3\text{Cl}$  observed, but K could not be measured. Values marked with (\*) are cited in this paper as "Koppel and Taft, unpublished data".
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- 78DAV/LAU Davidson, W. R., Lau, Y. K., Kebarle, P., *Can. J. Chem.* **56**, 1016 (1978). HPMS.
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- 91DEC/GAL Decouzon, M., Gal, J.-F., Maria, P.-C., *J. Org. Chem.* **56**, 3669 (1991). FT-ICR.
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- 80DEF/MCI DeFrees, D. J., McIver, Jr., R. T., Hehre, W. J., *J. Am. Chem. Soc.* **102**, 3334 (1980). ICR. Bracketing.
- 85DEF/MCL DeFrees D. J., McLean, A. D., *J. Chem. Phys.* **82**, 333 (1985).
- 93DEL Del Bene, J. E., *J. Phys. Chem.* **97**, 107 (1993). *Ab initio* calculation.
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- 88DIX/GOL Dixon, D. A., Gole, J. L., Komornicki, A., *J. Phys. Chem.* **92**, 2134 (1988). PA's calculated from *ab initio* molecular orbital theory.
- 84DIX/KOM Dixon, D. A., Komornicki, A., Kraemer, W. P., *J. Chem. Phys.* **81**, 3603 (1984). PA's of CO at O, CO at C,  $\text{H}_2\text{CO}$  calculated at the CI-SDQ level of theory and  $\text{PA}(\text{H}_2)$  at the CI-SD level.
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- 80DOI/MCM Doiron, C. E., McMahon, T. B., *Inorg. Chem.* **19**, 3037 (1980). ICR. Bracketing.
- 81DOI/MCM Doiron, C. E., McMahon, T. B., *Can. J. Chem.* **59**, 2689 (1981). ICR. Data relative to ethylene and  $\text{CH}_2(\text{CN})_2$ .
- 92DOT/IRA Dotan, I., Iraqi, M., Petrank, A., Lifshitz, C., *Rapid Commun. Mass Spectrom.* **6**, 579 (1992). SIFT.  $\Delta G^0$  values are determined for proton transfer reactions in two ways. First, the traditional way, forward and reverse rate constants are separately measured to obtain  $K_{\text{eq}}$ . Second, the rate constant in the endothermic direction is combined with the branching ratio for proton transfer and the calculated forward and reverse collision rates to derive  $K_{\text{eq}}$ . The results for both methods compare well. The tabulated values are those derived from equilibrium measurements.
- 93DOT/IRA Dotan, I., Iraqi, M., Lifshitz, C., *Int. J. Mass Spectrom. Ion Processes.* **124**, R21 (1993). ICR.  $\Delta G^0$  values obtained from the second method of 92DOT/IRA.
- 81DRU/MCM Drummond, D. F., McMahon, T. B., *J. Phys. Chem.* **85**, 3746 (1981). ICR.
- 80DYK/JON Dyke, J. M., Jonathan, N., Morris, A., Winter, M. J., *Mol. Phys.* **39**, 629 (1980).
- 81DYK/JON Dyke, J. M., Jonathan, N. B. H., Morris, A., Winter, M. J., *Mol. Phys.* **44**, 1059 (1981). Photoelectron spectroscopy. First adiabatic IP of  $\text{HO}_2 = (11.35 \pm 0.01) \text{ eV}$ .
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- =18.2 J (mol K)<sup>-1</sup>. Using  $\Delta_f H^0(\text{KOH})=-234.3$  kJ mol<sup>-1</sup>,  $\Delta_f H^0(\text{K}^+)=507.9$  kJ mol<sup>-1</sup>,  $S^0(\text{K}^+)=154.6$  J (mol K)<sup>-1</sup> and  $S^0(\text{KOH})=236.3$ , yields  $\text{PA}(\text{KOH})=1104.5$  kJ mol<sup>-1</sup> and  $\Delta S_p(\text{KOH})=16.6$  J (mol K)<sup>-1</sup>. Using  $\Delta_f H^0(\text{CsOH})=-259.4$  kJ mol<sup>-1</sup>,  $\Delta_f H^0(\text{Cs}^+)=451.8$  kJ mol<sup>-1</sup>,  $S^0(\text{Cs}^+)=169.8$  J (mol K)<sup>-1</sup> and  $S^0(\text{CsOH})=254.7$ , yields  $\text{PA}(\text{CsOH})=1117.9$  kJ mol<sup>-1</sup> and  $\Delta S_p(\text{CsOH})=22.6$  J (mol K)<sup>-1</sup>.
- 97EAS/SMI East, A. L. L., Smith, B. J., Radom, L., *J. Am. Chem. Soc.* **119**, 9014 (1997).
- 93EKE/HAG Ekeberg, D., Hagen, S. I., Hvistendahl, G., Schulze, C., Uggerud, E., Vedde, J., *Org. Mass Spectrom.* **28**, 1504 (1993). HPMS. Van't Hoff estimation of  $\Delta H^0$  and  $\Delta S^0$  over a rather limited temperature range in which clustering may have perturbed equilibrium. *Ab initio* calculations indicate  $\text{HFe}(\text{CO})_5^+$  is of  $C_{4v}$  symmetry with the proton attached to Fe.
- 84ELK/ARM Elkind, J. L., Armentrout, P. B., *J. Phys. Chem.* **88**, 5454 (1984). Determined  $D^0(\text{SiH}^+)=3.23\pm 0.04$  eV. Using  $\text{IP}(\text{Si})=8.15169$  eV gives  $\text{PA}(\text{Si})=(837.2\pm 4)$  kJ mol<sup>-1</sup>.
- 85ELK/ARM Elkind, J. L., Armentrout, P. B., *J. Phys. Chem.* **89**, 5626 (1985). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{VH}^+)=2.05\pm 0.06$  eV [(198±6) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{V})=6.743$  eV,  $\text{PA}(\text{V})=(859.4\pm 6)$  kJ mol<sup>-1</sup>.
- 86ELK/ARM Elkind, J. L., Armentrout, P. B., *Inorg. Chem.* **25**, 1078 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions.
- 86ELK/ARM2 Elkind, J. L., Armentrout, P. B., *J. Chem. Phys.* **84**, 4862 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D_{298}^0(\text{MnH}^+)=2.10\pm 0.15$  eV [(206±15) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{Mn})=7.434$  eV gives  $\text{PA}(\text{Mn})=(797\pm 15)$  kJ mol<sup>-1</sup>.
