

NIST20 EI MS Library



+40K Coverage

NIST/EPA/NIH GC-MS

NIST20 Tandem MS Library



2X Coverage

NIST LC-MS

MS Software



New Release

Quality Assurance

Why Upgrade to NIST20

- 350,643 spectra (44,021 new)
- 306,869 compounds (39,493 new)

Library Growth Concentrated in

- Human & plant metabolites
- Legal & illicit drugs
- General analytical interest

Gas Chromatography Retention Index and Methods Library

- 447,285 RI values
- 139,963 compounds

Comprehensive

- 30,999 compounds (17,191 new)
- 185,602 precursor ions (67,520 new)
- 1,320,464 spectra (745,638 new)
- Instruments Used: Ion Trap, Collision Cell

Wide Coverage

- Metabolites
- Pharmaceuticals
- Industrial Surfactants
- Glycans-Lipids-Sugars
- Pesticides
- Amino Acids, Di- & Tryptic Tri-Peptides

- Every new spectrum reviewed by two analysts.
- New compounds chosen for wide analytical interest.
- MS Search v. 2.4 with hybrid search
- AMDIS (GC-MS)
- MS Interpreter Major Revision

Email massspec@nist.gov

Web chemdata.nist.gov



Atomic Properties of the Elements

FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS[§]

1 second = 9 192 631 770 periods of radiation corresponding to the transition between the two hyperfine levels of the ground state of ¹³³Cs

speed of light in vacuum	<i>c</i>	299 792 458 m s ⁻¹	(exact)
Planck constant	<i>h</i>	6.626 070 15 × 10 ⁻³⁴ J Hz ⁻¹	(exact)
elementary charge	<i>e</i>	1.602 176 634 × 10 ⁻¹⁹ C	(exact)
Avogadro constant	<i>N_A</i>	6.022 140 76 × 10 ²³ mol ⁻¹	(exact)
Boltzmann constant	<i>k</i>	1.380 649 × 10 ⁻²³ J K ⁻¹	(exact)
electron volt	eV	1.602 176 634 × 10 ⁻¹⁹ J	(exact)
electron mass	<i>m_e</i>	9.109 383 70 × 10 ⁻³¹ kg	
energy equivalent	<i>m_ec²</i>	0.510 998 950 MeV	
proton mass	<i>m_p</i>	1.672 621 924 × 10 ⁻²⁷ kg	
energy equivalent	<i>m_pc²</i>	938.272 088 MeV	
fine-structure constant	<i>α</i>	1/137.035 999	
Rydberg energy	<i>R_∞hc</i>	13.605 693 1230 eV	
Newtonian constant of gravitation	<i>G</i>	6.674 × 10 ⁻¹¹ m ³ kg ⁻¹ s ⁻²	

§For the most accurate values of these and other constants, visit pml.nist.gov/constants.

