Backmatter

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A Background Data for the Chemical Elements

A.1 Periodic Table of the Elements

See ◘ Fig. A.1.

A.2 Historical Names of the Chemical Elements

See ◘ Table A.1.

A.3 Unified Numbering System for Metals and Alloys Standard Alphabetical Designation

The *Unified Numbering System for Metals and Alloys* (UNS) is the accepted alloy designation system in North America for commercially available metals and alloys and has also been accepted worldwide.[1] The UNS is managed jointly by ASTM International and SAE International. The standard code designation consists of five digits following the prefix letter identifying the alloy's family. Generally, UNS designations are simply expansions of the former designations (i.e., those of the American Iron and Steel Institute, Aluminum Association, Copper Development Association, etc.).

See ◘ Table A.2.

A.4 Names of Transfermium Elements 101–118

The *American Chemical Society* (ACS) has adopted the names listed in ◘ Table A.3 for elements 101–118. These names were adopted by the IUPAC International Union of Pure and Applied Chemistry and endorsed by the ACS Committee on Nomenclature. The new names differ in only two cases from the names supported by the ACS Committee on Nomenclature and adopted by the ACS publications in 1995. From September 1997, dubnium replaced hahnium for element 105 and bohrium replaced nielsbohrium for element 107.

A.5 Selected Physical Properties of the Elements

See ◘ Table A.4.

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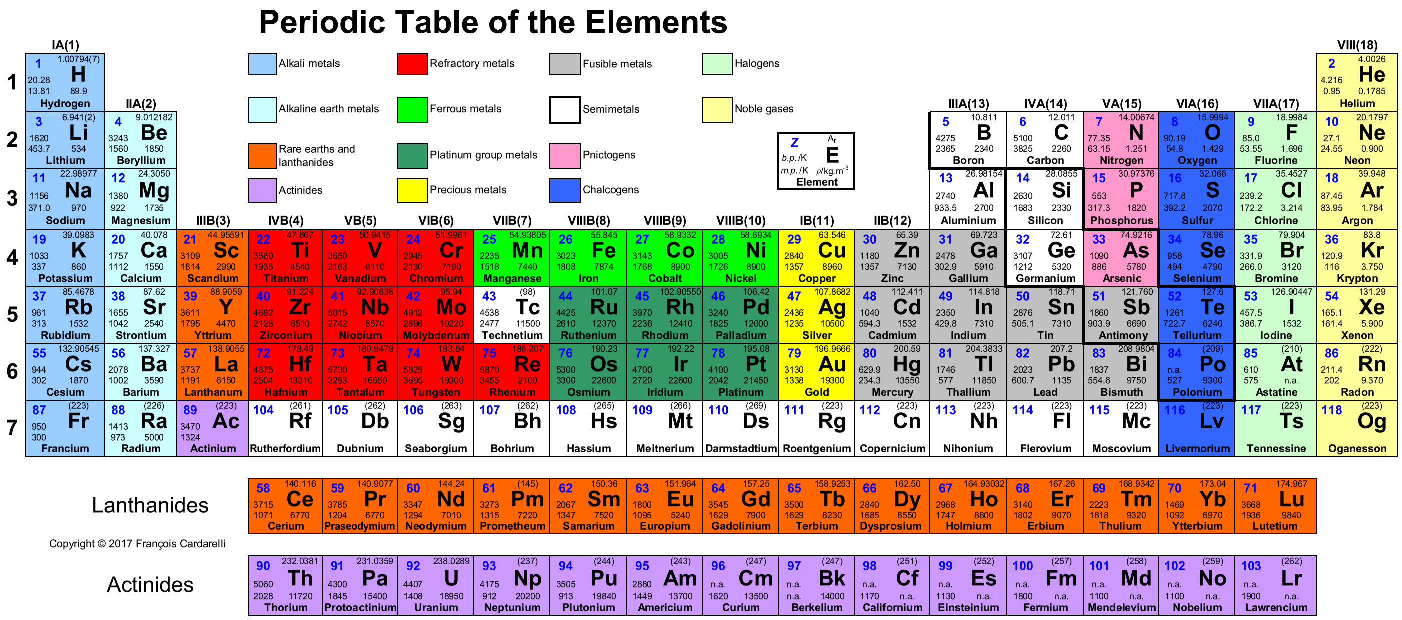
[1] Society of Automotive Engineers (SAE) Metals and Alloys in the Unified Numbering System, 7th edn. ASTM/SAE (1998).



Periodic Table of the Elements

- Alkali metals
- Alkaline earth metals
- Rare earths and lanthanides
- Actinides
- Refractory metals
- Ferrous metals
- Platinum group metals
- Precious metals
- Fusible metals
- Semimetals
- Pnictogens
- Chalcogens
- Halogens
- Noble gases

Z A_r
E
b.p. /K
m.p. /K ρ/kg.m^{-3}
Element

	IA(1)	IIA(2)	IIIB(3)	IVB(4)	VB(5)	VIB(6)	VIIB(7)	VIIIB(8)	VIIIB(9)	VIIIB(10)	IB(11)	IIB(12)	IIIA(13)	IVA(14)	VA(15)	VIA(16)	VIIA(17)	VIII(18)
1	1 **H** 1.00794(7) 20.28 13.81 89.9 Hydrogen																	2 **He** 4.0026 4.216 0.95 0.1785 Helium
2	3 **Li** 6.941(2) 1620 453.7 534 Lithium	4 **Be** 9.012182 3243 1560 1850 Beryllium											5 **B** 10.811 4275 2365 2340 Boron	6 **C** 12.011 5100 3825 2260 Carbon	7 **N** 14.00674 77.35 63.15 1.251 Nitrogen	8 **O** 15.9994 90.19 54.8 1.429 Oxygen	9 **F** 18.9984 85.0 53.55 1.696 Fluorine	10 **Ne** 20.1797 27.1 24.55 0.900 Neon
3	11 **Na** 22.98977 1156 371.0 970 Sodium	12 **Mg** 24.3050 1380 922 1735 Magnesium											13 **Al** 26.98154 2740 933.5 2700 Aluminium	14 **Si** 28.0855 2630 1683 2330 Silicon	15 **P** 30.97376 553 317.3 1820 Phosphorus	16 **S** 32.066 717.8 392.2 2070 Sulfur	17 **Cl** 35.4527 239.2 172.2 3.214 Chlorine	18 **Ar** 39.948 87.45 83.95 1.784 Argon
4	19 **K** 39.0983 1033 337 860 Potassium	20 **Ca** 40.078 1757 1112 1550 Calcium	21 **Sc** 44.95591 3109 1814 2990 Scandium	22 **Ti** 47.867 3560 1935 4540 Titanium	23 **V** 50.9415 3650 2163 6110 Vanadium	24 **Cr** 51.9961 2945 2130 7190 Chromium	25 **Mn** 54.93805 2235 1518 7440 Manganese	26 **Fe** 55.845 3023 1808 7874 Iron	27 **Co** 58.9332 3143 1768 8900 Cobalt	28 **Ni** 58.6934 3005 1726 8900 Nickel	29 **Cu** 63.546 2840 1357 8960 Copper	30 **Zn** 65.39 1180 1357 7130 Zinc	31 **Ga** 69.723 2478 302.9 5910 Gallium	32 **Ge** 72.61 3107 1212 5320 Germanium	33 **As** 74.9216 1090 886 5780 Arsenic	34 **Se** 78.96 958 494 4790 Selenium	35 **Br** 79.904 331.9 266.0 3120 Bromine	36 **Kr** 83.8 120.9 116 3.750 Krypton
5	37 **Rb** 85.4678 961 313 1532 Rubidium	38 **Sr** 87.62 1655 1042 2540 Strontium	39 **Y** 88.9059 3611 1795 4470 Yttrium	40 **Zr** 91.224 4682 2128 6510 Zirconium	41 **Nb** 92.90638 5015 2742 8570 Niobium	42 **Mo** 95.94 4912 2896 10220 Molybdenum	43 **Tc** (98) 4538 2477 11500 Technetium	44 **Ru** 101.07 4425 2610 12370 Ruthenium	45 **Rh** 102.90550 3970 2236 12410 Rhodium	46 **Pd** 106.42 3240 1825 12000 Palladium	47 **Ag** 107.8682 2436 1235 10500 Silver	48 **Cd** 112.411 1040 594.3 1532 Cadmium	49 **In** 114.818 2350 429.8 7310 Indium	50 **Sn** 118.71 2876 505.1 7310 Tin	51 **Sb** 121.760 1860 903.9 6690 Antimony	52 **Te** 127.6 1261 722.7 6240 Tellurium	53 **I** 126.90447 457.5 386.7 1532 Iodine	54 **Xe** 131.29 165.1 161.4 5.900 Xenon
6	55 **Cs** 132.90545 944 302 1870 Cesium	56 **Ba** 137.327 2078 1002 3590 Barium	57 **La** 138.9055 3737 1191 6150 Lanthanum	72 **Hf** 178.49 4875 2504 13310 Hafnium	73 **Ta** 180.9479 5730 3293 16650 Tantalum	74 **W** 183.84 5825 3695 19300 Tungsten	75 **Re** 186.207 5870 3455 2100 Rhenium	76 **Os** 190.23 5300 3300 22600 Osmium	77 **Ir** 192.22 4700 2720 22600 Iridium	78 **Pt** 195.08 4100 2042 21450 Platinum	79 **Au** 196.9666 3130 1338 19300 Gold	80 **Hg** 200.59 629.9 234.3 13550 Mercury	81 **Tl** 204.3833 1746 577 11850 Thallium	82 **Pb** 207.2 2023 600.7 1135 Lead	83 **Bi** 208.9804 1837 554.6 9750 Bismuth	84 **Po** (209) n.a. 527 9300 Polonium	85 **At** (210) 610 575 n.a. Astatine	86 **Rn** (222) 211.4 202 9.370 Radon
7	87 **Fr** (223) 950 300 Francium	88 **Ra** (226) 1413 973 5000 Radium	89 **Ac** (223) 3470 1324 Actinium	104 **Rf** (261) Rutherfordium	105 **Db** (262) Dubnium	106 **Sg** (263) Seaborgium	107 **Bh** (262) Bohrium	108 **Hs** (265) Hassium	109 **Mt** (266) Meitnerium	110 **Ds** (269) Darmstadtium	111 **Rg** (223) Roentgenium	112 **Cn** (223) Copernicium	113 **Nh** (223) Nihonium	114 **Fl** (223) Flerovium	115 **Mc** (223) Moscovium	116 **Lv** (223) Livermorium	117 **Ts** (223) Tennessine	118 **Og** (223) Oganesson

Lanthanides	58 **Ce** 140.116 3715 1071 6770 Cerium	59 **Pr** 140.9077 3785 1204 6770 Praseodymium	60 **Nd** 144.24 3347 1294 7010 Neodymium	61 **Pm** (145) 3273 1315 7220 Prometheum	62 **Sm** 150.36 2067 1347 7520 Samarium	63 **Eu** 151.964 1800 1095 5240 Europium	64 **Gd** 157.25 3545 1629 7900 Gadolinium	65 **Tb** 158.9253 3500 1629 8230 Terbium	66 **Dy** 162.50 2840 1685 8550 Dysprosium	67 **Ho** 164.93032 2968 1747 8800 Holmium	68 **Er** 167.26 3140 1802 9070 Erbium	69 **Tm** 168.9342 2223 1818 9320 Thulium	70 **Yb** 173.04 1469 1092 6970 Ytterbium	71 **Lu** 174.967 3668 1936 9840 Lutetium
Actinides	90 **Th** 232.0381 5060 2028 11720 Thorium	91 **Pa** 231.0359 4300 1845 15400 Protoactinium	92 **U** 238.0289 4407 1408 18950 Uranium	93 **Np** (237) 4175 912 20200 Neptunium	94 **Pu** (244) 3505 913 19840 Plutonium	95 **Am** (243) 2880 1449 13700 Americium	96 **Cm** (247) n.a. 1620 13500 Curium	97 **Bk** (247) n.a. n.a. 14000 Berkelium	98 **Cf** (251) n.a. 1170 n.a. Californium	99 **Es** (252) n.a. 1130 n.a. Einsteinium	100 **Fm** (257) n.a. 1800 n.a. Fermium	101 **Md** (258) n.a. 1100 n.a. Mendelevium	102 **No** (259) n.a. 1100 n.a. Nobelium	103 **Lr** (262) n.a. 1900 n.a. Lawrencium

Fig. A.1 The periodic table. *b.p.* boiling point, *m.p.* melting point, *n.a.* not available

Table A.1 Obsolete, historical, and other names of the chemical elements

Obsolete, historical, or other names and symbol	IUPAC name
Actinon (An)	Radon-219
Alabamine	Astatine
Aluminum	Aluminium
Argentum	Silver
Arsenicum	Arsenic
Aurum	Gold
Azote (Az)	Nitrogen
Caesium	Cesium
Cassiopeium	Lutetium
Celtium (Ct)	Hafnium
Columbium (Cb)	Niobium
Cuprum	Copper
Didynium (Dm)	Neodymium and praseodymium
Eka-aluminium	Gallium
Eka-caesium	Francium
Eka-silicon	Germanium
Pelopium	Niobium
Dianium	Niobium
Ilminium	Niobium
Emanation (Em)	Radon
Erythronium	Vanadium
Ferrum	Iron
Glucinium (Gl)	Beryllium
Hydrargyrum	Mercury
Illinium (Il)	Promethium
Kalium	Potassium
Masurium (Ma)	Technetium
Misch metal	Cerium impure
Natrium	Sodium
Niton	Radon-222
Panchromium	Vanadium
Plumbum	Lead
Stannum	Tin

Table A.1 (*continued*)

Obsolete, historical, or other names and symbol	IUPAC name
Stibium	Antimony
Sulphur	Sulfur
Thoron (Tn)	Radon-220
Virginium (Vi)	Francium
Wolfram	Tungsten

IUPAC International Union of Pure and Applied Chemistry

Table A.2 Unified Numbering System for Metals and Alloys alphabetical designation

UNS designation	Description
AXXXXX	Aluminum and aluminum alloys
CXXXXX	Copper and copper alloys
DXXXXX	Specified mechanical property steels
EXXXXX	Rare earth and rare earth like metals and alloys
FXXXXX	Cast irons and cast steels
GXXXXX	AISI and SAE carbon and alloy steels
HXXXXX	AISI and SAE H-steels
JXXXXX	Cast steels
KXXXXX	Miscellaneous steels and ferrous alloys
LXXXXX	Low-melting metals and alloys
MXXXXX	Miscellaneous nonferrous metals and alloys
NXXXXX	Nickel and nickel alloys
PXXXXX	Precious metals and alloys
RXXXXX	Reactive and refractory metals and alloys
SXXXXX	Heat- and corrosion-resistant stainless steels
TXXXXX	Tool steels, wrought and cast
WXXXXX	Welding filler metals
ZXXXXX	Zinc and zinc alloys

Table A.3 Names of transfermium elements

Element	Name	Symbol	Previous proposed name(s)	CAS RN
101	Mendelevium	Md	Mendelevium	7440-11-1
102	Nobelium	No	Nobelium	10028-14-5
103	Lawrencium	Lr	Lawrencium	22537-19-5
104	Rutherfordium	Rf	Kurchatovium	53850-36-5
105	Dubnium	Db	Hahnium, joliotium	53850-35-4
106	Seaborgium	Sg	Seaborgium	54038-81-2
107	Bohrium	Bh	Nielsbohrium	54037-14-8
108	Hassium	Hs	Hahnium	54037-57-9
109	Meitnerium	Mt	Meitnerium	54038-01-6
110	Darmstadtium	Ds	Ununnilium	54083-77-1
111	Roentgenium	Rg	Unununium	54386-24-2
112	Copernicium	Cn	Ununbium	54084-26-3
113	Nihonium	Nh	Ununtrium	54084-70-7
114	Flevorium	Fl	Ununquadium	54085-16-4
115	Moscovium	Mc	Ununpentium	54085-64-2
116	Livermorium	Lv	Ununhexium	54100-71-9
117	Tennessine	Ts	Ununseptium	87658-56-8
118	Oganesson	Og	Ununoctium	54144-19-3

CAS RN Chemical Abstracts Service Registry Number

Table A.4 Properties of the elements

Element name (IUPAC)	Actinium	Aluminium (aluminum)	Americium	Antimony	Argon (gas)
Relative abundance in Earth's crust (mg/kg)	5.5×10^{-10}	82,300	n. r.	0.2	3.5
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2 \cdot$ g^{-1}]	0.79000	0.00300	n. a.	0.01600	0.00600
Thermal neutron capture cross section (σ_{th}/10^{-28} m^2)	810	0.233	74	5.4	0.65
Absolute magnetic susceptibility (χ_m/10^{-6})	n. a.	1.6752	56.0229	−5.8081	−0.0009
Mass magnetic susceptibility ($4\pi\chi_m$/10^{-9} kg$^{-1} \cdot$ m^3)	n. a.	7.80	51.50	−10.90	−6.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	4.50	n. a.	5.10	n. r.
Electrical resistivity (ρ/μΩ · cm) (293.15 K)	n. a.	2.6548	68	39	n. r.
Coefficient of linear thermal expansion (α/10^{-6} K^{-1}) (0–100 °C)	14.9	23.03	n. a.	8.5	n. a.
Specific heat capacity (c_p/J · kg$^{-1} \cdot$ K^{-1}) (300 K)	n. a.	903	n. a.	205	524
Thermal conductivity (k/W · m$^{-1} \cdot$ K^{-1}) (300 K)	12	237	10 (estimated)	24.3	0.0177
Latent molar enthalpy of vaporization (L_{vap}/kJ · mol^{-1})	n. a.	294	238.5	193.43	15.580
Latent molar enthalpy of fusion (L_{fus}/kJ · mol^{-1})	n. a.	10.711	14.4	19.89	1.185
Boiling point (°C)	3196.9	2466.9	2606.9	1634.9	−185.9
Melting point (°C)	1046.9	660.323	993.9	630.7	−189.20
Poisson ratio (ν)	n. a.	0.345	n. a.	0.250	n. r.
Bulk or compression modulus (K/GPa)	n. a.	75.18	n. a.	n. a.	n. r.
Coulomb's or shear modulus (G/GPa)	n. a.	27.8	n. a.	20.7	n. r.
Young's or elastic modulus (E/GPa)	25.0	70.2	n. a.	54.7	n. r.
Density (ρ/kg · m^{-3}) (298.15 K)	10,060	2698.9	13,670	6696	1.784
Phase transition temperature (α to β) (°C)	n. a.	Room temperature at 20.5 GPa	1074	n. a.	−189.2
Lattice parameters (pm)	$a = 531.11$	$a = 404.96$	$a = 346.80$ $c = 1124.00$	$a = 336.90$ $b = 533.00$	$a = 531.09$
***Strukturbericht* designation and structure type**	A1 (Cu)	A1 (Cu)	A3′ (Mg)	A7 (α-As)	A1 (Cu)
Pearson symbol	*cF*4	*cF*4	*hP*4	*hR*2	*cF*4
Space group (Hermann–Mauguin)	$Fm3m$	$Fm3m$	$P6_3/mmc$	$R\bar{3}m$	$Fm3m$
Crystal space lattice	fcc	fcc	hcp	Rhombic	fcc
Electronegativity (Pauling)	1.10	1.61	1.30	2.05	n. a.
Electronic ground state	$^2D_{3/2}$	$^2P_{1/2}$	$^8S_{7/2}$	$^4S_{3/2}$	$^2S_{1/2}$
Electronic configuration (ground state)	[Rn]$6d^17s^2$	[Ne]$3s^23p^1$	[Rn]$5f^76d^07s^2$	[Kr]$4d^{10}5s^25p^3$	[Ne]$3s^23p^6$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	(227)	26.981538(2)	(243)	121.760(1)	39.948(1)
Atomic number (Z)	89	13	95	51	18
Symbol (IUPAC)	Ac	Al	Am	Sb	Ar
CAS RN	7440-34-8	7429-90-5	7440-35-9	7440-36-0	7440-37-1
Element name (IUPAC)	Actinium	Aluminium (aluminum)	Americium	Antimony	Argon (gas)

Table A.4 *(continued)*

Element name (IUPAC)	Arsenic (α)	Astatine (α)	Barium	Berkelium	Beryllium (α)
Relative abundance in Earth's crust (mg/kg)	1.8	n. r.	425	n. r.	2.8
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.02000	n. a.	0.00270	n. a.	0.00030
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	4.3	n. a.	1.3	710	0.0092
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	−1.7932	n. a.	3.2318	n. a.	−1.8526
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	−3.90	n. a.	11.30	n. a.	−12.60
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	n. r.	6.49	n. a.	9.00
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	26	n. r.	50	n. a.	4.266
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	4.7	n. a.	18.1	n. a.	11.6
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	329	n. a.	205	n. a.	1.825
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	50	1.7	18.4	10 (estimated)	194–210
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	118.1	n. a.	140.3	n. a.	308.8
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	24.44	n. a.	7.66	n. a.	12.22
Boiling point (°C)	615.9	n. a.	1636.9	n. a.	2969.9
Melting point (°C)	816.9	n. a.	728.9	n. a.	1282.9
Poisson ratio (ν)	n. a.	n. r.	0.280	n. a.	0.075
Bulk or compression modulus (K/GPa)	n. a.	n. r.	10.3	n. a.	110
Coulomb's or shear modulus (G/GPa)	n. a.	n. r.	4.86	n. a.	156
Young's or elastic modulus (E/GPa)	22	n. r.	12.8	n. a.	318
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	5778	n. a.	3594	14,790	1847.70
Phase transition temperature (α to β) (°C)	n. a.	n. a.	370	n. a.	1254
Lattice parameters (pm)	$a = 413.18$ $\alpha = 54°10'$	n. a.	$a = 502.30$	n. a.	$a = 228.59$ $c = 358.42$
***Strukturbericht* designation and structure type**	A7 (α-As)	n. a.	A2 (W)	n. a.	A3 (Mg)
Pearson symbol	*hR*2	n. a.	*cI*2	*n. a.*	*hP*2
Space group (Hermann–Mauguin)	$R\bar{3}m$	n. a.	*Im*3*m*	n. a.	$P6_3/mmc$
Crystal space lattice	Rhombic	n. a.	bcc	n. a.	hcp
Electronegativity (Pauling)	2.18	2.20	0.89	1.30	1.57
Electronic ground state	$^4S_{3/2}$	$^3P_{3/2}$	$^1S_0$	$^6H_{15/2}$	$^1S_0$
Electronic configuration (ground state)	$[\mathrm{Ar}]3d^{10}4s^24p^3$	$[\mathrm{Xe}]4f^{14}5d^{10}6s^26p^5$	$[\mathrm{Xe}]6s^2$	$[\mathrm{Rn}]5f^96d^07s^2$	$[\mathrm{He}]2s^2$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	74.92160(2)	(210)	137.327(7)	(247)	9.012182(3)
Atomic number (Z)	33	85	56	97	4
Symbol (IUPAC)	As	At	Ba	Bk	Be
CAS RN	7440-38-2	7440-68-8	7440-39-3	7440-40-6	7440-41-7
Element name (IUPAC)	Arsenic (α)	Astatine (α)	Barium	Berkelium	Beryllium (α)

Table A.4 *(continued)*

Element name (IUPAC)	Bismuth	Bohrium	Boron (β)	Bromine (liquid, Br_2)	Cadmium	Calcium (α)
Relative abundance in Earth's crust (mg/kg)	0.0085	n. r.	10	2.4	0.15	41,500
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.00060	n. a.	24.00000	0.02000	14.00000	0.00370
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	0.034	n. a.	755	6.8	2450	0.43
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	−1.3186	n. a.	−1.6200	−1.2176	−1.5832	1.7022
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	−1.70	n. a.	−8.70	−4.90	−2.30	13.80
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	4.60	n. a.	n. a.	n. r.	4.30	4.17
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	106.8	n. a.	6.500	n. r.	6.83	3.43
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	13.4	n. a.	5.0	n. a.	29.8	22.3
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	123	n. a.	1.107	947	231	647
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	7.87	n. a.	27.6	0.122	96.8	200
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	151	n. a.	480	29.96	99.9	154.7
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	10.89	n. a.	50.20	10.55	6.41	8.5395
Boiling point (°C)	1559.9	n. a.	3657.9	58.8	764.9	1495.0
Melting point (°C)	271.4	n. a.	2299.9	−7.3	321.0	838.9
Poisson ratio (ν)	0.330	n. a.	n. a.	n. r.	0.300	0.310
Bulk or compression modulus (K/GPa)	34.965	n. a.	185.53	n. r.	51	17.45
Coulomb's or shear modulus (G/GPa)	12.8	n. a.	n. a.	n. r.	24	7.85
Young's or elastic modulus (E/GPa)	34	n. a.	440	n. r.	62.6	19.6
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	9747	n. a.	2340	3122.60	8650	1550
Phase transition temperature (α to β) (°C)	n. a.	n. a.	n. a.	−153	n. a.	464
Lattice parameters (pm)	$a = 474.60$ $\alpha = 57.23°$	n. a.	$a = 1014.5$ $\alpha = 65°12'$	$a = 668.00$ $b = 449.00$ $c = 874.00$	$a = 297.94$ $b = 561.86$	$a = 558.84$
***Strukturbericht* designation and structure type**	A7 (α-As)	n. a.	A_g (β-B)	A14 (I_2)	A3 (Mg)	A1 (Cu)
Pearson symbol	*hR*2	n. a.	*hR*105	*oC*8	*hP*2	*cF*4
Space group (Hermann–Mauguin)	$R\bar{3}m$	n. a.	$R\bar{3}m$	*Cmca*	$P6_3/mmc$	*Fm*3*m*
Crystal space lattice	Rhombic	n. a.	Rhombic	Orthorhombic	hcp	fcc
Electronegativity (Pauling)	2.02	n. a.	2.04	2.96	1.69	1.00
Electronic ground state	$^4S_{3/2}$	n. a.	$^2P_{1/2}$	$^3P_{3/2}$	$^1S_0$	$^1S_0$
Electronic configuration (ground state)	$[Xe]4f^{14}5d^{10}6s^26p^3$	$[Rn]5f^{14}6d^57s^2$	$[He]2s^22p^1$	$[Ar]3d^{10}4s^24p^5$	$[Kr]4d^{10}5s^2$	$[Ar]4s^2$
Relative atomic mass ($^{12}C = 12.000$) (IUPAC 2001)[a]	208.98038(2)	(262)	10.811(7)	79.904(1)	112.411(8)	40.078(4)
Atomic number (Z)	83	107	5	35	48	20
Symbol (IUPAC)	Bi	Bh	B	Br	Cd	Ca
CAS RN	7440-69-9	54037-14-8	7440-42-8	7726-95-6	7440-43-9	7440-70-2
Element name (IUPAC)	Bismuth	Bohrium	Boron (β)	Bromine (liquid, Br_2)	Cadmium	Calcium (α)

Table A.4 *(continued)*

Element name (IUPAC)	Californium	Carbon (diamond)	Carbon (graphite)	Cerium (β)	Cesium
Relative abundance in Earth's crust (mg/kg)	n. r.	200	200	66.5	3
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\text{cm}^2 \cdot \text{g}^{-1}$]	n. a.	0.00015	0.00015	0.00210	0.07700
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	2900	0.0035	0.0035	0.6	29
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	−1.7332	−1.1150	144.2580	0.4173
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1} \cdot$ m^3)	n. a.	−6.20	−6.20	220.00	2.80
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	n. a.	n. a.	8.70	6.00
Electrical resistivity ($\rho/\mu\Omega \cdot$ cm) (293.15 K)	n. a.	1011	1.375	82.8	18.8
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	n. a.	1.2	n. a.	8.5	97.0
Specific heat capacity (c_p/J $\cdot$ kg$^{-1} \cdot$ K^{-1}) (300 K)	n. a.	509	709	192	236
Thermal conductivity (k/W $\cdot$ m$^{-1} \cdot$ K^{-1}) (300 K)	n. a.	990–2320	5.70 (⊥) 1960 (‖)	11.4	35.9
Latent molar enthalpy of vaporization (L_{vap}/kJ $\cdot$ mol^{-1})	n. a.	n. a.	n. a.	398.00	63.9
Latent molar enthalpy of fusion (L_{fus}/kJ $\cdot$ mol^{-1})	n. a.	117	117	5.23	2.087
Boiling point (°C)	n. a.	5.100	n. a.	3425.9	674.82
Melting point (°C)	n. a.	3.820	n. a.	798.9	28.4
Poisson ratio (ν)	n. a.	n. a.	n. a.	0.248	0.295
Bulk or compression modulus (K/GPa)	n. a.	444	n. a.	21.5	2.693
Coulomb's or shear modulus (G/GPa)	n. a.	n. a.	n. a.	13.5	0.67
Young's or elastic modulus (E/GPa)	n. a.	980	n. a.	33.6	1.69
Density (ρ/kg $\cdot$ m^{-3}) (298.15 K)	n. a.	3513	2260	8240	1873
Phase transition temperature (α to β) (°C)	n. a.	n. a.	n. a.	61	n. a.
Lattice parameters (pm)	n. a.	$a = 356.69$	$a = 246.16$ $c = 670.90$	$a = 368.10$ $c = 1185.7$	$a = 614.10$
Strukturbericht designation and structure type	n. a.	A4 (diamond)	A9 (graphite)	A3′ (α-La)	A2 (W)
Pearson symbol	n. a.	*cF*8	*hP*4	*hP*4	*cI*2
Space group (Hermann–Mauguin)	n. a.	$F\bar{3}md$	$P6_3/mmc$	$P6_3/mmc$	$Im3m$
Crystal space lattice	n. a.	Cubic	Hexagonal	dhcp	bcc
Electronegativity (Pauling)	1.30	2.55	2.55	1.12	0.79
Electronic ground state	$^5I_8$	$^3P_0$	$^3P_0$	$^3H_4$	$^2S_{1/2}$
Electronic configuration (ground state)	[Rn]$5f^{10}6d^07s^2$	[He]$2s^22p^2$	[He]$2s^22p^2$	[Xe]$5d^16s^24f^1$	[Xe]$6s^1$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	(251)	12.0107(8)	12.0107(8)	140.116(1)	132.90545(2)
Atomic number (Z)	98	6	6	58	55
Symbol (IUPAC)	Cf	C	C	Ce	Cs
CAS RN	7440-71-3	7782-40-3	7440-44-0	7440-45-1	7440-46-2
Element name (IUPAC)	Californium	Carbon (diamond)	Carbon (graphite)	Cerium (β)	Cesium

Table A.4 *(continued)*

Element name (IUPAC)	Chlorine (gas, Cl_2)	Chromium	Cobalt (ε)	Copper	Curium
Relative abundance in Earth's crust (mg/kg)	145	102	25	60	n. r.
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.33000	0.02100	0.21000	0.02100	n. a.
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	35.5	3.1	37.2	3.78	60
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	−0.00184	25.4612	n. r.	−0.7708	n. a.
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	−7.20	+44.5	Ferromagnetic	−1.08	n. a.
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. r.	2.14	6.60	4.38	n. a.
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	n. r.	12.7	6.24	1.7241	n. a.
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	n. a.	6.2	13.4	16.5	n. a.
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	479	459.8	421	384.7	n. a.
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	0.0089	93.7	99.2	401	10 (estimated)
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	20.410	348.78	382.4	300.7	395.70
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	6.406	20.90	15.50	13.263	14.64
Boiling point (°C)	−33.97	2671.9	2731.2	2566.9	n. a.
Melting point (°C)	−101.0	1856.9	1454.9	1084.62	n. a.
Poisson ratio (ν)	n. r.	0.210	0.320	0.343	n. a.
Bulk or compression modulus (K/GPa)	n. r.	160.2	181.5	142.45	n. a.
Coulomb's or shear modulus (G/GPa)	n. r.	115.3	82	48.3	n. a.
Young's or elastic modulus (E/GPa)	n. r.	279	211	129.8	n. a.
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	3214	7190	8900	8960	13,300
Phase transition temperature (α to β) (°C)	−100.97	38.35	440.1120	n. a.	n. a.
Lattice parameters (pm)	$a = 624.00$ $b = 448.00$ $c = 826.00$	$a = 288.46$	$a = 250.71$ $c = 406.94$	$a = 361.51$	n. a.
***Strukturbericht* designation and structure type**	A14 (I_2)	A2 (W)	A3 (Mg)	A1 (Cu)	n. a.
Pearson symbol	*oC*8	*cI*2	*hP*2	*cF*4	n. a.
Space group (Hermann–Mauguin)	*Cmca*	*Im*3*m*	$P6_3/mmc$	*Fm*3*m*	n. a.
Crystal space lattice	Orthorhombic	bcc	hcp	fcc	n. a.
Electronegativity (Pauling)	3.16	1.66	1.88	1.90	1.30
Electronic ground state	$^3P_{3/2}$	$^7S_3$	$^4F_{9/2}$	$^2S_{1/2}$	$^9D_2$
Electronic configuration (ground state)	$[\mathrm{Ne}]3s^2 3p^5$	$[\mathrm{Ar}]3d^5 4s^1$	$[\mathrm{Ar}]3d^7 4s^2$	$[\mathrm{Ar}]3d^{10} 4s^1$	$[\mathrm{Rn}]5f^7 6d^1 7s^2$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	35.4527(9)	51.9961(6)	58.933200(9)	63.546(3)	(247)
Atomic number (Z)	17	24	27	29	96
Symbol (IUPAC)	Cl	Cr	Co	Cu	Cm
CAS RN	7782-50-5	7440-47-3	7440-48-4	7440-50-8	7440-51-9
Element name (IUPAC)	Chlorine (gas, Cl_2)	Chromium	Cobalt (ε)	Copper	Curium

Table A.4 *(continued)*

Element name (IUPAC)	Darmstadtium	Dubnium	Dysprosium (α)	Einsteinium	Erbium
Relative abundance in Earth's crust (mg/kg)	n. r.	n. r.	5.2	n. r.	3.5
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2\cdot$g^{-1}]	n. a.	n. a.	2.00000	n. a.	0.36000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	n. a.	n. a.	920–1100	160	160–170
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	n. a.	3708.5449	n. a.	2719.8641
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1}\cdot$m^3)	n. a.	n. a.	5450.00	n. a.	3770.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	n. a.	n. a.	n. a.	2.01
Electrical resistivity (ρ/μΩ · cm) (293.15 K)	n. a.	n. a.	92.6	n. a.	87
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	n. a.	n. a.	9.9	n. a.	12.2
Specific heat capacity (c_p/J · kg$^{-1}\cdot$K^{-1}) (300 K)	n. a.	n. a.	170.5	n. a.	168
Thermal conductivity (k/W · m$^{-1}\cdot$K^{-1}) (300 K)	n. a.	n. a.	10.7	n. a.	14.5
Latent molar enthalpy of vaporization (L_{vap}/kJ · mol^{-1})	n. a.	n. a.	280	n. a.	280
Latent molar enthalpy of fusion (L_{fus}/kJ · mol^{-1})	n. a.	n. a.	11.06	9.40	19.90
Boiling point (°C)	n. a.	n. a.	2561.9	n. a.	2862.9
Melting point (°C)	n. a.	n. a.	1411.9	n. a.	1528.9
Poisson ratio (ν)	n. a.	n. a.	0.237	n. a.	0.237
Bulk or compression modulus (K/GPa)	n. a.	n. a.	40.5	n. a.	44.4
Coulomb's or shear modulus (G/GPa)	n. a.	n. a.	24.7	n. a.	28.3
Young's or elastic modulus (E/GPa)	n. a.	n. a.	61.4	n. a.	69.9
Density (ρ/kg · m^{-3}) (298.15 K)	n. a.	n. a.	8551	n. a.	9066
Phase transition temperature (α to β) (°C)	n. a.	n. a.	1381	n. a.	n. a.
Lattice parameters (pm)	n. a.	n. a.	$a = 359.15$ $c = 565.01$	n. a.	$a = 355.92$ $c = 558.50$
***Strukturbericht* designation and structure type**	n. a.	n. a.	A3 (Mg)	n. a.	A3 (Mg)
Pearson symbol	n. a.	n. a.	*hP*2	n. a.	*hP*2
Space group (Hermann–Mauguin)	n. a.	n. a.	$P6_3/mmc$	n. a.	$P6_3/mmc$
Crystal space lattice	n. a.	n. a.	hcp	n. a.	hcp
Electronegativity (Pauling)	n. a.	n. a.	1.22	1.30	1.24
Electronic ground state	n. a.	$^3F_{3/2}$	$^5I_8$	$^5I_{15/2}$	$^3H_6$
Electronic configuration (ground state)	[Rn]$5f^{14}6d^87s^2$	[Rn]$5f^{14}6d^37s^2$	[Xe]$5d^06s^24f^{10}$	[Rn]$5f^{11}6d^07s^2$	[Xe]$5d^06s^24f^{12}$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	(269)	(262)	162.500(1)	(252)	167.259(3)
Atomic number (Z)	110	105	66	99	68
Symbol (IUPAC)	Ds	Db	Dy	Es	Er
CAS RN	54083-77-1	53850-35-4	7429-91-6	7429-92-7	7440-52-0
Element name (IUPAC)	Darmstadtium	Dubnium	Dysprosium (α)	Einsteinium	Erbium