- 86ELK/ARM3 Elkind, J. L., Armentrout, P. B., *J. Phys. Chem.* **90**, 5736 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{FeH}^+)=2.12\pm 0.06$  eV [(204.5±6) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{Fe})=7.9024$  eV gives  $\text{PA}(\text{Fe})=(754\pm 8)$  kJ mol<sup>-1</sup>.
- 86ELK/ARM4 Elkind, J. L., Armentrout, P. B., *J. Phys. Chem.* **90**, 6576 (1986). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{CoH}^+)=1.98\pm 0.06$  eV [(191.0±9) kJ mol<sup>-1</sup>],  $D^0(\text{NiH}^+)=1.68\pm 0.08$  eV [(162.1±8) kJ mol<sup>-1</sup>] and  $D^0(\text{CuH}^+)=0.92\pm 0.13$  eV [(88.8±13) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{Co})=7.8810$  eV gives  $\text{PA}(\text{Co})=(742.7\pm 6)$  kJ mol<sup>-1</sup>. Using  $\text{IP}(\text{Ni})=7.6398$  eV gives  $\text{PA}(\text{Ni})=(737\pm 11)$  kJ mol<sup>-1</sup>. Using  $\text{IP}(\text{Cu})=7.72638$  eV gives  $\text{PA}(\text{Cu})=(655.3\pm 13)$  kJ mol<sup>-1</sup>.
- 87ELK/ARM Elkind, J. L., Armentrout, P. B., *J. Chem. Phys.* **86**, 1868 (1987). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{CrH}^+)=1.37\pm 0.09$  eV [(132.2±9) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{Cr})=6.76664$  eV gives  $\text{PA}(\text{Cr})=(791.3\pm 9)$  kJ mol<sup>-1</sup>.
- 88ELK/ARM Elkind, J. L., Armentrout, P. B., *Int. J. Mass Spectrom. Ion Processes* **83**, 259 (1988). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{TiH}^+)=2.31\pm 0.11$  eV [(222.9±11) kJ mol<sup>-1</sup>]. Using  $\text{IP}(\text{Ti})=6.8282$  eV gives  $\text{PA}(\text{Ti})=(876\pm 11)$  kJ mol<sup>-1</sup>.
- 89ELK/SUN Elkind, J. L., Sunderlin L. S., Armentrout, P. B., *J. Phys. Chem.* **93**, 3151 (1989). Heats of formation of metal hydrides from determinations of the onset energies of endothermic reactions. Derived  $D^0(\text{ScH}^+)=2.44\pm 0.09$  eV [(235.4±9) kJ mol<sup>-1</sup>],  $D^0(\text{YH}^+)=2.66\pm 0.06$  eV [(256.6±6) kJ mol<sup>-1</sup>],  $D^0(\text{LaH}^+)=2.48\pm 0.09$  eV [(239.3±9) kJ mol<sup>-1</sup>], and  $D^0(\text{LuH}^+)=2.11\pm 0.16$  eV [(203.6±15) kJ mol<sup>-1</sup>]. Using the following data, the corresponding PA values are deduced:  $\text{IP}(\text{Sc})=6.56144$  eV,  $\text{PA}(\text{Sc})=(914.4\pm 9)$  kJ mol<sup>-1</sup>;  $\text{IP}(\text{Y})=6.217$  eV,  $\text{PA}(\text{Y})=(967\pm 6)$  kJ mol<sup>-1</sup>;  $\text{IP}(\text{La})=5.577$  eV,  $\text{PA}(\text{La})=(1013.3\pm 9)$  kJ mol<sup>-1</sup>;  $\text{IP}(\text{Lu})=5.42585$  eV,  $\text{PA}(\text{Lu})=(992.1\pm 15)$  kJ mol<sup>-1</sup>.
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- 79ELL/EAD Ellenberger, M. R., Eades, R. A., Thomsen, M. W., Farneth, W. E., Dixon, D. A., *J. Am. Chem. Soc.* **101**, 7151 (1979). ICR. Bracketing.
- 96EWI/ZHA Ewing, N. P., Zhang, X., Cassidy, C. J., *J. Mass Spectrom.* **31**, 1345 (1996) FT-ICR bracketing.
- 81FAH/FEH Fahey, D. W., Fehsenfeld, F. C., Ferguson, E. E., *J. Chem. Phys.* **75**, 669 (1981). Flowing afterglow. Observation of  $\text{Si}^+ + \text{H}_2\text{O} \rightarrow \text{SiOH}^+ + \text{H}$  gives  $\Delta_f H$  of  $\text{SiOH}^+ < 778$  kJ mol<sup>-1</sup> (185.9 kcal mol<sup>-1</sup>) or  $\text{PA}(\text{SiO}) > 653$  kJ mol<sup>-1</sup> (156 kcal mol<sup>-1</sup>).  $\text{SiOH}^+$  transfers a proton to  $\text{NH}_3$ ;  $\text{PA}(\text{SiO}) < \text{PA}(\text{NH}_3)$ . Because these limits are so wide, data not given in the tables.
- 78FAR/MCM Farid, R., McMahon, T. B., *Int. J. Mass Spectrom. Ion Phys.* **27**, 163 (1978). ICR. Bracketing.
- 74FEH/FER Fehsenfeld, F. C., Ferguson, E. E., *J. Chem. Phys.* **60**, 5132 (1974). Flowing afterglow. Using  $\Delta_f H^0(\text{HCl})=-92.5$  kJ mol<sup>-1</sup> and  $\text{IP}(\text{HCl})=12.75$  eV, and assuming the second titled reaction is exothermic, gives  $\text{PA}(\text{HCl}) \geq 519$  kJ mol<sup>-1</sup>.
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- 87FER/JEN Fernandez, M. T., Jennings, K. R., Mason, R. S., *J. Chem. Soc., Faraday Trans.* **83**, 159 (1987). HPMS. See 92PAR/ FER for a reassessment of this paper's data.
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- 84FLA/MAQ Flammang, R., Maquestiau, A., Catalan, J., Perez, P., Elguero, J., *Org. Mass Spectrom.* **19**, 627 (1984). Relative proton affinities estimated by kinetic method, observation of the relative importances of modes of dissociation of proton-bound dimers (see 81MCL/CAM):  $\text{PA}(\text{Pyrazole}) < \text{PA}(\text{Indazole}) < \text{PA}(\text{1-Methylindazole}) < \text{PA}(\text{Imidazole}) < \text{PA}(\text{2-Methylindazole}) < \text{PA}(\text{Benzimidazole})$ .
- 78FON/HUD Foner, S. N., Hudson, R. L., *J. Chem. Phys.* **68**, 3169 (1978).
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- 75FOS/BEA Foster, M. S., Beauchamp, J. L., *Inorg. Chem.* **14**, 1229 (1975). ICR. Equilibrium observed between HF and N<sub>2</sub>.