Group 1 IA	1 ¹ S _{1/2} H Hydrogen 1.008 1s 13.5984	2 IIA	FREQUENTLY USED FUNDAMENTAL PHYSICAL CONSTANTS [§]										13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIII He Helium 4.0026 1s ² 24.5874																
			<p>speed of light in vacuum <i>c</i> 299 792 458 m s⁻¹ (exact)</p> <p>Planck constant <i>h</i> 6.626 070 15 × 10⁻³⁴ J Hz⁻¹ (exact)</p> <p>elementary charge <i>e</i> 1.602 176 634 × 10⁻¹⁹ C (exact)</p> <p>Avogadro constant <i>N_A</i> 6.022 140 76 × 10²³ mol⁻¹ (exact)</p> <p>Boltzmann constant <i>k</i> 1.380 649 × 10⁻²³ J K⁻¹ (exact)</p> <p>electron volt eV 1.602 176 634 × 10⁻¹⁹ J (exact)</p> <p>electron mass <i>m_e</i> 9.109 383 70 × 10⁻³¹ kg</p> <p>energy equivalent <i>m_ec²</i> 0.510 998 950 MeV</p> <p>proton mass <i>m_p</i> 1.672 621 924 × 10⁻²⁷ kg</p> <p>energy equivalent <i>m_pc²</i> 938.272 088 MeV</p> <p>fine-structure constant <i>α</i> 1/137.035 999</p> <p>Rydberg energy <i>R_∞hc</i> 13.605 693 1230 eV</p> <p>Newtonian constant of gravitation <i>G</i> 6.674 × 10⁻¹¹ m³ kg⁻¹ s⁻²</p>																															
2 ² S _{1/2} ³ S _{1/2}	3 ³ S _{1/2} ⁴ S ₀ Li Lithium 6.94 1s ² 2s 5.3917	4 ¹ S ₀ Be Beryllium 9.0122 1s ² 2s ² 9.3227											5 ² P _{1/2}	6 ³ P ₀	7 ⁴ S _{3/2}	8 ³ P ₂	9 ² P _{3/2}	10 ¹ S ₀ Ne Neon 20.180 1s ² 2s ² 2p ⁶ 21.5645																
3 ² S _{1/2} ² S _{1/2}	11 ² S _{1/2} ³ S _{1/2} Na Sodium 22.990 [Ne]3s	12 ¹ S ₀ Mg Magnesium 24.305 [Ne]3s ² 7.6462	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 ² P _{1/2} Al Aluminum 26.982 [Ne]3s ² 3p 5.9888	14 ³ P ₀ Si Silicon 28.085 [Ne]3s ² 3p ² 8.1517	15 ⁴ S _{3/2} P Phosphorus 30.974 [Ne]3s ² 3p ³ 10.4867	16 ³ P ₂ S Sulfur 32.06 [Ne]3s ² 3p ⁴ 10.3600	17 ³ P ₂ Cl Chlorine 35.45 [Ne]3s ² 3p ⁵ 12.9676	18 ¹ S ₀ Ar Argon 39.948 [Ne]3s ² 3p ⁶ 15.7596																
4 ³ S _{1/2} ² S _{1/2}	19 ³ S _{1/2} K Potassium 39.098 [Ar]4s 4.3407	20 ¹ S ₀ Ca Calcium 40.078 [Ar]4s ² 6.1132	21 ² D _{3/2}	22 ³ F ₂	23 ⁴ F _{3/2}	24 ⁷ S ₃	25 ⁶ S _{5/2}	26 ⁵ D ₄	27 ⁴ F _{9/2}	28 ³ F ₄	29 ² S _{1/2}	30 ¹ S ₀	31 ² P _{1/2}	32 ³ P ₀	33 ⁴ S _{3/2}	34 ³ P ₂	35 ² P _{3/2}	36 ¹ S ₀ Kr Krypton 83.798 [Ar]3d ¹⁰ 4s ⁴ 4p ⁶ 13.9996																