Table A.4 *(continued)*

Element name (IUPAC)	Europium	Fermium	Fluorine (gas, F_2)	Francium	Gadolinium (α)
Relative abundance in Earth's crust (mg/kg)	2	n. r.	585	n. r.	6.2
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	6.00000	n. a.	0.00020	n. a.	73.00000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	4.300–4.600	5800	0.0096	n. a.	49,000
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	115.1540	n. a.	n. a.	n. a.	n. r.
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	276.00	n. a.	n. a.	n. a.	Ferromagnetic
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	n. a.	n. r.	n. a.	1.76
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	90	n. a.	n. r.	n. a.	134
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	35.0	n. a.	n. a.	n. a.	9.4
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	182.3	n. a.	1.648	n. a.	235.9
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	13.9	n. a.	0.0279	15 (estimated)	10.6
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	176	3.3	6.620	n. a.	301.5
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	9.21	1.02	0.510	n. a.	10.50
Boiling point (°C)	1596.9	n. a.	−188.12	676.9	3265.9
Melting point (°C)	821.9	n. a.	−219.66	26.9	1312.9
Poisson ratio (ν)	0.152	n. a.	n. r.	n. a.	0.259
Bulk or compression modulus (K/GPa)	8.3	n. a.	n. r.	n. a.	37.9
Coulomb's or shear modulus (G/GPa)	7.9	n. a.	n. r.	n. a.	21.8
Young's or elastic modulus (E/GPa)	18.2	n. a.	n. r.	n. a.	54.8
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	5243	n. a.	1696	n. a.	7901
Phase transition temperature (α to β) (°C)	n. a.	n. a.	−227.60	n. a.	1235
Lattice parameters (pm)	$a = 458.27$	n. a.	$a = 550.00$	n. a.	$a = 363.36$ $c = 578.10$
***Strukturbericht* designation and structure type**	A2 (W)	n. a.	C34 (α-F)	n. a.	A3 (Mg)
Pearson symbol	*cI*2	n. a.	*mC*8	n. a.	*hP*2
Space group (Hermann–Mauguin)	*Im*3*m*	n. a.	*C*2/*c*	n. a.	$P6_3/mmc$
Crystal space lattice	bcc	n. a.	Monoclinic	n. a.	hcp
Electronegativity (Pauling)	n. a.	1.30	3.98	0.70	1.20
Electronic ground state	$^8S_{7/2}$	$^3H_6$	$^3P_{3/2}$	$^2S_{1/2}$	$^9D_2$
Electronic configuration (ground state)	$[\mathrm{Xe}]5d^06s^24f^7$	$[\mathrm{Rn}]5f^{12}6d^07s^2$	$[\mathrm{He}]2s^22p^5$	$[\mathrm{Rn}]7s^1$	$[\mathrm{Xe}]5d^16s^24f^7$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	151.964(1)	(257)	18.9984032(3)	(223)	157.25(3)
Atomic number (Z)	63	100	9	87	64
Symbol (IUPAC)	Eu	Fm	F	Fr	Gd
CAS RN	7440-53-1	7440-72-4	7782-41-4	7440-73-5	7440-54-2
Element name (IUPAC)	Europium	Fermium	Fluorine (gas, F_2)	Francium	Gadolinium (α)

Table A.4 *(continued)*

Element name (IUPAC)	Gallium	Germanium	Gold	Hafnium
Relative abundance in Earth's crust (mg/kg)	19	1.5	0.004	3
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2 \cdot$ g^{-1}]	0.01500	0.01100	0.17000	0.20000
Thermal neutron capture cross section (σ_{th}/10^{-28} m^2)	2.9	2.2	98.7	104
Absolute magnetic susceptibility (χ_m/10^{-6})	−1.4102	−0.6354	−2.7366	5.6136
Mass magnetic susceptibility ($4\pi\chi_m$/10^{-9} kg$^{-1} \cdot$ m^3)	−3.00	−1.50	−1.78	+5.3
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	n. a.	4.00	3.82
Electrical resistivity (ρ/μΩ · cm) (293.15 K)	27	450,000	2.35	35.5
Coefficient of linear thermal expansion (α/10^{-6} K^{-1}) (0–100 °C)	18.3	5.75	14.16	5.9
Specific heat capacity (c_p/J · kg$^{-1} \cdot$ K^{-1}) (300 K)	371	322	129	141.75
Thermal conductivity (k/W · m$^{-1} \cdot$ K^{-1}) (300 K)	40.6	58.6	317	23
Latent molar enthalpy of vaporization (L_{vap}/kJ · mol^{-1})	254	334	334	575.5
Latent molar enthalpy of fusion (L_{fus}/kJ · mol^{-1})	5.594	36.9447	12.78	27.196
Boiling point (°C)	2402.9	2829.9	2856.9	4690.0
Melting point (°C)	29.7646	937.5	1064.18	2229.9
Poisson ratio (ν)	0.470	0.320	0.420	0.260
Bulk or compression modulus (K/GPa)	51.02	74.9	177.6	109
Coulomb's or shear modulus (G/GPa)	6.67	29.6	26	56
Young's or elastic modulus (E/GPa)	9.81	79.9	78.5	141
Density (ρ/kg · m^{-3}) (298.15 K)	5907	5323	19,320	13,310
Phase transition temperature (α to β) (°C)	n. a.	n. a.	n. a.	1760
Lattice parameters (pm)	$a = 451.86$ $b = 765.70$ $c = 452.58$	$a = 565.74$	$a = 407.82$	$a = 319.46$ $c = 505.11$
***Strukturbericht* designation and structure type**	A11 (α-Ga)	A4 (diamond)	A1 (Cu)	A3 (Mg)
Pearson symbol	*oC*8	*cF*8	*cF*4	*hP*2
Space group (Hermann–Mauguin)	*Cmca*	*Fd*3*m*	*Fm*3*m*	$P6_3/mmc$
Crystal space lattice	Orthorhombic	Cubic	fcc	hcp
Electronegativity (Pauling)	1.81	2.01	2.54	1.30
Electronic ground state	$^2P_{1/2}$	$^3P_0$	$^2S_{1/2}$	$^3F_2$
Electronic configuration (ground state)	[Ar]$3d^{10}4s^24p^1$	[Ar]$3d^{10}4s^24p^2$	[Xe]$5d^{10}6s^14f^{14}$	[Xe]$5d^26s^24f^{14}$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	69.723(1)	72.64(1)	196.96655(2)	178.49(2)
Atomic number (Z)	31	32	79	72
Symbol (IUPAC)	Ga	Ge	Au	Hf
CAS RN	7440-55-3	7440-56-4	7440-57-5	7440-58-6
Element name (IUPAC)	Gallium	Germanium	Gold	Hafnium

Table A.4 *(continued)*

Element name (IUPAC)	Hassium	Helium (gas)	Holmium	Hydrogen (gas, H_2)	Indium
Relative abundance in Earth's crust (mg/kg)	n. r.	0.008	1.3	1400	0.25
Thermal neutron mass absorption coefficient [$(\mu/\rho)/cm^2 \cdot g^{-1}$]	n. a.	0.00010	0.15000	0.11000	0.60000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	n. a.	0.007	65	0.332	194
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	−0.00008	3842.3624	−0.0002	−0.8144
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1}\cdot$m^3)	n. a.	−5.90	5490.00	−24.80	−1.40
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	n. r.	1.71	n. r.	5.20
Electrical resistivity ($\rho/\mu\Omega\cdot$cm) (293.15 K)	n. a.	n. r.	81.4	n. r.	8.37
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	n. a.	n. a.	11.2	n. a.	24.8
Specific heat capacity (c_p/J$\cdot$kg$^{-1}\cdot$K^{-1}) (300 K)	n. a.	5.197	164.9	14.386	233
Thermal conductivity (k/W$\cdot$m$^{-1}\cdot$K^{-1}) (300 K)	n. a.	0.152	16.2	0.1815	81.6
Latent molar enthalpy of vaporization (L_{vap}/kJ$\cdot$mol^{-1})	n. a.	0.083	71	0.904	231.8
Latent molar enthalpy of fusion (L_{fus}/kJ$\cdot$mol^{-1})	n. a.	0.0138	16.80	0.117	3.27
Boiling point (°C)	n. a.	−269.2	2694.9	−252.85	2079.9
Melting point (°C)	n. a.	−272.2	1473.9	−259.05	156.5985
Poisson ratio (ν)	n. a.	n. r.	0.231	n. r.	0.450
Bulk or compression modulus (K/GPa)	n. a.	n. r.	40.2	n. r.	38.46
Coulomb's or shear modulus (G/GPa)	n. a.	n. r.	26.3	n. r.	3.68
Young's or elastic modulus (E/GPa)	n. a.	n. r.	64.8	n. r.	10.6
Density (ρ/kg$\cdot$m^{-3}) (298.15 K)	n. a.	0.1785	8795	0.08988	7310
Phase transition temperature (α to β) (°C)	n. a.	−269.20	n. a.	−271.90	n. a.
Lattice parameters (pm)	n. a.	$a = 347.00$	$a = 357.78$ $c = 561.78$	$a = 533.80$	$a = 325.30$ $c = 494.70$
***Strukturbericht* designation and structure type**	n. a.	A3 (Mg)	A3 (Mg)	A1 (Cu)	A6 (In)
Pearson symbol	n. a.	*hP*2	*hP*2	*cF*4	*tI*2
Space group (Hermann–Mauguin)	n. a.	$P6_3/mmc$	$P6_3/mmc$	$Fm3m$	$I4/mmm$
Crystal space lattice	n. a.	hcp	hcp	fcc	Tetragonal
Electronegativity (Pauling)	n. a.	Nil	1.23	2.20	1.78
Electronic ground state	n. a.	$^1S_0$	$^4I_{15/2}$	$^2S_{1/2}$	$^2P_{1/2}$
Electronic configuration (ground state)	$[Rn]5f^{14}6d^6 7s^2$	$1s^2$	$[Xe]5d^0 6s^2 4f^{11}$	$1s^1$	$[Kr]4d^{10}5s^2 5p^1$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	(265)	4.002602(2)	164.93032(2)	1.00794(7)	114.818(3)
Atomic number (Z)	108	2	67	1	49
Symbol (IUPAC)	Hs	He	Ho	H	In
CAS RN	54037-57-9	7440-59-7	7440-60-0	1333-74-0	7440-74-6
Element name (IUPAC)	Hassium	Helium (gas)	Holmium	Hydrogen (gas, H_2)	Indium

Table A.4 *(continued)*

Element name (IUPAC)	Iodine (solid, I_2)	Iridium	Iron	Krypton (gas)	Lanthanum (α)
Relative abundance in Earth's crust (mg/kg)	0.45	0.001	56,300	0.0001	39
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.01800	0.80000	0.01500	0.13000	0.02300
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	6.2	425	2.56	25	8.98
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	−1.7654	3.0101	n. r.	−0.0013	5.3790
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	−4.50	+1.67	Ferromagnetic	−4.40	11.00
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	4.27	6.51	n. r.	2.18
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	2×10^{15}	5.3	9.71	n. r.	57
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	n. a.	6.8	11.8	n. a.	4.9
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	429	129.95	447	246.8	195.1
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	0.449	146.5	80.2	0.0088	13.5
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	41.6	604.1	340.4	9.080	402.1
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	15.78	41.124	15.20	1.370	8.37
Boiling point (°C)	184.4	4129.9	2749.9	−153.4	3456.9
Melting point (°C)	113.6	2409.9	1534.9	−157.2	920.9
Poisson ratio (ν)	n. a.	0.262	0.291	n. r.	0.280
Bulk or compression modulus (K/GPa)	0.0787	387.6	169.8	n. r.	27.9
Coulomb's or shear modulus (G/GPa)	n. a.	209	81.6	n. r.	14.3
Young's or elastic modulus (E/GPa)	n. a.	528	208.2	n. r.	36.6
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	4930	22,650	7874	37,493	6145
Phase transition temperature (α to β) (°C)	n. a.	n. a.	914.1391	−193	868
Lattice parameters (pm)	$a = 726.97$ $b = 479.03$ $c = 979.42$	$a = 383.91$	$a = 286.65$	$a = 581.00$	$a = 377.40$ $c = 1217.10$
Strukturbericht designation and structure type	A14 (I_2)	A1 (Cu)	A2 (W)	A1 (Cu)	A3′ (α-La)
Pearson symbol	*oC*8	*cF*4	*cI*2	*cF*4	*hP*4
Space group (Hermann–Mauguin)	*Cmca*	*Fm*3*m*	*Im*3*m*	*Fm*3*m*	$P6_3/mmc$
Crystal space lattice	Orthorhombic	fcc	bcc	fcc	dhcp
Electronegativity (Pauling)	2.66	2.20	1.83	n. a.	1.10
Electronic ground state	$^3P_{3/2}$	$^4F_{9/2}$	$^5D_4$	$^1S_0$	$^2D_{3/2}$
Electronic configuration (ground state)	$[\mathrm{Kr}]4d^{10}5s^25p^5$	$[\mathrm{Xe}]5d^76s^24f^{14}$	$[\mathrm{Ar}]3d^64s^2$	$[\mathrm{Ar}]3d^{10}4s^24p^6$	$[\mathrm{Xe}]5d^16s^24f^0$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	126.90447(3)	192.217(3)	55.845(2)	83.798(2)	138.9055(2)
Atomic number (Z)	53	77	26	36	57
Symbol (IUPAC)	I	Ir	Fe	Kr	La
CAS RN	7553-56-2	7439-88-5	7439-89-6	7439-90-9	7439-91-0
Element name (IUPAC)	Iodine (solid, I_2)	Iridium	Iron	Krypton (gas)	Lanthanum (α)

Table A.4 *(continued)*

Element name (IUPAC)	Lawrencium	Lead	Lithium (β)	Lutetium	Magnesium
Relative abundance in Earth's crust (mg/kg)	n. r.	14	20	0.8	23,300
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	n. a.	0.00030	n. a.	0.22000	0.00100
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	n. a.	0.171	0.045	84	0.063
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	−1.3548	1.0879	0.9397	0.9405
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	n. a.	−1.50	+25.6	1.20	+6.8
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	4.28	4.35	n. a.	4.25
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	n. a.	20.648	8.55	79	4.38
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)		29.1	56.0	125.0	26.10
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	n. a.	129	3.547	154	1.025
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	n. a.	35.3	84.7	16.4	156
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	n. a.	179.5	147.109	414	128.7
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	n. a.	4.81	2.93	22.00	8.477
Boiling point (°C)	n. a.	1746.0	1346.97	3394.9	1089.9
Melting point (°C)	n. a.	327.46	180.54	1662.9	648.9
Poisson ratio (ν)	n. a.	0.440	0.362	0.261	0.291
Bulk or compression modulus (K/GPa)	n. a.	45.8	11.402	47.6	35.6
Coulomb's or shear modulus (G/GPa)	n. a.	5.59	4.24	27.2	17.3
Young's or elastic modulus (E/GPa)	n. a.	16.1	4.91	68.6	44.7
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	n. a.	11,350	534	9840	1738
Phase transition temperature (α to β) (°C)	n. a.	n. a.	−201.15	n. a.	n. a.
Lattice parameters (pm)	n. a.	$a = 495.02$	$a = 350.93$	$a = 350.52$ $c = 554.94$	$a = 320.94$ $c = 521.07$
***Strukturbericht* designation and structure type**	n. a.	A1 (Cu)	A2 (W)	A3 (Mg)	A3 (Mg)
Pearson symbol	n. a.	*cF*4	*cI*2	*hP*2	*hP*2
Space group (Hermann–Mauguin)	n. a.	$Fm3m$	$Im3m$	$P6_3/mmc$	$P6_3/mmc$
Crystal space lattice	n. a.	fcc	bcc	hcp	hcp
Electronegativity (Pauling)	n. a.	2.33	0.98	1.27	1.31
Electronic ground state	$^2D_{5/2}$	$^3P_0$	$^2S_{1/2}$	$^2D_{3/2}$	$^1S_0$
Electronic configuration (ground state)	$[\mathrm{Rn}]5f^{14}6d^{1}7s^{2}$	$[\mathrm{Xe}]4f^{14}5d^{10}6s^{2}6p^{2}$	$[\mathrm{He}]2s^{1}$	$[\mathrm{Xe}]5d^{1}6s^{2}4f^{14}$	$[\mathrm{Ne}]3s^{2}3p^{0}$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	(262)	207.2(1)	6.941(2)	174.967(1)	24.3050(6)
Atomic number (Z)	103	82	3	71	12
Symbol (IUPAC)	Lr	Pb	Li	Lu	Mg
CAS RN	22537-19-5	7439-92-1	7439-93-2	7439-94-3	7439-95-4
Element name (IUPAC)	Lawrencium	Lead	Lithium (β)	Lutetium	Magnesium

Table A.4 *(continued)*

Element name (IUPAC)	Manganese	Meitnerium	Mendelevium	Mercury	Molybdenum
Relative abundance in Earth's crust (mg/kg)	950	n. r.	n. r.	0.085	1.2
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.08300	n. a.	n. a.	0.63000	0.00900
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	13.3	n. a.	n. a.	374	2.6
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	71.6388	n. a.	n. a.	−2.2637	9.5154
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	+121	n. a.	n. a.	−2.10	+11.7
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	0.40	n. a.	n. a.	1.00	4.35
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	144	n. a.	n. a.	94.1	5.2
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	21.7	n. a.	n. a.	62.0	5.43
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	479	n. a.	n. a.	138	251
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	7.82	n. a.	n. a.	8.34	142
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	231.11	n. a.	n. a.	59.1	595
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	12.06	n. a.	n. a.	2.324	37.48
Boiling point (°C)	2061.9	n. a.	n. a.	356.6	4678.9
Melting point (°C)	1243.9	n. a.	n. a.	−38.9	2621.85
Poisson ratio (ν)	0.240	n. a.	n. a.	n. r.	0.293
Bulk or compression modulus (K/GPa)	139.67	n. a.	n. a.	n. r.	261.2
Coulomb's or shear modulus (G/GPa)	79.5	n. a.	n. a.	n. r.	125.6
Young's or elastic modulus (E/GPa)	191	n. a.	n. a.	n. r.	324.8
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	7440	n. a.	n. a.	13,546	10,220
Phase transition temperature (α to β) (°C)	710, 1090, 1136	n. a.	n. a.	−38.836	n. a.
Lattice parameters (pm)	$a = 891.39$	n. a.	n. a.	$a = 300.50$ $a = 70.53°$	$a = 314.68$
***Strukturbericht* designation and structure type**	A12 (α-Mn)	n. a.	n. a.	A10 (α-Hg)	A2 (W)
Pearson symbol	*cI*58	n. a.	n. a.	*hR*1	*cI*2
Space group (Hermann–Mauguin)	$I\bar{4}3m$	n. a.	n. a.	$R\bar{3}m$	$Im3m$
Crystal space lattice	Cubic	n. a.	n. a.	Rhombic	bcc
Electronegativity (Pauling)	1.55	n. a.	n. a.	2.00	2.16
Electronic ground state	$^6S_{5/2}$	n. a.	$^2F_{7/2}$	$^1S_0$	$^7S_3$
Electronic configuration (ground state)	$[\mathrm{Ar}]3d^5 4s^2$	$[\mathrm{Rn}]5f^{14} 6d^7 7s^2$	$[\mathrm{Rn}]5f^{13} 6d^0 7s^2$	$[\mathrm{Xe}]4f^{14} 5d^{10} 6s^2 6p^0$	$[\mathrm{Kr}]4d^5 5s^1$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	54.938049(9)	(266)	(258)	200.59(2)	95.94(1)
Atomic number (Z)	25	109	101	80	42
Symbol (IUPAC)	Mn	Mt	Md	Hg	Mo
CAS RN	7439-96-5	54038-01-6	7440-11-1	7439-97-6	7439-98-7
Element name (IUPAC)	Manganese	Meitnerium	Mendelevium	Mercury	Molybdenum

Table A.4 *(continued)*

Element name (IUPAC)	Neodymium (α)	Neon (gas)	Neptunium	Nickel	Niobium	Nitrogen (gas, N_2)
Relative abundance in Earth's crust (mg/kg)	41.5	0.005	n. r.	84	20	19
Thermal neutron mass absorption coefficient $[(\mu/\rho)/\mathrm{cm}^2\cdot\mathrm{g}^{-1}]$	0.11000	0.00600	n. a.	0.02600	0.00400	0.04800
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	49	0.04	180	37.2	1.15	1.91
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	267.6477	−0.0003	n. a.	n. r.	18.8226	−0.0010
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1}\cdot$m^3)	480.00	−4.10	n. a.	Ferromagnetic	+27.6	−10.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	1.64	n. r.	n. a.	6.92	2.633	n. r.
Electrical resistivity ($\rho/\mu\Omega\cdot$cm) (293.15 K)	64	n. r.	122	6.844	15.22	n. r.
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	6.7	n. a.	n. a.	13.3	7.07	n. a.
Specific heat capacity (c_p/J$\cdot$kg$^{-1}\cdot$K^{-1}) (300 K)	190.3	1.030	n. a.	471	265.75	1.041
Thermal conductivity (k/W$\cdot$m$^{-1}\cdot$K^{-1}) (300 K)	16.5	0.0493	6.3	90.7	53.7	0.02958
Latent molar enthalpy of vaporization (L_{vap}/kJ$\cdot$mol^{-1})	289	1.710	336	377.5	689.9	5.577
Latent molar enthalpy of fusion (L_{fus}/kJ$\cdot$mol^{-1})	7.14	0.335	3.20	17.16	29.30	0.720
Boiling point (°C)	3067.9	−246.1	3901.9	2731.9	4741.9	−195.85
Melting point (°C)	1020.9	−248.67	639.9	1452.9	2467.9	−210.05
Poisson ratio (ν)	0.281	n. r.	n. a.	0.312	0.397	n. r.
Bulk or compression modulus (K/GPa)	31.8	n. r.	n. a.	177.3	170.3	n. r.
Coulomb's or shear modulus (G/GPa)	16.3	n. r.	n. a.	76	37.5	n. r.
Young's or elastic modulus (E/GPa)	41.4	n. r.	68.0	199.5	104.9	n. r.
Density (ρ/kg$\cdot$m^{-3}) (298.15 K)	7007	0.89994	20,250	8902	8570	1.2506
Phase transition temperature (α to β) (°C)	863	−248.59	280	358	n. a.	−237.54
Lattice parameters (pm)	a = 365.82 c = 1179.66	a = 446.20	a = 472.30 b = 488.70 c = 666.30	a = 352.38	a = 330.07	a = 566.1
***Strukturbericht* designation and structure type**	A3′ (α-La)	A1 (Cu)	A_c (α-Np)	A1 (Cu)	A2 (W)	n. a. (α-N)
Pearson symbol	*hP*4	*cF*4	*oP*8	*cF*4	*cI*2	*cP*8
Space group (Hermann–Mauguin)	$P6_3/mmc$	*Fm*3*m*	*Pnma*	*Fm*3*m*	*Im*3*m*	*Pa*3
Crystal space lattice	dhcp	Cubic	Orthorhombic	fcc	bcc	Cubic
Electronegativity (Pauling)	1.14	1.14	1.36	1.91	1.60	3.04
Electronic ground state	$^5I_4$	$^1S_0$	$^6L_{11/2}$	$^3F_4$	$^6D_{1/2}$	$^4S_{3/2}$
Electronic configuration (ground state)	[Xe]$5d^0 6s^2 4f^4$	[He]$2s^2 2p^6$	[Rn]$5f^4 6d^1 7s^2$	[Ar]$3d^8 4s^2$	[Kr]$4d^4 5s^1$	[He]$2s^2 2p^3$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	144.24(3)	20.1797(6)	237.0482	58.6934(2)	92.90638(2)	14.00674(7)
Atomic number (Z)	60	10	93	28	41	7
Symbol (IUPAC)	Nd	Ne	Np	Ni	Nb	N
CAS RN	7440-00-8	7440-01-9	7439-99-8	7440-02-0	7440-03-1	7727-37-9
Element name (IUPAC)	Neodymium (α)	Neon (gas)	Neptunium	Nickel	Niobium	Nitrogen (gas, N_2)

Table A.4 *(continued)*

Element name (IUPAC)	Nobelium	Osmium	Oxygen (gas, O_2)	Palladium	Phosphorus (P_4)
Relative abundance in Earth's crust (mg/kg)	n. r.	0.0015	461,000	0.015	1050
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	n. a.	0.02300	0.00001	0.02300	0.00200
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	n. a.	15	0.00028	6.9	0.18
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	1.0786	0.1518	62.8817	−1.6366
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	n. a.	+0.6	+1335	+65.74	−11.30
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	4.10	n. r.	3.77	n. a.
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	n. a.	8.12	n. r.	10.8	1×10^{17}
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	n. a.	4.57	n. a.	11.76	n. a.
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	n. a.	129.84	920	244	744.5
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	n. a.	87.6	0.02674	71.8	0.235
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	n. a.	746	6.820	362	56.5
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	n. a.	57.855	0.445	16.736	2.64
Boiling point (°C)	n. a.	5026.9	−183.05	2963.9	279.9
Melting point (°C)	n. a.	3126.85	−219.05	1554.9	44.15
Poisson ratio (ν)	n. a.	0.250	n. r.	0.394	n. a.
Bulk or compression modulus (K/GPa)	n. a.	383	n. r.	187	n. a.
Coulomb's or shear modulus (G/GPa)	n. a.	223	n. r.	43.6	n. a.
Young's or elastic modulus (E/GPa)	n. a.	558.6	n. r.	121	30.4
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	n. a.	22,590	1429	12,020	1820
Phase transition temperature (α to β) (°C)	n. a.	n. a.	−249.38	n. a.	n. a.
Lattice parameters (pm)	n. a.	$a = 269.87$ $c = 431.97$	$a = 540.3$ $b = 342.9$ $c = 508.6$ $\beta = 132.53°$	$a = 389.03$	$a = 331.36$ $b = 1047.8$ $c = 437.63$
***Strukturbericht* designation and structure type**	n. a.	A3 (Mg)	n. a. (α-O)	A1 (Cu)	P (white)
Pearson symbol	n. a.	*hP*2	*mC*4	*cF*4	*cP*8
Space group (Hermann–Mauguin)	n. a.	$P6_3/mmc$	$C2m$	$Fm3m$	$Cmca$
Crystal space lattice	n. a.	hcp	Monoclinic	fcc	Orthorhombic
Electronegativity (Pauling)	n. a.	2.20	3.44	2.20	2.19
Electronic ground state	$^1S_0$	$^5D_4$	$^3P_2$	$^1S_0$	$^4S_{3/2}$
Electronic configuration (ground state)	$[Rn]5f^{14}6d^07s^2$	$[Xe]5d^66s^24f^{14}$	$[He]2s^22p^4$	$[Kr]4d^{10}5s^0$	$[Ne]3s^23p^3$
Relative atomic mass ($^{12}C = 12.000$) (IUPAC 2001)[a]	(259)	190.23(3)	15.9994(3)	106.42(1)	30.973761(2)
Atomic number (Z)	102	76	8	46	15
Symbol (IUPAC)	No	Os	O	Pd	P
CAS RN	10028-14-5	7440-04-2	7782-44-7	7440-05-3	7723-14-0
Element name (IUPAC)	Nobelium	Osmium	Oxygen (gas, O_2)	Palladium	Phosphorus (P_4)

Table A.4 *(continued)*

Element name (IUPAC)	Platinum	Plutonium	Polonium	Potassium	Praseodymium (α)
Relative abundance in Earth's crust (mg/kg)	0.005	n. r.	2×10^{-10}	20,900	9.2
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2 \cdot$ g^{-1}]	0.02000	n. a.	n. a.	0.01800	0.02900
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	10	1.7	0.5	2.1	11.4
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	20.8246	50.0485	n. a.	0.4596	227.9878
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1} \cdot$ m^3)	+12.2	+31.70	n. a.	6.70	423.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	3.92	+18.405	n. a.	5.70	1.71
Electrical resistivity ($\rho/\mu\Omega \cdot$ cm) (293.15 K)	9.81	146	140	6.15	68
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	9.1	55.0	n. a.	83.0	6.8
Specific heat capacity (c_p/J $\cdot$ kg$^{-1} \cdot$ K^{-1}) (300 K)	131.47	133	n. a.	754	193
Thermal conductivity (k/W $\cdot$ m$^{-1} \cdot$ K^{-1}) (300 K)	71.6	6.74	20	102.4	12.5
Latent molar enthalpy of vaporization (L_{vap}/kJ $\cdot$ mol^{-1})	510.5	333.5	102.91	76.735	331
Latent molar enthalpy of fusion (L_{fus}/kJ $\cdot$ mol^{-1})	22.175	2.90	10.00	2.334	6.89
Boiling point (°C)	3826.9	3231.9	961.9	766.39	3511.9
Melting point (°C)	1771.9	640.9	253.9	63.65	930.9
Poisson ratio (ν)	0.397	0.180	n. a.	0.350	0.281
Bulk or compression modulus (K/GPa)	284.9	42.4	n. a.	4.201	28.8
Coulomb's or shear modulus (G/GPa)	60.9	34.5	n. a.	1.28	14.8
Young's or elastic modulus (E/GPa)	172.4	87.5	26	3.175	37.3
Density (ρ/kg $\cdot$ m^{-3}) (298.15 K)	21,450	19,840	9320	862	6773
Phase transition temperature (α to β) (°C)	n. a.	122	54	n. a.	795
Lattice parameters (pm)	$a = 392.36$	$a = 618.30$ $b = 482.20$ $c = 1096.30$ $\beta = 101.79°$	$a = 336.60$	$a = 533.10$	$a = 367.21$ $c = 1183.26$
***Strukturbericht* designation and structure type**	A1 (Cu)	n. a. (α-Pu)	A$_h$ (α-Po)	A2 (W)	A3′ (α-La)
Pearson symbol	*cF*4	*mP*16	*cP*1	*cI*2	*hP*4
Space group (Hermann–Mauguin)	$Fm3m$	$P2_1/m$	$Pm3m$	$Im3m$	$P6_3/mmc$
Crystal space lattice	fcc	Monoclinic	Cubic	bcc	dhcp
Electronegativity (Pauling)	2.28	1.28	2.00	0.82	1.13
Electronic ground state	$^3D_3$	$^7F_0$	$^3P_2$	$^2S_{1/2}$	$^4I_{9/2}$
Electronic configuration (ground state)	$[Xe]5d^9 6s^1 4f^{14}$	$[Rn]5f^5 6d^0 7s^2$	$[Xe]4f^{14} 5d^{10} 6s^2 6p^4$	$[Ar]4s^1$	$[Xe]5d^0 6s^2 4f^3$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	195.078(2)	(244)	(209)	39.0983(1)	140.90765(2)
Atomic number (Z)	78	94	84	19	59
Symbol (IUPAC)	Pt	Pu	Po	K	Pr
CAS RN	7440-06-4	7440-07-5	7440-08-6	7440-09-7	7440-10-0
Element name (IUPAC)	Platinum	Plutonium	Polonium	Potassium	Praseodymium (α)

Table A.4 *(continued)*

Element name (IUPAC)	Promethium (*α*)	Protoactinium	Radium	Radon (gas)	Rhenium
Relative abundance in Earth's crust (mg/kg)	n. r.	1.4×10^{-6}	9×10^{-7}	4×10^{-13}	0.0007
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	n. a.	n. a.	n. a.	n. a.	0.16000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	8000	500	20	0.7	90
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	n. a.	39.7509	n. a.	n. a.	7.6276
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	n. a.	32.50	n. a.	n. a.	+4.56
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. a.	n. a.	n. a.	n. r.	4.50
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	50 (estimated)	17.7	100	n. r.	17.3
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	n. a.	n. a.	n. a.	n. a.	6.63
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	185 (estimated)	n. a.	n. a.	n. a.	136
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	17.9 (estimated)	47 (estimated)	18.6 (estimated)	0.00364 (estimated)	71.2
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	289	481	113	18.100	714.8
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	7.13	12.34	8.50	3.247	34.08
Boiling point (°C)	2726.9	4000.0	1139.9	−61.75	5596.9
Melting point (°C)	1167.9	1839.9	699.9	−71.2	3184.85
Poisson ratio (ν)	0.280	n. a.	n. a.	n. r.	0.260
Bulk or compression modulus (K/GPa)	33	n. a.	n. a.	n. r.	379
Coulomb's or shear modulus (G/GPa)	18	n. a.	n. a.	n. r.	181
Young's or elastic modulus (E/GPa)	46.0	76.0	13.2	n. r.	520
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	7220	15,370	c. 5000	9073	21,020
Phase transition temperature (α to β) (°C)	890	1170	n. a.	n. a.	n. a.
Lattice parameters (pm)	$a = 365.00$ $c = 1165.00$	$a = 392.21$	$a = 514.80$	n. a.	$a = 276.08$ $c = 445.80$
Strukturbericht designation and structure type	A3′ (*α*-La)	A_a (*α*-Pa)	A2 (W)	n. a.	A3 (Mg)
Pearson symbol	*hP*4	*tI*2	*cI*2	n. a.	*hP*2
Space group (Hermann–Mauguin)	$P6_3/mmc$	$I4/mmm$	$Im3m$	n. a.	$P6_3/mmc$
Crystal space lattice	dhcp	Tetragonal	bcc	n. a.	hcp
Electronegativity (Pauling)	n. a.	1.50	0.89	n. a.	1.90
Electronic ground state	$^6H_{5/2}$	$^4K_{11/2}$	$^1S_0$	$^1S_0$	$^6S_{5/2}$
Electronic configuration (ground state)	$[\mathrm{Xe}]5d^0 6s^2 4f^5$	$[\mathrm{Rn}]5f^2 6d^1 7s^2$	$[\mathrm{Rn}]7s^2$	$[\mathrm{Xe}]4f^{14} 5d^{10} 6s^2 6p^6$	$[\mathrm{Xe}]5d^5 6s^2 4f^{14}$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	(145)	231.03588(2)	(226)	(222)	186.207(1)
Atomic number (Z)	61	91	88	86	75
Symbol (IUPAC)	Pm	Pa	Ra	Rn	Re
CAS RN	7440-12-2	7440-13-3	7440-14-4	10043-92-2	7440-15-5
Element name (IUPAC)	Promethium (*α*)	Protoactinium	Radium	Radon (gas)	Rhenium

Table A.4 (*continued*)

Element name (IUPAC)	Rhodium	Roentgenium	Rubidium	Ruthenium	Rutherfordium	Samarium (*α*)
Relative abundance in Earth's crust (mg/kg)	0.001	n. r.	90	0.001	n. r.	7.05
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.63000	n. a.	0.00300	0.00900	n. a.	47.00000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	145	n. a.	0.38	2.6	n. a.	5900
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	13.4308	n. a.	0.3170	5.3353	n. a.	66.4249
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1} \cdot$ m^3)	+13.60	n. a.	2.60	+5.42	n. a.	111.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	4.30	n. a.	4.80	4.10	n. a.	1.48
Electrical resistivity ($\rho/\mu\Omega \cdot$ cm) (293.15 K)	4.51	n. a.	12.5	7.6	n. a.	88
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	8.5	n. a.	90.0	9.6	n. a.	n. a.
Specific heat capacity (c_p/J $\cdot$ kg$^{-1} \cdot$ K^{-1}) (300 K)	243	n. a.	363.435	238	n. a.	181
Thermal conductivity (k/W $\cdot$ m$^{-1} \cdot$ K^{-1}) (300 K)	150	n. a.	58.2	117	n. a.	13.3
Latent molar enthalpy of vaporization (L_{vap}/kJ $\cdot$ mol^{-1})	494	n. a.	75.77	595.6	n. a.	165
Latent molar enthalpy of fusion (L_{fus}/kJ $\cdot$ mol^{-1})	26.5935	n. a.	2.198	38.59	n. a.	8.92
Boiling point (°C)	3696.9	n. a.	697.24	4150.0	n. a.	1790.9
Melting point (°C)	1963.9	n. a.	39.5	2336.9	n. a.	1076.9
Poisson ratio (ν)	0.260	n. a.	0.300	0.250	n. a.	0.274
Bulk or compression modulus (K/GPa)	276	n. a.	2.935	286	n. a.	37.8
Coulomb's or shear modulus (G/GPa)	147	n. a.	0.91	173	n. a.	19.5
Young's or elastic modulus (E/GPa)	379	n. a.	2.35	432	n. a.	49.7
Density (ρ/kg $\cdot$ m^{-3}) (298.15 K)	12,410	n. a.	1532	12,370	n. a.	7520
Phase transition temperature (α to β) (°C)	n. a.	n. a.	n. a.	n. a.	n. a.	922
Lattice parameters (pm)	$a = 380.32$	n. a.	$a = 570.50$	$a = 270.58$ $c = 428.16$	n. a.	$a = 362.86$ $c = 2620.70$
***Strukturbericht* designation and structure type**	A1 (Cu)	n. a.	A2 (W)	A3 (Mg)	n. a.	C19 (*α*-Sm)
Pearson symbol	*cF*4	n. a.	*cI*2	*hP*2	n. a.	*hR*3
Space group (Hermann–Mauguin)	$Fm3m$	n. a.	$Im3m$	$P6_3/mmc$	n. a.	$R\bar{3}m$
Crystal space lattice	fcc	n. a.	bcc	hcp	n. a.	Rhombic
Electronegativity (Pauling)	2.28	n. a.	0.82	2.20	n. a.	1.17
Electronic ground state	$^4F_{9/2}$	n. a.	$^2S_{1/2}$	$^5F_5$	$^3F_2$	$^7F_0$
Electronic configuration (ground state)	[Kr]$4d^8 5s^1$	[Rn]$5f^{14} 6d^{10} 7s^1$	[Kr]$5s^1$	[Kr]$4d^7 5s^2$	[Rn]$5f^{14} 6d^2 7s^2$	[Xe]$5d^0 6s^2 4f^6$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	102.90550(2)	(272)	85.4678(3)	101.07(2)	(261)	150.36(3)
Atomic number (Z)	45	111	37	44	104	62
Symbol (IUPAC)	Rh	Rg	Rb	Ru	Rf	Sm
CAS RN	7440-16-6	n. a.	7440-17-7	7440-18-8	53850-36-5	7440-19-9
Element name (IUPAC)	Rhodium	Roentgenium	Rubidium	Ruthenium	Rutherfordium	Samarium (*α*)