- 75FOS/BEA2 Foster, M. S., Beauchamp, J. L., *J. Am. Chem. Soc.* **97**, 4814 (1975). ICR. Bracketing.
- 75FOS/BEA3 Foster, M. S., Beauchamp, J. L., *J. Am. Chem. Soc.* **97**, 4808 (1975). ICR. Bracketing.
- 74FOS/WIL Foster, M. S., Williamson, A. D., Beauchamp, J. L., *Int. J. Mass Spectrom. Ion Phys.* **15**, 429 (1974). Temperature of 320 K assumed.
- 89FOX/WLO Fox, A., Wlodek, S., Hopkinson, A. C., Lien, M. H., Sylvain, M., Rodriguez, C., Bohme, D. K., *J. Phys. Chem.* **93**, 1549 (1989). Selected ion flow tube bracketing study. PA(SiO) bracketed with CH<sub>3</sub>CN, allene and H<sub>2</sub>S. PA(SiS) bracketed with HCN, H<sub>2</sub>S and H<sub>2</sub>O. Molecular orbital calculations (MP4/6-31G\*\*//6-31G\*\*) suggest that protonation preferably occurs on the O and S ends, with SiOH<sup>+</sup> being linear and SiSH<sup>+</sup> being bent. Compare results of calculations with that of 92BRU/GRE.
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- 79FRE/HAR Freeman, C. G., Harland, P. W., McEwan, M. J., *Int. J. Mass Spectrom. Ion Phys.* **30**, 285 (1979). Flowing afterglow. Bracketing.
- 75FRE/KEB<sup>11</sup> French, M., Kebarle, P., *Can. J. Chem.* **53**, 2668 (1975). HPMS. Determination of activation energy of (C<sub>2</sub>H<sub>5</sub><sup>+</sup> + CH<sub>4</sub> ⇌ C<sub>2</sub>H<sub>5</sub><sup>+</sup> + H<sub>2</sub> + CH<sub>4</sub>) as 44 kJ mol<sup>-1</sup> (10.5 kcal mol<sup>-1</sup>). Taking this as reaction enthalpy, PA(C<sub>2</sub>H<sub>4</sub>) = 681.7 kJ mol<sup>-1</sup>, Δ<sub>r</sub>H<sup>0</sup>(C<sub>2</sub>H<sub>4</sub>) = 52.3 kJ mol<sup>-1</sup> and Δ<sub>r</sub>H<sup>0</sup>(C<sub>2</sub>H<sub>6</sub>) = -84.1 kJ mol<sup>-1</sup> yields PA(C<sub>2</sub>H<sub>6</sub>) = 589.3 kJ mol<sup>-1</sup>.
- 87FRE/KNI Freeman, C. G., Knight, J. S., Love, J. G., McEwan, M. J., *Int. J. Mass Spectrom. Ion Processes* **80**, 255 (1987). SIFT measurements. ΔG<sup>0</sup> values for HOC<sup>+</sup> reacting with O<sub>2</sub> (≈4 kJ mol<sup>-1</sup>) and Kr (≈0 kJ mol<sup>-1</sup>) were inferred from a comparison of proton transfer reaction efficiencies. From these values and standard entropies of relevant species, ΔH<sup>0</sup> values were determined and a PA(CO at O) = (427 ± 8) kJ mol<sup>-1</sup> was suggested.
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- 89GAL/SPE Galli, C., Speranza, M., *Org. Mass Spectrom.* **24**, 139 (1989). Fourier transform ICR. GB's determined from proton transfer equilibria. Only the final measured GB values the arenes are tabulated. The reference bases employed in the GB measurements are listed, along with their GB values from the previous evaluation, but no thermochemical data is reported for the equilibria of any arene with these reference bases. Tabulated GB values for these arenes are adjusted according to the GB values of the reference bases in this present evaluation. Temperature not indicated.
- 92GAR/RUT van Garderen, H. F., Ruttink, P. J. A., Burgers, P. C., McGibbon, G. A., Terlouw, J. K., *Int. J. Mass Spectrom. Ion Processes* **121**, 159 (1992). *Ab initio* calculations at SDCl/6-31G\*\*//6-31G\*\* level of theory, including ZPVE corrections.
- 83GAU/HOU Gaumann, T., Houriet, R., Stahl, D., Tabet, J.-C., Heinrich, N., Schwarz, H., *Org. Mass Spectrom.* **18**, 215 (1983). ICR. Details not given. Authors conclude that C<sub>6</sub>H<sub>5</sub><sup>+</sup> formed upon protonation of 1,3-C<sub>6</sub>H<sub>8</sub> and 1,4-C<sub>6</sub>H<sub>8</sub> has methylcyclopentenyl structure.
- 91GLO/TWI Glosik, J., Twiddy, N. D., Javahery, G., Ferguson, E. E., *Int. J. Mass Spectrom. Ion Processes* **109**, 75 (1991). Selected ion flow tube study. Direct measure of equilibrium constant, ΔS<sup>0</sup> calculated from known spectral data for the protonated ions and statistical thermodynamics to obtain ΔH<sup>0</sup> for titled reaction.
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- 76GOR/MUN Goren, A., Munson, B., *J. Phys. Chem.* **80**, 2848 (1976). Relative values for heats of formation of alkyl ions from hydride transfer equilibrium constant determinations; absolute values assigned relative to Δ<sub>r</sub>H<sup>0</sup>(t-C<sub>4</sub>H<sub>9</sub><sup>+</sup>) = 711 kJ mol<sup>-1</sup>. PA values derived using same data under 75SOL/FIE.
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- 94GRU/CAL Grutzmacher, H.-F., Caltapanides, A., *Am Soc. Mass Spectrom.* **5**, 826 (1994). Bracketing of PAs using MIKE spectra of proton-bound heterodimers. The observed substituent effects indicate O protonation for the benzamides examined.
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- 91GUO/GRA Guo, Y., Grabowski, J. J., *J. Am. Chem. Soc.* **113**, 5923 (1991). Flowing afterglow bracketing measurement of gas phase acidity of the phenyl radical (1552 or 371 kcal mol<sup>-1</sup>) by observing/not observing proton transfer from acids to o-benzyne radical anion (o-C<sub>6</sub>H<sub>4</sub><sup>-</sup>). From this value and an EA(C<sub>6</sub>H<sub>4</sub>) = 12.9 kcal mol<sup>-1</sup>, the values Δ<sub>r</sub>H<sup>0</sup>(o-C<sub>6</sub>H<sub>4</sub><sup>-</sup>) = 385 kJ mol<sup>-1</sup> (92 kcal mol<sup>-1</sup>) and Δ<sub>r</sub>H<sup>0</sup>(o-C<sub>6</sub>H<sub>4</sub>) = 439 kJ mol<sup>-1</sup> (105 kcal mol<sup>-1</sup>) were derived and ultimately a PA(o-C<sub>6</sub>H<sub>4</sub>) = 841 kJ mol<sup>-1</sup> (201 kcal mol<sup>-1</sup>). For comparison, see 91RIV/ING where Δ<sub>r</sub>H<sup>0</sup>(o-C<sub>6</sub>H<sub>4</sub>) = (440 ± 10) kJ mol<sup>-1</sup> is proposed. Refer also to 90KLO.