5 ² S _{1/2} ¹ S ₀	37 ² S _{1/2} Rb Rubidium 85.468 [Kr]5s 4.1771	38 ¹ S ₀ Sr Strontium 87.62 [Kr]5s ² 5.6949	39 ² D _{3/2}	40 ³ F ₂	41 ⁶ D _{1/2}	42 ⁷ S ₃	43 ⁶ S _{5/2}	44 ⁵ F ₅	45 ⁴ F _{9/2}	46 ¹ S ₀	47 ² S _{1/2}	48 ¹ S ₀	49 ² P _{1/2}	50 ³ P ₀	51 ⁴ S _{3/2}	52 ³ P ₂	53 ² P _{3/2}	54 ¹ S ₀ Xe Xenon 131.29 [Kr]4d ¹⁰ 5s ² 5p ⁶ 12.1298																
6 ² S _{1/2} ¹ S ₀	55 ² S _{1/2} Cs Cesium 132.91 [Xe]6s 3.8939	56 ¹ S ₀ Ba Barium 137.33 [Xe]6s ² 5.2117	57 ² D _{3/2}	58 ¹ G ₄	59 ⁴ I _{9/2}	60 ⁵ I ₄	61 ⁶ H _{5/2}	62 ⁷ F ₀	63 ⁸ S _{7/2}	64 ⁹ D ₂	65 ⁶ H _{15/2}	66 ⁵ I ₈	67 ⁴ I _{15/2}	68 ³ H ₆	69 ² F _{7/2}	70 ¹ S ₀	71 ² D _{3/2}	72 ³ F ₂	73 ⁴ F _{3/2}	74 ⁵ D ₀	75 ⁶ S _{5/2}	76 ⁵ D ₄	77 ⁴ F _{9/2}	78 ³ D ₃	79 ² S _{1/2}	80 ¹ S ₀	81 ² P _{1/2}	82 ³ P ₀	83 ⁴ S _{3/2}	84 ³ P ₂	85 ² P _{3/2}	86 ¹ S ₀ Rn Radon (222) [Hg]6p ⁶ 10.7485		
7 ² S _{1/2} ¹ S ₀	87 ² S _{1/2} Fr Francium (223) [Rn]7s 4.0727	88 ¹ S ₀ Ra Radium (226) [Rn]7s ² 5.2784	89 ² D _{3/2}	90 ³ F ₂	91 ⁴ K _{11/2}	92 ⁵ L ₆	93 ⁶ L _{11/2}	94 ⁷ F ₀	95 ⁸ S _{7/2}	96 ⁹ D ₂	97 ⁶ H _{15/2}	98 ⁵ I ₈	99 ⁴ I _{15/2}	100 ³ H ₆	101 ² F _{7/2}	102 ¹ S ₀	103 ² P _{1/2}	104 ³ F ₂	105 ⁴ F _{3/2}	106 ⁰	107 ^{5/2}	108 ⁴	109 ⁵	110 ⁴	111 ⁵	112 ⁶	113 ⁵	114 ⁶	115 ⁵	116 ⁶	117 ⁵	118 ⁶	119 ⁵	120 ⁶
Lanthanides	57 ² D _{3/2} La Lanthanum 138.91 [Xe]5d6s ² 5.5769	58 ¹ G ₄ Ce Cerium 140.12 [Xe]4f5d6s ² 5.5386	59 ⁴ I _{9/2} Pr Praseodymium 140.91 [Xe]4f6s ² 5.4702	60 ⁵ I ₄ Nd Neodymium 144.24 [Xe]4f6s ² 5.5250	61 ⁶ H _{5/2} Pm Promethium (145) [Xe]4f6s ² 5.577	62 ⁷ F ₀ Sm Samarium 150.36 [Xe]4f6s ² 5.6437	63 ⁸ S _{7/2} Eu Europium 151.96 [Xe]4f6s ² 5.6704	64 ⁹ D ₂ Gd Gadolinium 157.25 [Xe]4f5d6s ² 5.8638	65 ⁶ H _{15/2} Tb Terbium 158.93 [Xe]4f6s ² 5.8638	66 ⁵ I ₈ Dy Dysprosium 162.50 [Xe]4f6s ² 5.9391	67 ⁴ I _{15/2} Ho Holmium 164.93 [Xe]4f12s ² 6.0215	68 ³ H ₆ Er Erbium 167.26 [Xe]4f12s ² 6.1077	69 ² F _{7/2} Tm Thulium 168.93 [Xe]4f13s ² 6.1843	70 ¹ S ₀ Yb Ytterbium 173.05 [Xe]4f13s ² 6.2542	71 ² D _{3/2} Lu Lutetium 174.97 [Xe]4f14s6s ² 5.4259	72 ³ F ₂ Hf Hafnium 178.49 [Xe]4f14s5d6s ² 6.8251	73 ⁴ F _{3/2} Ta Tantalum 180.95 [Xe]4f14s5d6s ² 7.5496	74 ⁵ D ₀ W Tungsten 183.84 [Xe]4f14s5d6s ² 7.8640	75 ⁶ S _{5/2} Re Rhenium 186.21 [Xe]4f14s5d6s ² 7.8335	76 ⁵ D ₄ Os Osmium 190.23 [Xe]4f14s5d6s ² 8.4382	77 ⁴ F _{9/2} Ir Iridium 192.22 [Xe]4f14s5d6s ² 8.9670	78 ³ D ₃ Pt Platinum 195.08 [Xe]4f14s5d96s ¹ 8.9588	79 ² S _{1/2} Au Gold 196.97 [Xe]4f14s5d106s ¹ 9.2256	80 ¹ S ₀ Hg Mercury 200.59 [Xe]4f14s5d106s ² 10.4375	81 ² P _{1/2} Tl Thallium 204.38 [Hg]6p 6.1083	82 ³ P ₀ Pb Lead 207.2 [Hg]6p ² 7.4167	83 ⁴ S _{3/2} Bi Bismuth 208.98 [Hg]6p ³ 7.2855	84 ³ P ₂ Po Polonium (209) [Hg]6p ⁴ 8.414	85 ² P _{3/2} At Astatine (210) [Hg]6p ⁵ 9.3175	86 ¹ S ₀ Rn Radon (222) [Hg]6p ⁶ 10.7485				
Actinides	89 ² D _{3/2} Ac Actinium (227) [Rn]6d7s ² 5.3802	90 ³ F ₂ Th Thorium 232.04 [Rn]6d7s ² 6.3067	91 ⁴ K _{11/2} Pa Protactinium 231.04 [Rn]5f6d7s ² 5.89	92 ⁵ L ₆ U Uranium 238.03 [Rn]5f36d7s ² 6.1941	93 ⁶ L _{11/2} Np Neptunium (237) [Rn]5f46d7s ² 6.2655	94 ⁷ F ₀ Pu Plutonium (244) [Rn]5f7s ² 6.0258	95 ⁸ S _{7/2} Am Americium (243) [Rn]5f7s ² 5.9738	96 ⁹ D ₂ Cm Curium (247) [Rn]5f76d7s ² 5.9914	97 ⁶ H _{15/2} Bk Berkelium (247) [Rn]5f97s ² 6.1978	98 ⁵ I ₈ Cf Californium (251) [Rn]5f107s ² 6.2817	99 ⁴ I _{15/2} Es Einsteinium (252) [Rn]5f117s ² 6.3676	100 ³ H ₆ Fm Fermium (257) [Rn]5f127s ² 6.50	101 ² F _{7/2} Md Mendelevium (288) [Rn]5f137s ² 6.58	102 ¹ S ₀ No Nobelium (259) [Rn]5f147s ² 6.66	103 ² P _{1/2} Lr Lawrencium (260) [Rn]5f147s2p 4.96	104 ³ F ₂ Rf Rutherfordium (261) [Rn]5f146d7s ² 6.02	105 ⁴ F _{3/2} Db Dubnium (269) [Rn]5f146d7s ² 6.8	106 ⁰ Sg Seaborgium (269) [Rn]5f146d7s ² 7.8	107 ^{5/2} Bh Bohrium (270) [Rn]5f146d7s ² 7.7	108 ⁴ Hs Hassium (269) [Rn]5f146d7s ² 7.6	109 ⁵ Mt Meitnerium (278) [Rn]5f146d7s ² 7.6	110 ⁴ Ds Darmstadtium (281) [Rn]5f146d7s ² 7.6	111 ⁵ Rg Roentgenium (282) [Rn]5f146d7s ² 7.6	112 ⁶ Cn Copernicium (285) [Rn]5f146d7s ² 7.6	113 ⁵ Nh Nihonium (286) [Rn]5f146d7s ² 7.6	114 ⁶ Fl Flerovium (289) [Rn]5f146d7s ² 7.6	115 ⁵ Mc Moscovium (289) [Rn]5f146d7s ² 7.6	116 ⁶ Lv Livermorium (293) [Rn]5f146d7s ² 7.6	117 ⁵ Ts Tennessine (294) [Rn]5f146d7s ² 7.6	118 ⁶ Og Oganesson (294) [Rn]5f146d7s ² 7.6				

Atomic Number: 58
Ground State: ¹G₄
Symbol: Ce
Name: Cerium
Standard Atomic Weight: 140.12
Ground-state Configuration: [Xe]4f5d6s²
Ionization Energy (eV): 5.5386

†Based upon ¹²C. () indicates the mass number of the longest-lived isotope.