Table A.4 *(continued)*

Element name (IUPAC)	Scandium (*α*)	Seaborgium	Selenium (*γ*)	Silicon	Silver
Relative abundance in Earth's crust (mg/kg)	22	n. r.	0.05	0.00200	0.075
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.25000	n. a.	0.05600	171	0.20000
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	27.2	n. a.	11.7	−0.2965	63.6
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	20.9314	n. a.	−1.5247	−1.60	−1.8967
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	+88	n. a.	−4.00	n. a.	−2.27
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	2.80	n. a.	n. a.		4.10
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	61	n. a.	106	10,0000	1.59
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	10.2	n. a.	37.0	2.56	19.1
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	567.7	n. a.	321	712	235
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	15.8	n. a.	2.04	83.7	429
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	332.7	n. a.	95.48	359	258
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	14.10	n. a.	6.28	50.66	11.95
Boiling point (°C)	2830.9	n. a.	685.0	3281.9	2162.9
Melting point (°C)	1540.9	n. a.	216.9	1409.9	961.78
Poisson ratio (*ν*)	0.279	n. a.	0.450	0.420	0.367
Bulk or compression modulus (*K*/GPa)	56.6	n. a.	8.621	98	105.3
Coulomb's or shear modulus (*G*/GPa)	29.7	n. a.	6.46	80.5	30.3
Young's or elastic modulus (*E*/GPa)	74.4	n. a.	58	113	82.7
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	2989	n. a.	4790	2329	10,500
Phase transition temperature (*α* to *β*) (°C)	950	n. a.	n. a.	n. a.	n. a.
Lattice parameters (pm)	*a* = 330.88 *c* = 526.80	n. a.	*a* = 436.59 *c* = 495.37	*a* = 543.102	a = 408.57
***Strukturbericht* designation and structure type**	A3 (Mg)	n. a.	A8 (*γ*-Se)	A4 (diamond)	A1 (Cu)
Pearson symbol	*hP*2	n. a.	*hP*3	*cF*8	*cF*4
Space group (Hermann–Mauguin)	$P6_3/mmc$	n. a.	$P3_121$	$F\bar{3}md$	$Fm3m$
Crystal space lattice	hcp	n. a.	Hexagonal	Cubic	fcc
Electronegativity (Pauling)	1.36	n. a.	2.55	1.90	1.93
Electronic ground state	$^2D_{3/2}$	n. a.	$^3P_2$	$^3P_0$	$^2S_{1/2}$
Electronic configuration (ground state)	$[\mathrm{Ar}]4s^24p^1$	$[\mathrm{Rn}]5f^{14}6d^47s^2$	$[\mathrm{Ar}]3d^{10}4s^24p^4$	$[\mathrm{Ne}]3s^23p^2$	$[\mathrm{Kr}]4d^{10}5s^1$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	44.955910(8)	(263)	78.96(3)	28.0855(3)	107.8682(2)
Atomic number (*Z*)	21	106	34	14	47
Symbol (IUPAC)	Sc	Sg	Se	Si	Ag
CAS RN	7440-20-2	54038-81-2	7782-49-2	7440-21-3	7440-22-4
Element name (IUPAC)	Scandium (*α*)	Seaborgium	Selenium (*γ*)	Silicon	Silver

Table A.4 *(continued)*

Element name (IUPAC)	Sodium	Strontium	Sulfur (α)	Tantalum	Technetium
Relative abundance in Earth's crust (mg/kg)	23,600	370	350	2	n. r.
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.00700	0.00500	0.00550	0.04100	n. a.
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}$ m^2)	0.53	1.2	0.52	20.5	22
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	0.6801	0.2668	−1.0213	14.1805	31.2978
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}$ kg$^{-1} \cdot$ m^3)	+8.8	+1.32	−6.20	+10.7	34.20
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	5.50	3.82	n. a.	3.50	n. a.
Electrical resistivity ($\rho/\mu\Omega \cdot$ cm) (293.15 K)	4.2	23	2×10^{15}	12.45	22.6
Coefficient of linear thermal expansion ($\alpha/10^{-6}$ K^{-1}) (0–100 °C)	70.6	23.0	74.33	6.6	n. a.
Specific heat capacity (c_p/J $\cdot$ kg$^{-1} \cdot$ K^{-1}) (300 K)	1.225	301	706	140	708
Thermal conductivity (k/W $\cdot$ m$^{-1} \cdot$ K^{-1}) (300 K)	141	35.3	0.269	57.5	0.206
Latent molar enthalpy of vaporization (L_{vap}/kJ $\cdot$ mol^{-1})	97.424	136.9	45	732.8	585.2
Latent molar enthalpy of fusion (L_{fus}/kJ $\cdot$ mol^{-1})	2.602	8.40	1.235	36.57	33.29
Boiling point (°C)	897.38	1383.9	444.7	5424.9	4876.9
Melting point (°C)	97.83	768.9	112.9	2995.9	2171.9
Poisson ratio (v)	0.340	0.280	n. a.	0.342	0.260
Bulk or compression modulus (K/GPa)	7.407	12.54	7.692	196.3	31.06
Coulomb's or shear modulus (G/GPa)	2.53	6.03	n. a.	69.2	162.00
Young's or elastic modulus (E/GPa)	6.8	15.7	17.80	185.7	407.00
Density (ρ/kg $\cdot$ m^{-3}) (298.15 K)	971.2	2540	2070	16,654	11,500
Phase transition temperature (α to β) (°C)	−268	235, 540	93.55	n. a.	n. a.
Lattice parameters (pm)	$a = 429.06$	$a = 608.49$	$a = 104.64$ $b = 1286.60$ $c = 2448.60$	$a = 330.31$	$a = 273.80$ $c = 439.30$
***Strukturbericht* designation and structure type**	A2 (W)	A1 (Cu)	A16 (α-S)	A2 (W)	A3 (Mg)
Pearson symbol	*cI*2	*cF*4	*oF*128	*cI*2	*hP*2
Space group (Hermann–Mauguin)	*Im*3*m*	*Fm*3*m*	*Fddd*	*Im*3*m*	$P6_3/mmc$
Crystal space lattice	bcc	fcc	Orthorhombic	bcc	hcp
Electronegativity (Pauling)	0.93	0.95	2.58	1.50	1.90
Electronic ground state	$^2S_{1/2}$	$^1S_0$	$^3P_2$	$^4F_{3/2}$	$^6S_{5/2}$
Electronic configuration (ground state)	[Ne]$3s^1 3p^0$	[Kr]$5s^2$	[Ne]$3s^2 3p^4$	[Xe]$5d^3 6s^2 4f^{14}$	[Kr]$4d^5 5s^2$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	22.989770(2)	87.62(1)	32.065(5)	180.9479(1)	98.9062
Atomic number (Z)	11	38	16	73	43
Symbol (IUPAC)	Na	Sr	S	Ta	Tc
CAS RN	7440-23-5	7440-24-6	7704-34-9	7440-25-7	7440-26-8
Element name (IUPAC)	Sodium	Strontium	Sulfur (α)	Tantalum	Technetium

Table A.4 *(continued)*

Element name (IUPAC)	Tellurium	Terbium (*α*)	Thallium	Thorium	Thulium
Relative abundance in Earth's crust (mg/kg)	0.001	1.2	0.85	9.6	0.52
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2 \cdot$ g^{-1}]	0.01300	0.09000	0.00600	0.01000	0.25000
Thermal neutron capture cross section (σ_{th}/10^{-28} m^2)	5.4	23	3.4	7.4	105
Absolute magnetic susceptibility (χ_m/10^{-6})	−1.9366	8905.8650	−2.8290	6.7151	1476.0658
Mass magnetic susceptibility ($4\pi\chi_m$/10^{-9} kg$^{-1} \cdot$ m^3)	−3.90	13,600.00	−3.00	+7.2	1990.00
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	n. a.	n. a.	5.20	+3.567	1.95
Electrical resistivity (ρ/µΩ · cm) (293.15 K)	436,000	114	18	15.7	79
Coefficient of linear thermal expansion (α/10^{-6} K^{-1}) (0–100 °C)	27.0	7.0	30.0	11.4–12.5	11.6
Specific heat capacity (c_p/J · kg$^{-1} \cdot$ K^{-1}) (300 K)	202	172	130	118	160
Thermal conductivity (k/W · m$^{-1} \cdot$ K^{-1}) (300 K)	2.35	11.1	46.1	54	16.8
Latent molar enthalpy of vaporization (L_{vap}/kJ · mol^{-1})	114.1	293	165	514.1	247
Latent molar enthalpy of fusion (L_{fus}/kJ · mol^{-1})	17.49	10.15	4.14	13.81	16.84
Boiling point (°C)	989.9	3122.9	1456.9	4787.9	1946.9
Melting point (°C)	449.6	1355.9	303.5	1749.984	1544.9
Poisson ratio (ν)	0.180	0.261	0.450	0.270	0.213
Bulk or compression modulus (K/GPa)	20.833	38.7	28.5	53.8	44.5
Coulomb's or shear modulus (G/GPa)	16.7	22.1	2.7	30.8	30.5
Young's or elastic modulus (E/GPa)	47.1	55.7	7.9	78.3	74
Density (ρ/kg · m^{-3}) (298.15 K)	6240	8229	11,850	11,720	9321
Phase transition temperature (α to β) (°C)	n. a.	1289	230	1360	n. a.
Lattice parameters (pm)	a = 445.66 c = 592.64	a = 360.55 c = 569.66	a = 345.66 c = 552.48	a = 508.51	a = 353.75 c = 555.40
***Strukturbericht* designation and structure type**	A8 (γ-Se)	A3 (Mg)	A3 (Mg)	A1 (Cu)	A3 (Mg)
Pearson symbol	*hP*3	*hP*2	*hP*2	*cF*4	*hP*2
Space group (Hermann–Mauguin)	$P3_121$	$P6_3/mmc$	$P6_3/mmc$	$Fm3m$	$P6_3/mmc$
Crystal space lattice	Hexagonal	hcp	hcp	fcc	hcp
Electronegativity (Pauling)	2.10	1.20	1.62	1.30	1.25
Electronic ground state	$^3P_2$	$^6H_{15/2}$	$^2P_{1/2}$	$^3F_2$	$^2F_{7/2}$
Electronic configuration (ground state)	[Kr]$4d^{10}5s^25p^4$	[Xe]$5d^06s^24f^9$	[Xe]$4f^{14}5d^{10}6s^26p^1$	[Rn]$6d^27s^2$	[Xe]$5d^06s^24f^{13}$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	127.60(3)	158.92534(2)	204.3833(2)	232.0381(1)	168.93421(2)
Atomic number (Z)	52	65	81	90	69
Symbol (IUPAC)	Te	Tb	Tl	Th	Tm
CAS RN	13494-80-9	7440-27-9	7440-28-0	7440-29-1	7440-30-4
Element name (IUPAC)	Tellurium	Terbium (*α*)	Thallium	Thorium	Thulium

▪ **Table A.4** *(continued)*

Element name (IUPAC)	Tin (β)	Titanium	Tungsten	Uranium	Vanadium
Relative abundance in Earth's crust (mg/kg)	2.3	5650	1.25	2.7	950
Thermal neutron mass absorption coefficient [(μ/ρ)/cm$^2 \cdot$ g^{-1}]	0.00200	0.04400	0.03600	0.00500	0.03300
Thermal neutron capture cross section (σ_{th}/10^{-28} m^2)	0.63	6.1	18.4	7.57	5.06
Absolute magnetic susceptibility (χ_m/10^{-6})	−1.8004	14.4874	7.0495	32.5727	30.7844
Mass magnetic susceptibility (4$\pi\chi_m$/10^{-9} kg$^{-1} \cdot$ m^3)	−3.10	+40.1	+4.59	+21.6	+62.8
Temperature coefficient of electrical resistivity (10^{-3} K^{-1})	4.65	3.80	4.80	+2.82	3.90
Electrical resistivity (ρ/μΩ · cm) (293.15 K)	11	42	5.65	30.8	24.8
Coefficient of linear thermal expansion (α/10^{-6} K^{-1}) (0–100 °C)	21.1	8.35	4.59	12.6	8.3
Specific heat capacity (c_p/J · kg$^{-1} \cdot$ K^{-1}) (300 K)	229	537.8	132	116	489
Thermal conductivity (k/W · m$^{-1} \cdot$ K^{-1}) (300 K)	66.6	21.9	174	27.6	30.7
Latent molar enthalpy of vaporization (L_{vap}/kJ · mol^{-1})	296.10	428.9	806.8	417.1	451.8
Latent molar enthalpy of fusion (L_{fus}/kJ · mol^{-1})	7.08	19.41	52.31	9.1420	21.50
Boiling point (°C)	2269.9	3286.9	5656.9	3773.9	3376.9
Melting point (°C)	231.93	1668.0	3413.85	1132.4	1886.9
Poisson ratio (ν)	0.357	0.361	0.280	0.250	0.365
Bulk or compression modulus (K/GPa)	58.2	108.4	311	97.9	158.73
Coulomb's or shear modulus (G/GPa)	18.4	45.6	160.6	70.6	46.7
Young's or elastic modulus (E/GPa)	49.9	120.2	411	177	127.6
Density (ρ/kg · m^{-3}) (298.15 K)	7298	4540	19,300	18,950	6160
Phase transition temperature (α to β) (°C)	13	882	n. a.	662, 770	n. a.
Lattice parameters (pm)	a = 581.97 c = 317.49	a = 295.030 c = 468.312	a = 316.522	a = 285.38 b = 586.80 c = 495.57	a = 302.28
***Strukturbericht* designation and structure type**	A5 (β-Sn)	A3 (Mg)	A2 (W)	A20 (α-U)	A2 (W)
Pearson symbol	*tI*4	*hP*2	*cI*2	*oC*4	*cI*2
Space group (Hermann–Mauguin)	$I4_1/amd$	$P6_3/mmc$	$Im3m$	$Cmcm$	$Im3m$
Crystal space lattice	Tetragonal	hcp	bcc	Orthorhombic	bcc
Electronegativity (Pauling)	1.96	1.54	2.36	1.38	1.63
Electronic ground state	$^3P_0$	$^3F_2$	$^5D_0$	$^5L_6$	$^4F_{3/2}$
Electronic configuration (ground state)	[Kr]$4d^{10}5s^25p^2$	[Ar]$3d^24s^2$	[Xe]$5d^46s^24f^{14}$	[Rn]$5f^36d^17s^2$	[Ar]$3d^34s^2$
Relative atomic mass (^{12}C = 12.000) (IUPAC 2001)[a]	118.710(7)	47.867(1)	183.84(1)	238.02891(3)	50.9415(1)
Atomic number (Z)	50	22	74	92	23
Symbol (IUPAC)	Sn	Ti	W	U	V
CAS RN	7440-31-5	7440-32-6	7440-33-7	7440-61-1	7040-62-2
Element name (IUPAC)	Tin (β)	Titanium	Tungsten	Uranium	Vanadium

Table A.4 *(continued)*

Element name (IUPAC)	Xenon (gas)	Ytterbium	Yttrium	Zinc	Zirconium
Relative abundance in Earth's crust (mg/kg)	0.00001	3.2	33	70	165
Thermal neutron mass absorption coefficient [$(\mu/\rho)/\mathrm{cm}^2 \cdot \mathrm{g}^{-1}$]	0.08300	0.07600	0.00600	0.00550	0.00660
Thermal neutron capture cross section ($\sigma_{th}/10^{-28}\ \mathrm{m}^2$)	25	35	1.28	1.1	0.184
Absolute magnetic susceptibility ($\chi_m/10^{-6}$)	−1.2113	3.2701	23.6851	−1.2539	8.6979
Mass magnetic susceptibility ($4\pi\chi_m/10^{-9}\ \mathrm{kg}^{-1} \cdot \mathrm{m}^3$)	−4.30	5.90	66.60	−2.21	+16.8
Temperature coefficient of electrical resistivity ($10^{-3}\ \mathrm{K}^{-1}$)	n. r.	1.30	2.71	4.17	4.40
Electrical resistivity ($\rho/\mu\Omega \cdot \mathrm{cm}$) (293.15 K)	n. r.	29	57	5.916	41
Coefficient of linear thermal expansion ($\alpha/10^{-6}\ \mathrm{K}^{-1}$) (0–100 °C)	n. a.	25.0	10.8	25.0	5.78
Specific heat capacity ($c_p/\mathrm{J} \cdot \mathrm{kg}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	158	145	298	389	278
Thermal conductivity ($k/\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1}$) (300 K)	0.00569	34.9	17.2	121	22.7
Latent molar enthalpy of vaporization ($L_{vap}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	40.66	159	365	123.6	573
Latent molar enthalpy of fusion ($L_{fus}/\mathrm{kJ} \cdot \mathrm{mol}^{-1}$)	1.81	7.66	11.43	7.322	21.28
Boiling point (°C)	−108.04	1192.9	3337.9	906.9	4376.9
Melting point (°C)	−111.76	823.9	1521.9	419.527	1854.7
Poisson ratio (ν)	n. r.	0.207	0.243	0.249	0.380
Bulk or compression modulus (K/GPa)	n. r.	30.5	41.2	69.4	89.8
Coulomb's or shear modulus (G/GPa)	n. r.	9.9	25.6	41.9	36.5
Young's or elastic modulus (E/GPa)	n. r.	23.9	63.5	104.5	97.1
Density ($\rho/\mathrm{kg} \cdot \mathrm{m}^{-3}$) (298.15 K)	3540	6965	4469	7133	6506
Phase transition temperature (α to β) (°C)	−185	−3	1485	n. a.	862
Lattice parameters (pm)	$a = 635.00$	$a = 364.82$ $c = 573.18$	$a = 364.82$ $c = 573.18$	$a = 266.48$ $c = 494.69$	$a = 323.17$ $c = 574.76$
***Strukturbericht* designation and structure type**	A1 (Cu)	A3 (Mg)	A3 (Mg)	A3 (Mg)	A3 (Mg)
Pearson symbol	*cF*4	*hP*2	*hP*2	*hP*2	*hP*2
Space group (Hermann–Mauguin)	$Fm3m$	$P6_3/mmc$	$P6_3/mmc$	$P6_3/mmc$	$P6_3/mmc$
Crystal space lattice	fcc	hcp	hcp	hcp	hcp
Electronegativity (Pauling)	n. a.	1.11	1.22	1.65	1.33
Electronic ground state	$^1S_0$	$^1S_0$	$^2D_{3/2}$	$^1S_0$	$^3F_2$
Electronic configuration (ground state)	$[\mathrm{Kr}]4d^{10}5s^25p^6$	$[\mathrm{Xe}]5d^06s^24f^{14}$	$[\mathrm{Kr}]4d^15s^2$	$[\mathrm{Ar}]3d^{10}4s^2$	$[\mathrm{Kr}]4d^25s^2$
Relative atomic mass ($^{12}\mathrm{C} = 12.000$) (IUPAC 2001)[a]	131.293(6)	173.04(3)	88.90585(2)	65.409(4)	91.224(2)
Atomic number (Z)	54	70	39	30	40
Symbol (IUPAC)	Xe	Yb	Y	Zn	Zr
CAS RN	7040-63-3	7040-64-4	7040-65-5	7040-66-6	7040-67-7
Element name (IUPAC)	Xenon (gas)	Ytterbium	Yttrium	Zinc	Zirconium

bcc body-centered cubic, *CAS RN* Chemical Abstracts Service Registry Number, *dhcp* double hexagonal close packed, *fcc* face-centered cubic, *hcp* hexagonal close packed, *IUPAC* International Union of Pure and Applied Chemistry, *n. a.* not available, *n. r.* not relevant

[a] Values in *parentheses* indicate that all isotopes of the element are unstable

A.6 Geochemical Classification of the Elements

See ◘ Table A.5.

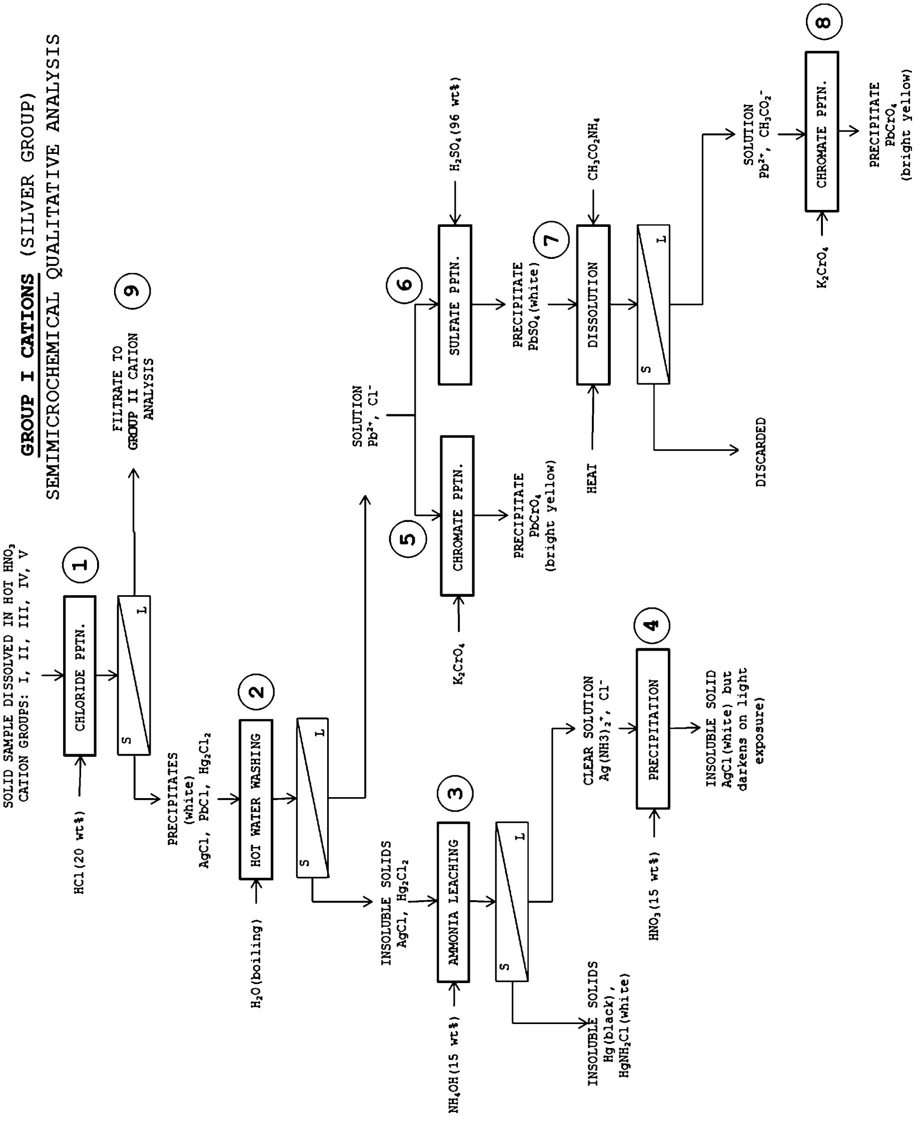
◘ **Table A.5** Geochemical classification of the elements. (After Goldschmidt, B. *J. Chem. Soc.* (1937) 55)

Classes	**Description**	**Examples**
Lithophilic	Affinity for silicate materials	O, Si, Al, Mg, Ca, Na, K, Ti, Zr, Hf, Nb, Ta, W, Sn, U
Siderophilic	Affinity for iron	Fe, Co, Ni, platinum group metals
Chalcophilic	Affinity for sulfur-forming sulfides, sulfosalts, and chalcogenides	Cu, Fe, Co, Ni, Hg, Cd, Os, Ir, Pt, Ru, Rh, Pd, Zn, Re, As, Sb, Se, Te
Hydrophilic	Affinity for water and aqueous solutions (i.e., brines, geothermal fluids)	H, O, Na, K, Li, Cl, F, Mg
Atmophilic	Gaseous elements	H, O, N, He, Ar, rare gases
Biophilic	Animals and plants	C, H, O, N, P

B Charts for Semimicrochemical Qualitative Identification of Metal Cations

B.1 Group I Cations: Silver Group

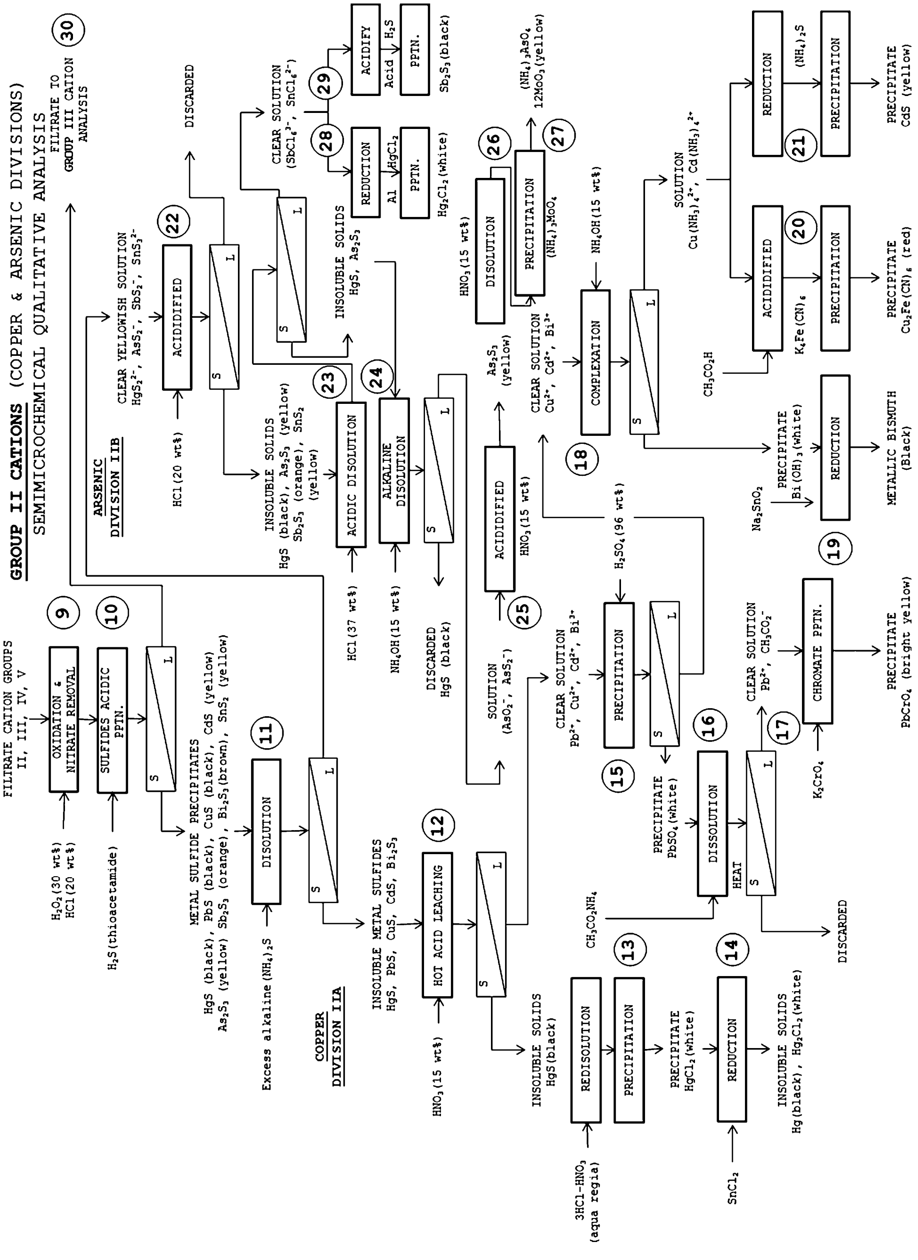
See ◘ Fig. B.1.



◘ **Fig. B.1** Identification chart for group I cations. *PPTN.* precipitation

B.2 Group II Cations: Copper and Arsenic Divisions

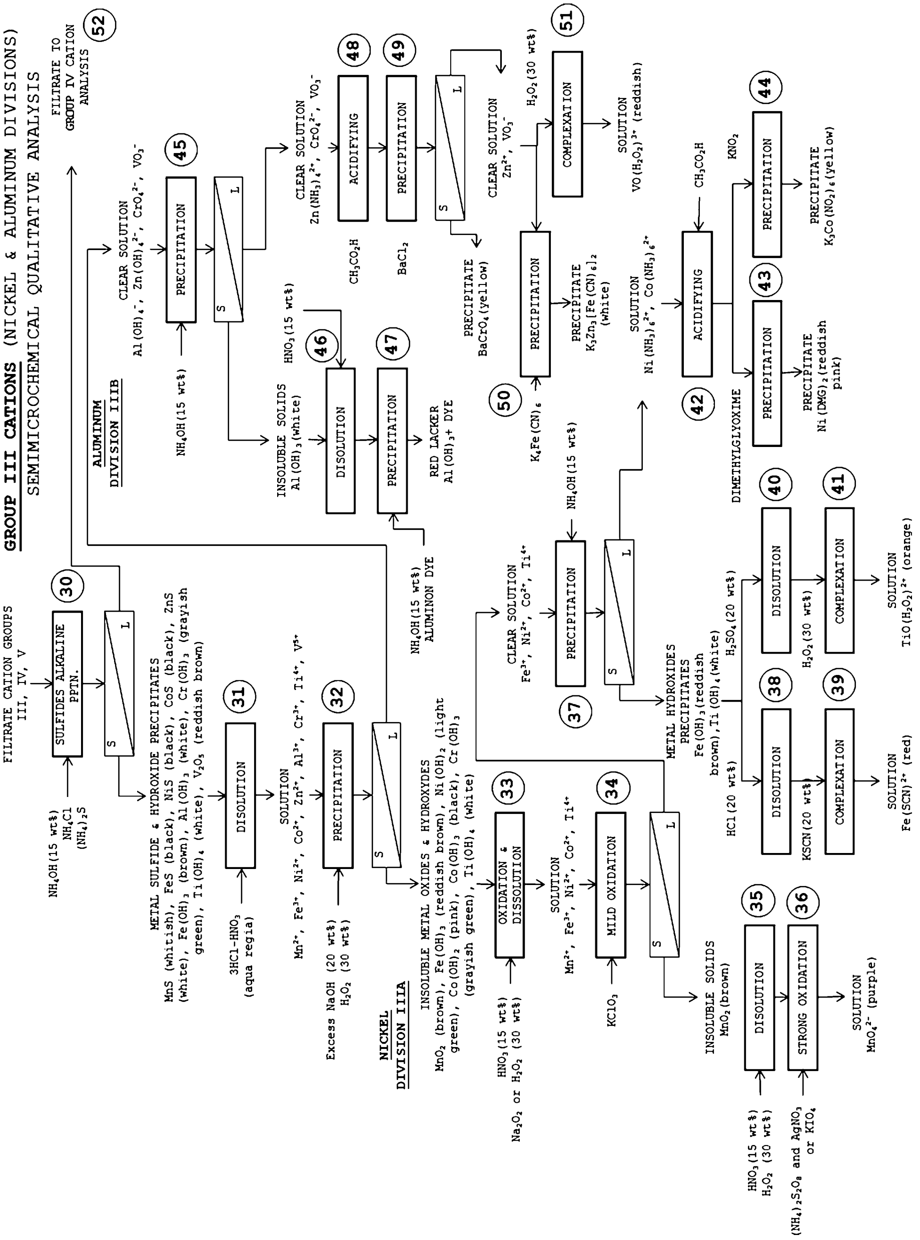
See ◘ Fig. B.2.



◘ **Fig. B.2** Identification chart for group II cations. *PPTN.* precipitation

B.3 Group III Cations: Nickel and Aluminum Divisions

See ■ Fig. B.3.



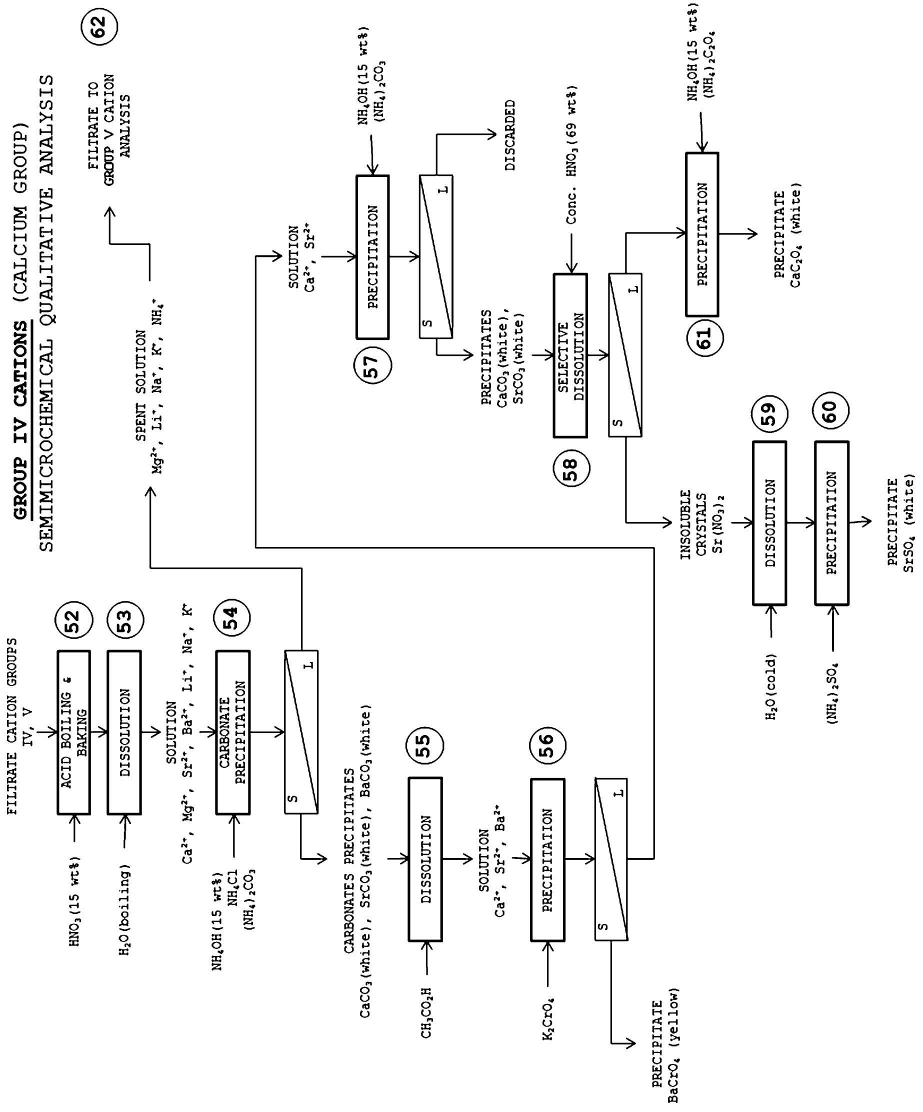
■ **Fig. B.3** Identification chart for group III cations. *PPTN*. precipitation

B.4 Group IV Cations: Calcium Group

See ◘ Fig. B.4.

B.5 Group V Cations: Sodium Group

See ◘ Fig. B.5.