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- 84SMI/ADA Smith, D., Adams, N. G., Ferguson, E. E., *Int. J. Mass Spectrom. Ion Processes* **61**, 15 (1984). SIFT measurement of the reaction  $C_2H_2^+ + H_2 = C_2H_3^+ + H$  yielded  $\Delta H^0 = 6.7 kJ mol^{-1}$ . This combined with data in 88LIA/BAR yields a  $\Delta_f H^0(C_2H_3^+) = 1116.7 kJ mol^{-1}$ , which finally yields a  $PA(C_2H_2) = 641.4 kJ mol^{-1}$ .
- 85SMI/ADA Smith, D., Adams, N. G., *J. Phys. Chem.* **89**, 3964 (1985). SIFT. Rate constant of proton transfer from  $HCS^+$  to  $C_2H_5OH$  is 50% of collision rate constant; rate constant of proton transfer to  $CH_3SH$  is 30% of collision rate constant.
- 94SMI/CHY Smith, R. L., Chyall, L. J., Chou, P. K., Kentamaa, H. I., *J. Am. Chem. Soc.* **116**, 781 (1994). FT-ICR bracketing. Title ion generated from ring opened ionized cyclo-butanone by  $\cdot CH_2CH_2CH_2CO^+ + CH_2 = C = O \rightleftharpoons \cdot CH_2CH_2CH_2CH_2CO^+ + CO$ .
- 78SMI/MUN Smith, D. E., Munson, B., *J. Am. Chem. Soc.* **100**, 497 (1978). Bracketing.  $CH_3F < SO_2F_2 < SO_2 < HSO_3F < C_2H_4 < H_2O < H_2SO_4 \sim CF_3SO_3H < H_2S$ .
- 93SMI/RAD Smith, B. J., Radom, L., *J. Am. Chem. Soc.* **115**, 4885 (1993). *Ab initio* calculations at the G2 level.
- 95SMI/RAD Smith, B. J., Radom, L., *J. Phys. Chem.* **99**, 6468 (1995). Various *ab initio* procedures compared and evaluated. Tabulated values for each molecule correspond to the most rigorous method applied to that molecule.
- 75SOL/FIE Solomon, J. J., Field, F. H., *J. Am. Chem. Soc.* **97**, 2625 (1975). Heats of formation of alkyl ions from hydride transfer equilibria; related to the  $\Delta_f H^0(t-C_4H_9^+) = 711 kJ/mol$  and  $\Delta_f H^0(iso-C_4H_{10}) = -134.3 kJ mol^{-1}$ . Using  $\Delta_f H^0(2\text{-methyl-2-pentene}) = -66.9 kJ mol^{-1}$  and  $\Delta_f H^0(2\text{-methyl pentane}) = -174.1 kJ mol^{-1}$  gives  $PA(2\text{-methyl-2-pentene}) = 807.8 kJ mol^{-1}$ . Using  $\Delta_f H^0(2,3\text{-dimethyl-2-butene}) = -69.5 kJ mol^{-1}$  and  $\Delta_f H^0(2,3\text{-dimethyl butane}) = 176.1 kJ mol^{-1}$  gives  $PA(2,3\text{-dimethyl-2-butene}) = 813.9 kJ mol^{-1}$ .
- 76SOL/FIE Solomon, J. J., Field, F. H., *J. Am. Chem. Soc.* **98**, 1567 (1976). Hydride transfer equilibrium constant determined for  $t-C_4H_9^+$  and  $i-C_3H_7^+$  with alkyl molecules. Using  $\Delta_f H^0(t-C_4H_9^+) = 711 kJ mol^{-1}$ ,  $\Delta_f H^0(C_3H_7^+) = 804.3 kJ mol^{-1}$ ,  $\Delta_f H^0(i-C_4H_{10}) = (-134.4 \pm 0.4) kJ mol^{-1}$  and  $\Delta_f H^0(C_3H_8) = (-104.6 \pm 0.4) kJ mol^{-1}$  the following are derived: using  $\Delta_f H^0(1\text{-methyl cyclopentene}) = -4.2 kJ mol^{-1}$  and  $\Delta_f H^0(\text{methyl cyclopentane}) = -105.9 kJ mol^{-1}$  gives  $PA(1\text{-methyl cyclopentene}) = 813.2 kJ mol^{-1}$ ; using  $\Delta_f H^0(\text{norborn-2-ene}) = (87.9 \pm 4.2) kJ mol^{-1}$  and  $\Delta_f H^0(\text{norbornane}) = (-50.2 \pm 4.2) kJ mol^{-1}$  gives  $PA(\text{norbornane}) = 829.1 kJ mol^{-1}$ ;  $\Delta_f H^0(c-C_5H_{10}) = -78.2 kJ mol^{-1}$  and  $\Delta_f H^0(c-C_5H_8) = 36.0 kJ mol^{-1}$  gives  $PA[(c-C_5H_8)] = 762.1 kJ mol^{-1}$ . Values for  $n$   $\Delta_f H^0(2\text{-methyl norbornane})$  and  $\Delta_f H^0(2\text{-methyl norborn-2-ene})$  were estimated in the following way. Since the difference  $\Delta_f H^0(i-C_4H_{10}) - \Delta_f H^0(C_3H_8) = (-134.4 \pm 0.4) kJ mol^{-1} - (-104.6 \pm 0.4) kJ mol^{-1} = -29.8 \pm 0.4 kJ mol^{-1}$ , the difference  $\Delta_f H^0(c-C_5H_9CH_3) - \Delta_f H^0(c-C_5H_{10}) = (-105.9 \pm 0.4) kJ mol^{-1} - (-78.2 \pm 0.4) kJ mol^{-1} = -27.7 \pm 0.4 kJ mol^{-1}$ , and the difference  $\Delta_f H^0(c-C_4H_7CH_3) - \Delta_f H^0(c-C_4H_8) = (28.5 \pm 0.4) kJ mol^{-1} - (-31 kJ mol^{-1}) = 59.5 \pm 0.4 kJ mol^{-1}$ , then the difference  $\Delta_f H^0(2\text{-methyl norbornane}) - \Delta_f H^0(\text{norbornane}) = (-50.2 \pm 0.4) kJ mol^{-1}$  is estimated to be  $-30 kJ mol^{-1}$  putting  $\Delta_f H^0(2\text{-methyl norbornane}) = (-80 \pm 4) kJ mol^{-1}$ . Similarly, since the difference  $\Delta_f H^0(i-C_4H_8) - \Delta_f H^0(C_3H_6) = (-16.7 \pm 0.4) kJ mol^{-1} - (20.1 \pm 0.4) kJ mol^{-1} = -36.8 kJ mol^{-1}$ , the difference  $\Delta_f H^0(c-C_5H_7CH_3) - \Delta_f H^0(c-C_5H_8) = (36.0 \pm 0.4) kJ mol^{-1} - (-40.2 kJ mol^{-1}) = 76.2 \pm 0.4 kJ mol^{-1}$ , and the difference  $\Delta_f H^0(1\text{-methyl cyclohexene}) - \Delta_f H^0(\text{cyclo hexene}) = (-43.1 \pm 0.4) kJ mol^{-1} - (-38.5 kJ mol^{-1}) = -4.6 \pm 0.4 kJ mol^{-1}$ , then the difference  $\Delta_f H^0(2\text{-methyl norborn-2-ene}) - \Delta_f H^0(\text{norborn-2-ene}) = (87.9 kJ mol^{-1})$  is estimated as  $-38 kJ mol^{-1}$ , putting  $\Delta_f H^0(2\text{-methyl norborn-2-ene}) = (50 \pm 4) kJ mol^{-1}$ . All of this puts  $PA(2\text{-methyl norborn-2-ene}) = (845 \pm 6) kJ mol^{-1}$ .
- 75SOL/HAR Solka, B. H., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.* **17**, 379 (1975). Equilibrium:  $CH_3CHOH^+ + CH_3SH$ ,  $\Delta G^0 = -2.1 kJ mol^{-1} (-0.5 kcal mol^{-1})$ ,  $CH_3SH_2^+ + C_2H_5CHO$ ,  $\Delta G^0 = -8.4 kJ mol^{-1} (-2 kcal mol^{-1})$ ,  $CH_3SH_2^+ + (CH_3)_2O$ ,  $\Delta G^0 = -16.7 kJ mol^{-1} (-4 kcal mol^{-1})$ .
- 72SOL/POR Solomon, J. J., Porter, R. F., *J. Am. Chem. Soc.* **94**, 1443 (1972). Bracketing.
- 74STA/BEA Staley, R. H., Beauchamp, J. L., *J. Am. Chem. Soc.* **96**, 6252 (1974). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.
- 74STA/BEA2 Staley, R. H., Beauchamp, J. L., *J. Am. Chem. Soc.* **96**, 1604 (1974). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.
- 75STA/BEA Staley, R. H., Beauchamp, J. L., *J. Chem. Phys.* **62**, 1998 (1975). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.
- 76STA/KLE Staley, R. H., Kleckner, J. E., Beauchamp, J. L., *J. Am. Chem. Soc.* **98**, 2081 (1976). ICR. Data relative to TAFT scale; temperature assumed to be 320 K.
- 77STA/TAA Staley, R. H., Taagepera, M., Henderson, W. G., Koppel, I., Beauchamp, J. L., Taft, R. W., *J. Am. Chem. Soc.* **99**, 326 (1977). ICR. Data related to TAFT scale; temperature assumed to be 320 K.
- 77STA/WIE Staley, R. H., Wieting, R. D., Beauchamp, J. L., *J. Am. Chem. Soc.* **99**, 5964 (1977). ICR. Data related to TAFT scale; temperature assumed to be 320 K.
- 79STE/BEA Stevens, A. E., Beauchamp, J. L., *J. Am. Chem. Soc.* **101**, 245 (1979). ICR. Bracketing:  $CH_3CH=CH_2 < (CO)_3MnCH_3 - CH_3OH < CH_3CHO$ .

- 81STE/BEA Stevens, A. E., Beauchamp, J. L., *J. Am. Chem. Soc.* **103**, 190 (1981). ICR. Compounds related to gas phase basicity scale, but no experimental details given; (bracketing or equilibrium?). From proton affinity cited here for  $(C_3H_5)_2Ni$ , also given in (76COR/BEA), it would appear that results given here correspond to the contracted 300 K scale, and therefore the usual correction to 320 has been made. However, there is still an unexplained discrepancy of  $1.3 \text{ kcal mol}^{-1}$  for  $(C_3H_5)_2Ni$  results. Entropy corrections unknown.
- 80STO/CAM Stone, J. A., Camicioli, J. R. M., Baird, M. C., *Inorg. Chem.* **19**, 3128 (1980). ICR. Bracketing.
- 86STO/LI Stone, J. A., Li, X., Turner, P. A., *Can. J. Chem.* **64**, 2021 (1986). HPMS. Temperature dependence of proton-transfer equilibria.
- 82STO/SPL Stone, J. A., Splinter, D. E., Kong, S. Y., *Can. J. Chem.* **60**, 910 (1982). HPMS.
- 84STO/SPL Stone, J. A., Splinter, D. E., *Int. J. Mass Spectrom. Ion Processes.* **59**, 169 (1984). Bracketing.
- 77SUM/POL Summerhays, K. D., Pollack, S. K., Taft, R. W., Hehre, W. J., *J. Am. Chem. Soc.* **99**, 4585 (1977). ICR. Data related to TAFT scale; temperature assumed to be 350 K.
- 86SUN/KUL Sunner, J. A., Kulatunga, R., Kebarle, P., *Anal. Chem.* **58**, 1312 (1986). HPMS measurement of temperature-dependent proton transfer equilibria to obtain  $\Delta G^0$ ,  $\Delta H^0$  and  $\Delta S^0$  with respect to unspecified bases. Also estimated PA and GB of triethanolamine [102-71-6] to be 975 and  $941 \text{ kJ mol}^{-1}$ , respectively.