◘ **Fig. B.4** Identification chart for group IV cations

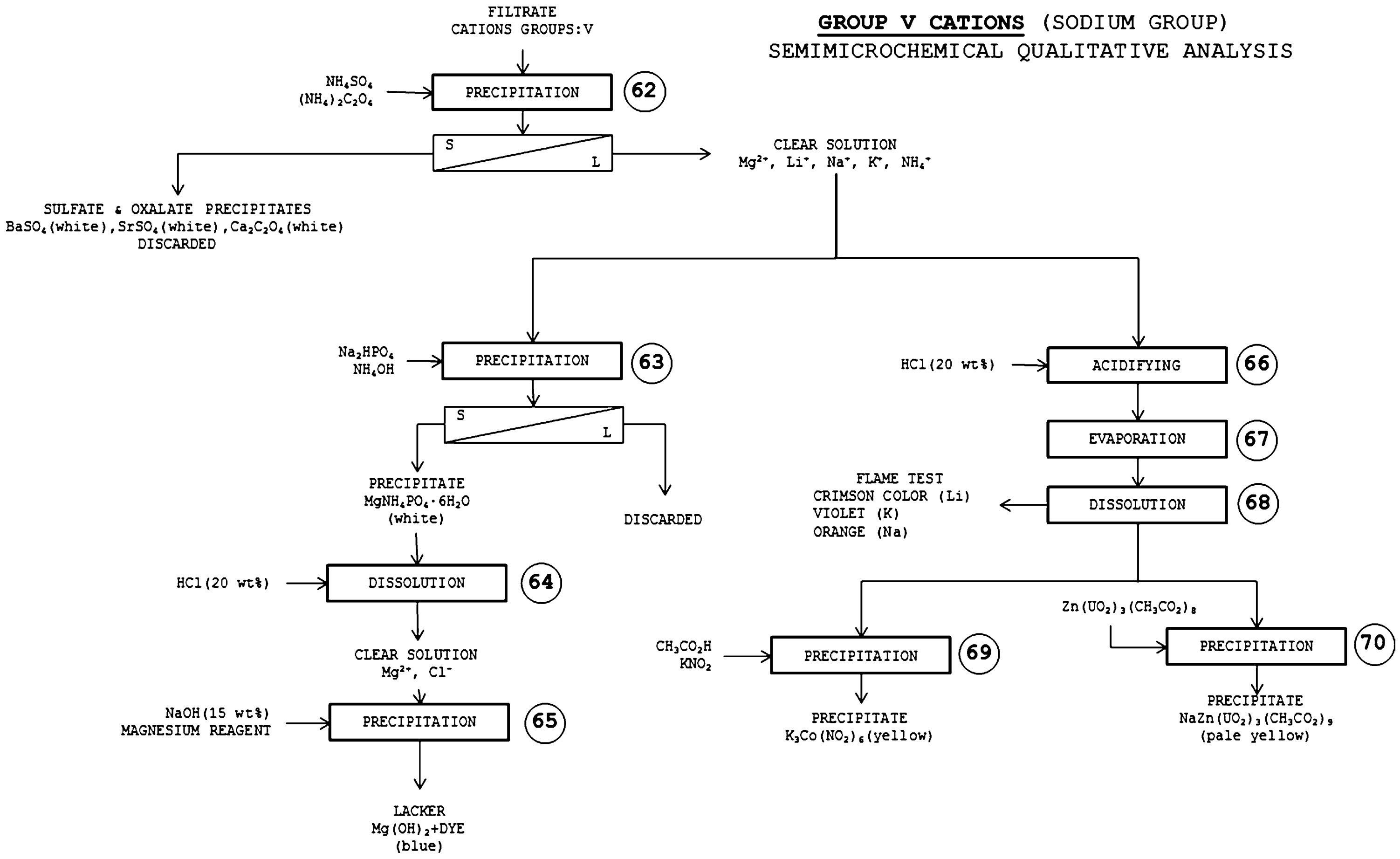


Fig. B.5 Identification chart for group V cations

C NIST Thermochemical Data for Pure Substances

Table C.1 NIST molar thermodynamic properties of pure substances (298.15 K and 100 kPa). (From Wagman, D.D., et al. The NBS Tables of Chemical Thermodynamic Properties *J. Phys. Chem. Ref. Data*, 11, Suppl. 2 (1982))

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
Ag(s)	0.0	0.0	42.55	25.351
Ag(g)	284.55	245.65	172.997	20.786
Ag^+(g)	1021.73	–	–	–
Ag_2CO_3(s)	−505.8	−436.8	167.4	112.26
Ag_2O(s)	−31.05	−11.20	121.3	65.86
Ag_2S(s) (argentite)	−32.59	−40.67	144.01	76.53
AgCN(s)	146.0	156.9	107.19	66.73
AgCNS(s)	87.9	101.39	131.0	63.0
AgCl(s) (cerargyrite)	−127.068	−109.789	96.2	50.79
AgBr(s)	−100.37	−96.90	107.1	52.38
AgI(s)	−61.83	−66.19	115.5	56.82
$AgNO_3$(s)	−124.39	−33.47	140.92	93.05
Ag_3PO_4(s)	–	−879.0	–	–
Ag_2CrO_4(s)	−731.74	−641.76	217.6	142.26
Ag_2SO_4(s)	−715.88	−618.41	200.4	131.38
Al(s)	0.0	0.0	28.33	24.35
Al(g)	326.4	285.7	164.54	21.38
Al^{3+}(g)	5483.17	–	–	–
$Al(OH)_3$	−1276.0	–	–	–
$AlCl_3$(s)	−704.2	−628.8	110.67	91.84
$AlCl_3$(g)	−583.2	–	–	–
Al_2O_3(s) (alumina)	−1675.7	−1582.3	50.92	79.04
B(s)	0.0	0.0	5.86	11.09
BF_3(g)	−1137.00	−1120.35	254.01	50.46
$BaCO_3$(s)	−1216.3	−1137.6	112.1	85.35
BaC_2O_4(s)	−1368.6	–	–	–
$BaCrO_4$(s)	−1446.0	−1345.22	158.6	–

Table C.1 (*continued*)

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
BaF_2(s)	−1207.1	−1156.8	96.36	71.21
$BaSO_4$(s)	−1473.2	−1362.2	132.2	101.75
Bi(s)	0.0	0.0	56.74	25.52
Bi_2S_3(s)	−143.1	−140.6	200.4	122.2
Br_2(l)	0.0	0.0	152.231	75.689
Br_2(g)	30.907	3.110	245.463	36.02
Br(g)	111.88	82.429	174.91	20.786
Br^-(g)	−219.07	–	–	–
C(s) (graphite)	0.0	0.0	5.740	8.527
C(s) (diamond)	1.895	2.900	2.377	6.113
C(g)	716.682	671.257	158.096	20.838
CO(g)	−110.525	−137.168	197.674	29.42
CO_2(g)	−393.509	−394.359	213.74	37.11
$COCl_2$(g)	−218.8	−204.6	283.53	57.66
CH_4(g)	−74.81	−50.72	186.264	35.309
C_2H_2(g)	226.73	209.20	200.94	43.93
C_2H_4(g)	52.25	68.12	219.45	43.56
C_2H_6(g)	−84.68	−32.82	229.60	52.63
C_3H_6(g)	20.2	62.72	266.9	64.0
C_3H_8(g)	−104.5	−23.4	269.9	7.0
C_4H_{10}(g)	−126.5	−17.15	310.1	97.4
C_5H_{12}(g)	−146.5	−8.37	348.9	120.2
C_8H_{18}(g)	−208.5	16.40	466.7	189.0
CH_3OCH_3(g)	−184.05	−112.59	266.38	64.39
CH_3OH(g)	−200.66	−162.00	239.70	43.89
CH_3OH(l)	−238.66	−166.36	126.8	81.6
C_2H_5OH(g)	−235.10	−168.49	282.70	65.44
C_2H_5OH(l)	−277.69	−174.78	160.7	111.46
CH_3COOH(l)	−484.51	−389.9	159.8	124.3
$(CH_3)_2O$(g)	−184.05	−112.59	266.38	64.39
CH_3CHO(l)	−192.30	−128.20	160.2	–
CH_3Cl(g)	−80.83	−57.37	234.58	40.75
$CHCl_3$(g)	−103.14	−70.34	295.71	65.69

Table C.1 *(continued)*

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
CCl_4(l)	−135.44	−65.27	216.40	131.75
C_6H_6(g)	82.9	129.7	269.2	81.6
C_6H_6(l)	49.0	124.7	172.	
C_6H_{12}(l)	−156.3	26.7	204.4	157.7
CaO(s)	−635.09	−604.03	39.75	42.80
$Ca(OH)_2$(s)	−986.09	−898.49	83.39	87.49
$CaCO_3$(s) (calcite)	−1206.92	−1128.79	92.9	81.88
$CaCO_3$(s) (aragonite)	−1207.13	−1127.75	88.7	81.25
CaC_2O_4(s)	−1360.6	–	–	–
CaF_2(s)	−1219.6	−1167.3	68.87	67.03
$Ca_3(PO_4)_2$(s)	−4109.9	−3884.7	240.91	231.58
$CaSO_4$(s)	−1434.11	−1321.79	106.7	99.66
Cd(s)	0.0	0.0	51.76	25.98
Cd(g)	2623.54	–	–	–
Cd^{2+}(g)	112.01	77.41	167.746	20.786
$Cd(OH)_2$(s)	−560.7	−473.6	96.0	–
CdS(s)	−161.9	−156.5	64.9	–
Cl_2(g)	0.0	0.0	223.066	33.907
Cl(g)	121.679	105.680	165.198	21.840
Cl^-(g)	−233.13	–	–	–
ClO_2(g)	102.5	120.5	256.84	41.97
Cu(s)	0.0	0.0	33.150	24.35
Cu(g)	338.32	298.58	166.38	20.786
CuC_2O_4(s)	–	−661.8	–	–
$CuCO_3 \cdot Cu(OH)_2$(s)	−1051.4	−893.6	186.2	–
Cu_2O(s)	−168.6	−146.0	93.14	63.64
CuO(s)	−157.3	−129.7	42.63	42.30
$Cu(OH)_2$(s)	−449.8	–	–	–
Cu_2S(s)	−79.5	−86.2	120.9	76.32
CuS(s)	−53.1	−53.6	66.5	47.82
F_2(g)	0.0	0.0	202.78	31.30
F(g)	78.99	61.91	158.754	22.744
F^-(g)	−255.39	–	–	–

Table C.1 (*continued*)

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
Fe(s)	0.0	0.0	27.28	25.10
Fe(g)	416.3	370.7	180.490	25.677
Fe^{2+}(g)	2749.93	–	–	–
Fe^{3+}(g)	5712.8	–	–	–
$Fe_{0.947}O$(s)	−266.27	−245.12	57.49	48.12
Fe_2O_3(s)	−824.2	−742.2	87.40	103.85
Fe_3O_4(s)	−1118.4	−1015.4	146.4	143.43
$Fe(OH)_3$(s)	−823.0	−696.5	106.7	–
Fe_3C(s)	25.1	20.1	104.6	105.9
$FeCO_3$(s) (siderite)	−740.57	−666.67	92.9	82.13
FeS(s) (pyrrhotite)	−100.0	−100.4	60.29	50.54
FeS_2(s)	−178.2	−166.9	52.93	62.17
H_2(g)	0.0	0.0	130.684	28.824
H(g)	217.965	203.247	114.713	20.784
H^+(g)	1536.202	–	–	–
H_2O(g)	−241.818	−228.572	188.825	33.577
H_2O(l)	−285.830	−237.129	69.91	75.291
H_2O_2(g)	−136.31	−105.57	232.7	43.1
H_2O_2(l)	−187.78	−120.35	109.6	89.1
H_2S(g)	−20.63	−33.56	205.79	34.23
H_2SO_4(l)	−813.989	−690.003	156.904	138.91
HF(g)	−271.1	−273.2	173.779	29.133
HCl(g)	−92.307	−95.299	186.908	29.12
HBr(g)	−36.40	−53.45	198.695	29.142
HI(g)	26.48	1.70	206.594	29.158
HCN(g)	135.1	124.7	201.78	35.86
Hg(l)	0.0	0.0	76.02	27.983
$HgCl_2$(s)	−224.3	−178.6	146.0	–
Hg_2Br_2(s)	−206.90	−181.075	218.0	–
Hg_2Cl_2(s)	−265.22	−210.745	192.5	–
HgS(s) (red)	−58.2	−50.6	82.4	48.41
HgS(s) (black)	−53.6	−47.7	88.3	–
Hg_2SO_4(s)	−743.12	−625.815	200.66	131.96

Table C.1 (*continued*)

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
I_2(s)	0.0	0.0	116.135	54.438
I_2(g)	62.438	19.327	260.69	36.90
I(g)	106.838	70.250	180.791	20.786
I^-(g)	−197.0	–	–	–
ICl(g)	17.78	−5.46	247.551	35.56
K(s)	0.0	0.0	64.18	29.58
K(g)	89.24	60.59	160.336	20.786
K^+(g)	514.26	–	–	–
KF(s)	−567.27	−537.75	66.57	49.04
KCl(s)	−436.747	−409.14	82.59	51.30
KBr(s)	−393.798	−380.66	95.90	52.30
KI(s)	−327.900	−324.892	106.32	52.93
$KClO_4$(s)	−432.75	−303.09	151.0	112.38
KNO_3(s)	−494.63	−394.86	133.05	96.40
Mg(s)	0.0	0.0	32.68	24.89
Mg^{2+}(g)	2348.504	–	–	–
MgF_2(s)	−1123.4	−1070.2	57.24	61.59
$MgCO_3$(s)	−1095.8	−1012.1	65.7	75.52
$Mg(OH)_2$(s)	−924.54	−833.51	63.18	77.03
Mn(s)	0.0	0.0	32.01	26.32
MnO_2(s)	−520.03	−465.14	53.05	54.14
MnS(s) (green)	−214.2	−218.4	78.2	49.96
N_2(g)	0.0	0.0	191.61	29.125
N(g)	472.704	455.563	153.298	20.786
NH_3(g)	−46.11	−16.45	192.45	35.06
NH_4Cl(s)	−314.43	−202.87	94.6	84.1
NO(g)	90.25	86.55	210.761	29.844
NO_2(g)	33.18	51.31	240.06	37.20
N_2O(g)	82.05	104.20	219.85	38.45
N_2O_4(g)	9.16	97.89	304.29	77.28
N_2O_4(l)	−19.50	97.54	209.2	142.7
N_2O_5(g)	11.3	115.1	355.7	84.5
N_2O_5(s)	−43.1	113.9	178.2	143.1

Table C.1 (*continued*)

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
NOCl(g)	51.71	66.08	261.69	44.69
NOBr(g)	82.17	82.42	273.66	45.48
Na(s)	0.0	0.0	51.21	28.24
Na(g)	107.32	76.761	153.712	20.786
Na^+(g)	609.358	–	–	–
NaF(s)	−573.647	−543.494	51.46	46.86
NaCl(s)	−411.153	−384.138	72.13	50.50
NaBr(s)	−361.062	−348.983	86.82	51.38
NaI(s)	−287.78	−286.06	98.53	52.09
Na_2CO_3(s)	−1130.68	−1044.44	134.98	112.30
$NaNO_2$(s)	−358.65	−284.55	103.8	–
$NaNO_3$(s)	−467.85	−367.00	116.52	92.88
Na_2O(s)	−414.22	−375.46	75.06	69.12
NiS(s)	−82.0	−79.5	52.97	47.11
O_2(g)	0.0	0.0	205.138	29.355
O_3 (ozone)	142.7	163.2	238.93	39.20
O(g)	249.170	231.731	161.055	21.912
P(s) (white)	0.0	0.0	41.09	23.840
P(g)	314.64	278.25	163.193	20.786
PH_3(g)	5.4	13.4	210.23	37.11
PCl_3(g)	−287.0	−267.8	311.78	71.84
PCl_5(g)	−374.9	−305.0	364.58	112.80
Pb(s)	0.0	0.0	64.81	26.44
Pb(g)	195.0	161.9	175.373	20.786
$PbBr_2$(s)	−278.9	−261.92	161.5	80.12
$PbCl_2$(s)	−359.41	−314.10	−136.0	–
PbO(s) (minium)	−218.99	−189.93	66.5	45.81
PbO(s) (litharge)	−217.32	−187.89	68.70	45.77
PbO_2(s)	−277.4	−217.33	68.6	64.64
Pb_3O_4(s)	−718.4	−601.2	211.3	146.9
$Pb(OH)_2$(s)	–	−452.2	–	–
PbS(s) (galena)	−100.4	−98.7	91.2	49.50
$PbSO_4$(s)	−919.94	−813.14	148.57	103.207

Table C.1 (*continued*)

Chemical substance	$\Delta_f H^0$ (kJ · mol^{-1})	$\Delta_f G^0$ (kJ · mol^{-1})	S^0 (J · K^{-1} · mol^{-1})	C_p^0 (J · K^{-1} · mol^{-1})
S(s) (rhombic)	0.0	0.0	31.80	22.64
S(s) (monoclinic)	0.33	–	–	–
S(g)	278.805	238.250	167.821	23.673
SF_6(g)	−1209.		−1105.3	291.82
SO_2(g)	−296.830	−300.194	248.22	39.87
SO_3(g)	−395.72	−371.06	256.76	50.67
SO_3(l)	−441.04	−373.75	113.8	–
SO_2Cl_2(g)	−364.0	−320.0	311.94	77.0
Sn(s) (white)	0.0	0.0	51.55	26.99
Sn(s) (gray)	−2.09	0.13	44.14	25.77
SnO(s)	−285.8	−256.9	56.5	44.31
SnO_2(s)	−580.7	−519.6	52.3	52.59
SnS(s)	−100.0	−98.3	77.0	49.25
Tl(s)	0.0	0.0	64.18	26.32
Tl^+(g)	777.764	–	–	–
Tl^{3+}(g)	5639.2	–	–	–
Zn(s)	0.0	0.0	41.63	25.40
Zn^{2+}(g)	2782.78	–	–	–
ZnO(s)	−348.28	−318.30	43.64	40.25
ZnS(s) (wurtzite)	−192.63	–	–	–
ZnS(s) (sphalerite)	−205.98	−201.29	57.7	46.0

g gas, *l* liquid, *s* crystalline solid

D Hydrogen-like Atom Spectra

D.1 Historical Background

As expected from its simple structure, the atomic spectrum of the hydrogen atom is the simplest of all the elements. The well-known H_α, H_β, H_γ, H_δ, etc., lines that appear in the visible region were first studied in the spectrum of the Sun, and their wave numbers (v) were measured with great accuracy by early spectroscopists. In 1885, J.J. Balmer pointed out that the wave numbers of spectral lines can be expressed by the simple mathematical relationship

$$v = 1/\lambda = k\ [n^2/(n^2 - 4)],$$

where k is a constant and n a positive integer equal to 3, 4, 5, 6, etc., for spectral lines H_α, H_β, H_γ, H_δ, etc., respectively. This equation, which has become of fundamental importance, can be rewritten in the form

$$v = 1/\lambda = R_\mathrm{H}\ [n^2/(2^2 - n^2)].$$

Close examination of the Balmer equation shows that it consists of two terms: the first term is a constant, or series term, and the second is a variable, and is referred to as a current term. Hence, the series of lines where the series term is 2 were named the Balmer series. At that time the constant was called the Rydberg constant and was equal to 109,677.76 cm^{-1} for the hydrogen atom. The remarkable accuracy with which this straightforward equation reproduced the actual wave numbers of the spectral lines lead W. Ritz to introduce in 1908 the Ritz combination principle, which is only a generalization of the Balmer formula: *the wave number of any spectral line may be represented as the combination of two terms, one of which is constant and the other variable throughout each spectral series*. Because this basic principle applies over the entire spectrum of electromagnetic radiation, from X-rays to infrared radiation, it was an important milestone in the development of the important concept of electronic energy levels. The phrase “spectral term” as today used in modern spectroscopy has the specific meaning introduced by the Ritz combination principle.

D.2 The Classical Bohr Model for Hydrogen-like Atoms

The hydrogen atom is the simplest atom, and can be modeled with relatively simple classical mechanics considerations. The theoretical explanation of the atomic spectrum of hydrogen was provided by a young Danish scientist named Niels Bohr. In 1911, the New Zealand physicist Ernest Rutherford, on the basis of the alpha particle scattering experiments of his colleagues Hans Geiger and Ernest Marsden, had proposed the nuclear model of the atom. Bohr was working in Rutherford’s laboratory at the time and saw how to incorporate this new viewpoint of the atom and the quantization condition of Planck into a successful theory for the hydrogen atom. The Bohr model of the electronic energy levels of the hydrogen atom is based on four postulates:

1. The electron in the atom has only a fixed number of stationary states of motion. In each of these states it has a fixed energy.
2. When the electron is in a particular state of motion (in a particular orbital), it does not radiate. When it moves from a state of higher energy to one of lower energy, it emits a quantum of light. The energy of this light equals the difference between the energies of the two states.
3. In any of these states the electron moves in a closed circular motion around the atomic nucleus, which has infinite mass compared with the mass of the electron.
4. The angular momentum of the electron in its stable orbits is quantized. Only orbits for which the angular momentum has values that are integer multiples of a quantum of angular momentum are allowed.

By extension, a ***hydrogen-like atom*** or ***hydrogenic ion*** (i.e., or sometimes ***hydrogenoid*** ion) is a cation having a structure isoelectronic with that of the neutral hydrogen atom (i.e., with only one electron of rest mass $m_1 = m_0$ and electric charge $Q_1 = -e$ in a closed circular orbit of radius r around the atomic nucleus of mass $m_2 = M$ and electric charge $Q_2 = +Ze$, where Z is the atomic number of the corresponding chemical element, i.e., number of protons). Some examples of common hydrogen-like cations are He^+, Li^{2+}, and Be^{3+}. The electrostatic attractive force existing between the two opposite point charges is given by Coulomb's law:

$$F_e = -(1/4\pi\varepsilon_0)Q_1Q_2/r^2 = Ze^2/4\pi\varepsilon_0 r^2,$$

where F_e is the electrostatic force in newtons (N), Q_1 and Q_2 are electrostatic charges of the electron and nucleus respectively in coulombs (C), ε_0 is the permittivity of a vacuum ($8.8541878 \times 10^{-12}$ F · m^{-1}) and r is the orbital radius in meters (m).

The gravitational force existing between the two point masses is given by Newton's law:

$$F_g = -Gm_1m_2/r^2 = -Gm_0M/r^2,$$

where F_g is the gravitation force in newtons (N), m_0 and M are the masses of the electron and nucleus respectively in kilograms (kg), G is the gravitational constant (6.67408×10^{-11} N · kg^{-2} · m^2), and r is the orbital radius in meters (m).

Newton's second law of motion states that the sum of all the external forces applied on the electron are equal to the first time derivative of the linear momentum:

$$F_e + F_g = \mathrm{d}p/\mathrm{d}t = m_0\mathrm{d}v_G/\mathrm{d}t = m_0a_G.$$

But because of the great difference between the electron and nucleon (proton, neutron) rest masses ($M_p/m_0 = 1836.15267389$), the ratio of the electrostatic force to the gravitational force is the biggest known ratio in the universe! Using $Z = 1$, $e = 1.6021766208 \times 10^{-19}$ C, and $m_0 = 9.10938356 \times 10^{-31}$ kg, and $M_p = 1.672621898 \times 10^{-27}$ for the hydrogen atom, we obtain $F_e/F_g = (Ze^2/4\pi\varepsilon_0 Gm_0M) = 2.3 \times 10^{39}$. Therefore, in the following calculations, we will always ignore the gravitational force ($F_g = 0$). Hence, the fundamental Newton's second law of motion becomes

$$F_e = m_0\mathrm{d}v_G/\mathrm{d}t = m_0a_G.$$

To remain in a circular orbit, the electron must be experiencing a centripetal acceleration. The acceleration vector ($\boldsymbol{a}_\mathrm{G}$) can be decomposed into two orthogonal vector components – a tangential acceleration ($\boldsymbol{a}_\mathrm{N}$) and a normal centripetal acceleration ($\boldsymbol{a}_\mathrm{T}$) – and hence the normal acceleration for a centripetal circular motion is given by

$$a_\mathrm{G} = -v^2/r e_\mathrm{r}.$$

where v is the velocity of the electron in meters per second ($\mathrm{m \cdot s^{-1}}$).

Therefore, substituting the expression for the Coulomb force in Newton's second law, we obtain

$$m_0 v^2/r = Ze^2/4\pi\varepsilon_0 r^2.$$

Hence, it is possible to express the kinetic (K) energy of the orbiting electron:

$$K = 1/2 m_0 v^2 = Ze^2/8\pi\varepsilon_0 r.$$

For simplicity, we assumed that the mass of the atomic nucleus is infinite so its position remains fixed. But to take it into account, we can correct this approximation by introducing the reduced mass. A more precise model considers the two point masses rotating around the common mass center. In that case, the mass of the electron must be replaced by the reduced mass of the electron–nucleus system, denoted μ and defined by

$$\mu = m_0 M/(m_0 + M).$$

Therefore,

$$K = 1/2 \mu v^2 = Ze^2/8\pi\varepsilon_0 r.$$

On the other hand, the potential energy is given by

$$V = -Ze^2/4\pi\varepsilon_0 r,$$

the negative sign indicating that energy must be provided to an electron to bring it far away from the nucleus. Therefore, the calculation of the mechanical energy (E) of the electron–nucleus system consists in summing the potential (V) and kinetic (K) energies of the orbiting electron:

$$E = K + V = Ze^2/8\pi\varepsilon_0 r - Ze^2/4\pi\varepsilon_0 r = -Ze^2/8\pi\varepsilon_0 r.$$

Note that the energy of a bound atom is negative, since it is lower than the energy of the separated electron and proton, which is taken arbitrarily as zero as an absolute reference.

At this point, Bohr made an assumption that departs radically from the concepts of classical mechanics. Bohr's assumption, called the quantum hypothesis, asserts that the angular momentum for a point mass, $\boldsymbol{L} = \boldsymbol{rp} = mvr$, can take only certain values, which are whole-number multiples of the quantity $h/2\pi$, which was later confirmed by Louis de Broglie. This assumption gives the Bohr quantization relationship:

$$\mu v r = n\hbar = nh/2\pi,$$

where n is an integer called the ***principal quantum number,*** with $n = 1, 2, 3$, etc., excluding $n = 0$, since the electron is not in a circular orbit. Hence, we can rearrange the preceding equation, solving for r, to obtain the following expression:

$$1/2\mu v^2 = n^2\hbar^2/2\mu r^2 = n^2h^2/8\pi^2\mu r^2 = Ze^2/8\pi\varepsilon_0 r.$$

Therefore, it is now possible to express the Bohr radius for any hydrogen-like atom as a function of the quantized principal number (n):

$$r_n = 4\pi\varepsilon_0 n^2\hbar^2/Z\mu e^2 = n^2h^2\varepsilon_0/\pi\mu Ze^2.$$

Since r_n is a fundamental constant, this equation predicts that the orbital radius increases in direct proportion to the square of the quantum number, n^2, and decreases in inverse proportion to the atomic number, Z. In the case of the hydrogen atom ($Z = 1$) and $n = 1$, we obtain the so-called first Bohr radius, denoted a_0:

$$a_0 = r_1 = 4\pi\varepsilon_0\hbar^2/m_0e^2 = h^2\varepsilon_0/\pi m_0e^2 = 5.2917721067 \times 10^{-11}\ \text{m}.$$

Thus, the allowed orbital radii are then given by

$$r_n = n^2a_0,$$

and the sizes of the orbits in the hydrogen atom are predicted to be a_0, $4a_0$, $9a_0$, $16a_0$, $25a_0$, etc. Furthermore, the orbits in He^+ (Z = 2) for any value of n are predicted to be half as large as the comparable orbits in H. Although the radius equation is an interesting result, the more important equation concerned the energy of the electron, because this correctly predicted the line spectra of one-electron atoms. Introducing the new quantities into the total energy equation, we obtain the energy of a quantum level n:

$$E_n = -Ze^2/8\pi\varepsilon_0 r_n = -\mu e^4/2(4\pi\varepsilon_0)^2\hbar^2(Z^2/n^2) = -2\pi\mu e^4/(4\pi\varepsilon_0)^2h^2(Z^2/n^2).$$

For the one-electron hydrogenic atom, the lowest energy occurs when $n = 1$. This energy state is called the ground or fundamental state. The highest energy state would be n = infinity, with r = infinity (i.e., zero potential energy since infinite separation of the electron from the nucleus), $v = 0$ (zero kinetic energy of the electron), and therefore $E_n = 0$. Therefore, it requires an energy of 13.6 eV, which corresponds to the ionization energy of hydrogen, to remove the electron from the vicinity of the nucleus and turn a neutral hydrogen atom into a positive cation and a (stationary) free electron. If the atom receives sufficient energy, as in a gas discharge tube, its electron may jump to a higher orbit ($p > 1$) with corresponding higher energy by the supply of energy $E_n - E_p$. This represents an excited state. The only way the atom can assume a lower-energy state is through emission of energy in the form of electromagnetic radiation. The energy of this radiation is equal to the energy difference between the high state and the lower state characterized by their principal quantum numbers n and p. If we express this energy change involved during the electronic transition, we obtain the equation

$$E_p - E_n = \mu e^4/2(4\pi\varepsilon_0)^2\hbar^2Z^2(1/n^2 - 1/p^2) = 2\pi\mu e^4/(4\pi\varepsilon_0)^2h^2Z^2(1/n^2 - 1/p^2).$$

We assume that p is always at least one integer value greater than n; that is, $p > n$. The lower state, n, may be either the ground state ($n = 1$) or any other excited state with a lower value than the original state, p. Since the energy of electromagnetic radiation is conventionally not given a sense of sign, the equation has been formulated here in terms of the absolute value. For clarity, it is possible to introduce a new quantity, called the Rydberg, denoted Ry and expressed in joules, that corresponds to the first ionization energy of the hydrogen atom:

$$\mathrm{Ry} = m_0 e^4/(4\pi\varepsilon_0)^2\hbar^2 = 2\pi m_0 e^4/(4\pi\varepsilon_0)^2 h^2 = 13.6\,\mathrm{eV}.$$

Therefore,

$$E_p - E_n = \mathrm{Ry}(\mu/m_0)Z^2(1/n^2 - 1/p^2).$$

From Planck, we know that $E = hc\overline{\nu}$ and hence if we divide the preceding equation by hc, we obtain the expression for the wave number of the absorbed/emitted electromagnetic radiation. If we introduce a new spectroscopic quantity called the spectral term denoted T_{np} with the dimension of a wave number and defined by

$$T_{np} = (E_p - E_n)/hc,$$

the corresponding electronic transition, we obtain the equation

$$\begin{aligned} T_{np} = \upsilon_{np} &= \mu e^4/2(4\pi\varepsilon_0)^2\hbar^3 c Z^2(1/n^2 - 1/p^2) \\ &= 2\pi\mu e^4/(4\pi\varepsilon_0)^2 h^3 c Z^2(1/n^2 - 1/p^2). \end{aligned}$$

Introducing a new quantity called the Rydberg constant (R_∞) defined by

$$R_\infty = m_0 e^4/2(4\pi\varepsilon_0)^2\hbar^3 c = 2\pi m_0 e^4/(4\pi\varepsilon_0)^2 h^3 c = 109{,}737\,\mathrm{cm}^{-1}$$

and

$$\mathrm{Ry} = R_\infty hc$$

into the spectral term equation, we obtain the well-known ***Balmer–Ritz equation*** that Rydberg and Ritz discovered experimentally:

$$T_{np} = R_\infty hc[M/(m_0 + M)]Z^2(1/n^2 - 1/p^2) = \mathrm{Ry}[M/(m_0 + M)]Z^2(1/n^2 - 1/p^2).$$

This general equation represents the wave number for the series of transitions from various excited states to the same lower state. With use of the correct reduced mass and the appropriate value of Z, the preceding expression may be used to generate the wave number of the transitions in any hydrogenic atom or ion. The constant appearing in the Balmer–Ritz formula for spectral lines gives the Rydberg constant for an atom with atomic number Z, denoted RZ:

$$R_\mathrm{Z} = R_\infty/(1 + m_0/M) = \mu Z^2 e^4/2(4\pi\varepsilon_0)^2\hbar^3 c = 2\pi\mu Z^2 e^4/(4\pi\varepsilon_0)^2 h^3 c.$$

Table D.1 Spectral series for the hydrogen atom

Spectral series historical name and year of discovery	Ground state	Spectral region	Spectral lines (measured)
Lyman series (named after T. Lyman; 1904–1906)	$n = 1$	Far UV	2 → 1: 121.57 nm 3 → 1: 102.57 nm 4 → 1: 97.253 nm ∞ → 1: 91.15 nm
Balmer series (named after J.J. Balmer; 1885)	$n = 2$	Visible	3 → 2: 656.2852 nm (red) 4 → 2: 486.133 nm (cyan) 5 → 2: 434.047 nm (violet) 6 → 2: 410.174 nm 7 → 2: 397.072 nm 8 → 2: 388.9049 nm 9 → 2: 383.5384 nm
Ritz–Paschen series (named after F. Paschen; 1916)	$n = 3$	Near IR	8 → 3: 954.62 nm 7 → 3: 1004.98 nm 6 → 3: 1093.8 nm 5 → 3: 1281.81 nm 4 → 3: 1875.01 nm
Brackett series (named after F.S. Brackett; 1922)	$n = 4$	IR	6 → 4: 2630 nm 5 → 4: 4050 nm
Pfund series (named after A.H. Pfund; 1924)	$n = 5$	Far IR	6 → 5: 7400 nm

For heavy hydrogen-like ions, $M \gg m_0$, the two constants R_Z and R_∞ are very similar. In the case of the hydrogen atom ($Z = 1$), we obtain the Rydberg constant for the hydrogen atom denoted R_H:

$$\begin{aligned} R_H &= m_0 e^4/(1 + m_0/M_p)(4\pi\varepsilon_0)^2\hbar^3 c \\ &= 2\pi m_0 e^4/(1 + m_0/M_p)(4\pi\varepsilon_0)^2 h^3 c = 109{,}677\ \mathrm{cm}^{-1}. \end{aligned}$$

Initially the spectral lines of the hydrogen atom were recorded in the visible range by Balmer, and substitution of other values of n in the equation gives frequencies that predict other series of line spectra for hydrogen, which had not been observed at the time Balmer did his experiments. Balmer's elucidation of the series for which $n = 2$ was simply a result that visible light was the most readily observed kind of electromagnetic radiation with the spectroscopes available in the late nineteenth century. Other series predicted by the equation fall either in the ultraviolet region or in the infrared region, and are more difficult to observe experimentally. With better instrumentation and the impetus of the Bohr equation, the line spectra reported in Table D.1 were subsequently discovered, in addition to the Balmer series.

D.3 Isotopic Effect

The Balmer–Ritz equation demonstrates the impact of the isotopic effect on atomic spectral lines. In 1931, H.C. Urey devised a method for the concentration of any possible heavy hydrogen isotopes by the fractional distillation of 4 L of liquid hydrogen down to 1 mL and measured the spectrum of the residual gas. The result was a set of lines displaced slightly from the hydrogen spectrum. This amounted to the discovery of deuterium (^{2}H or D), or heavy hydrogen, for which Urey was awarded the 1934 Nobel Prize in Chemistry. If the mass of the deuteron as assumed to be twice that of the proton, the Rydberg constant for a deuterium atom is $R_D = 109{,}707\ \mathrm{cm}^{-1}$. Therefore, precise measurements of the wave number shift of spectral terms can provide information on the isotopic composition by means of the equation

$$T_{np} = R_\infty hc[M/(m_0 + M)]Z^2(1/n^2 - 1/p^2) = \mathrm{Ry}[M/(m_0 + M)]Z^2(1/n^2 - 1/p^2).$$

D.4 Structure Fine Constant

Regarding the velocity of the orbiting electron and the quantification condition $mvr = n\hbar$, we can write the linear velocity of the electron in circular motion around of a nucleus of atomic number Z as follows:

$$v_\mathrm{e} = (e^2/4\pi\varepsilon_0\hbar)(Z/n).$$

If we compare the linear velocity of the electron given by the preceding equation with the speed of light in a vacuum, c, we can introduce the dimensionless ratio (v_e/c) defined as follows:

$$v_\mathrm{e}/c = (e^2/4\pi\varepsilon_0\hbar c)(Z/n) = \alpha(Z/n) = (Z/137n).$$

The new constant denoted α is called the fine structure constant and is equal to 1/137.036.

D.5 Positronium and Muonium Atoms

Another interesting example involving reduced mass concerns positronium, a short-lived combination of an electron and a positron, the electron's antiparticle. The electron and positron mutually annihilate with a half-life of approximately 10^{-7} s, and positronium decays into gamma rays of 1.011 MeV. The reduced mass of positronium is half the mass of the electron. Thus, the ionization energy is 6.80 eV, half that of a hydrogen atom.

D.6 Spectroscopic Notation and Transition Selection Rules

A shorthand notation for the possible electronic energy levels in an atom involves specifying the principal quantum number of the least tightly bound electron, the total electronic angular momentum due to spin, the total electronic orbital angular momentum, and the total electronic angular momentum, defined as follows:

$$n, L = l_1 + l_2 + l_3 \ldots; \quad S = s_1 + s_2 + s_3 \ldots; \quad \text{and} \quad J = L + S.$$

The notation is known as ***L–S coupling*** or ***Russell–Saunders coupling*** notation since the total electronic angular momentum is simply the vector sum of the electronic orbital and spin angular momenta. The notation is written as follows:

$$n^{2S+1}L_J.$$

The number $(2S + 1)$ is known as the multiplicity of the electronic state. Therefore, the electronic states for which $(2S + 1) = 1, 2$, and 3 are named singlet, doublet, and triplet respectively. For historical reasons, $L = 0$ is referred to as a S state, $L = 1$ is a P state, $L = 2$ is a D state, $L = 3$ is a F state, meaning sharp, principal, diffuse, and fundamental, and the alphabet is followed thereafter with use of uppercase G, H, I, J, and K. As an example of an application of this notation, the ground state of the hydrogen atom is $1^2\mathrm{S}_{1/2}$. Since a photon carries energy and angular momentum, any electronic transition from one allowed energy level to another must conserve energy and angular momentum for the atom–photon system. Thus, restrictions on the allowed changes in multiplicity and orbital and total angular momentum can be partially understood. These restrictions are known as selection rules, and they are

$$\Delta S = 0, \quad \Delta L \pm 1 \quad \text{and} \quad \Delta J \pm 1, 0,$$

with $J = 0$ to $J = 0$ forbidden. Any allowed (dipole) transition between two electronic states must obey these selection rules. This is called the ***Laporte spin selection rule*** (**dipolar electric moment selection rule**). Notice that the magnetic quantum number does not appear in the spectroscopic notation. The reason is that effects on electronic energies in atoms due to quantum number m are realized only if the atom is placed in an external magnetic field (***Zeeman effect***). Nevertheless, the selection rule still applies, and is written

$$\Delta m \pm 1, 0.$$

D.7 Nomenclature of Atom Electron Energies and X-ray Emission Lines

The new notation for X-ray emission lines and absorption edges called the International Union of Pure and Applied Chemistry (IUPAC) nomenclature replaces the ***Siegbahn nomenclature*** by a system based on the energy-level designation. The IUPAC X-ray nomenclature has the advantage of being simple and easy to extend to any kind of transition.

The electronic states occurring as initial and final states of a process involving the absorption or emission of X-ray radiation are called X-ray levels. This term is used here with the same meaning as in the description of many-electron states in atomic spectroscopy (i.e., as part of the conceptual hierarchy, configuration, term and level). It represents a many-electron state which, in the purely atomic case, has total angular momentum $(J = L + S)$ as a well-defined quantum number. The word "term" in atomic spectroscopy denotes a set of levels that have the same electronic configuration and the same value of the quantum numbers for total spin S and total orbital angular momentum L (see ◘ Table D.2).

Table D.2 X-ray emission line nomenclature. (International Union of Pure and Applied Chemistry and Siegbahn)

Designation and lower electron energy level			**Higher electron energy level**																		
			$\mathbf{L_1}$	$\mathbf{L_2}$	$\mathbf{L_3}$	$\mathbf{M_1}$	$\mathbf{M_2}$	$\mathbf{M_3}$	$\mathbf{M_4}$	$\mathbf{M_5}$	$\mathbf{N_1}$	$\mathbf{N_2}$	$\mathbf{N_3}$	$\mathbf{N_4}$	$\mathbf{N_5}$	$\mathbf{N_6}$	$\mathbf{N_7}$	$\mathbf{O_1}$	$\mathbf{O_2}$	$\mathbf{O_3}$	$\mathbf{O_4}$
			$^2S_{1/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2S_{1/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2S_{1/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$	$^2D_{5/2}$	$^2F_{5/2}$	$^2F_{7/2}$	$^2S_{1/2}$	$^2P_{1/2}$	$^2P_{3/2}$	$^2D_{3/2}$
K series	K	$^2S_{1/2}$	*n.a.*	$K\alpha_2$	$K\alpha_1$	*n.a.*	$K\beta_3$	$K\beta_1$	$K\beta_5$		*n.a.*	$K\beta_2$		$K\beta_4$		*n.a.*	*n.a.*	*n.a.*	$K\delta_2$	$K\delta_1$	*n.a.*
L series	L_1	$^2S_{1/2}$	*n.a.*				$L\beta_4$	$L\beta_3$	$L\beta_{10}$	$L\beta_9$	*n.a.*	$L\gamma_2$	$L\gamma_3$	*n.a.*	$L\gamma 1_1$	*n.a.*	*n.a.*	*n.a.*	$L\gamma'_4$		*n.a.*
	L_2	$^2P_{1/2}$		*n.a.*	*n.a.*	L_η	*n.a.*	$L\beta_{17}$	$L\beta_1$	*n.a.*	$L\gamma_5$	*n.a.*	*n.a.*	$L\gamma_1$	*n.a.*	L_ν		$L\gamma_8$	*n.a.*	*n.a.*	$L\gamma_6$
	L_3	$^2P_{3/2}$		*n.a.*	*n.a.*	L_l	*n.a.*	L_σ	$L\alpha_2$	$L\alpha^1$	$L\beta_6$	*n.a.*	*n.a.*	$L\beta_{15}$	$L\beta 2$	$L\beta'_{6,7}$		$L\beta_7$	*n.a.*	*n.a.*	$L\beta_5$
M series	M_1	$^2S_{1/2}$				L_ℓ															
	M_2	$^2P_{1/2}$			L_t																
	M_3	$^2P_{3/2}$			$K\beta_{3,4}$									$M\gamma_2$	$M\gamma_1$						
	M_4	$^2D_{3/2}$										$M\zeta_{1,2}$				$M\beta_1$					
	M_5	$^2D_{5/2}$											$M\zeta_2$			$M\alpha_2$	$M\alpha 1$				
N series	N_1	$^2S_{1/2}$																			
	N_2	$^2P_{1/2}$																			

n.a. transition not allowed because of the electronic transition rules: $\Delta S = 0$, $\Delta L \pm 1$ and $\Delta J \pm 1, 0$

D.8 X-ray Emission Lines

See Table D.3.

Table D.3 X-ray emission lines (electronvolts)

Z	Element	Line									
		$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$K\beta_3$	$L\alpha_1$	$L\alpha_2$	$L\beta_1$	$L\beta_2$	$L\gamma_1$	$M\alpha_1$
		K-L_3	K-L_2	K-M_3	K-M_2	K-L_3	L_3-M_5	L_2-M_4	L_3-N_5	L_2-N_4	M_5-N_7
1	H	13.60									
2	He	24.59									
3	Li	54.75									
4	Be	108.50									
5	B	183.30									
6	C	277.00									
7	N	392.40									
8	O	524.90									
9	F	676.80									
10	Ne	848.60	848.60								
11	Na	1040.98	1040.98	1071.10							
12	Mg	1253.60	1253.60	1302.20							
13	Al	1486.70	1486.27	1557.45							
14	Si	1739.98	1739.38	1835.94							
15	P	2013.70	2012.70	2139.10							
16	S	2307.84	2306.64	2464.04							
17	Cl	2622.39	2620.78	2815.60							
18	Ar	2957.70	2955.63	3190.50							
19	K	3313.80	3311.10	3589.60							
20	Ca	3691.68	3688.09	4012.70		341.30	341.30	344.90			
21	Sc	4090.60	4086.10	4460.50		395.40	395.40	399.60			
22	Ti	4510.84	4504.86	4931.81		452.20	452.20	458.40			
23	V	4952.20	4944.64	5427.29		511.30	511.30	519.20			
24	Cr	5414.72	5405.51	5946.71		572.80	572.80	582.80			
25	Mn	5898.75	5887.65	6490.45		637.40	637.40	648.80			
26	Fe	6403.84	6390.84	7057.98		705.00	705.00	718.50			
27	Co	6930.32	6915.30	7649.43		776.20	776.20	791.40			
28	Ni	7478.15	7460.89	8264.66		851.50	851.50	868.80			
29	Cu	8047.78	8027.83	8905.29		929.70	929.70	949.80			
30	Zn	8638.86	8615.78	9572.00		1011.70	1011.70	1034.70			

Table D.3 (*continued*)

Z	Element	Line									
		$K\alpha_1$	$K\alpha_2$	$K\beta_1$	$K\beta_3$	$L\alpha_1$	$L\alpha_2$	$L\beta_1$	$L\beta_2$	$L\gamma_1$	$M\alpha_1$
		$K\text{-}L_3$	$K\text{-}L_2$	$K\text{-}M_3$	$K\text{-}M_2$	$K\text{-}L_3$	$L_3\text{-}M_5$	$L_2\text{-}M_4$	$L_3\text{-}N_5$	$L_2\text{-}N_4$	$M_5\text{-}N_7$
31	Ga	9251.74	9224.82	10,264.20		1097.92	1097.92	1124.80			
32	Ge	9886.42	9855.32	10,982.10		1188.00	1188.00	1218.50			
33	As	10,543.72	10,507.99	11,726.20		1282.00	1282.00	1317.00			
34	Se	11,222.40	11,181.40	12,495.90		1379.10	1379.10	1419.23			
35	Br	11,924.20	11,877.60	13,291.40		1480.43	1480.43	1525.90			
36	Kr	12,649.00	12,598.00	14,112.00		1586.00	1586.00	1636.60			
37	Rb	13,395.30	13,335.80	14,961.30		1694.13	1692.56	1752.17			
38	Sr	14,165.00	14,097.90	15,835.70		1806.56	1804.74	1871.72			
39	Y	14,958.40	14,882.90	16,737.80		1922.56	1920.47	1995.84			
40	Zr	15,775.10	15,690.90	17,667.80		2042.36	2039.90	2124.40	2219.40	2302.70	
41	Nb	16,615.10	16,521.00	18,622.50		2165.89	2163.00	2257.40	2367.00	2461.80	
42	Mo	17,479.34	17,374.30	19,608.30		2293.16	2289.85	2394.81	2518.30	2623.50	
43	Tc	18,367.10	18,250.80	20,619.00		2424.00	2420.00	2538.00	2674.00	2792.00	
44	Ru	19,279.20	19,150.40	21,656.80		2558.55	2554.31	2683.23	2836.00	2964.50	
45	Rh	20,216.10	20,073.70	22,723.60		2696.74	2692.05	2834.41	3001.30	3143.80	
46	Pd	21,177.10	21,020.10	23,818.70		2838.61	2833.29	2990.22	3171.79	3328.70	
47	Ag	22,162.92	21,990.30	24,942.40		2984.31	2978.21	3150.94	3347.81	3519.59	
48	Cd	23,173.60	22,984.10	26,095.50		3133.73	3126.91	3316.57	3528.12	3716.86	
49	In	24,209.70	24,002.00	27,275.90		3286.94	3279.29	3487.21	3713.81	3920.81	
50	Sn	25,271.30	25,044.00	28,486.00		3443.98	3435.42	3662.80	3904.86	4131.12	
51	Sb	26,359.10	26,110.80	29,725.60		3604.72	3595.32	3843.57	4100.78	4347.79	
52	Te	27,472.30	27,201.70	30,995.70		3769.33	3758.80	4029.58	4301.70	4570.90	
53	I	28,612.00	28,317.20	32,294.70		3937.65	3926.04	4220.72	4507.50	4800.90	
54	Xe	29,779.00	29,458.00	33,624.00		4109.90					
55	Cs	30,972.80	30,625.10	34,986.90		4286.50	4272.20	4619.80	4935.90	5280.40	
56	Ba	32,193.60	31,817.10	36,378.20		4466.26	4450.90	4827.53	5156.50	5531.10	
57	La	33,441.80	33,034.10	37,801.00		4650.97	4634.23	5042.10	5383.50	5788.50	833.00
58	Ce	34,719.70	34,278.90	39,257.30		4840.20	4823.00	5262.20	5613.40	6052.00	883.00
59	Pr	36,026.30	35,550.20	40,748.20		5033.70	5013.50	5488.90	5850.00	6322.10	929.00
60	Nd	37,361.00	36,847.40	42,271.30		5230.40	5207.70	5721.60	6089.40	6602.10	978.00
61	Pm	38,724.70	38,171.20	43,826.00		5432.50	5407.80	5961.00	6339.00	6892.00	–
62	Sm	40,118.10	39,522.40	45,413.00		5636.10	5609.00	6205.10	6586.00	7178.00	1081.00
63	Eu	41,542.20	40,901.90	47,037.90		5845.70	5816.60	6456.40	6843.20	7480.30	1131.00

Table D.3 (*continued*)

Z	Element	Line									
		Kα_1	Kα_2	Kβ_1	Kβ_3	Lα_1	Lα_2	Lβ_1	Lβ_2	Lγ_1	Mα_1
		K-L_3	K-L_2	K-M_3	K-M_2	K-L_3	L_3-M_5	L_2-M_4	L_3-N_5	L_2-N_4	M_5-N_7
64	Gd	42,996.20	42,308.90	48,697.00		6057.20	6025.00	6713.20	7102.80	7785.80	1185.00
65	Tb	44,481.60	43,744.10	50,382.00		6272.80	6238.00	6978.00	7366.70	8102.00	1240.00
66	Dy	45,998.40	45,207.80	52,119.00		6495.20	6457.70	7247.70	7635.70	8418.80	1293.00
67	Ho	47,546.70	46,699.70	53,877.00		6719.80	6679.50	7525.30	7911.00	8747.00	1348.00
68	Er	49,127.70	48,221.10	55,681.00		6948.70	6905.00	7810.90	8189.00	9089.00	1406.00
69	Tm	50,741.60	49,772.60	57,517.00		7179.90	7133.10	8101.00	8468.00	9426.00	1462.00
70	Yb	52,388.90	51,354.00	59,370.00		7415.60	7367.30	8401.80	8758.80	9780.10	1521.40
71	Lu	54,069.80	52,965.00	61,283.00		7655.50	7604.90	8709.00	9048.90	10,143.40	1581.30
72	Hf	55,790.20	54,611.40	63,234.00		7899.00	7844.60	9022.70	9347.30	10,515.80	1644.60
73	Ta	57,532.00	56,277.00	65,223.00		8146.10	8087.90	9343.10	9651.80	10,895.20	1710.00
74	W	59,318.24	57,981.70	67,244.30		8397.60	8335.20	9672.35	9961.50	11,285.90	1775.40
75	Re	61,140.30	59,717.90	69,310.00		8652.50	8586.20	10,010.00	10,275.20	11,685.40	1842.50
76	Os	63,000.50	61,486.70	71,413.00		8911.70	8841.00	10,355.30	10,598.50	12,095.30	1910.20
77	Ir	64,895.60	63,286.70	73,560.80		9175.10	9099.50	10,708.30	10,920.30	12,512.60	1979.90
78	Pt	66,832.00	65,112.00	75,748.00		9442.30	9361.80	11,070.70	11,250.50	12,942.00	2050.50
79	Au	68,803.70	66,989.50	77,984.00		9713.30	9628.00	11,442.30	11,584.70	13,381.70	2122.90
80	Hg	70,819.00	68,895.00	80,253.00		9988.80	9897.60	11,822.60	11,924.10	13,830.10	2195.30
81	Tl	72,871.50	70,831.90	82,576.00		10,268.50	10,172.80	12,213.30	12,271.50	14,291.50	2270.60
82	Pb	74,969.40	72,804.20	84,936.00		10,551.50	10449.50	12,613.70	12,622.60	14,764.40	2345.50
83	Bi	77,107.90	74,814.80	87,343.00		10,838.80	10,730.91	13,023.50	12,979.90	15,247.70	2422.60
84	Po	79,290.00	76,862.00	89,800.00		11,130.80	11,015.80	13,447.00	13,340.40	15,744.00	
85	At	81,520.00	78,950.00	92,300.00		11,426.80	11,304.80	13,876.00		16,251.00	
86	Rn	83,780.00	81,070.00	94,870.00		11,727.00	11,597.90	14,316.00		16,770.00	
87	Fr	86,100.00	83,230.00	97,470.00		12,031.30	11,895.00	14,770.00	14,450.00	17,303.00	
88	Ra	88,470.00	85,430.00	100,130.00		12,339.70	12,196.20	15,235.80	14,841.40	17,849.00	
89	Ac	90,884.00	87,670.00	102,850.00		12,652.00	12,500.80	15,713.00		18,408.00	
90	Th	93,350.00	89,953.00	105,609.00		12,968.70	12,809.60	16,202.20	15,623.70	18,982.50	2996.10
91	Pa	95,868.00	92,287.00	108,427.00		13,290.70	13,122.20	16,702.00	16,024.00	19,568.00	3082.30
92	U	98,439.00	94,665.00	111,300.00		13,614.70	13,438.80	17,220.00	16,428.30	20,167.10	3170.80
93	Np	101,059.00				13,944.10	13,759.70	17,750.20	16,840.00	20,784.80	
94	Pu	103,734.00				14,278.60	14,084.20	18,293.70	17,255.30	21,417.30	
95	Am	105,970.00				14,617.20	14,411.90	18,852.00	17,676.50	22,065.20	
96	Cm	108,759.00				14,954.00					3525.00

▣ **Table D.3** (*continued*)

Z	Element	Line									
		Kα_1	Kα_2	Kβ_1	Kβ_3	Lα_1	Lα_2	Lβ_1	Lβ_2	Lγ_1	Mα_1
		K-L$_3$	K-L$_2$	K-M$_3$	K-M$_2$	K-L$_3$	L$_3$-M$_5$	L$_2$-M$_4$	L$_3$-N$_5$	L$_2$-N$_4$	M$_5$-N$_7$
97	Bk	111,698.00				15,307.00					3616.00
98	Cf	114,801.00				15,655.00					3709.00
99	Es	119,080.00				16,036.00					
100	Fm	122,190.00				16,402.00					
101	Md	125,390.00				16,768.00					
102	No	128,660.00				17,139.00					
103	Lr	132,020.00				17,500.00					

D.9 X-ray Energy Levels

See ▣ Table D.4.

Table D.4 X-ray energy levels (electronvolts)

Z	Element	Line																							
		K	L_1	L_2	L_3	M_1	M^2	M_3	M_4	M_5	N_1	N_2	N_3	N_4	N_5	N_6	N_7	O_1	O_2	O_3	O_4	O_5	P_1	P_2	P_3
1	H	13.59811																							
2	He	24.58678																							
3	Li	54.75																							
4	Be	111.00																							
5	B	188.00		4.70																					
6	C	283.80		6.40																					
7	N	401.60		9.20																					
8	O	532.00	23.70	7.10																					
9	F	685.40	31.00	8.60																					
10	Ne	866.90	45.00	18.30																					
11	Na	1072.10	63.30	31.10																					
12	Mg	1305.00	89.40	51.40																					
13	Al	1559.60	117.70	73.10																					
14	Si	1838.90	148.70	99.20																					
15	P	2145.50	189.30	132.20																					
16	S	2472.00	229.20	164.80																					
17	Cl	2822.40	270.20	201.60	200.00	17.50	6.80																		
18	Ar	3202.90	320.00	247.30	245.20	25.30	12.40																		
19	K	3607.40	377.10	296.30	293.60	33.90	17.80																		
20	Ca	4038.10	437.80	350.00	346.40	43.70	25.40																		
21	Sc	4492.80	500.40	406.70	402.20	53.80	32.30		6.60																

Table D.4 (*continued*)

Z	Element	Line																							
		K	L_1	L_2	L_3	M_1	M^2	M_3	M_4	M_5	N_1	N_2	N_3	N_4	N_5	N_6	N_7	O_1	O_2	O_3	O_4	O_5	P_1	P_2	P_3
22	Ti	4966.40	563.70	461.50	455.50	60.30	34.60		3.70																
23	V	5465.10	628.20	520.50	512.90	66.50	37.80		2.20																
24	Cr	5989.20	694.60	583.70	574.50	74.10	42.50		2.30																
25	Mn	6539.00	769.00	651.40	640.30	83.90	48.60	48.60	3.30																
26	Fe	7112.00	846.10	721.10	708.10	92.90	54.00	54.00	3.60																
27	Co	7708.90	925.60	793.60	778.60	100.70	59.50	59.50	2.90																
28	Ni	8332.80	1008.10	871.90	854.70	111.80	68.10	68.10	3.60																
29	Cu	8978.90	1096.10	951.00	931.10	119.80	73.60	73.60	1.60																
30	Zn	9658.60	1193.60	1042.80	1019.70	135.90	86.60	86.60	8.10																
31	Ga	10,367.10	1297.70	1142.30	1115.40	158.10	106.80	102.90	17.40																
32	Ge	11,103.10	1414.30	1247.80	1216.70	180.00	127.90	120.80	28.70																
33	As	11,866.70	1526.50	1358.60	1323.10	203.50	146.40	140.50	41.20	41.20		2.50	2.50												
34	Se	12,657.80	1653.90	1476.20	1435.80	231.50	168.20	161.90	56.70	56.70		5.60	5.60												
35	Br	13,473.70	1782.00	1596.00	1549.90	256.50	189.30	181.50	70.10	69.00	27.30	5.20	4.60												
36	Kr	14,325.60	1921.00	1727.20	1674.90		222.70	213.80	88.90	88.90	24.00	10.60	10.60												
37	Rb	15,199.70	2065.10	1863.90	1804.40	322.10	247.40	238.50	111.80	110.30	29.30	14.80	14.00												
38	**Sr**	16,104.60	2216.30	2006.80	1939.60	357.50	279.80	269.10	135.00	133.10	37.70	19.90	19.90												
39	Y	17,038.40	2372.50	2155.50	2080.00	393.60	312.40	300.30	159.60	157.40	45.40	25.60	25.60												
40	Zr	17,997.60	2531.60	2306.70	2222.30	430.30	344.20	330.50	182.40	180.00	51.30	28.70	28.70												
41	Nb	18,985.60	2697.70	2464.70	2370.50	468.40	378.40	363.00	207.40	204.60	58.10	33.90	33.90	3.20											
42	Mo	19,999.50	2865.50	2625.10	2520.20	504.60	409.70	392.30	230.30	227.00	61.80	34.80	34.80	1.80											

Table D.4 *(continued)*

Z	Element	Line																							
		K	L_1	L_2	L_3	M_1	M^2	M_3	M_4	M_5	N_1	N_2	N_3	N_4	N_5	N_6	N_7	O_1	O_2	O_3	O_4	O_5	P_1	P_2	P_3
43	Tc	21,044.00	3042.50	2793.20	2676.90		444.90	425.00	256.40	252.90		38.90	38.90	2.00											
44	Ru	22,117.20	3224.00	2966.90	2837.90	585.00	482.80	460.60	283.60	279.40	74.90	43.10	43.10	2.50											
45	Rh	23,219.90	3411.90	3146.10	3003.80	627.10	521.00	496.20	311.70	307.00	81.00	47.90	47.90	1.50											
46	Pd	24,350.30	3604.30	3330.30	3173.30	669.90	559.10	531.50	340.00	334.70	86.40	51.10	51.10	3.30											
47	Ag	25,514.00	3805.80	3523.70	3351.10	717.50	602.40	571.40	372.80	366.70	95.20	62.60	55.90	9.30											
48	Cd	26,711.20	4018.00	3727.00	3537.50	770.20	650.70	616.50	410.50	403.70	107.60	66.90	66.90												
49	In	27,939.90	4237.50	3938.00	3730.10	825.60	702.20	664.30	450.80	443.10	121.90	77.40	77.40	16.20	16.20			0.10	0.80	0.80					
50	Sn	29,200.10	4464.70	4156.10	3928.80	883.80	756.40	714.40	493.30	484.80	136.50	88.60	88.60	23.90	23.90			0.90	1.10	1.10					
51	Sb	30,491.20	4698.30	4380.40	4132.20	943.70	811.90	765.60	536.90	527.50	152.00	98.40	98.40	31.40	31.40			6.70	2.10	2.10					
52	Te	31,813.80	4939.20	4612.00	4341.40	1006.00	869.70	818.70	582.50	572.10	168.30	110.20	110.20	39.80	39.80			11.60	2.30	2.30					
53	I	33,169.40	5188.10	4852.10	4557.10	1072.10	930.50	874.60	631.30	619.40	186.40	122.70	122.70	49.60	49.60			13.60	3.30	3.30					
54	Xe	34,561.40	5452.80	5103.70	4782.20		999.00	937.00		672.30		146.70	146.70												
55	Cs	35,984.60	5714.30	5359.40	5011.90	1217.10	1065.00	997.60	739.50	725.50	230.80	172.30	161.60	78.80	76.50			22.70	13.10	11.40					
56	Ba	37,440.60	5988.80	5623.60	5247.00	1292.80	1136.70	1062.20	796.10	780.70	253.00	191.80	179.70	92.50	89.90			39.10	16.60	14.60					
57	La	38,924.60	6266.30	5890.60	5482.70	1361.30	1204.40	1123.40	848.50	831.70	270.40	205.80	191.40	98.90	0.10			32.30	14.40						
58	Ce	40,443.00	6548.80	6164.20	5723.40	1434.60	1272.80	1185.40	901.30	883.30	289.60	223.30	207.20	110.00	2.00			37.80	19.80						
59	Pr	41,990.60	6834.80	6440.40	5964.30	1511.00	1337.40	1242.20	951.10	931.00	304.50	236.30	217.60	113.20	1.50			37.40	22.30						
60	Nd	43,568.90	7126.00	6721.50	6207.90	1575.30	1402.80	1297.40	999.90	977.70	315.20	243.30	224.60	117.50				37.50	21.10						
61	Pm	45,184.00	7427.90	7012.80	6459.30		1471.40	1356.90	1051.50	1026.90		242.00	242.00	120.40											
62	Sm	46,834.20	7736.80	7311.80	6716.20	1722.80	1540.70	1419.80	1106.00	1080.20	345.70	265.60	247.40	129.00	5.50			37.40	21.30						
63	Eu	48,519.00	8052.00	7617.10	6976.90	1800.00	1613.90	1480.60	1160.60	1130.90	360.20	283.90	256.60	133.20	0.00			31.80	22.00						

Table D.4 *(continued)*

Z	Element	Line K	L_1	L_2	L_3	M_1	M^2	M_3	M_4	M_5	N_1	N_2	N_3	N_4	N_5	N_6	N_7	O_1	O_2	O_3	O_4	O_5	P_1	P_2	P_3
64	Gd	50,239.10	8375.60	7930.30	7242.80	1880.80	1688.30	1544.00	1217.20	1185.20	375.80	288.50	270.90	140.50	0.10			36.10	20.30						
65	Tb	51,995.70	8708.00	8251.60	7514.00	1967.50	1767.70	1611.30	1275.00	1241.20	397.90	310.20	385.00	147.00	147.00	2.60		39.00	25.40	25.40					
66	Dy	53,788.50	9045.80	8580.60	7790.10	2046.80	1841.80	1675.60	1332.50	1294.90	416.30	331.80	292.90	154.20	154.20	4.20		62.90	26.30	26.30					
67	Ho	55,617.70	9394.20	8917.80	8071.10	2128.30	1922.80	1741.20	1391.50	1351.40	435.70	343.50	306.60	161.00	161.00	3.70		51.20	20.30	20.30					
68	Er	57,485.50	9751.30	9264.30	8357.90	2206.50	2005.80	1811.80	1453.30	1409.30	449.10	366.20	320.00	176.70	167.60	4.30		59.80	29.40	29.40					
69	Tm	59,389.60	10,115.70	9616.90	8648.00	2306.80	2089.80	1884.50	1514.60	1467.70	471.70	385.90	336.60	179.60	179.60	5.30		53.20	32.30	32.30					
70	Yb	61,332.30	10,486.40	9978.20	8943.60	2398.10	2173.00	1949.80	1576.30	1527.80	487.20	396.70	343.50	198.10	184.90	6.30		54.10	23.40	23.40					
71	Lu	63,313.80	10,870.40	10,348.60	9244.10	2491.20	2263.50	2023.60	1639.40	1588.50	506.20	410.10	359.30	204.80	195.00	6.90		56.80	28.00	28.00					
72	Hf	65,350.80	11,270.70	10,739.40	9560.70	2600.90	2365.40	2107.60	1716.40	1661.70	538.10	437.00	380.40	223.80	213.70	17.10		64.90	38.10	30.60					
73	Ta	67,416.40	11,681.50	11,136.10	9881.10	2708.00	2468.70	2194.00	1793.20	1735.10	565.50	464.80	404.50	241.30	229.30	25.00	25.00	71.10	44.90	36.40	5.70				
74	W	69,525.00	12,099.80	11,544.00	10,206.80	2819.60	2574.90	2281.00	1871.60	1809.20	595.00	491.60	425.30	258.80	245.40	36.50	33.60	77.10	46.80	35.60	6.10				
75	Re	71,676.40	12,526.70	11,958.70	10,535.30	2931.70	2681.60	2367.30	1948.90	1882.90	625.00	517.90	444.40	273.70	260.20	40.60	40.60	82.80	45.60	34.60	3.50				
76	Os	73,870.80	12,968.00	12,385.00	10,870.90	3048.50	2792.20	2457.20	2030.80	1960.10	654.30	546.50	468.20	289.40	272.80	46.30	46.30	83.70	58.00	45.40					
77	Ir	76,111.00	13,418.50	12,824.10	11,215.20	3173.70	2908.70	2550.70	2116.10	2040.40	690.10	577.10	494.30	311.40	294.90	63.40	60.50	95.20	63.00	50.50	3.80				
78	Pt	78,394.80	13,879.90	13,272.60	11,563.70	3296.00	3026.50	2645.40	2201.90	2121.60	722.00	609.20	519.00	330.80	313.30	74.30	71.10	101.70	65.30	51.70	2.20				
79	Au	80,724.90	14,352.80	13,733.60	11,918.70	3424.90	3147.80	2743.00	2291.10	2205.70	758.80	643.70	545.40	352.00	333.90	86.40	82.80	107.80	71.70	53.70	2.50				
80	Hg	83,102.30	14,839.30	14,208.70	12,283.90	3561.60	3278.50	2847.10	2384.90	2294.90	800.30	676.90	571.00	378.30	359.80	102.20	98.50	120.30	80.50	57.60	6.40				
81	Tl	85,530.40	15,346.70	14,697.90	12,657.50	3704.10	3415.70	2956.60	2485.10	2389.30	845.50	721.30	609.00	406.60	386.20	122.80	118.50	136.30	99.60	75.40	15.30	13.10			
82	Pb	88,004.50	15,860.80	15,200.00	13,035.20	3850.70	3554.20	3066.40	2585.60	2484.00	893.60	763.90	644.50	435.20	412.90	142.90	138.10	147.30	104.80	86.00	21.80	19.20	3.10	0.70	
83	Bi	90,525.90	16,387.50	15,711.10	13,418.60	3999.10	3696.30	3176.90	2687.60	2579.60	938.20	805.30	678.90	463.60	440.00	161.90	157.40	159.30	116.80	92.80	26.50	24.40		2.70	

Table D.4 *(continued)*

Z	Element	Line																								
		K	L_1	L_2	L_3	M_1	M^2	M_3	M_4	M_5	N_1	N_2	N_3	N_4	N_5	N_6	N_7	O_1	O_2	O_3	O_4	O_5	P_1	P_2	P_3
84	Po	93,105.00	16,939.30	16,244.30	13,813.80	4149.40	3854.10	3301.90	2798.00	2683.00	995.30	851.00	705.00	500.20	473.40										
85	At	95,729.90	17,493.00	16,784.70	14,213.50	4317.00	4008.00	3426.00	2908.70	2786.70	1042.00	886.00	740.00	533.20											
86	Rn	98,404.00	18,049.00	17,337.10	14,619.40	4482.00	4159.00	3538.00	3021.50	2892.40	1097.00	929.00	768.00	566.60											
87	Fr	101,137.00	18,639.00	17,906.50	15,031.20	4652.00	4327.00	3663.00	3136.20	2999.90	1153.00	980.00	810.00	603.30	577.00						31.40	31.40			
88	Ra	103,921.90	19,236.70	18,484.30	15,444.40	4822.00	4489.50	3791.80	3248.40	3104.90	1208.40	1057.60	879.10	635.90	602.70	298.90	298.90	254.40	200.40	152.80	67.20	67.20	43.50	18.80	
89	Ac	106,755.30	19,840.00	19,083.20	15,871.00	5002.00	4656.00	3909.00	3370.20	3219.00	1269.00	1080.00	890.00	674.90											
90	Th	109,650.90	20,472.10	19,693.20	16,300.30	5182.30	4830.40	4046.10	3490.80	3332.00	1329.50	1168.20	967.30	714.10	676.40	344.40	335.20	290.20	229.40	181.80	94.30	87.90	59.50	49.00	43.00
91	Pa	112,601.40	21,104.60	20,313.70	16,733.10	5366.90	5000.90	4173.80	3611.20	3441.80	1387.10	1224.30	1006.70	743.40	708.20	371.20	359.50	309.60	222.90	222.90	94.10	94.10			
92	U	115,606.10	21,757.40	20,947.60	17,166.30	5548.00	5182.20	4303.40	3727.60	3551.70	1440.80	1272.60	1044.90	780.40	737.70	391.30	380.90	323.70	259.30	195.10	105.00	96.30	70.70	42.30	32.30
93	Np	118,678.00	22,426.80	21,600.50	17,610.00	5723.20	5366.20	4434.70	3850.30	3665.80	1500.70	1327.70	1086.80	815.90	770.30	415.00	404.40		283.40	206.10	109.30	101.30			
94	Pu	121,818.00	23,097.20	22,266.20	18,056.80	5932.90	5541.20	4556.60	3972.60	3778.10	1558.60	1372.10	1114.80	848.90	801.40	445.80	432.40	351.90	274.10	206.50	116.00	105.40			
95	Am	125,027.00	23,772.90	22,944.00	18,504.10	6120.50	5710.20	4667.00	4092.10	3886.90	1617.10	1411.80	1135.70	878.70	827.60						115.80	103.30			
96	Cm	128,220.00	24,460.00	23,779.00	18,930.00	6288.00	5895.00	4797.00	4227.00	3971.00	1643.00	1440.00	1154.00					385.00							
97	Bk	131,590.00	25,275.00	24,385.00	19,452.00	6556.00	6147.00	4977.00	4366.00	4132.00	1755.00	1554.00	1235.00	398.00											
98	Cf	135,960.00	26,110.00	25,250.00	19,930.00	6754.00	6359.00	5109.00	4497.00	4253.00	1799.00	1616.00	1279.00	419.00											
99	Es	139,490.00	26,900.00	26,020.00	20,410.00	6977.00	6574.00	5252.00	4630.00	4374.00	1868.00	1680.00	1321.00	435.00											
100	Fm	143,090.00	27,700.00	26,810.00	20,900.00	7205.00	6793.00	5397.00	4766.00	4498.00	1937.00	1747.00	1366.00	454.00											
101	Md	146,780.00	28,530.00	27,610.00	21,390.00	7441.00	7019.00	5546.00	4903.00	4622.00	2010.00	1814.00	1410.00	472.00											
102	No	150,540.00	29,380.00	28,440.00	21,880.00	7675.00	7245.00	5688.00	5037.00	4741.00	2078.00	1876.00	1448.00	484.00											
103	Lr	154,380.00	30,240.00	29,280.00	22,360.00	7900.00	7460.00	5710.00	5150.00	4860.00	2140.00	1930.00	1480.00	490.00											

E Crystal Field Theory (CFT)

E.1 Introduction

Crystal field theory (CFT) was originally developed by the German physicist Hans Bethe in 1929 by applying the knowledge of both group theory and quantum mechanics to electrostatic theory. It was further improved in 1935 by John H. Van Vleck, and by Leslie Orgel in the 1940s to allow room for some covalency in the atomic interactions. These modifications are often referred to as ***ligand field theory***.[1] This theory was originally and successfully used to explain the color properties and magnetic behavior of ionic solids incorporating traces of first-row transition metal cations; that is, Sc ($Z = 21$) through Zn ($Z = 30$). All of these transition metals are characterized by subshell *d* electrons (see ◘ Table E.1). Crystal field theory can also be used to predict magnetic and spectral properties of ionic solids but cannot be applied to ligands forming strong covalent bonds such as sulfides, borides, and carbides.

In crystal field theory the main assumptions are that the attractive and repulsive forces that hold ions together are electrostatic in nature (i.e., there are no covalent interactions) and that the metal cation M^{n+} is surrounded by a given number of opposite-sign anions or electric dipoles, called **ligands** (L), to balance electrostatic charges and the system forms a transition metal complex in which ligands and cations are treated as simple point charges.

The number of ligands depends on the ratio of ionic radii of anions and cations (***Pauling's rules***), and is called the **coordination number** (CN). The polyhedral assembly adopts a minimum energy by optimizing its geometrical structure called a **coordination polyhedron**. Usually the octahedron (coordination number 6) and the tetrahedron (coordination number 4) are the most common coordination polyhedrons found for transition metals. The ligand point charges represent the crystal electrical field perturbing the *d* orbitals of the metal cation containing nonbonding electrons.