- 93SUN/SQU Sunderlin, L. S., Squires, R. R., *Chem. Phys. Lett.* **212**, 307 (1993). Energy-resolved CID used to obtain the dissociation energies of  $H_2O-NO_2^+$  [ $(61.9 \pm 10) \text{ kJ mol}^{-1}$ ,  $(14.8 \pm 2.3) \text{ kcal mol}^{-1}$ ] and of  $CH_3OH-NO_2^+$  [ $(80.3 \pm 10) \text{ kJ mol}^{-1}$ ,  $(19.2 \pm 2.3) \text{ kcal mol}^{-1}$ ]. Combined with  $\Delta_f H^0(H_2O)$  and  $\Delta_f H^0(CH_3OH)$  and a revised  $\Delta_f H^0(NO_2^+)$  yielded  $PA(HNO_3) = (743.5 \pm 10) \text{ kJ mol}^{-1}$  and  $PA(CH_3NO_3) = (732 \pm 10) \text{ kJ mol}^{-1}$ . Compare with 94CAC/ATT.
- 91SZU/MCM Szulejko, J. E., McMahon, T. B., *Int. J. Mass Spectrom Ion Processes* **109**, 279 (1991). HPMS and temperature dependence of proton transfer equilibrium constants.
- 93SZU/MCM Szulejko, J. E., McMahon, T. B., *J. Am. Chem. Soc.* **115**, 7839 (1993). HPMS and temperature dependence of proton transfer equilibrium constants.
- 72TAA/HEN Taagepera, M., Henderson, W. G., Brownlee, R. T. C., Beauchamp, J. L., Holtz, D., Taft, R. W., *J. Am. Chem. Soc.* **94**, 1369 (1972).
- 81TAA/SUM Taagepera, M., Summerhays, K. D., Hehre, W. J., Topsom, R. D., Pross, A., Radom, L., Taft, R. W., *J. Org. Chem.* **46**, 891 (1981). ICR. See comments under TAFT.
- TAFT ICR. Unpublished compiled list of values of gas phase basicities measured by several workers, notably including Taft, R. W., McIver, R., Hehre, W. J., and co-workers. Here referred to as the "TAFT list". Most of the data given on the list have been published elsewhere, and are listed here with the appropriate reference. (See: 75ARN, 72ARN/JON, 76COO/KAT, 82DEF/HEH, 80DEF/MCI, 76DEV/WOL, 74HEH/MCI, 72HEN/TAA, 79LOC/HUN, 83MCI, 82PAU/HEH, 82PAU/HEH(2), 82PIE/HEH, 82PIE/HEH(2), 79PIE/POL, 77POL/DEV, 80POL/HEH, 81POL/RAI, 77POL/WOL, 77SUM/POL, 75TAF, 83TAF, 73TAF/TAA, 77WOL/ABB, 75WOL/HAR, 77WOL/STA) Values cited as "TAFT" either have not been published, or the publication has not been identified for the current compilation. All data from these various publications have been assumed to have been taken at 320 K, rather than the originally reported 300 K (R. W. Taft, personal communication). As a result of the uncertainty in the actual temperature(s) at which measurements were made, and the great length of the free energy scale represented by these results, there may be some uncertainty in the length of the scale. To minimize this problem, sections of the scale have been related to local standards (i.e.,  $H_2O$ , isobutene) wherever possible. Occasionally thermochemical scales from other laboratories have been related by the subsequent authors to this base scale; when this is the case, the notation given here is "Related to TAFT scale".
- 86TAFT Taft, R. W., Personal communication. A list (dated 10/9/86) of relative gas phase basicities of 310 compounds determined at the Department of Chemistry, University of California, Irvine, by R. W. Taft and collaborators. The list was submitted by R. W. Taft for inclusion in this update of proton affinity data. Experimental details of reference bases used in the measurements were not included. Many of the data have been published, or appeared in our 1984 published compilation of proton affinity data. Values appearing here represent only those species for which Taft *et al.* have revised their own earlier values, or for which determinations from the Irvine laboratory were not available previously. It is assumed that these data supersede any earlier values from this laboratory.
- 75TAF Taft, R. W., "Gas Phase Proton Transfer Equilibria", in "Proton Transfer Reactions," E. F. Caldin and V. Gold, Editors, p. 31 (1975). ICR. Data as reported corrected to 320 K. See comments under TAFT.
- 83TAF Taft, R. W., *Prog. Phys. Org. Chem.* **14**, 248 (1983). ICR. See comments under TAFT. Temperature correction of scale from 300 to 320 K were included in this 1983 review of the body of data referred to here as "TAFT scale".
- 86TAF/ANV Taft, R. W., Anvia, F., Taagepera, M., Catalan, J., Elguero, J., *J. Am. Chem. Soc.* **108**, 3237 (1986). ICR.
- 86TAF/GAL Taft, R. W., Gal, J.-F., Genbaldi, S., Maria, P.-C., *J. Am. Chem. Soc.* **108**, 861 (1986). ICR.
- 73TAF/TAA Taft, R. W., Taagepera, M., Summerhays, K. D., Mitsky, J., *J. Am. Chem. Soc.* **95**, 3811 (1973). ICR. See comments under TAFT.
- 78TAF/TAA Taft, R. W., Taagepera, M., Abboud, J. L. M., Wolf, J. F., DeFrees, D. J., Hehre, W. J., Bartmess, J. E., McIver, Jr., R. T., *J. Am. Chem. Soc.* **100**, 7765 (1978). Table I lists free energy changes for proton transfer relative to methanol. (Although data are cited as coming from 77WOL/STA, several compounds appear here that did not appear in that paper.) Data here corrected to 320 K and related to local standards.
- 78TAF/WOL Taft, R. W., Wolf, J. F., Beauchamp, J. L., Scorrano, G., Amett, E. M., *J. Am. Chem. Soc.* **100**, 1240 (1978). ICR. See comments under TAFT.

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- 76TAN/LIA Tang, I. N., Lian, M. S., Castleman, Jr., A. W., *J. Chem. Phys.* **65**, 4022 (1976). HPMS measurement of the equilibrium  $Sr^+H_2O \rightleftharpoons SrOH^+$  yielded  $\Delta H^0 = -144.3$  kJ mol<sup>-1</sup> ( $-34.5$  kcal mol<sup>-1</sup>) and  $\Delta S^0 = -131$  J (mol K)<sup>-1</sup> ( $-31.1$  cal (mol K)<sup>-1</sup>). Using  $\Delta_f H^0(SrOH) = -184.1$  kJ mol<sup>-1</sup>,  $\Delta_f H^0(Sr^+) = 712.6$  kJ mol<sup>-1</sup>,  $S^0(Sr^+) = 170.4$  J (mol K)<sup>-1</sup> and  $S^0(SrOH) = 246.4$  J (mol K)<sup>-1</sup> gives  $PA(SrOH) = 1019.4$  and  $\Delta S_p = -18$  J (mol K)<sup>-1</sup>.
- 78TAN/MAC Tanaka, K., Mackay, G. I., Bohme, D. K., *Can. J. Chem.* **56**, 193 (1978). Flowing afterglow.
- 89TIC/JAV Tichy, M., Javahery, G., Twiddy, N. D., Ferguson, E. E., *Int. J. Mass Spectrom. Ion Processes* **93**, 165 (1989).  $\Delta H^0$  and  $\Delta S^0$  values for proton-transfer reactions obtained from "van't Hoff" plots of ratios of forward and reverse rate constants versus reciprocal average center of mass kinetic energies in a selected-ion flow drift tube.
- 79TIE/AND Tiedemann, P. W., Anderson, S. L., Ceyer, S. T., Hirooka, T., Ng, C. Y., Mahan, B. H., Lee, Y. T., *J. Chem. Phys.* **71**, 605 (1979). Appearance energies of fragment ions from molecular clusters.
- 84TOL/BEA Tolbert M. A., Beauchamp, J. L., *J. Am. Chem. Soc.* **106**, 8117 (1984). Heat of formation of  $ScH^+$  through determination of onset energies of the endothermic reaction  $Sc^+ + H_2 = ScH^+ + H$ . Using  $IP(Sc) = (6.56144 \pm 0.00006)$  eV gives  $PA(Sc) = 907.5$  kJ mol<sup>-1</sup>.
- 89TOM/ABB Tomas, F., Abboud, J.-L. M., Laynez, J., Notario, R., Santos, L., Nilsson, S. O., Catalan, J., Claramunt R. M., Elguero, J., *J. Am. Chem. Soc.* **111**, 7348 (1989). ICR.
- 81TRA Traeger, J. C., *Org. Mass Spectrosc.* **16**, 193 (1981). Appearance potential of  $sec-C_4H_9^+$  from halogenated butanes, and correction to 298 K.
- 85TRA Traeger, J. C., *Org. Mass Spectrom.* **20**, 223 (1985). Appearance potential determinations of  $C_3H_5O^+$  by photoionization mass spectrometry.
- 85TRA2 Traeger, J. C., *Int. J. Mass Spectrom. Ion Processes* **66**, 271 (1985). AE measurements for  $HCO^+$  derived from  $H_2CO$ ,  $CH_3CHO$ ,  $C_2H_3CHO$ , glyoxal and  $HCOOH$ . A value of  $\Delta_f H^0(HCO^+, 298 K) = (825.6 \pm 2.7)$  kJ mol<sup>-1</sup> is deduced from the formation of  $HCO^+$  from  $HCOOH$ , yielding  $PA(CO) = (594 \pm 3)$  kJ mol<sup>-1</sup>.
- 96TRA Traeger, J. C., *Rapid Commun. Mass Spectrom.* **10**, 119 (1996). Threshold photoionization mass spectrometry. Determined  $\Delta_f H^0(t-C_4H_9^+, 298 K) = (711.4 \pm 1.1)$  kJ mol<sup>-1</sup>, yielding  $PA(i-C_4H_9) = (801.7 \pm 1.4)$  kJ mol<sup>-1</sup>.
- 93TRA/HOL Traeger, J. C., Holmes, J. L., *J. Phys. Chem.* **97**, 3453 (1993). Photoionization mass spectrometric appearance energy of  $CH_2OH^+$  from  $CH_3OH$  as 11.578 eV.
- 91TRA/KOM Traeger, J. C., Kompe, B. M., *Org. Mass Spectrom.* **26**, 209 (1991). Dissociative photoionization mass spectrometry of  $HCOOH$  and  $CF_3COOH$  used to obtain  $\Delta_f H^0(COOH^+, 298 K) = (600 \pm 3)$  kJ mol<sup>-1</sup> [(143.5  $\pm$  0.7) kcal mol<sup>-1</sup>] from appearance energy measurements (12.31 eV for  $HCOOH$  and 11.82 eV for  $CF_3COOH$ ) and using the following  $\Delta H_f^0$  values at 298 K:  $HCOOH$ ,  $-378.7$  kJ mol<sup>-1</sup>;  $H$ , 218 kJ mol<sup>-1</sup>;  $CF_3COOH$ ,  $-1030.5$  kJ mol<sup>-1</sup> and  $CF_3$ ,  $-460.2$  kJ mol<sup>-1</sup>. Compare with 89RUS/SCH.
- 81TRA/MCL Traeger, J. C., McLoughlin, R. G., *J. Am. Chem. Soc.* **103**, 3647 (1981). Appearance potentials of  $CH_3^+$ ,  $C_2H_3^+$ ,  $sec-C_3H_7^+$ , and  $t-C_4H_9^+$ ; evaluation and correction to 298 K.
- 82TRA/MCL Traeger, J. C., McLoughlin, R. G., Nicholson, A. J. C., *J. Am. Chem. Soc.* **104**, 5318 (1982). Appearance potentials of  $CH_3CO^+$  ions; correction to 298 K.
- 86TRA/MUN Tran, V. T., Munson, B., *Org. Mass Spectrom.* **21**, 41 (1986). HPMS. Bracketing.
- 78TSA Tsang, W., *Int. J. Chem. Kinet.* **10**, 41 (1978). Heats of formation of benzyl, tert-butyl radicals.
- 79VAJ/HAR Vajda, J. H., Harrison, A. G., *Int. J. Mass Spectrom. Ion Phys.* **30**, 293 (1979) HPMS.
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- 82VIL/FUT Villinger, H., Futrell, J. H., Howorka, F., Duric, N., Lindinger, W., *J. Chem. Phys.* **76**, 3529 (1982).
- 75VOG/BEA Vogt, J., Beauchamp, J. L., *J. Am. Chem. Soc.* **97**, 6682 (1975). ICR. Bracketing.
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- 78WAN/DES Wang, J.-S., DeStefano, A. J., Porter, R. F., *Inorg. Chem.* **17**, 1374 (1978). HPMS. Bracketing.
- 74WAR Wameck, P., *Z. Naturforsch.* **29a**, 350 (1974).
- 88WEB/HOU Weber, J., Houriet, R., *J. Phys. Chem.* **92**, 5926 (1988). ICR study of proton transfer equilibria. *Ab initio* calculations suggest that protonation occurs on the chalcogen atom in each case.
- 85WEI/PLA Weil, D. A., Platzner, I., Miller, L. L., Dixon, D. A., *Org. Mass Spectrom.* **20**, 115 (1985). ICR. Bracketing.  $GB(C_2H_4) < GB(COS) < GB(H_2O)$ .  $GB(COS) < GB(CS_2) - GB(H_2S) < GB(CH_3CCH)$ : This basicity value for  $CS_2$  is in good agreement with the value one would predict for a temperature of 320 K from the results of 77MAU/FIE.