Historically, crystal field theory was first applied to the two inorganic solid compounds manganese(II) oxide (MnO) and copper(I) chloride (CuCl). When applied to alkali metal cations containing a symmetric sphere of charge, calculations of energies are generally quite successful. The approach taken uses classical potential energy equations that take into account the attractive and repulsive interactions between charged particles; that is, Coulomb's or electrostatic law interactions.

$$E_{\text{binding}} = -q_1 q_2/(4\pi\varepsilon_0 r),$$

where q_1 and q_2 are the electric charges of the interacting ion expressed in coulombs (C) and r is the distance separating them in meters (m). This leads to the correct prediction that large cations of low charge, such as K^+ and Na^+, exhibit low polarization (***hard and soft acids and bases theory (HSAB)***) and hence should form few coordination compounds. For first-row transition metal cations that contain differing numbers of *d* electrons in orbitals that are not spherically symmetric, however, the situation is quite different. The shape and occupation of these *d* orbitals become important in an accurate description of the bond energy and properties of the transition metal compound. Therefore, to be able to understand and use crystal field

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[1] C.J. Ballhausen, *J. Chem. Ed.* 56(1979)194–197, 215–218, 357–361

Table E.1 First-row transition elements with their ground electronic state

	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
Atomic number (*Z*)	21	22	23	24	25	26	27	28	29	30
Ground state electronic structure	$[Ar]4s^23d^1$	$[Ar]4s^23d^2$	$[Ar]4s^23d^3$	$[Ar]4s^13d^5$	$[Ar]4s^23d^5$	$[Ar]4s^23d^6$	$[Ar]4s^23d^7$	$[Ar]4s^23d^8$	$[Ar]4s^13d^{10}$	$[Ar]4s^23d^{10}$
Oxidation states[a]	*3*	2, 3, *4*	2, 3, 4, *5*	2, *3*, 6	*2*, 3, 4, 6, 7	2, *3*	*2*, 3	*2*, 3	1, *2*	2

[a] The major stable oxidation state is given in *italic type*

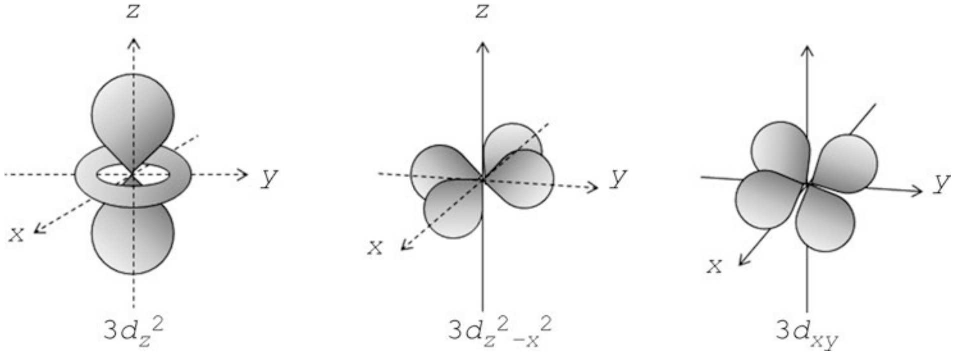

Fig. E.1 *d*-electron orbitals

theory, it is essential to have a clear picture of the shapes (i.e., angular dependence functions) of the *d* orbitals (see Fig. E.1).

E.2 Octahedral Crystal Field

If we consider a transition metal cation M^{n+} (e.g., Mn^{2+}) in its ground state, the free or isolated metal cation exhibits an electronic structure of $[Ar]4s^03d^5$, which is taken as the standard reference for the ground energy level. When the metal cation becomes surrounded by a spherical field of ligands (L^{q-}) (e.g., oxygen anions, O^{2-}), the negative electrostatic charge is distributed evenly on the surface of a sphere surrounding the cation with a radius equal to the M–L interatomic distance. The spherical symmetry of the free cation does not affect the degeneracy of the free cation 3*d* orbitals. The only effect of a spherical field is to raise the energy level of all 3*d* orbitals.

However, if the metallic cation is surrounded by only six ligands arranged toward the corners of an octahedron, this yields an octahedral symmetry called an ***octahedral ligand field*** (*Oh*)

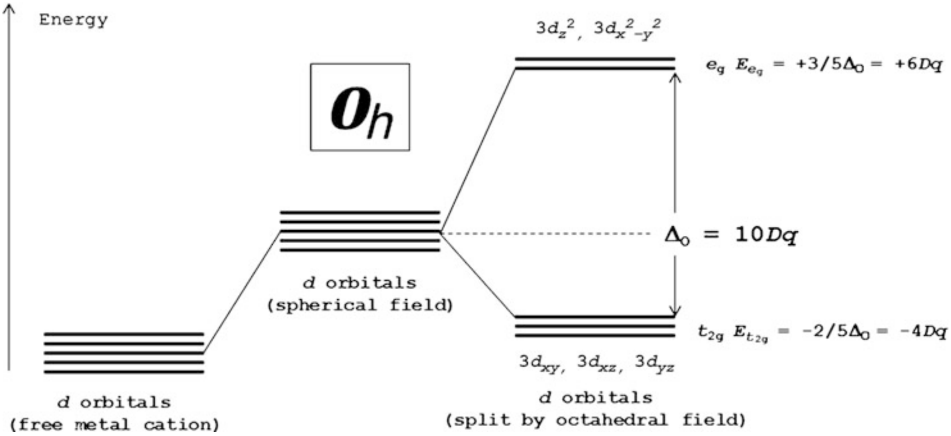

Fig. E.2 Octahedral crystal field splitting

in which a transition metal cation is hexacoordinated as ML_6 (e.g., MnO_6^{10-}). For simplicity, it is useful to consider a set of Cartesian coordinates (*xyz*) with the metal cation occupying the origin and the ligands oriented along the three major axes.

Because the electron density of each ligand donor exerts an electrostatic field toward the orbitals of the metal cation, the wave function increases the energy of electrons when the orbital is located in a region of high electron density, while it lowers it when the electron density is smaller. As the *s* orbitals are spherical, they are not affected by any type of crystal field geometry. The three 4*p* orbitals are still degenerate, and they still exhibit the same energy because each 4*p* orbital points toward two anion ligands at the corners of the octahedron. On the other hand, the electrostatic repulsion between electrons on the ligands and electrons in the 3*d* orbitals increases the energy of these orbitals.

Because the two 3*d* orbitals $3d_{x^2-y^2}$ and $3d_{z^2}$ on the metal cation point directly toward the six ligand anions and the three 3*d* orbitals 3*dxy*, 3*dxz*, and 3*dyz* lie between the ligands, the electron energy of the $3d_{x^2-y^2}$ and $3d_{z^2}$ orbitals increases much more than the energy of the 3*dxy*, 3*dxz*, and 3*dyz* orbitals. Therefore, the octahedral crystal field induces a splitting of energy levels called the ***crystal field splitting*** of the five 3*d* orbitals. As a result, the 3*dxy*, 3*dxz*, and 3*dyz* orbitals are now lower in energy than the $3d_{x^2-y^2}$ and $3d_{z^2}$ orbitals. By convention, the 3*dxy*, 3*dxz*, and 3*dyz* orbitals in an octahedral complex are denoted by the symbol $\boldsymbol{t_{2g}}$ according to a notation used in ***group theory***. On the other hand, the $3d_{x^2-y^2}$ and $3d_{z^2}$ orbitals are denoted by the symbol $\boldsymbol{e_g}$ (see ◘ Fig. E.2).

Because the two sets of 3*d* orbitals now differ, they are no longer degenerate and have distinct energy. Because of coulombic interactions, there is an electrostatic attraction between the positive cation nucleus and the ligand anions, and also an electrostatic repulsions between the electrons of M^{n+} and ligand electrons.

The ***splitting energy*** between the e_g and t_{2g} levels is called the octahedral ***crystal field stabilization energy*** (CFSE) and it is denoted by Δ_o, formerly denoted by 10 Dq. It is a measure of the crystal field strength and it is defined by the simple equation

$$\Delta_o = E_{e_g} - E_{t_{2g}} = 10\,\mathrm{Dq}.$$

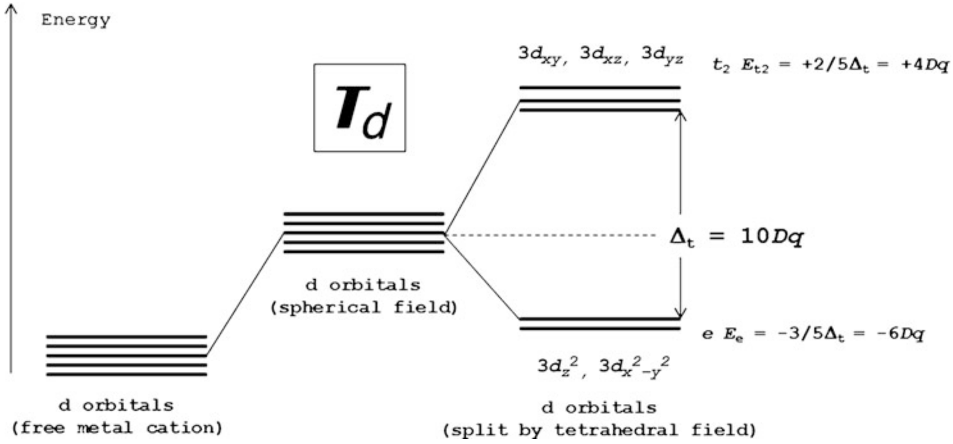

Fig. E.3 Tetrahedral crystal field splitting

When we redistribute the ligand charge from spherical to O_h, we do not change the total electrostatic potential energy of the system; therefore, the average energy of the t_{2g} and e_g orbitals in O_h must equal the energy of the original 3d orbitals in the spherical symmetry (see Fig. E.7):

$$0 = 3E_{t_{2g}} + 2E_{e_g}.$$

Therefore, the individual energies of each subelectronic level are given by the following equations:

$$E_{e_g} = +3/5\Delta_o = +6\,\mathrm{Dq},$$
$$E_{t_{2g}} = -2/5\Delta_o = -4\,\mathrm{Dq}.$$

As a general rule, the CFSE of an electronic configuration of the type $(t_{2g})p(e_g)q$ with p and q electrons respectively is simply given by the following equation:

$$\mathrm{CFSE} = 3q\Delta_o/5 - 2p\Delta_o/5 = (3q - 2p)\Delta_o/5 = (6q - 4p)\,\mathrm{Dq}.$$

The magnitude of the energy splitting of the t_{2g} and e_g orbitals is obtained from spectroscopic measurements, and it depends on the type of the metal cation, the cation valence, and the nature of the ligands.

E.3 Tetrahedral Crystal Field

If we consider a transition metal cation M^{n+}(e.g., Cu^{2+}) in its ground state, the free or isolated metal cation exhibits an electronic structure of $[Ar]4s^03d^9$, which is taken as the standard reference for the ground energy level. When the metal cation becomes surrounded by a spherical field of ligands (X^{q-}) (e.g., chloride anions, Cl^-), the negative electrostatic charge is distributed evenly on the surface of a sphere surrounding the cation with a radius equal to the M–X interatomic distance. The spherical symmetry of the free cation does not affect the degeneracy of the free cation 3*d* orbitals. The only effect of a spherical field is to raise the energy level of all 3*d* orbitals.

However, if the metallic cation is now surrounded by only four ligand anions arranged toward the corners of a tetrahedron, this yields a tetrahedral symmetry called a ***tetrahedral ligand field*** (T_d) in which a transition metal cation is tetracoordinated as MX_6 (e.g., $CuCl_4^{2-}$).

The electrostatic repulsions occurring between electrons that might be added to these orbitals and the electrons on the six ligand anions that surround the metal cation increase the energies of these orbitals. As previously, the 4*s* orbitals remains unaffected and the three 4*p* orbitals are still degenerate, but once again, the ligand anions in the crystal split the energy of the 3*d* orbitals on the transition metal cation. The tetrahedral crystal field splits these orbitals into the same t_2 and *e* sets of orbitals as does the octahedral crystal field (see ■ Fig. E.3).

But because the four ligands lie at alternating corners of a cube to form a tetrahedral geometry, the $3d_{x^2-y^2}$ and $3d_{z^2}$ orbitals of the metal cation point directly at the center of the cube and lie between the ligands, and the 3*dxy*, 3*dxz*, and 3*dyz* orbitals point toward the ligands. As a result, the splitting observed in a tetrahedral crystal field is the opposite of the splitting observed for an octahedral field. The two orbitals in the *e* set are now lower in energy than the three orbitals in the t_2 set.

The splitting energy between the *e* and t_2 levels is called the ***tetrahedral CFSE***, denoted by Δ_t (10 Dq) and defined as follows:

$$\Delta_t = E_{t_2} - E_e = 10\,\mathrm{Dq}.$$

Because the total energy of the system is zero,

$$0 = 3E_{t_2} + 2E_e.$$

Therefore, the individual energies of each subelectronic level is given by

$$E_{t_2} = +2/5\Delta_t = +4\,\mathrm{Dq},$$
$$E_e = -3/5\Delta_t = -6\,\mathrm{Dq}.$$

Because a tetrahedral complex has fewer ligands, the magnitude of the splitting is smaller. The difference between the energies of the t_2 and *e* orbitals in a tetrahedral complex (Δ_t) is slightly less than half that in analogous octahedral complexes (Δ_o):

$$\Delta_t = 4/9\Delta_o.$$

E.4 Factors Affecting the CFSE

The factors affecting the magnitude of the CFSE are as follows:

1. The ***valence*** or ***oxidation state*** of the metal cation: the higher the valence, the greater the CFSE. As a rule of thumb, the CFSE increases by approximately 50% when the oxidation state increases by one unit.

Table E.2 Jørgensen *f* and *g* factors for different anions. (Jørgensen, C.K. (1971) *Modern Aspects of Ligand Field Theory*. Elsevier, Amsterdam)

	Br^-	SCN^-	Cl^-	F^-	$C_2O_4^{2-}$	H_2O	NCS^-	NH_3	CN^-
f	0.72	0.73	0.78	0.90	0.99	1.00	1.02	1.25	1.70
Cation	Mn(II)	Ni(II)	Co(II)	V(II)	Fe(III)	Cr(III)	Co(III)	Mn(IV)	Mo(III)
g (cm^{-1})	8000	8700	9000	12,000	14,000	17,400	18,200	23,000	24,600

2. The ***nature*** of the metal cation. The CFSE increases from lighter to heavier transition metals ($3d < 4d < 5d$). For instance, it increases by approximately 50% on going from iron to ruthenium, and by approximately 25% on going from ruthenium to osmium.
3. The ***coordination number*** and the ***coordination polyhedron***. The octahedral CFSE is approximately 50% larger than the tetrahedral CFSE.
4. The ***nature of the ligands***.

E.5 The Spectrochemical Series

As mentioned previously, the splitting of *d* orbitals in the crystal field model depend not only on the geometry of the complex but also on the nature of the metal cation, the charge on this cation, and the ligands that surround the metal. When the coordination polyhedron and the metal cation are held constant, the ligands can be ordered by increasing field strength as follows:

$$\begin{aligned}&CO > CN^- > CH_3^-, C_6H_5^- > NO_2^- > NH_3 > SCN^- > H_2O > O^{2-} > OH^- >\\&F^-, N^{3-} > Cl^- > S^{2-} > Br^- > I^-.\end{aligned}$$

Ligands that give rise to large CFSEs are called ***strong-field ligands***, while the others are called ***weak-field ligands***.

Historically, because the CFSEs were measured directly by spectroscopic measurements based on absorption spectra of transition metal complexes, the series was called the ***ligand spectrochemical series***. The range of experimental values for a given geometry is wide. For instance, for an octahedral field, octahedral CFSE ranges from 100 kJ/mol for $Ni(H_2O)_6^{2+}$ to 520 kJ/mol for $Rh(CN)_6^{3-}$.

When the geometry and the ligands are held constant, the metals can be arranged according to a ***cation spectrochemical series***. The approximate order of this splitting decreases as follows.

$$\begin{aligned}&Pt^{4+} > Ir^{3+} > Pd^{4+} > Ru^{3+} > Rh^{3+} > Mo^{3+} > Co^{3+} > Cr^{3+} >\\&Fe^{3+} > V^{2+} > Fe^{2+} > Co^{2+} > Ni^{2+} > Mn^{2+}.\end{aligned}$$

Metal cations at one end of this series are called strong-field cations, because the splitting due to the crystal field is unusually strong, while cations at the other end are known as weak-field cations. Jørgensen[2] proposed a simple formula that allows the CFSE to be estimated:

$$\text{CFSE} = fg,$$

where the f is a function of the ligand and g is a function of the metal cation (see ◘ Table E.2).

E.6 High-Spin and Low-Spin Octahedral Complexes

Once the relative energies of the d orbitals in a transition metal complex are known, it is necessary to consider how these orbitals are filled with valence electrons so as to obtain the electron configuration. The following guidelines are used:

1. The system adopts the configuration of lowest possible energy.
2. The Pauli principle is obeyed.
3. Hund's rule is obeyed.

As for free metal cations, the degenerate orbitals are filled according to ***Hund's rule***; that is, the electrons occupy degenerate orbitals with the maximum number of parallel spins. This means that one unpaired electron is added to each of the degenerate orbitals in a subshell before a second electron is added to any orbital in the subshell. Electrons are added to a subshell with the same value of the spin quantum number until each orbital in the subshell has at least one electron.

In the case of octahedral transition metal cations with a $3d^1$, $3d^2$, or $3d^3$ electronic configuration, there is only one possible arrangement of electrons consistent with these simple guidelines (see ◘ Table E.3). The electrons in these arrangements occupy orbitals with $2/5\Delta_o$.

For octahedral complexes of transition metal cations with the electronic configuration $3d^4$, $3d^5$, $3d^6$, or $3d^7$, there are two possible arrangements consistent with the guidelines. The additional electron could be used to pair one of the electrons in the lower energy (t_{2g}) set of orbitals or it could be placed in one of the higher energy (e_g) orbitals. The system adopts the stabler arrangement, which depends on the relative magnitudes of Δ_o and P, where P is the ***pairing energy*** (i.e., the energy that must be added to the system to force two electrons to pair). There are two contributions to P: coulombic repulsion (i.e., the electrostatic repulsion between two electrons in the same region of space) and loss of exchange stabilization resulting from parallel spins (see ◘ Fig. E.4).

If $\Delta_o > P$, it is easier to pair two electrons than for one electron to occupy e_g. This leads to the minimum number of unpaired electrons, and is called the ***low-spin*** configuration.

If $\Delta_o < P$, it is easier for electrons to occupy e_g than to pair two electrons. This leads to the maximum number of unpaired electrons, and is called the ***high-spin*** configuration.

Finally, for octahedral complexes of transition metal cations with the electronic configuration $3d^8$, $3d^9$, or $3d^{10}$, there is again only one possibility.

Therefore, the choice between the high-spin and low-spin configuration narrows down to only octahedral complexes of transition metal cations with the electronic configuration $3d^4$, $3d^5$, $3d^6$, or $3d^7$.

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[2] JØrgensen, C.K. *Adv. Chem. Phys.* **5**(1963)33.

Table E.3 Octahedral complex configurations

3*d* electron configuration	High-spin state (low field)	Low-spin state (strong field)	High-spin/low-spin effect	Examples
$3d^0$	$(t_{2g})^0(e_g)^0$	$(t_{2g})^0(e_g)^0$	No	Sc^{3+} (colorless), Ti^{4+}, V^{5+}, Cr^{6+}
$3d^1$	1 $(t_{2g})^1(e_g)^0$	1 $(t_{2g})^1(e_g)^0$	No	Ti^{3+}, V^{4+}
$3d^2$	1 1 $(t_{2g})^2(e_g)^0$	1 1 $(t_{2g})^2(e_g)^0$	No	Ti^{2+}, V^{3+}
$3d^3$	1 1 1 $(t_{2g})^3(e_g)^0$	1 1 1 $(t_{2g})^3(e_g)^0$	No	V^{2+}, Cr^{3+}
$3d^4$	1 1 1 1 $(t_{2g})^3(e_g)^1$	11 1 1 $(t_{2g})^4(e_g)^0$	Yes	Cr^{2+}, Mn^{3+}
$3d^5$	1 1 1 1 1 $(t_{2g})^3(e_g)^2$	11 11 1 $(t_{2g})^5(e_g)^0$	Yes	Mn^{2+}, Fe^{3+}
$3d^6$	11 1 1 1 1 $(t_{2g})^4(e_g)^2$	11 11 11 $(t_{2g})^6(e_g)^0$	Yes	Fe^{2+}, Co^{3+}
$3d^7$	11 11 1 1 1 $(t_{2g})^5(e_g)^2$	11 11 11 1 $(t_{2g})^6(e_g)^1$	Yes	Co^{2+}, Ni^{3+}
$3d^8$	11 11 11 1 1 $(t_{2g})^6(e_g)^2$	11 11 11 1 1 $(t_{2g})^6(e_g)^2$	No	Ni^{2+}
$3d^9$	11 11 11 11 1 $(t_{2g})^6(e_g)^3$	11 11 11 11 1 $(t_{2g})^6(e_g)^3$	No	Cu^{2+}
$3d^{10}$	11 11 11 11 11 $(t_{2g})^6(e_g)^4$	11 11 11 11 11 $(t_{2g})^6(e_g)^4$	No	Zn^{2+} (colorless), Cu^{+}

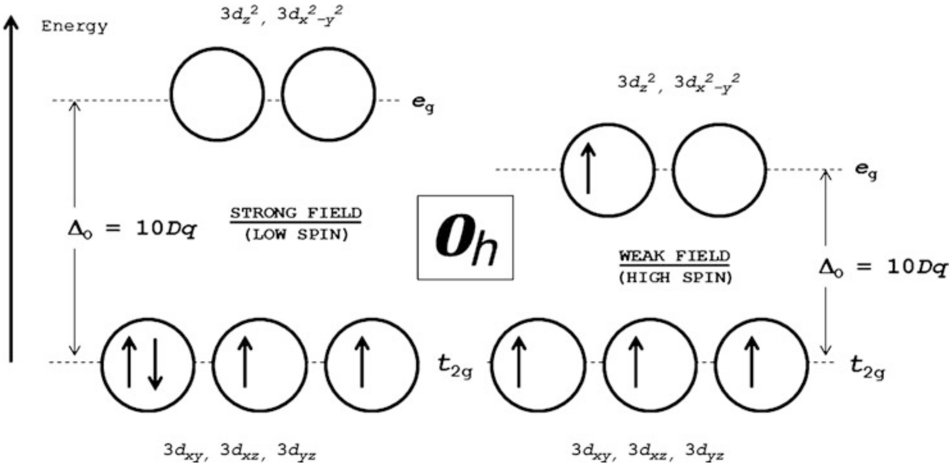
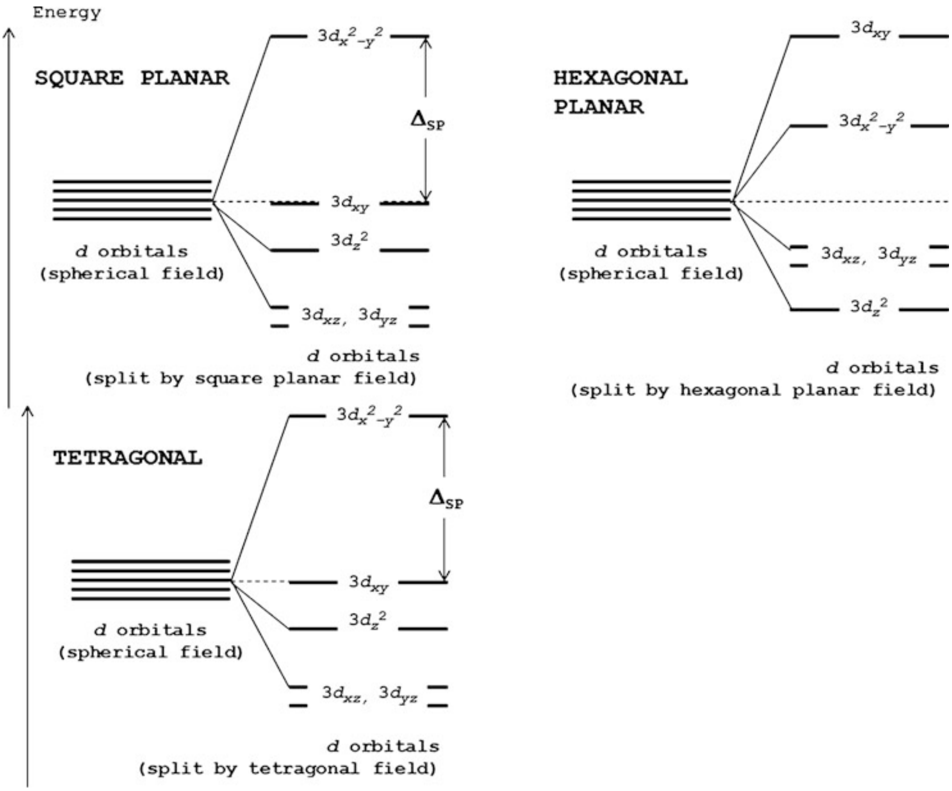


Fig. E.4 Low-spin and high-spin configurations



◘ **Fig. E.5** Square, tetragonal, and hexagonal crystal field splitting

As a result, we expect to find low-spin complexes among metal cations and ligands that lie toward the **high-field** end of the spectrochemical series. High-spin complexes are expected among metal cations and ligands that lie toward the **low-field** end of the series. The terms weak field and strong field give an indication of the splitting abilities of the ligand. For instance, water always gives rise to a small splitting of *d* orbitals for first-row transition metal cations and hence is referred to as a ***weak-field ligand***. Conversely, CN^- is a ***strong-field ligand***, since it causes a large splitting of the *d* orbitals. In conclusion, when metal cations with between four and seven electrons in the 3*d* orbitals form octahedral compounds, two possible electron allocations can occur, and this applies to the following transition metal cations: Cr(II), Mn(II), Mn(III), Fe(II), Co(II), Co(III), and Ni(III). These are referred to as either **weak field–strong field** or **high spin–low spin** configurations.

E.7 Other Crystal Field Splitting

In addition to tetrahedral and octahedral crystal field splitting, crystal field states corresponding to other symmetry environments are also found; for instance, square planar field, cubic field, hexagonal planar field, and tetragonal field (see ◘ Fig. E.5).

E.7.1 Tetragonal Crystal Field

A ***tetragonal crystal field*** complex is one containing either six ligands or five ligands and belonging to the D_{4h} or C_{4v} point group. For example, in the case of $[Co(NH_3)_4Cl_2^+]$, the ligand field strength of Cl^- is lower than that of NH_3, so $3d_{z^2}$ is stabilized compared with $d_{x^2-y^2}$, which is destabilized relative to the octahedral field. We can obtain the d-orbital splitting diagram for a tetragonal complex from that of the O_h complex by increasing or decreasing two bond lengths. An increase is called a tetragonal elongation. Pulling the z-axis ligands away makes d_{z^2} stabler. Further, it allows more room around the metal cation, so the ligands in the xy plane can move in closer, and thus $d_{x^2-y^2}$ becomes less stable. Similar electrostatic and geometric considerations allow us to conclude that dxy is destabilized and dxz and dyz are stabilized. The orbital degeneracy can be obtained directly from the character table. Finally, if instead of tetragonal elongation we perform tetragonal compression, the diagram will show reversed splitting.

E.8 Jahn–Teller Distortion Theorem

In a nonlinear molecule in an electronically degenerate state, distortion will occur to lower the symmetry, remove the degeneracy, and lower the electronic energy. The Jahn–Teller theorem[3] does not predict which types of distortions will occur, but the center of symmetry in a complex must remain constant.

E.9 Applications of Crystal and Ligand Field Theory

E.9.1 Assessment of Magnetic Properties

As discussed in Chap. 7, compounds in which all of the electrons are paired are diamagnetic and exhibit a negative magnetic susceptibility, while compounds that contain one or more unpaired electrons exhibit paramagnetism.

The force of attraction between paramagnetic complexes and a magnetic field is proportional to the number of unpaired electrons in the complex. We can therefore determine whether a complex is high spin or low spin by simply measuring the strength of the interaction between the complex and a magnetic field using a ***Gouy balance*** and determining the number of unpaired electrons by looking at the magnetic properties of a standard reference compound [e.g., mercury cobalt thiocyanate, $HgCo(SCN)_4$].

To predict the magnetic moment, we can use the simple formula

$$m = [4S(S+1)]^{1/2}\mu_B,$$

where S is the spin quantum number (1/2 for each unpaired electron).

An alternative representation is

$$m = [S(S+2)]^{1/2}\mu_B,$$

where n is the number of unpaired electrons. These simple formulas give good results for most first-row transition metal compounds, and they can be refined to include orbital contributions.

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[3] Jahn, H.A. and Teller, E. – *Proc. R. Soc. London,* Ser. A A236, 220, 1937.

E.9.2 Measurement of Ionic Radii

For a given oxidation state, the ionic radius decreases steadily on going from left to right in a transition series. Populating antibonding orbitals (i.e., filling the e_g levels in an octahedron) leads to an increase in ionic radius. Therefore, the ionic radius depends on the spin state of the metal (i.e., high spin or low spin).

E.10 Orgel Diagrams

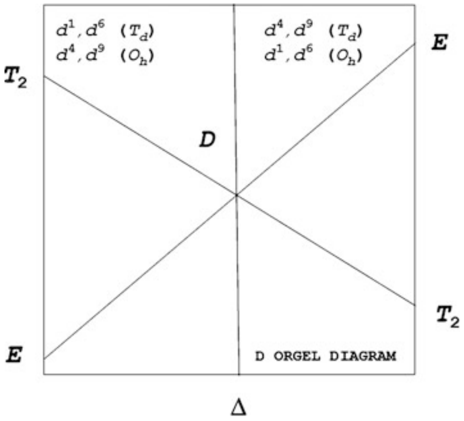
Orgel diagrams are correlation diagrams useful for showing the energy levels of electronic terms in high-spin octahedral and tetrahedral transition metal cations. They only show the spin-allowed transitions.

For complexes with D ground terms, only one electronic transition is expected, and the transition energy corresponds directly to *D*. The following high-spin configurations are considered with an Orgel diagram: d^1, d^4, d^6, and d^9. On the left-hand side of the diagram in ◘ Fig. E.6, tetrahedral (d^1, d^6), and octahedral (d^4, d^9) complexes are reported, while on the right-hand side of the diagram, tetrahedral (d^4, d^9) and octahedral (d^1, d^6) complexes are reported. For clarity, the *g* subscripts required for the octahedral complexes have been omitted.

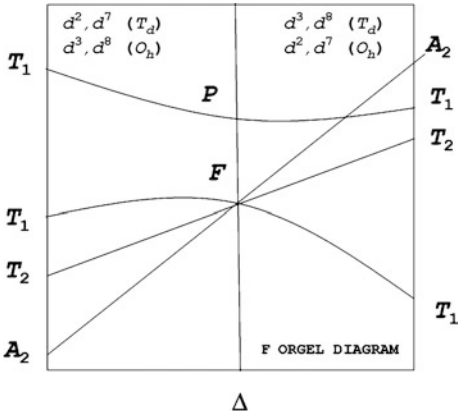
For complexes with F ground terms, three electronic transitions are expected, and *D* may not correspond directly to a transition energy. The following electronic configurations are considered: d^2, d^3, high-spin d^7, and d^8. On the left-hand side of the diagram in ◘ Fig. E.7, tetrahedral (d^2, d^7) and octahedral (d^3, d^8) complexes are reported, and on the right-hand side tetrahedral (d^3, d^8) and octahedral (d^2 and high-spin d^7) complexes are reported. Again for clarity, the *g* subscripts required for the octahedral complexes have been omitted.

On the left-hand side, the first transition corresponds to *D*, the equation to calculate the second contains expressions with both *D* and the configuration interaction (CI), and the third has expressions that contain Δ, CI, and the ***Racah parameter*** denoted by *B*′:

$4T_{2g} \rightarrow 4A_{2g}$ with transition energy Δ,
$4T_{1g}(F) \rightarrow 4A_{2g}$ with transition energy $= 9/5\Delta - CI$,
$4T_{1g}(P) \rightarrow 4A_{2g}$ with transition energy $= 6/5\Delta + 15B' + CI$.



◘ **Fig. E.6** Orgel diagram for complexes with D ground term



◘ **Fig. E.7** Orgel diagram for complexes with F and P ground terms

On the other hand, on the right-hand side of the diagram, the first transition can be unambiguously assigned to

$3T_{2g} \rightarrow 3T_{1g}$ with transition energy $4/5\Delta$ + CI.

But, depending on the size of the ligand field (Δ), the second transition may be due to

$3A_{2g} \rightarrow 3T_{1g}$ with transition energy $9/5D$ + CI (weak field),
$3T_{1g}(P) \rightarrow 3T_{1g}$ with transition energy $3/5D + 15B' + 2$CI (strong field).

E.11 Tanabe–Sugano Diagrams

An alternative method for calculation of the CFSE from atomic spectra uses ***Tanabe–Sugano*** diagrams,[4] which are able to predict the transition energies for both spin-allowed and spin-forbidden transitions, as well as for both strong-field (low-spin) and weak-field (high-spin) complexes. Most textbooks give Tanabe–Sugano diagrams only for octahedral complexes and a separate diagram is required for each configuration. In this representation, the energy of the electronic states is given on the y-axis and the ligand field strength increases on the x-axis from left to right. Linear lines are found when there are no other terms of the same type, and curved lines are found when two or more terms are repeated. This is as a result of the "noncrossing rule." The baseline in the Tanabe–Sugano diagram represents the lowest-energy or ground-term state (see ◘ Figures E.8–E.11).

E.12 Nephelauxetic Effect

The ***nephelauxetic effect*** consists in a reduction of the interelectronic repulsion because the electrons are delocalized somewhat onto the ligands. Ionic ligands such as fluoride anions give

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[4] Tanabe, Y.; and Sugano, S. *J. Phys. Soc. Japan* **9**(1954)753–766

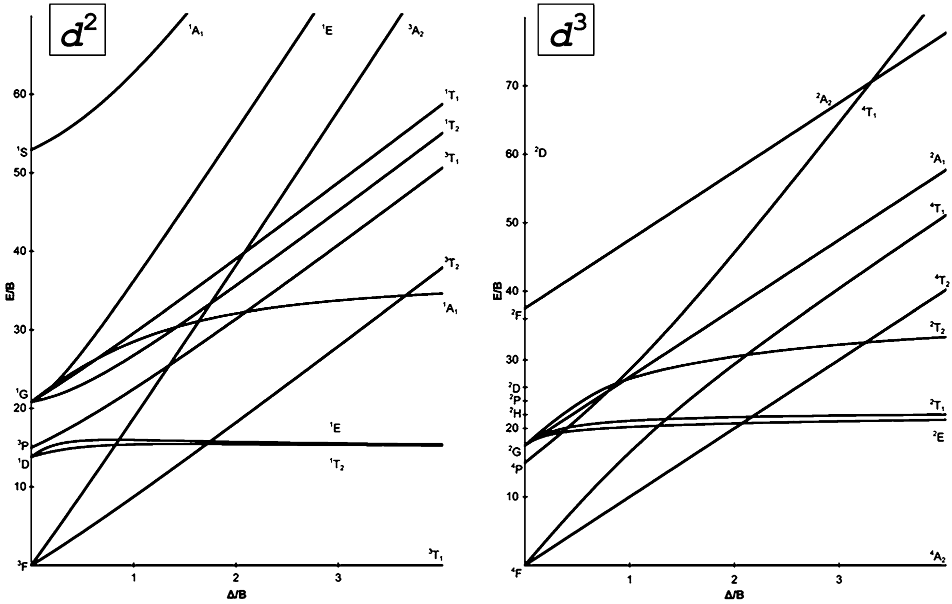


Fig. E.8 Tanabe–Sugano diagrams for d^2 and d^3 configurations

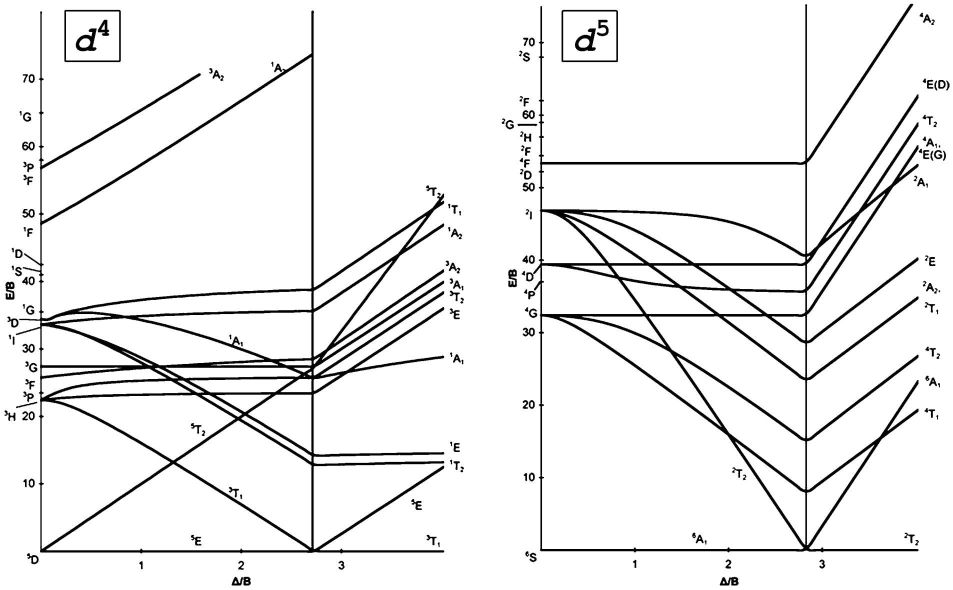
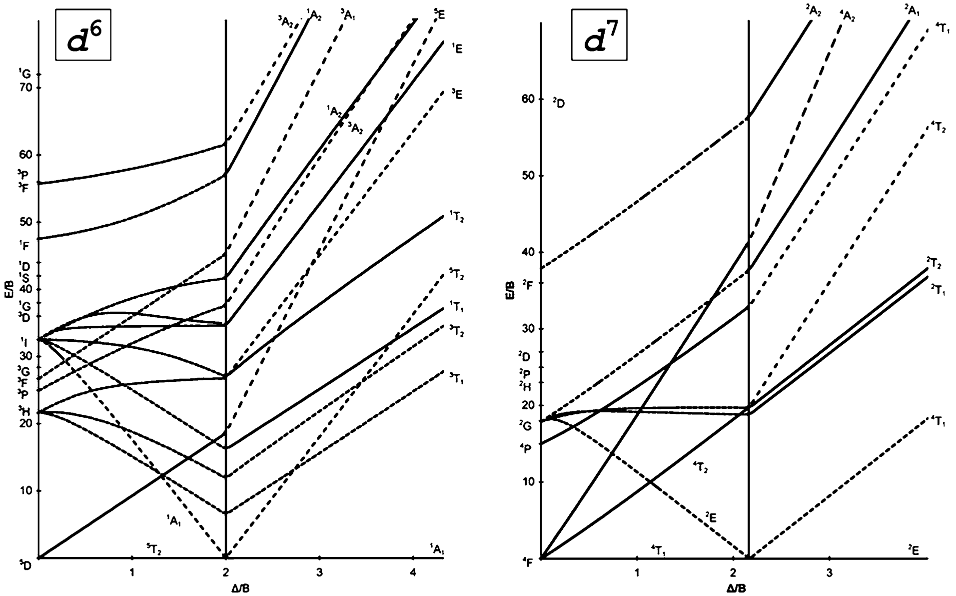
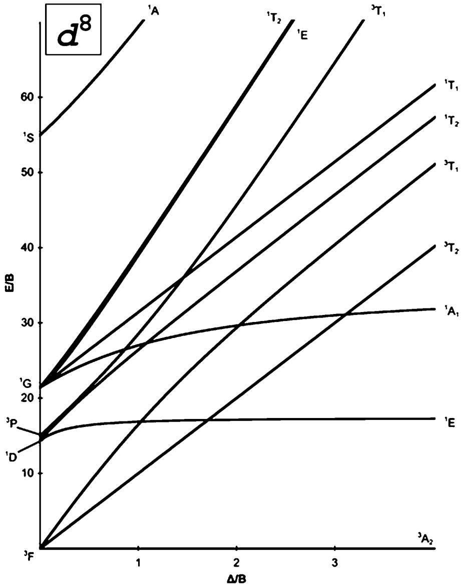


Fig. E.9 Tanabe–Sugano diagrams for d^4 and d^5 configurations



■ **Fig. E.10** Tanabe–Sugano diagrams for d^6 and d^7 configurations



■ **Fig. E.11** Tanabe–Sugano diagrams for d^8 configuration a small reduction in B, while covalently bonded ligands such as iodides give a large reduction in B. This can be exemplified by the so-called ***nephelauxetic series***, as follows:

$$F^- > H_2O > NH_3 > C_2O_4^{2-} > SCN^- > Cl^-, CN^- > Br^- > S^{2-}, I^-.$$

E.13 Further Reading

BALLHAUSEN, C.J. (1962) *Introduction to Ligand Field Theory*. McGraw Hill, New York.
FIGGIS, B.N. (1966) *Introduction to Ligand Fields*. Wiley, New York.
JØRGENSEN, C.K. (1971) *Modern Aspects of Ligand Field Theory*. Elsevier, Amsterdam.
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BURNS, R.G. (1993) *Mineralogical Applications of Crystal Field Theory, 2nd edn.* Cambridge University Press, London.