- 79WIB/FIS Wiberg, N., Fischer G., Bachhuber, H., *Z. Naturforsch.* **34b**, 1385 (1979). Ionization and appearance potentials in  $HN=NH$ ,  $H_2N=N$ , and  $N_2H_4$ .
- 80WIG/BEA Wight, C. A., Beauchamp, J. L., *J. Phys. Chem.* **84**, 2503 (1980). ICR: Related to TAFT scale; temperature corrected to 320 K.
- 76WIL/LEB Williamson, A. D., LeBreton, P. R., Beauchamp, J. L., *J. Am. Chem. Soc.* **98**, 2705 (1976). Thermochemical cycles based on appearance potentials of  $CH_2CFX^+$  and  $CH_3CFX$  ( $X=H,F$ ) from  $CH_3CFXCH_3$ , and  $IP(CH_2CFX)$ . Measured  $AE(CH_3CHFCH_3 \rightarrow CH_3CHF^+ + CH_3 + e^-) = 11.75$  eV and  $AE(CH_3CHFCH_3 \rightarrow CH_2CHF^+ + CH_4 + e^-) = 11.53$  eV; combining these quantities with  $IP(CH_2CHF) = 10.363$  eV and  $D_e(CH_3-H) = 438.1$  kJ mol<sup>-1</sup> yields  $PA(CH_2CHF) = 729$  kJ mol<sup>-1</sup>. Measured  $AE(CH_3CF_2CH_3 \rightarrow CH_3CF_2^+ + CH_3 + e^-) = 11.81$  eV and  $AE(CH_3CF_2CH_3 \rightarrow CH_2CF_2^+ + CH_4 + e^-) = 11.57$  eV; combining these quantities with  $IP(CH_2CF_2) = 10.29$  eV gives  $PA(CH_2CF_2) = 734$  kJ mol<sup>-1</sup>.
- 76WIL/LOS Willis, C., Lossing, F. P., Back, R. A., *Can. J. Chem.* **54**, 1 (1976). Heat of formation of  $N_2H^+$  as a fragment ion in  $N_2H_2$ .
- 75WIL/MCC Wilson, M. S., McCloskey, J. A., *J. Am. Chem. Soc.* **97**, 3436 (1975). HPMS. Bracketing: All compounds bracketed relative to  $NH_3$ ,  $CH_3NH_2$ ,  $(CH_3)_2NH$ , and  $(CH_3)_3N$ .
- 88WLO/ROD Wlodek, S., Rodriguez, C. F., Lien, M. H., Hopkinson, A. C., Bohme, D. K., *Chem. Phys. Lett.* **143**, 385 (1988). Selected ion flow tube measurement. An approximate empirical relationship between reaction efficiency and  $\Delta G^0$  suggested that proton transfer from  $SiNH_2^+$  to  $NH_3$  was close to isoergic. Also observed no proton transfer from  $SiNH_2^+$  to  $(CH_3)_2S$  nor  $(CH_3)_2CO$ .

- 77WOL/ABB Wolf, J. F., Abboud, J. L. M., Taft, R. W., *J. Org. Chem.* **42**, 3316 (1977). ICR. Results given in figure form.
- 76WOL/DEV Wolf, J. F., Devlin, J. L., DeFrees, D. J., Taft, R. W., Hehre, W. J., *J. Am. Chem. Soc.* **98**, 5097 (1976).
- 90WOL/GRU Wolf, R., Grutzmacher, H. F., *New J. Chem.* **14**, 379 (1990). FT-ICR. GB values obtained from proton-transfer equilibria at an assumed temperature of 320 K.
- 75WOL/HAR Wolf, J. F., Harch, P. G., Taft, R. W., *J. Am. Chem. Soc.* **97**, 2904 (1975). ICR: Related to TAFT scale. Data corrected from 300 to 350 K.
- 77WOL/STA Wolf, J. F., Staley, R. H., Koppel, I., Taagepera, M., McIver, Jr., R. T., Beauchamp, J. L., Taft, R. W., *J. Am. Chem. Soc.* **99**, 5417 (1977). ICR. Data corrected from 300 to 350 K (R. W. Taft, personal communication).
- 92WU/FEN Wu, Z., Fenselau, C., *Rapid Commun. Mass Spectrom.* **6**, 403 (1992). PA(arginine) reported using the kinetic method employing 1,1,3,3-tetramethylguanidine (TMG), 1,5-diazabicyclo[4.3.0]non-5-ene (DBN) and 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) as reference bases. The relevant rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation.
- 92WU/FEN2 Wu, Z., Fenselau, C., *J. Am. Soc. Mass Spectrom.* **3**, 863 (1992). Proton affinities are reported from measured dissociation kinetics of proton-bound dimers. The relevant rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation. The results are tabulated as GB values at an unknown effective temperature.
- 93WU/FEN Wu, Z., Fenselau, C., *Tetrahedron* **49**, 9197 (1993). GB values obtained from MIKE measurements and by applying the kinetic method. The relevant rate data were reanalyzed using the current GB values of reference bases as determined in this present evaluation. GB values are reported at unknown effective *T*.
- 94WU/FEN Wu, Z., Fenselau, C., *Rapid Commun. Mass Spectrom.* **8**, 777 (1994). Kinetic method. As much as possible, the relevant rate data were reanalyzed using the current PA values of reference bases as determined in this present evaluation.  $\Delta S_p$  values also determined.
- 93WU/LEB Wu, J., Lebrilla, C. B., *J. Am. Chem. Soc.* **115**, 3270 (1993). ICR bracketing. Also molecular orbital calculations using the semi-empirical AM1 package.
- 73YAM/KEB Yamdagni, R., Kebarle, P., *J. Am. Chem. Soc.* **95**, 3504 (1973). HPMS.
- 76YAM/KEB Yamdagni, R., Kebarle, P., *J. Am. Chem. Soc.* **98**, 1320 (1976). HPMS. Data assumed to have been superseded by data in 79LAU, when species studied have been duplicated. Other data corrected to 79LAU scale; free energy change values multiplied by 1.05.
- 96ZHA/STO Zhang, W., Stone, J. A., Brook, M. A., McGibbon, G. A., *J. Am. Chem. Soc.* **118**, 5764 (1996). HPMS.
- 93ZHA/ZIM Zhang, K., Zimmerman, D. M., Chung-Phillips, A., Cassady, C. J., *J. Am. Chem. Soc.* **115**, 10812 (1993). FT-ICR. Bracketing by gas-basicity. Calculations indicate glycine protonates at the amino group and that diglycine protonates on N-terminal amino group with H bonding to carbonyl of amide moiety.