F Crystallography and Crystallochemistry

F.1 Direct Space Lattice Parameters

A crystal is a periodic array of ordered entities (e.g., ions, atoms, molecules) in three dimensions. The repeating unit is imagined to be a unit cell whose volume and shape are designated by the three vectors representing the length and direction of the cell edges as three unit vectors of translation.

A space lattice is defined by either the three unit lattice vectors **a**, **b**, and **c** or the set of the six lattice parameters: a, b, c, α, β, and γ, where the last three quantities represent the plane angles between the cell edges. The International Union of Crystallography has standardized the notation and definition of space lattice parameters, and this international standard nomenclature is listed below:

$\alpha \equiv \angle(b, c)$ and plane A ≡ (b, c)
$\beta \equiv \angle(c, a)$ and plane B ≡ (c, a)
$\gamma \equiv \angle(a, b)$ and plane C ≡ (a, b)

There are seven possible space lattices that entirely describe both inorganic and organic crystalline materials. These are called the seven crystal systems (i.e., cubic, tetragonal, hexagonal, trigonal, orthorhombic, monoclinic, and triclinic).

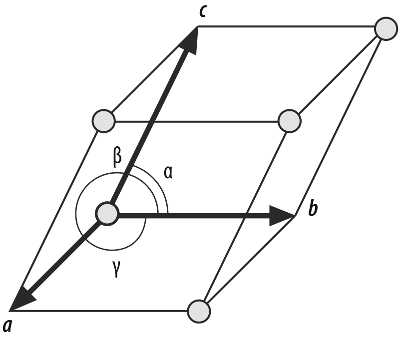
F.2 Symmetry Elements

See ◘ Table F.1.

F.3 The Seven Crystal Systems

See ◘ Table F.3.

The five platonic polyhedrons are listed in ◘ Table F.2.



◘ **Fig. F.1** International Union of Crystallography standardized notation for space lattice parameters

Table F.1 Symmetry element notation

Symmetry element	Notation		Symmetry operation
	International Hermann–Mauguin	Old Schoenflies–Fedorov	
Center	1	C_i	Center of inversion
Reflection plane (mirror)	m	C_s	Single reflection plane of symmetry
n-fold rotation axis	n	C_n	n-fold rotation axis with $n = 2, 3, 4$, and 6, the angle of rotation, A, expressed in radians is given by A (rad) = $2\pi/n$
Inversion axis	n	C_{ni}	Vertical n-fold rotation axis followed, by an inversion by a symmetry center lying on the axis (2 = m, 3, 4 =, 6)
Glide plane	a, b, c, n, d	–	Reflection in a plane followed by a translation according to a vector parallel to the plane. Translation in the **a** direction: a, Translation in the **b** direction: b, Translation in the **c** direction: c, Translation in the 1/2(**a** + **b**) or face diagonal direction: n, Translation in the 1/2(**a** + **b** + **c**) or volume diagonal direction: d
Screw axis	n_m	–	Vertical n-fold axis, followed by a translation parallel to the axis
Rotary-reflection axis	$\sim n$	S_n	Point group with an n-fold axis of rotary reflection

Table F.2 Five Platonic regular polyhedrons

Regular polyhedron	Description	Volume	Surface area	No. of faces	No. of edges	No. of vertices
Tetrahedron	Equilateral triangle	$a^3\sqrt{2}/12$	$a^2\sqrt{3}$	4	6	4
Octahedron	Equilateral triangle	$a^3\sqrt{2}/3$	$2a^2\sqrt{3}$	8	12	6
Hexahedron (cube)	Square	a^3	$6a^2$	6	12	8
Pentagonal dodecahedron	Regular pentagon	$a^3(15 + 7\sqrt{5})/4$	$3a^2[5(5 + 2\sqrt{5})]^{1/2}$	12	30	20
Icosahedron	Equilateral triangle	$5a^3(3 + \sqrt{5})/12$	$5a^2\sqrt{3}$	20	30	12

■ **Table F.3** The seven crystal systems

Crystal system	**Synonyms, old names**	**Symbol**	**Geometrical description**	**Symmetry**		**Lattice parameters (IUCr) (edge length, interaxial angles)**
				Hermann–Mauguin	**Schoenflies–Fedorov**	
Cubic	Isometric	C (c)	Cube	$m3m$	O_h	$a = b = c$ $\alpha = \beta = \gamma = \pi/2$ rad
Hexagonal		H (h)	Upright prism with a regular hexagonal base	$6/mmm$	D_{6h}	$a = b \neq c$ $\alpha = \beta = \pi/2$ rad and $\gamma = 2\pi/3$ rad
Tetragonal	Quadratic	T (t)	Upright prism with a square base	$4/mmm$	D_{4h}	$a = b \neq c$ $\alpha = \beta = \gamma = \pi/2$ rad
Rhombohedral	Trigonal	R (h)	Prism with each face equal to identical lozenges	$3m$	D_{3d}	$a = b = c$ $\alpha = \beta = \gamma \neq \pi/2$ rad
Orthorhombic	Orthogonal	O (o)	Upright prism with a rectangular base	mmm	D_{2h}	$a \neq b \neq c$ $\alpha = \beta = \gamma = \pi/2$ rad
Monoclinic	Clinorhombic	M (m)	Inclined prism with a rectangular base	$2/m$	C_{2h}	$a \neq b \neq c$ $\alpha = \gamma = \pi/2$ rad and $\beta > 2\pi/3$ rad
Triclinic	Anorthic	T (a)	Uneven prism	1	C	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq \pi/2$ rad

IUCr International Union of Crystallography

F.4 Conversion of a Rhombohedral to a Hexagonal Lattice

The rhombohedral unit cell is defined by three equal-length unit translations a, and the plane angle between them, α. The rhombohedral latticespace latticeparameters parameters can be converted to hexagonal lattice parameters with use of the following equations:

$$a_\mathrm{H} = 2a_\mathrm{R}\sin(\alpha/2),$$

$$c_\mathrm{H} = 3(a_\mathrm{R}^2 - 2a_\mathrm{H}^2/3)^{1/2}.$$

F.5 The 14 Bravais Space Lattices

See ■ Table F.4.

Table F.4 The 14 Bravais space lattices

Crystal system	Bravais space lattice	ASTM notation	Hermann–Mauguin symbol	Pearson notation
Cubic	Primitive cell	C	*P*	*cP*1
	Body centered	B	*I*	*cI*2
	Face centered	F	*F*	*cF*4
Hexagonal	Primitive cell	H	*P*	*hP*2
Tetragonal	Primitive cell	T	*P*	*tP*1
	Body centered	U	*I*	*tI*2
Rhombohedral	Primitive cell	R	*R*	*hR*1
Orthorhombic	Primitive cell	O	*P*	*oP*1
	Base centered	Q	*A*, *B*, *C*	*oA*2
	Body centered	P	*I*	*oI*2
	Face centered	S	*F*	*oF*4
Monoclinic	Primitive cell	M	*P*	*mP*1
	Base centered	N	*A*, *B*, *C*	*mP*2
Triclinic	Primitive cell	A	*P*	*aP*1

A, *B*, *C* faces orthogonal to lattice vectors **a**, **b**, and **c** respectively, *F* face centered (from German *flächenzentriert*), *I* body centered (from German *innenzentriert*), *P* primitive

Table F.5 Characteristics of close-packed-arrangements

Parameters	Simple cubic	Body-centered cubic	Face-centered cubic	Hexagonal close packed
Notation	sc, *P*	bcc, *I*	fcc, *F*	hcp
Unit cell volume	a^3	a^3	a^3	$a^2c\sqrt{3}/2$
Number of entities per unit cell	1	2	4	2
Primitive cell volume	a^3	$a^3/2$	$a^3/4$	$a^2c\sqrt{3}/12$
Number of first-neighbor entities (coordination number)	6	8	12	12
Number of second-neighbor entities	12	6	6	12
Smallest distance between first neighbors	a	$a\sqrt{3}/2 \cong 0.866a$	$a/\sqrt{2} \cong 0.707a$	a
Smallest distance between second neighbors	$a\sqrt{2} = 1.414a$	a	a	$a\sqrt{3}$
Packing fraction	$\pi/6 \cong 0.524$	$\pi\sqrt{3}/8 \cong 0.680$	$\pi\sqrt{2}/6 \cong 0.740$	$\pi\sqrt{2}/6 \cong 0.740$

F.6 Characteristics of Close-Packed Arrangements

See ■ Table F.5.

F.7 The 32 Classes of Symmetry

The Schoenflies-Fedorov notation is listed in ■ Table F.6.

They are ten elements of symmetry in crystalscrystals. These ten symmetry operators can be combined in 32 ways to produce the 32 point groups given in ■ Table F.7.

■ **Table F.6** Schoenflies–Fedorov point group crystal notation

Notation	Description
C_n	Point group with a single n-fold rotation axis
C_{nh}	Point group with a single vertical n-fold rotation axis, together with a horizontal mirror plane
C_{nv}	Point group with a single vertical n-fold rotation axis, together with a vertical mirror plane
D_n	Point group with a single vertical n-fold rotation axis, together with a twofold rotation axis perpendicular to it
V	Alternative symbol to D_2
O	Holohedral cubic point group
T	Tetartohedral cubic point groups
S_n	Point group with an n-fold axis of rotary reflection
i	Center of inversion
s	Single plane of symmetry
d	Diagonal reflection plane, bisecting the angle between two horizontal axes

■ **Table F.7** The 32 classes of symmetry

Crystal system	Hermann–Mauguin symbol	Schoenflies–Fedorov symbol	Crystal morphology, and names of classes according to Von Grothcrystal	Typical mineral	Class no.
Cubic	$m3m$	O_h	Cubic hexaoctahedral (holohedral)	Galena, PbS	32
	$\bar{4}3m$	T_d	Cubic hexatetrahedral (tetrahedral)	Sphalerite, ZnS	31
	$m3$	T_h	Cubic dyakisdodecahedral (diploidal or pyritohedral)	Pyrite, FeS_2	30
	432	O	Cubic pentagonal icositetrahedral (gyroidal or plagiohedral)	Cuprite, Cu_2O	29
	23	T	Cubic tetrahedral pentagonal dodecahedral (tetartohedral)	Ullmannite, NiSSb	28

Table F.7 (*continued*)

Crystal system	Hermann–Mauguin symbol	Schoenflies–Fedorov symbol	Crystal morphology, and names of classes according to Von Grothcrystal	Typical mineral	Class no.
Hexagonal	$6/mmm$	D_{6h}	Dihexagonal dipyramidal (holohedral)	Beryl, $Be_3Al_2[Si_6O_{18}]$	27
	$6mm$	C_{6v}	Dihexagonal pyramidal (hemimorphic)	Greenockite, CdS	26
	$6/m$	C_{6h}	Hexagonal dipyramidal (pyramidal)	Apatite, $Ca_5(PO_4)_3(F,OH, Cl)$	25
Hexagonal	622	D_6	Hexagonal trapezohedral (trapezohedral)	Kalsilite	24
	6	C_6	Hexagonal pyramidal (tetartohedral)	Nepheline, $KNa_3Si_4Al_4O_{16}$	23
	$\bar{6}m2$	D_{3h}	Ditrigonal dipyramidal (trigonal holohedral)	Benitoite, $BaTiSi_3O_9$	22
	$\bar{6}$	C_{3n}	Trigonal–dipyramidal	Silver orthophosphate, Ag_2HPO_4	19
Trigonal (rhombohedral)	$\bar{3}m$	C_{3d}	Hexagonal scalenoedral (ditrigonal pyramidal, holohedral)	Calcite, $CaCO_3$	21
	$3m$	C_{3v}	Ditrigonal pyramidal (hemimorphic hemihedral)	Tourmaline	20
	32	D_3	Trigonal trapezohedral	α-Quartz, SiO_2	18
	$\bar{3}$	$S_5 = C_{3i}$	Trigonal rhombohedral	Dolomite, $CaMg(CO_3)_2$	17
	3	C_3	Trigonal–pyramidal (tetartohedral)	Sodium periodate, $NaIO_4$	16
Tetragonal	$4/mmm$	D_{4h}	Ditetragonal dipyramidal (holohedral)	Zircon, $ZrSiO_4$	15
	$4mm$	C_{4v}	Ditetragonal pyramidal (hemimorphic hemihedral)	Diaboleite, $2Pb(OH)_2 \cdot CuCl_2 \cdot 6H_2O$	14
	$4/m$	C_{4h}	Tetragonal dipyramidal (paramorphic hemihedral)	Scheelite, $CaWO_4$	13
	422	D_4	Tetragonal trapezohedral (enantiomorphic hemihedral)	Phosgenite, $NiSO_4$	12
	$\bar{4}2m$	$V_4 = D_{2d}$	Tetragonal scalenohedral (sphenoidal, hemihedral of the second sort)	Chalcopyrite, $CuFeS_2$	11
	4	C_4	Tetragonal pyramidal (tetartohedral)	Wulfenite, $PbMoO_4$	10
	$\bar{4}$	S_4	Tetragonal disphenoidal (ogdohedral)	Cahnite, $Ca_4B_2As_2O_{12} \cdot 4H_2O$	9

Table F.7 *(continued)*

Crystal system	Hermann–Mauguin symbol	Schoenflies–Fedorov symbol	Crystal morphology, and names of classes according to Von Grothcrystal	Typical mineral	Class no.
Orthorhombic	*mmm*	$V_h = D_{2h}$	Orthorhombic dipyramidal (holohedral)	Barite, $BaSO_4$	8
	*mm*2	C_{2v}	Orthorhombic pyramidal (hemimorphic hemihedral)	Topaz	7
	222	$V = D_2$	Orthorhombic disphenoidal (enantiomorphic hemihedral)	Sulfur, S_8	6
Monoclinic	2/*m*	C_{2h}	Rhomboidal prismatic (holohedral)	Gypsum, $CaSO_4$	5
	m	$C_{h1} = CS$	Monoclinic domatic (clinohedral, hemihedral)	Clinohedrite, $CaZnHSiO_5$	4
	2	C_2	Monoclinic sphenoidal (hemimorphic hemihedral)	Tartaric acid	3
Triclinic	$\bar{1}$	*Ci*	Triclinic pinacoidal (holohedral)	Axinite, $CuSO_4$	2
	1	C_1	Triclinic asymmetric (pedial, hemihedral)	Calcium thiosulfate, CaS_2O_3	1

F.8 *Strukturbericht* Structures

See Tables F.8–F.13.

Table F.8 *Strukturbericht* designations for pure elementspure elements (i.e., A type)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
A_a	α-Protoactinium	Tetragonal	*I*4/*mmm*	*tI*2
A_b	β-Uranium	Tetragonal	*P*4*nm*	*tP*30
A_c	α-Neptunium	Orthorhombic	*Pmcn*	*oP*8
A_d	β-Neptunium	Tetragonal	$P42_1$	*tP*4
A_e	β-$TiCu_3$	Orthorhombic	*Cmcm*	*oC*4
A_f	$HgSn_{10}$	Hexagonal	*P*6/*mmm*	*hP*1
A_g	γ-Boron	Tetragonal	*P*4*n*2	*tP*50
A_h	α-Polonium	Cubic	$Pm\bar{3}m$	*cP*1
A_i	β-Polonium	Rhombohedral	$R\bar{3}m$	*tR*1
A_k	α-Selenium	Monoclinic	$P2_1/n$	*mP*32
A_l	β-Selenium	Monoclinic	$P2_1/a$	*mP*32

Table F.8 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
A1	Copper	Cubic (fcc)	$Fm\bar{3}m$	*cF*4
A2	Tungsten	Cubic (bcc)	$Im\bar{3}m$	*cI*2
A3	Magnesium	Hexagonal (hcp)	$P6_3/mmc$	*hP*2
A4	Diamond	Cubic	$Fd\bar{3}m$	*cF*8
A5	*β*-Tin (white)	Tetragonal	$I4/amd$	*tI*4
A6	Indium	Tetragonal	$F4/mmm$	*tF*4
A7	*α*-Arsenic	Rhombohedral	$R\bar{3}m$	*hR*2
A8	*γ*-Selenium	Trigonal	$P3_221$	*hP*3
A9	Graphite	Hexagonal	$P6_3/mmc$	*hP*4
A10	*α*-Mercury	Rhombohedral	$R3m$	*hR*1
A11	*α*-Gallium	Orthorhombic	$Cmca$	*oC*8
A12	*α*-Manganese	Cubic	$I43m$	*cI*58
A13	*β*-Manganese	Cubic	$P4_13$	*cP*20
A14	Iodine (I_2)	Orthorhombic	$Pm\bar{3}n$	*cP*8
A15	*β*-Tungsten (W_3O), or Cr_3Si	Cubic	$Pm\bar{3}n$	*cP*8
A16	*α*-Sulfur (S_4)	Orthorhombic	$Fddd$	*oF*128
A17	Phosphorus (black)	Orthorhombic	$Cmca$	*oC*8
A19	Polonium	Monoclinic	n. a.	n. a.
A20	*α*-Uranium	Orthorhombic	$Cmcm$	*oC*4

bcc body-centered cubic, *fcc* face-centered cubic, *hcp* hexagonal close packed, *n. a.* not available

Table F.9 *Strukturbericht* designations for binary compoundsbinary compounds (AX type)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
B_a	CoU	Cubic	$I2_13$	*cI*16
B_b	*ζ*-AgZn	Hexagonal	$P\bar{3}$	*hP*9
B_c	CaSi	Orthorhombic	$Cmmc$	*oC*8
B_d	*η*-NiSi	Orthorhombic	$Pbnm$	*oP*8
B_e	CdSb	Orthorhombic	$Pbca$	*oP*16
B_f	CrB	Orthorhombic	$Cmcm$	*oC*8
B_g	MoB	Tetragonal	$I4/amd$	*tI*16
B_h	WC	Hexagonal	$P\bar{6}/mmm$	*hP*2

Table F.9 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
B_i	γ-MoC	Hexagonal	$P6_3/mmc$	$hP8$
B_k	BN	Hexagonal	$P6_3/mmc$	$hP4$
B_l	AsS (realgar)	Monoclinic	$P2_1n$	$mP32$
B_m	TiB	Orthorhombic	$Pnma$	$oP8$
B1	NaCl (halite, rock salt)	Cubic	$Fm\bar{3}m$	$cF8$
B2	CsCl	Cubic	$Pm\bar{3}m$	$cP2$
B3	ZnS (sphalerite)	Cubic	$F\bar{4}3m$	$cF8$
B4	ZnS (wurtzite)	Hexagonal	$P6_3mc$	$hP4$
$B8_1$	α-NiAs	Hexagonal	$P6_3/mmc$	$hP4$
$B8_2$	β-Ni_2In	Hexagonal	$P6_3/mmc$	$hP4$
B9	HgS (cinnabar)	Hexagonal	$P3_121$	$hP6$
B10	LiOH (lithine)	Tetragonal	$P4/nmm$	$tP4$
B11	PbO (massicot)	Tetragonal	$P4/nmm$	$tP4$
B12	BN	Hexagonal	$P6_3mc$	$hP4$
B13	NiS (millerite)	Hexagonal	$R\bar{3}m$	$hR6$
B16	GeS	Orthorhombic	$Pnma$	$oP8$
B17	PtS (cooperite)	Tetragonal	$P4_2/mmc$	$tP4$
B18	CuS (covellite)	Hexagonal	$P6_3/mmc$	$hP12$
B19	AuCd	Orthorhombic	$Pmcm$	$oP4$
B20	FeSi	Cubic	$P2_13$	$cP8$
B21	CO	Cubic	$P2_13$	$cP8$
B24	TlF	Orthorhombic	$Fmmm$	$oF8$
B26	CuO	Monoclinic	n. a.	n. a.
B27	FeB	Orthorhombic	$Pbnm$	$oP8$
B29	SnS	Orthorhombic	$Pmcn$	$oP8$
B31	MnP	Orthorhombic	$Pbnm$	$oP8$
B32	NaTl	Cubic	$Fd\bar{3}m$	$cF16$
B33	CrB	Orthorhombic	$Cmcm$	$oC8$
B34	PdS	Tetragonal	$P4_2/m$	$tP16$
B35	CoSn	Hexagonal	$P6/mmm$	$hP6$
B37	TlSe	Tetragonal	$I4/mcm$	$tI16$

n. a. not available

Table F.10 *Strukturbericht* designations for ternary compounds (A_2X or AX_2 type)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
C_a	Mg_2Niternary compounds	Hexagonal	$P6_222$	*hP*18
C_b	Mg_2Cu	Orthorhombic	*Fddd*	*oF*48
C_c	$ThSi_2$	Tetragonal	*I*4/*amd*	*tI*12
C_e	$CoGe_2$	Orthorhombic	*Aba*	*oA*24
C_g	ThC_2	Monoclinic	*C*2/*c*	*mC*12
C_h	Cu_2Te	Hexagonal	*P*6/*mmm*	*hP*6
C_k	$LiZn_2$	Hexagonal	$P6_3/mmc$	*hP*3
C1	CaF_2 (fluorite)	Cubic	$Fm\bar{3}m$	*cF*12
$C1_b$	MgAgAs	Cubic	$F4\bar{3}m$	*cF*12
C2	FeS_2 (pyrite)	Cubic	$Pa\bar{3}$	*cP*12
C3	Cu_2O (cuprite)	Cubic	$Pn\bar{3}m$	*cP*6
C4	TiO_2 (rutile)	Tetragonal	$P4_2/mmm$	*tP*6
C5	TiO_2 (anatase)	Tetragonal	$I4_1/amd$	*tI*6
C6	CdI_2	Hexagonal	*P*3*m*1	*hP*3
C7	MoS_2 (molybdenite)	Hexagonal	$P6_3/mmc$	*hP*6
C8	SiO_2 (quartz)	Hexagonal	$R3_12_1$	*hR*9
C9	SiO_2 (β-cristobalite)	Cubic	$P4_32_12$	*cP*12
C10	SiO_2 (β-tridymite)	Hexagonal	$P6_3/mmc$	*hP*12
$C11_a$	CaC_2	Tetragonal	*I*4/*mmm*	*tI*6
$C11_b$	$MoSi_2$	Tetragonal	*I*4/*mmm*	*tI*6
C12	$CaSi_2$	Rhombohedral	$R\bar{3}m$	*hR*6
C14	$MgZn_2$ (laves)	Hexagonal	$P6_3/mmc$	*hP*12
C15	$MgCu_2$ (laves)	Cubic	$Fd\bar{3}m$	*cF*24
$C15_b$	$AuBe_5$	Cubic	$F4\bar{3}m$	*cF*24
C16	Al_2Cu	Tetragonal	*I*4/*mcm*	*tI*12
C18	FeS_2 (marcasite)	Orthorhombic	*Pnnm*	*oP*6
C19	α-Sm	Hexagonal	$R\bar{3}m$	*hR*3
C21	TiO_2 (brookite)	Orthorhombic	*Pbca*	*oP*24
C22	Fe_2P	Hexagonal	*P*26*m*	*hP*9
C23	$PbCl_2$	Orthorhombic	*Pnma*	*oP*12
C24	$HgBr_2$	Orthorhombic	$Cmc2_1$	*oC*12
C25	$HgCl_2$	Orthorhombic	*Pnma*	*oP*16

Table F.10 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
C28	$HgCl_2$	Orthorhombic	n. a.	n. a.
C29	SrH_2	Orthorhombic	n. a.	n. a.
C32	AlB_2	Hexagonal	*P6/mmm*	*hP*3
C33	Bi_2Te_3S	Hexagonal	$R\bar{3}m$	*hR*5
C34	$AuTe_2$ (calaverite)	Monoclinic	*C*2/*m*	*mC*6
C35	$CaCl_2$	Orthorhombic	n. a.	n. a.
C36	$MgNi_2$	Hexagonal	$P6_3/mmc$	*hP*24
C37	Co_2Si	Orthorhombic	*Pbnm*	*oP*12
C38	Cu_2Sb	Tetragonal	*P*4/*nmm*	*tP*6
C40	$CrSi_2$	Hexagonal	$P6_222$	*hP*9
C42	SiS_2	Orthorhombic	*Icma*	*oI*12
C43	ZrO_2 (baddeleyite)	Monoclinic	$P2_1c$	*mP*12
C44	GeS_2	Orthorhombic	*Fdd*2	*oF*72
C46	$AuTe_2$ (krennerite)	Orthorhombic	*Pma*2	*oP*24
C49	$ZrSi_2$	Orthorhombic	*Cmcm*	*oC*12
C54	TiS_2	Orthorhombic	*Fddd*	*oF*24

n. a. not available

Table F.11 *Strukturbericht* designations for quaternary compoundsquaternary compounds (A_3X or AX_3 type)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D0_a$	β-$TiCu_3$	Orthorhombic	*Pmmn*	*oP*8
$D0_b$	γ-Ag_3Ga	Hexagonal	*P*3	*hP*9
$D0_c$	U_3Si	Tetragonal	*I*4/*mcm*	*tI*16
$D0_d$	Mn_3As	Orthorhombic	*Pmmn*	*oP*16
$D0_2$	$CoAs_3$ (skutterudite)	Cubic	*Im*3	*cI*32
$D0_3$	BiF_3 or $BiLi_3$	Cubic	$Fm\bar{3}m$	*cF*16
$D0_4$	$CrCl_3$	Hexagonal	$P3_112$	*hP*24
$D0_5$	BiI_3	Rhombohedral	$R\bar{3}$	*hR*8
$D0_9$	ReO_3 or Cu_3N	Cubic	$Pm\bar{3}m$	*cP*4
$D0_{11}$	Fe_3C	Orthorhombic	*Pnma*	*oP*16
$D0_{14}$	AlF_3	Rhombohedral	$R\bar{3}2$	*hR*8

Table F.11 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D0_{15}$	$AlCl_3$	Monoclinic	*C2/m*	*mC*16
$D0_{18}$	Na_3As	Hexagonal	$P6_3/mmc$	*hP*8
$D0_{19}$	Mg_3Cd	Hexagonal	$P6_3/mmc$	*hP*8
$D0_{20}$	$NiAl_3$	Orthorhombic	*Pnma*	*oP*16
$D0_{21}$	Cu_3P	Hexagonal	*P3c1*	*hP*24
$D0_{22}$	$TiAl_3$	Tetragonal	*I4/mmm*	*tI*8
$D0_{23}$	$ZrAl_3$	Tetragonal	*I4/mmm*	*tI*16
$D0_{24}$	$TiNi_3$	Hexagonal	$P6_3/mmc$	*hP*16

Table F.12 *Strukturbericht* designations for penternary compoundscompounds (A_4X or AX_4 type)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D1_3$	$BaAl_4$	Tetragonal	*I4/mmm*	*tI*10
$D1_a$	$MoNi_4$	Tetragonal	*I4/m*	*tI*10
$D1_b$	UAl_4	Orthorhombic	*Imma*	*oI*20
$D1_c$	$PtSn_4$	Orthorhombic	*Aba*2	*oC*20
$D1_d$	$PtPb_4$	Tetragonal	*P4/nbm*	*tP*10
$D1_e$	UB_4	Tetragonal	*P4/mbm*	*tP*20
$D1_f$	Mn_4B	Orthorhombic	*Fddd*	*oF*40
$D1_g$	B_4C	Rhombohedral	$R\bar{3}m$	*tR*15

Table F.13 *Strukturbericht* designations for other compounds

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D2_a$	$TiBe_{12}$	Hexagonal	*P6/mmm*	*hP*13
$D2_b$	$ThMn_{12}$	Tetragonal	*I4/mcm*	*tI*26
$D2_c$	U_6Mn	Tetragonal	*I4/mcm*	*tI*28
$D2_d$	$CaCu_5$	Hexagonal	*C6/mmm*	*hC*6
$D2_e$	$BaHg_{11}$	Cubic	$Pm\bar{3}m$	*cP*36
$D2_f$	UB_{12}	Cubic	$Fm\bar{3}m$	*cF*52
$D2_g$	Fe_8N	Tetragonal	*I4/mmm*	*tI*18
$D2_h$	Al_6Mn	Orthorhombic	*Cmcm*	*oC*28
$D2_1$	CaB_6	Cubic	$Pm\bar{3}m$	*cP*7

Table F.13 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D2_3$	$NaZn_{13}$	Cubic	$Fm\bar{3}c$	*cF*112
$D5_a$	U_3Si_2	Tetragonal	$P4/mbm$	*tP*10
$D5_b$	Pt_2Sn_3	Hexagonal	$P6/mmc$	*hR*10
$D5_c$	Pu_2C_3	Cubic	$I\bar{4}3d$	*cI*40
$D5_e$	Ni_3Si_2	Rhombohedral	$R\bar{3}2$	*hR*5
$D5_1$	α-Al_2O_3	Rhombohedral	$R\bar{3}c$	*hR*10
$D5_2$	La_2O_3	Hexagonal	$P3m1$	*hP*5
$D5_3$	Mn_2O_3	Cubic	$Ia3$	*cI*80
$D5_8$	Sb_2S_3	Orthorhombic	$Pbnm$	*oP*20
$D5_9$	Zn_3P_2	Tetragonal	$P4/nmc$	*tP*40
$D5_{10}$	Cr_3C_2	Orthorhombic	$Pbnm$	*oP*20
$D5_{13}$	Ni_2Al_3	Hexagonal	$C3m1$	*hC*5
$D5_{19}$	Al_3Ni_2	n. a.	n. a.	n. a.
$D7_a$	Ni_3Sn_4	Monoclinic	$C2/m$	*mC*14
$D7_b$	Ta_3B_4	Orthorhombic	$Immm$	*oI*14
$D7_1$	Al_4C_3	Rhombohedral	$R\bar{3}m$	*hR*7
$D7_2$	Co_3S_4	Cubic	$Fd\bar{3}m$	*cF*56
$D7_3$	Th_3P_4	Cubic	$I\bar{4}3d$	*cI*26
$D8_a$	Th_6Mn_{23}	Cubic	$Fm\bar{3}m$	*cF*116
$D8_b$	V_3Ni_2	Tetragonal	$P4/mnm$	*tP*30
$D8_c$	$Mg_2Cu_6Al_5$	Cubic	$Pm3m$	*cP*39
$D8_d$	Co_2Al_9	Monoclinic	$P2_1/a$	*mP*22
$D8_e$	$Mg_{32}(Al,Zn)_{49}$	Cubic	$Im\bar{3}m$	*cI*162
$D8_f$	Ir_3Sn_7	Cubic	$Im\bar{3}m$	*cI*40
$D8_g$	Mg_5Ga_3	Orthorhombic	$Ibam$	*oI*28
$D8_h$	W_2B_5	Hexagonal	$P6_3/mmc$	*hP*14
$D8_i$	Mo_2B_5	Rhombohedral	$R3m$	*hR*7
$D8_k$	Th_7S_{12}	Hexagonal	$P6_3/m$	*hP*19
$D8_l$	B_3Cr_5	Tetragonal	$I4/mcm$	*tI*32
$D8_m$	Si_3W_5	Tetragonal	$I4/mcm$	*tI*32
$D8_1$	Fe_3Zn_{10}	Cubic	$Im3m$	*cI*52
$D8_2$	Cu_5Zn_8	Cubic	$I43m$	*cI*52
$D8_3$	Cu_9Al_4	Cubic	$P43m$	*cP*52

Table F.13 (*continued*)

Designation	Typical example	Crystal system	Hermann–Mauguin symbol	Pearson symbol
$D8_4$	$Cr_{23}C_6$	Cubic	$Fm\bar{3}m$	*cF*116
$D8_5$	Fe_7W_6	Rhombohedral	$R\bar{3}m$	*hR*13
$D8_6$	$Cu_{15}Si_4$	Cubic	$I43d$	*cI*76
$D8_8$	Mn_5Si_3	Hexagonal	$P6_3/mcm$	*hP*16
$D8_9$	Co_9S_8	Cubic	$Fm\bar{3}m$	*cF*68
$D8_{10}$	Cr_5Al_8	Rhombohedral	$R3m$	*hR*26
$D8_{11}$	Co_2Al_5	Hexagonal	$P6_3/mcm$	*hP*28
$D10_1$	Cr_7C_3	Hexagonal	$P31c$	*hP*80
$D10_2$	Fe_3Th_7	Hexagonal	$P6_3/mcm$	*hP*20
$E0_1$	PbClF	Tetragonal	$P4/nmm$	*tP*6
$E0_7$	FeAsS	Monoclinic	$B2_1/d$	*mB*24
$E1_a$	$MgCuAl_2$	Orthorhombic	$Cmcm$	*oC*16
$E1_b$	$AuAgTe_4$ (sylvanite)	Monoclinic	$P2/c$	*mP*12
$E1_1$	$CuFeS_2$ (chalcopyrite)	Tetragonal	$I42d$	*tI*16
$E2_1$	$CaTiO_3$ (perovskite)	Cubic	$Pm3m$	*cP*5
$E2_4$	Sn_2S_3	Orthorhombic	$Pnma$	*oP*20
E3	Al_2CdS_4	Tetragonal	$I4$	*tI*14
$E9_a$	Al_7Cu_2Fe	Tetragonal	$P4/mnc$	*tP*40
$E9_b$	$FeMg_3Al_8Si_6$	Hexagonal	$P62m$	*hP*18
$E9_c$	Mn_3Al_9Si	Hexagonal	$P6_3/mmc$	*hP*26
$E9_d$	$AlLi_3N_2$	Cubic	$Ia3$	*cI*96
$E9_e$	$CuFe_2S_3$ (cubanite)	Orthorhombic	$Pnma$	*oP*24
$E9_3$	Fe_3W_3C	Cubic	$Fd\bar{3}m$	*cF*112
$F0_1$	NiSSb (ullmannite)	Cubic	$P2_13$	*cP*12
$F5_a$	$KFeS_2$	Monoclinic	$C2/c$	*mC*16
$F5_1$	$CrNaS_2$	Rhombohedral	$R\bar{3}m$	*hR*4
$F5_6$	CuS_2Sb	Orthorhombic	$Pnma$	*oP*16
$G0_6$	$KClO_3$	Monoclinic	$P2_1/m$	*mP*10
$H1_1$	Al_2MgO_4 (spinel)	Cubic	$Fd\bar{3}m$	*cF*56
$H2_4$	Cu_3S_4V (sulvanite)	Cubic	$P43m$	*cP*8
$H2_5$	$AsCu_3S_4$ (enargite)	Orthorhombic	$Pmn2_1$	*oP*16
$H2_6$	$FeCu_2SnS_4$ (stannite)	Tetragonal	$I42m$	*tI*16
$L1_a$	Pt_3Cu	Cubic	$Fm\bar{3}c$	*cF*32

Table F.13 (*continued*)

Designation	**Typical example**	**Crystal system**	**Hermann–Mauguin symbol**	**Pearson symbol**
$L1_0$	CuAu	Tetragonal	$C4/mmm$	$tC4$
$L1_2$	Cu_3Au	Cubic	$Pm\bar{3}m$	$cP4$
$L2_a$	δ-TiCu	Tetragonal	$P4/mmm$	$tP2$
$L2_1$	$AlCu_2Mn$	Cubic	$Fm\bar{3}m$	$cF16$
$L2_2$	Sb_2Tl_7	Cubic	$Im\bar{3}m$	$cI54$
L′1	Fe_4N	Cubic	$Pm\bar{3}m$	$cP5$
L′2	Martensite	Tetragonal	$I4/mmm$	$tI3$
$L'2_b$	ThH_2	Tetragonal	$I4/mmm$	$tI6$
L′3	Fe_2N	Hexagonal	$P6_3/mmc$	$hP3$
$L'6_0$	$CuTi_3$	Tetragonal	$P4/mmm$	$tP4$
L′6	No name	Tetragonal	$F4/mmm$	$tF4$

n. a. not available

F.9 The 230 Space Groups

See Tables F.14–F.23.

Table F.14 Triclinic space groups

Ordered number	**Space group (Hermann–Mauguin)**
001	$P\,1$
002	$P\,1$

Table F.15 Monoclinic space groups

Ordered number	**Space group (Hermann–Mauguin)**
003	$P\,2$
004	$P\,2_1$
005	$C\,2$
006	$P\,m$
007	$P\,c$
008	$C\,m$
009	$C\,c$
010	$P\,2/m$

Table F.15 (*continued*)

Ordered number	Space group (Hermann–Mauguin)
011	$P\,2_1/m$
012	$C\,2/m$
013	$P\,2/c$
014	$P\,2_1/c$
015	$C\,2/c$

Table F.16 Orthorhombic space groups

Ordered number	Space group (Hermann–Mauguin)
016	$P\,2\,2\,2$
017	$P\,2\,2\,2_1$
018	$P\,2_1\,2_1\,2$
019	$P\,2_1\,2_1\,2_1$
020	$C\,2\,2\,2_1$
021	$C\,2\,2\,2$
022	$F\,2\,2\,2$
023	$I\,2\,2\,2$
024	$I\,2_1\,2_1\,2_1$
025	$P\,m\,m\,2$
026	$P\,m\,c\,2_1$
027	$P\,c\,c\,2$
028	$P\,m\,a\,2$
029	$P\,c\,a\,2_1$
030	$P\,n\,c\,2$
031	$P\,m\,n\,2_1$
032	$P\,b\,a\,2$
033	$P\,n\,a\,2_1$
034	$P\,n\,n\,2$
035	$C\,m\,m\,2$
036	$C\,m\,c\,2_1$
037	$C\,c\,c\,2$
038	$A\,m\,m\,2$
039	$A\,b\,m\,2$
040	$A\,m\,a\,2$

Table F.16 (*continued*)

Ordered number	**Space group (Hermann–Mauguin)**
041	*A b a* 2
042	*F m m* 2
043	*F d d* 2
044	*I m m* 2
045	*I b a* 2
046	*I m a* 2
047	*P m m m*
048	*P n n n*
049	*P c c m*
050	*P b a n*
051	*P m m a*
052	*P n n a*
053	*P m n a*
054	*P c c a*
055	*P b a m*
056	*P c c n*
057	*P b c m*
058	*P n n m*
059	*P m m n*
060	*P b c n*
061	*P b c a*
062	*P n m a*
063	*C m c m*
064	*C m c a*
065	*C m m m*
066	*C c c m*
067	*C m m a*
068	*C c c a*
069	*F m m m*
070	*F d d d*
071	*I m m m*
072	*I b a m*
073	*I b c a*
074	*I m m a*

Table F.17 Tetragonal space groups

Ordered number	Space group (Hermann–Mauguin)
075	$P\,4$
076	$P\,4_1$
077	$P\,4_2$
078	$P\,4_3$
079	$I\,4$
080	$I\,4_1$
081	$P\,\bar{4}$
082	$I\,\bar{4}$
083	$P\,4/m$
084	$P\,4_2/m$
085	$P\,4/n$
086	$P\,4_2/n$
087	$I\,4/m$
088	$I\,4_1/a$
089	$P\,4\,2\,2$
090	$P\,4\,2_1\,2$
091	$P\,4_1\,2\,2$
092	$P\,4_1\,2_1\,2$
093	$P\,4_2\,2\,2$
094	$P\,4_2\,2_1\,2$
095	$P\,4_3\,2\,2$
096	$P\,4_3\,2_1\,2$
097	$I\,4\,2\,2$
098	$I\,4_1\,2\,2$
099	$P\,4\,m\,m$
100	$P\,4\,b\,m$
101	$P\,4_2\,c\,m$
102	$P\,4_2\,n\,m$
103	$P\,4\,c\,c$
104	$P\,4\,n\,c$
105	$P\,4_2\,m\,c$
106	$P\,4_2\,b\,c$
107	$I\,4\,m\,m$
108	$I\,4\,c\,m$

Table F.17 (*continued*)

Ordered number	**Space group (Hermann–Mauguin)**
109	$I\,4_1\,m\,d$
110	$I\,4_1\,c\,d$
111	$P\,\bar{4}\,2\,m$
112	$P\,\bar{4}\,2\,c$
113	$P\,\bar{4}\,2_1\,m$
114	$P\,\bar{4}\,2_1\,c$
115	$P\,\bar{4}\,m\,2$
116	$P\,\bar{4}\,c\,2$
117	$P\,\bar{4}\,b\,2$
118	$P\,\bar{4}\,n\,2$
119	$I\,\bar{4}\,m\,2$
120	$I\,\bar{4}\,c\,2$
121	$I\,\bar{4}\,2\,m$
122	$I\,\bar{4}\,2\,d$
123	$P\,4/m\,m\,m$
124	$P\,4/m\,c\,c$
125	$P\,4/n\,b\,m$
126	$P\,4/n\,n\,c$
127	$P\,4/m\,b\,m$
128	$P\,4/m\,n\,c$
129	$P\,4/n\,m\,m$
130	$P\,4/n\,c\,c$
131	$P\,4_2/m\,m\,c$
132	$P\,4_2/m\,c\,m$
133	$P\,4_2/n\,b\,c$
134	$P\,4_2/n\,n\,m$
135	$P\,4_2/m\,b\,c$
136	$P\,4_2/m\,n\,m$
137	$P\,4_2/n\,m\,c$
138	$P\,4_2/n\,c\,m$
139	$I\,4/m\,m\,m$
140	$I\,4/m\,c\,m$
141	$I\,4_1/a\,m\,d$
142	$I\,4_1/a\,c\,d$

Table F.18 Trigonal space groups

Ordered number	**Space group (Hermann–Mauguin)**
143	$P\ 3$
144	$P\ 3_1$
145	$P\ 3_2$
146	$R\ 3$
147	$P\ 3$
148	$R\ 3$
149	$P\ 31\ 2$
150	$P\ 3\ 2_1$
151	$P\ 3_1\ 1\ 2$
152	$P\ 3_1\ 2\ 1$
153	$P\ 32_1\ 2$
154	$P\ 32\ 2_1$
155	$R\ 3\ 2$
156	$P\ 3\ m\ 1$
157	$P\ 3\ 1\ m$
158	$P\ 3\ c\ 1$
159	$P\ 3\ 1\ c$
160	$R\ 3\ m$
161	$R\ 3\ c$
162	$P\ \bar{3}\ 1\ m$
163	$P\ \bar{3}\ 1\ c$
164	$P\ \bar{3}\ m\ 1$
165	$P\ \bar{3}\ c\ 1$
166	$R\ \bar{3}\ m$
167	$R\ \bar{3}\ c$

Table F.19 Hexagonal space groups

Ordered number	**Space group (Hermann–Mauguin)**
168	$P\ 6$
169	$P\ 6_1$
170	$P\ 6_5$
171	$P\ 6_2$
172	$P\ 6_4$

Table F.19 (*continued*)

Ordered number	Space group (Hermann–Mauguin)
173	$P\,6_3$
174	$P\,\bar{6}$
175	$P\,6/m$
176	$P\,6_3/m$
177	$P\,6\,2\,2$
178	$P\,6_1\,2\,2$
179	$P\,6_5\,2\,2$
180	$P\,6_2\,2\,2$
181	$P\,6_4\,2\,2$
182	$P\,6_3\,2\,2$
183	$P\,6\,m\,m$
184	$P\,6\,c\,c$
185	$P\,6_3\,c\,m$
186	$P\,6_3\,m\,c$
187	$P\,\bar{6}\,m\,2$
188	$P\,\bar{6}\,c\,2$
189	$P\,\bar{6}\,2\,m$
190	$P\,\bar{6}\,2\,c$
191	$P\,6/m\,m\,m$
192	$P\,6/m\,c\,c$
193	$P\,6_3/m\,c\,m$
194	$P\,6_3/m\,m\,c$

Table F.20 Cubic space groups

Ordered number	Space group (Hermann–Mauguin)
195	$P\,2\,3$
196	$F\,2\,3$
197	$I\,2\,3$
198	$P\,2_1\,3$
199	$I\,2_1\,3$
200	$P\,m\,\bar{3}$
201	$P\,n\,\bar{3}$
202	$F\,m\,\bar{3}$

Table F.20 (*continued*)

Ordered number	Space group (Hermann–Mauguin)
203	$F d \bar{3}$
204	$I m \bar{3}$
205	$P a \bar{3}$
206	$I a \bar{3}$
207	$P 4 3 2$
208	$P 4_2 3 2$
209	$F 4 3 2$
210	$F 4_1 3 2$
211	$I 4 3 2$
212	$P 4_3 3 2$
213	$P 4_1 3 2$
214	$I 4_1 3 2$
215	$P 4 3 m$
216	$F 4 3 m$
217	$I \bar{4} 3 m$
218	$P \bar{4} 3 n$
219	$F \bar{4} 3 c$
220	$I \bar{4} 3 d$
221	$P m \bar{3} m$
222	$P n \bar{3} n$
223	$P m \bar{3} n$
224	$P n \bar{3} m$
225	$F m \bar{3} m$
226	$F m \bar{3} c$
227	$F d \bar{3} m$
228	$F d \bar{3} c$
229	$I m \bar{3} m$
230	$I a \bar{3} d$

F.10 Crystallographic Calculations

F.10.1 Theoretical Crystal Density

The theoretical density, ρ, expressed in kilograms per cubic meter, of a crystalcrystal having a number Z of entities with atomic (or molecular) molar mass M, expressed in kilograms per mole, placed in a space lattice structure having a unit cell of volume V, expressed in cubic meters, is given by the following equation,

$$\rho_{\text{theoretical}} = ZM/N_{\text{A}}V_{\text{cell}},$$

where N_{A} is Avogadro's number (i.e., $6.022140857 \times 10^{23}$ mol^{-1}).

F.10.2 Lattice Point and Vector Position

A lattice point, {M}, which describes the position of a microscopic entity (e.g., electrons, ions, atoms, molecules, or clusters), is located in the crystalcrystal space lattice by giving the number of unit translations, along each of the three distinct translation directions, by which it is displaced from the point {O} as a fixed origin. Therefore, each lattice point is entirely described by a set of three coordinates (u, v, w) or by the single position vector $\mathbf{V}$:

$$\mathbf{V} = \mathbf{OM} = u\mathbf{a} + v\mathbf{b} + w\mathbf{c}.$$

Sometimes the lattice point coordinates are denoted by the designation $\cdot\, uvw \,\cdot$, (e.g., $\cdot\, 320 \,\cdot$)

F.10.3 Scalar Product

The scalar product of two vectors is a scalar quantity represented as $\mathbf{V}_1 \cdot \mathbf{V}_2$ and is defined by the following equation:

$$\mathbf{V}_1 \cdot \mathbf{V}_2 = |\mathbf{V}_1| \cdot |\mathbf{V}_2| \cos(\mathbf{V}_1, \mathbf{V}_2) = |\mathbf{V}_1| \cdot |\mathbf{V}_2| \cos\theta,$$

where θ is the plane angle measured counterclockwise between the two vectors and expressed in radians. Introducing the set of six vector coordinates, we can express the scalar product analytically as

$$\begin{aligned}\mathbf{V}_1 \cdot \mathbf{V}_2 = [&u_1u_2\mathbf{a}_2 + v_1v_2\mathbf{b}_2 + w_1w_2\mathbf{c}_2 + (u_1v_2 + v_1u_2)\mathbf{ab}\cos\gamma \\ &+ (u_1w_2 + w_1u_2)\mathbf{ac}\cos\beta + (w_1v_2 + v_1w_2)\mathbf{bc}\cos\alpha].\end{aligned}$$

Finally, the scalar product can be also written as a matrix product:

$$\mathbf{V}_1 \cdot \mathbf{V}_2 = (u_1v_1w_1) \cdot \begin{vmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{vmatrix} \cdot \begin{vmatrix} u_2 \\ v_2 \\ w_2 \end{vmatrix}.$$

F.10.4 Vector or Cross Product

The vector product of two vectors is a vector quantity represented as $\mathbf{V}_1 \times \mathbf{V}_2$ or $\mathbf{V}_1 \wedge \mathbf{V}_2$ and is defined by the following equation:

$$\mathbf{V}_1 \times \mathbf{V}_2 = |\mathbf{V}_1| \times |\mathbf{V}_2| \sin(\mathbf{V}_1, \mathbf{V}_2) = |\mathbf{V}_1| \times |\mathbf{V}_2| \sin\theta,$$

where θ is the plane angle measured counterclockwise between the two vectors and expressed in radians. Introducing the set of the six vector coordinates, we can express the vector product analytically as

$$\mathbf{V}_1 \times \mathbf{V}_2 = [(v_1 w_2 - w_1 v_2)\mathbf{b} \times \mathbf{c} + (u_2 w_1 - u_1 w_2)\mathbf{c} \times \mathbf{a} + (u_1 v_2 - u_2 v_1)\mathbf{a} \times \mathbf{b}].$$

Finally, the vector product can also be written as a matrix determinant:

$$\mathbf{V}_1 \times \mathbf{V}_2 = \begin{vmatrix} \mathbf{a} & \mathbf{b} & \mathbf{c} \\ u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \end{vmatrix}.$$

F.10.5 Mixed Product and Cell Multiplicity

The mixed product of three vectors is a scalar quantity represented as $(\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3)$ and is defined to be equal to

$$\mathbf{V}_1 \cdot (\mathbf{V}_2 \times \mathbf{V}_3) = (\mathbf{V}_1 \times \mathbf{V}_2) \cdot \mathbf{V}_3.$$

The vector product can also be written as a matrix product:

$$(\mathbf{V}_1, \mathbf{V}_2, \mathbf{V}_3) = \underbrace{\begin{vmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{vmatrix}}_{\text{cell multiplicity}} (\mathbf{a}, \mathbf{b}, \mathbf{c}).$$

The ***multiplicity of the cell,*** m, is a dimensionless physical quantity equal to the number of entities (e.g., electrons, ions, atoms, molecules) contained in the crystalcrystal lattice structure (see ◘ Table F.21).

The rigorous deduction of entities (e.g., ions, atoms, molecules) contained inside the unit cell depends only on their particular locations in the crystal space lattice, so:

1. Entities located on the corners are counted as one eighth (1/8), because they are shared by eight other neighboring cells.

Table F.21 Cell multiplicity

Class	Multiplicity	Name
Single unit cell	$m = 1$	Primitive cell
Multiple cell	$m = 2$	Double cell
	$m = 3$	Triple cell
	$m = 4$	Quadruple cell

2. Entities located on the edges of the lattice are counted as one quarter (1/4) because they are shared by four neighboring cells.
3. Entities located at the faces of the cell are counted as half (1/2) because they are shared by two adjacent cells.
4. Entities located inside the cell space lattice are counted as unity (1).

Therefore, the multiplicity, m, of the cell can be easily calculated from the number, N, of entities in each particular location (i.e., corners, edges, faces, interior):

$$m = N_{\text{inside}} + N_{\text{faces}}/2 + N_{\text{edges}}/4 + N_{\text{corners}}/8.$$

F.10.6 Unit Cell Volume

The unit cell volumespace lattice is given by the following general equation, which is calculated from the mixed product of the three lattice vectors:

$$V_{\text{unit cell}} = (\mathbf{a}, \mathbf{b}, \mathbf{c}) = abc(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}.$$

For particular space lattice see ◘ Table F.22.

Table F.22 Space latticespace lattice volume

System	Volume
Cubic	$V_C = a^3$
Tetragonal	$V_Q = a^2c$
Hexagonal	$V_H = a^2c\sqrt{3}/2 = 0.866a^2c$
Rhombohedral	$V_R = a^3(1 - 3\cos^2\alpha + 2\cos^3\alpha)^{1/2}$
Orthorhombic	$V_O = abc$
Monoclinic	$V_M = abc\sin\beta$
Triclinic	$V_T = abc\,(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$

Table F.23 Plane anglespace lattice between lattice planes

System	Plane angle
Cubic	$\cos\varphi = \dfrac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{\left(h_1^2 + k_1^2 + l_1^2\right)\left(h_2^2 + k_2^2 + l_2^2\right)}}$
Tetragonal	$\cos\varphi = \dfrac{\dfrac{h_1h_2 + k_1k_2}{a^2} + \dfrac{l_1l_2}{c^2}}{\sqrt{\left(\dfrac{h_1^2 + k_1^2}{a^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2 + k_2^2}{a^2} + \dfrac{l_2^2}{c^2}\right)}}$
Hexagonal	$\cos\varphi = \dfrac{h_1h_2 + k_1k_2 + \dfrac{h_1k_2 + h_2k_1}{2} + \dfrac{3a^2l_1l_2}{4c^2}}{\sqrt{\left(h_1^2 + k_1^2 + h_1k_1 + \dfrac{3a^2l_1^2}{4c^2}\right)\left(h_2^2 + k_2^2 + h_2k_2 + \dfrac{3a^2l_2^2}{4c^2}\right)}}$
Rhombohedral	$\cos\varphi = \dfrac{\left[\begin{array}{c}(h_1h_2 + k_1k_2 + l_1l_2)(\sin\alpha)^2 \\ +(k_1l_2 + k_2l_1 + l_1h_2 + l_2h_1 + h_1k_2 + k_1h_2)\left[(\cos\alpha)^2 - \cos\alpha\right]\end{array}\right]}{\sqrt{\begin{array}{l}\left[\left(h_1^2 + k_1^2 + l_1^2\right)(\sin\alpha)^2 + 2\left(h_1k_1 + k_1l_1 + h_1l_1\right)\right]\left[(\cos\alpha)^2 - \cos\alpha\right] \\ \times\left[\left(h_2^2 + k_2^2 + l_2^2\right)(\sin\alpha)^2 + (2h_2k_2 + k_2l_2 + h_2l_2)\right]\left[(\cos\alpha)^2 - \cos\alpha\right]\end{array}}}$
Orthorhombic	$\cos\varphi = \dfrac{\dfrac{h_1h_2}{a^2} + \dfrac{k_1k_2}{b^2} + \dfrac{l_1l_2}{c^2}}{\sqrt{\left(\dfrac{h_1^2}{a^2} + \dfrac{k_1^2}{b^2} + \dfrac{l_1^2}{c^2}\right)\left(\dfrac{h_2^2}{a^2} + \dfrac{k_2^2}{b^2} + \dfrac{l_2^2}{c^2}\right)}}$
Monoclinic	$\cos\varphi = \dfrac{\dfrac{h_1h_2}{a^2} + \dfrac{k_1k_2\left(\sin\beta^2\right)}{b^2} + \dfrac{l_1l_2}{c^2} - \dfrac{(h_2l_1 + h_1l_2)\cos\beta}{ac}}{\sqrt{\begin{array}{l}\left[\dfrac{h_1^2}{a^2} + \dfrac{k_1^2\left(\sin\beta^2\right)}{b^2} + \dfrac{l_1^2}{c^2} - \dfrac{2h_1l_1\cos\beta}{ac}\right] \\ \times\left[\dfrac{h_2^2}{a^2} + \dfrac{k_2^2\left(\sin\beta^2\right)}{b^2} + \dfrac{l_2^2}{c^2} - \dfrac{2h_2l_2\cos\beta}{ac}\right]\end{array}}}$
Triclinic	See the general formula in the text

F.10.7 Plane Angle Between Lattice Planes

One is also occasionally interested in computing the angle between planes. If φ is the angle between the plane with Miller indices (h_1, k_1, l_1) and the plane with Miller indices (h_2, k_2, l_2), then the basic equation to calculate this angle is (see Table F.23 and coefficients *sii* in Table F.24)

$$\cos\varphi = \frac{d_{h_1k_1l_1}d_{h_2k_2l_2}}{v^2}[s_{11}h_1h_2 + s_{22}k_1k_2 + s_{33}l_1l_2 + s_{23}(k_1l_2 + k_2l_1) + s_{13}(l_1h_2 + l_2h_1) + s_{12}(h_1k_2 + h_2k_1)].$$

F.11 Interplanar Spacing

See ■ Tables F.24 and F.25.

■ **Table F.24** General formula for the interplanar spacing

$(1/d_{hkl}) = (1/V)\cdot(s_{11}h^2 + s_{22}k^2 + s_{33}l^2 + 2s_{12}hk + 2s_{23}kl + 2s_{13}hl)^{1/2}$, where $V = abc\cdot(1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma)^{1/2}$	
$s_{11} = b^2c^2\sin^2\alpha$	$s_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$
$s_{22} = a^2c^2\sin^2\beta$	$s_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$
$s_{33} = a^2b^2\sin^2\gamma$	$s_{31} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$

■ **Table F.25** Interplanar spacing according to the type of crystalcrystal lattice

System	Interplanar spacing
Cubic	$\frac{1}{d_{hkl}} = \sqrt{\frac{h^2+k^2+l^2}{a^2}}$
Tetragonal	$\frac{1}{d_{hkl}} = \sqrt{\frac{h^2+k^2}{a^2} + \frac{l^2}{c^2}}$
Hexagonal	$\frac{1}{d_{hkl}} = \sqrt{\frac{4\left(k^2+hk+k^2\right)}{3a^2} + \frac{l^2}{c^2}}$
Rhombohedral	$\frac{1}{d_{hkl}} = \sqrt{\frac{\left(h^2+k^2+l^2\right)(\sin\alpha)^2 + 2\left(kh+kl+lh\right)\left(\cos\alpha^2 - \cos\alpha\right)}{a\left[1 - 3(\cos\alpha)^2 + 2(\cos\alpha)^3\right]}}$
Orthorhombic	$\frac{1}{d_{hkl}} = \sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}$
Monoclinic	$\frac{1}{d_{hkl}} = \sqrt{\frac{h^2}{a^2(\sin\beta)^2} + \frac{k^2}{b^2(\sin\beta)^2} + \frac{l^2}{c^2(\sin\beta)^2} - \frac{2hl\cos\beta}{ac(\sin\beta)^2}}$
Triclinic	See the general formula in Table F.24

F.12 Reciprocal Lattice Unit Cell

See Table F.26.

Table F.26 Definition of the reciprocal lattice

The three reciprocal lattice vectors are a*, b*, and c* defined by the nine relations below		
$\mathbf{a}\mathbf{a}^* = 1$	$\mathbf{b}\mathbf{a}^* = 0$	$\mathbf{c}\mathbf{a}^* = 0$
$\mathbf{a}\mathbf{b}^* = 0$	$\mathbf{b}\mathbf{b}^* = 1$	$\mathbf{c}\mathbf{b}^* = 0$
$\mathbf{a}\mathbf{c}^* = 0$	$\mathbf{b}\mathbf{c}^* = 0$	$\mathbf{c}\mathbf{c}^* = 1$

A condensed notation used by crystallographers is as follows: $\mathbf{a}_i\mathbf{b}_j = \delta_{ij}$, where δ_{ij} is the Kronecker operator (i.e., for $i = j$, $\delta_{ij} = 1$, and for $i \neq j$, $\delta_i = 0$). A slightly different notation is used in solid-state physics: $\mathbf{a}_i\mathbf{b}_j = 2\pi\delta_{ij}$

G Transparent Materials for Optical Windows

See ▣ Table G.1 and ▣ Fig. G.1.

▣ **Table G.1** Optical properties of window materials

Window material	**Long (IR) and short (UV) cutoffs**						**Refractive index (n_D)**	**Comments**
	Wavelength range (λ/μm)		**Wavenumber range (σ/cm^{-1})**		**Colour temperature (T/K)**			
LiF (lithium fluoride)	0.105	5.88	95,000	1700	27,531	493	1.40	Best VUV transmitter available
MgF_2 (Irtran-1)	0.115	8.00	87,000	1250	25,213	362	1.35	
SiO_2 (fused silica)	0.120	4.50	83,333	2222	24,150	644		
CaF_2 (fluorite; Irtran-3)	0.130	9.01	77,000	1110	22,315	322	1.434	Resists most acids and alkalis; withstands high pressure; insoluble in water
Al_2O_3 (sapphire)	0.140	6.50	71,429	1538	20,700	446	1.765	Hard crystal
BaF_2 (barium fluoride)	0.149	13.51	67,000	740	19,417	214	1.46	Brittle crystal; insoluble in water; good resistance to fluorine and fluorides
SiO_2 (quartz)	0.154	3.70	65,000	2700	18,837	782	1.549	Hard crystal, transparent in the visible range
$CaCO_3$ (calcite)	0.200	5.50	50,000	1818	14,490	527	1.572	
KCl (sylvite)	0.210	30.00	47,619	333	13,800	97	1.490	
CsI (cesium iodide)	0.250	80.00	40,000	125	11,592	36	1.74	Soft crystal; soluble in water; hydroscopic; offers an extended transmission range
C (diamond)	0.250	80.00	40,000	125	11,592	36	2.418	Phonon bands around 1900–2600 cm^{-1} except in type IIa diamonds; very useful for high-pressure or corrosive work
KBr (potassium bromide)	0.250	25.00	40,000	400	11,592	116	1.53	Very soft water-soluble crystal; low cost and good transmission range; fogs
KI (potassium iodide)	0.250	45.00	40,000	222	11,592	64		

Table G.1 (*continued*)

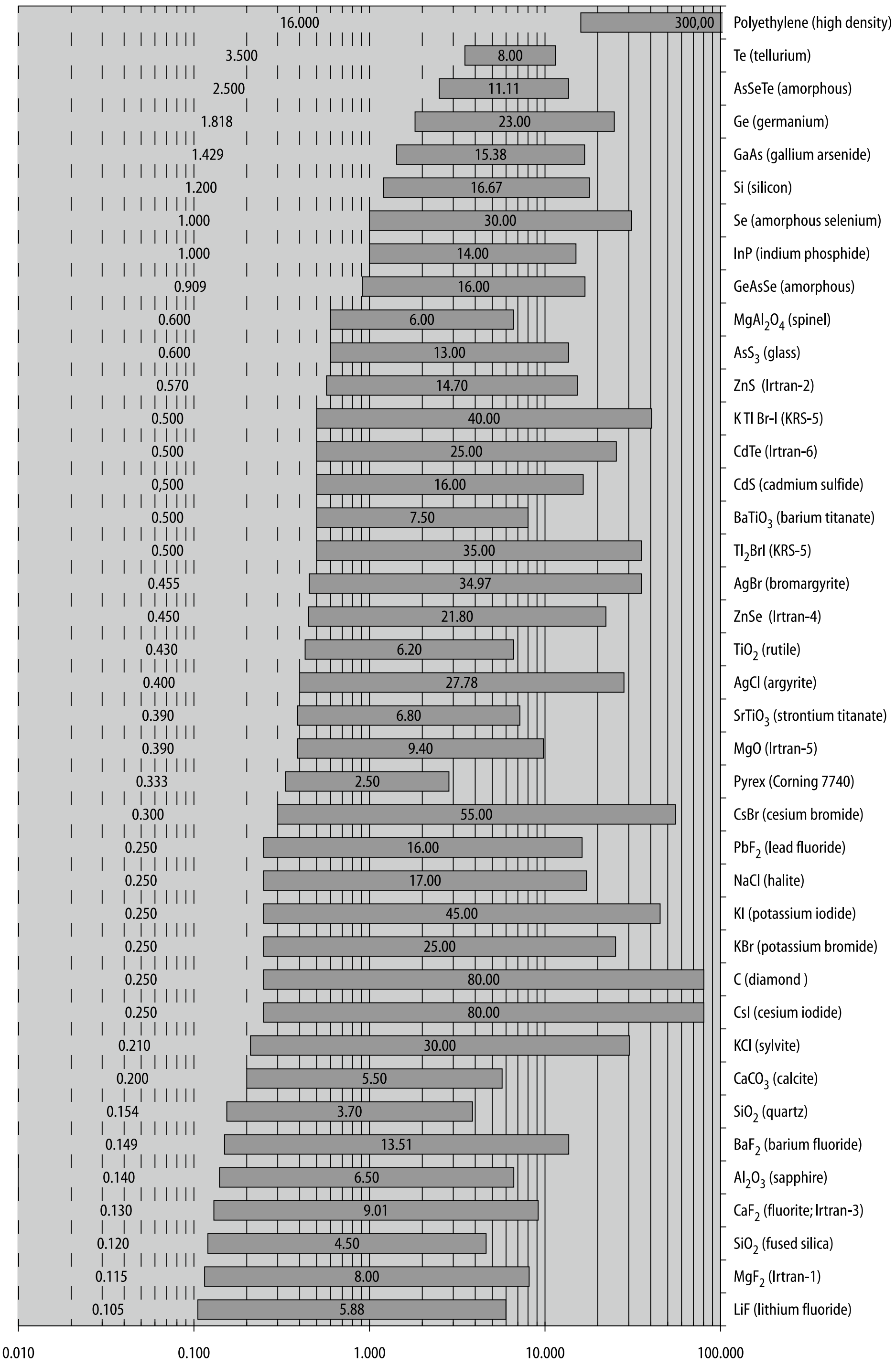
Window material	Long (IR) and short (UV) cutoffs						Refractive index (n_D)	Comments
	Wavelength range (λ/µm)		Wavenumber range (σ/cm^{-1})		Colour temperature (T/K)			
NaCl (halite)	0.250	17.00	40,000	588	11,592	170	1.544	Very soft water-soluble crystal; low cost and good transmission range; fogs
PbF_2 (lead fluoride)	0.250	16.00	40,000	625	11,592	181		
CsBr (cesium bromide)	0.300	55.00	33,333	182	9660	53		
Pyrex (Corning 7740)	0.333	2.50	30,000	4000	8694	1159	1.47	
MgO (Irtran-5)	0.390	9.40	25,641	1064	7431	308	1.735	
$SrTiO_3$ (strontium titanate)	0.390	6.80	25,641	1471	7431	426		
AgCl (argyrite)	0.400	27.78	25,000	360	7245	104	2.070	Soft crystal that is insoluble in water; darkens on exposure to UV radiation; will cold flow
TiO_2 (rutile)	0.430	6.20	23,256	1613	6740	467	2.755	
ZnSe (Irtran-4)	0.450	21.80	22,222	459	6440	133	2.890	Hard and brittle crystal; inert; ideal material for ATR
AgBr (bromargyrite)	0.455	34.97	22,000	286	6376	83	2.253	Soft crystal; insoluble in water; darkens on exposure to UV radiation; will creep
Tl_2BrI (KRS-5)	0.500	35.00	20,000	286	5796	83	2.370	Toxic
$BaTiO_3$ (barium titanate)	0.500	7.50	20,000	1333	5796	386		
CdS (cadmium sulfide)	0.500	16.00	20,000	625	5796	181	2.320	
CdTe (Irtran-6)	0.500	25.00	20,000	400	5796	116	2.670	Lower thermal conductivity than ZnSe (used with CO_2 lasers). Attacked by oxidizers

Table G.1 (*continued*)

Window material	Long (IR) and short (UV) cutoffs						Refractive index (n_D)	Comments
	Wavelength range (λ/μm)		Wavenumber range (σ/cm^{-1})		Colour temperature (T/K)			
TL(Br,I) (KRS-5)	0.500	40.00	20,000	250	5796	72	2.37	Toxic; soft crystal deforms under pressure; good ATR material, soluble in bases and insoluble in acids, toxic
ZnS (Irtran-2)	0.570	14.70	17,544	680	5084	197	2.356	Insoluble in water
AsS_3 (glass)	0.600	13.00	16,667	769	4830	223		
$MgAl_2O_4$ (spinel)	0.600	6.00	16,667	1667	4830	483	1.719	
GeAsSe (amorphous)	0.909	16.00	11,000	625	3188	181	2.50	Amorphous material transmitting IR radiation is a glass; insoluble in water; resistant to corrosion
InP (indium phosphide)	1.000	14.00	10,000	714	2898	207	3.100	
Se (amorphous selenium)	1.000	30.00	10,000	333	2898	97	2.500	
Si (silicon)	1.200	16.67	8330	600	2414	174	3.490	Hard and brittle crystal; inert; ideal material for far-IR
GaAs (gallium arsenide)	1.429	15.38	7000	650	2029	188	3.330	Hard crystal; can be made amorphous
Ge (germanium)	1.818	23.00	5500	435	1594	126	3.990	Hard and brittle crystal; insoluble in water; well suited for ATR
AsSeTe (amorphous)	2.500	11.11	4000	900	1159	261	2.80	Good for mid-IR fiber optics; chemically inert
Te (tellurium)	3.500	8.00	2857	1250	828	362	3.300	
Polyethylene (high density)	16.000	300.00	625	33	181	10	1.54	Excellent for far-IR; very cheap; attacked by few solvents; difficult to clean

Transmission region in which a sample 2 mm thick has 10% transmission. Irtran was a registered trademark of Eastman Kodak Company

ATR attenuated total reflection, *VUV* vacuum UV



■ **Fig. G.1** Electromagnetic transparency range of optical window materials

H Corrosion Resistance of Materials Toward Various Corrosive Media

Table H.1 Maximum operating temperature (°C) of metals for handling liquid metals under an inert atmosphere

Molten metal or alloy	Metallic container														
	316L	**Fe**	**Mn**	**Ti**	**Zr**	**Hf**	**Nb**	**Ta**	**Mo**	**W**	**Ag**	**Au**	**Pt**	**Rh**	**Ir**
Ag	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	1200	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.
Al	A	n. a.	n. a.	750	n. a.	n. a.	n. a.	A	n. a.	n. a.	A	A	n. a.	n. a.	A
Bi	A	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	560	n. a.	n. a.	A	A	A	A	470
Ca	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	1200	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	A
Cd	A	n. a.	n. a.	450	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	A
Ga	A	n. a.	n. a.	400	n. a.	n. a.	n. a.	400	400	n. a.	A	A	n. a.	n. a.	230
Hg	n. a.	n. a.	n. a.	150	n. a.	n. a.	n. a.	600	600	n. a.	A	A	A	550	550
In	A	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	A	n. a.	A	n. a.	360
K	1000	n. a.	n. a.	n. a.	600	600	n. a.	900	n. a.	n. a.	A	A	n. a.	260	260
Li	540	n. a.	n. a.	750	1000	1000	1000	1000	1200	1200	A	A	n. a.	n. a.	380
Mg	n. a.	n. a.	n. a.	850	A	A	1000	1150	n. a.	n. a.	A	A	n. a.	n. a.	A
Na	1000	n. a.	n. a.	600	600	600	n. a.	900	n. a.	n. a.	A	A	n. a.	290	290
NaK	n. a.	n. a.	n. a.	n. a.	600	600	n. a.	900	n. a.	n. a.	A	A	n. a.	n. a.	n. a.
Pb	n. a.	n. a.	n. a.	600	n. a.	n. a.	n. a.	1000	850	n. a.	A	A	A	A	n. a.
Sb	A	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.
Sn	A	n. a.	n. a.	600	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	A	n. a.	A	n. a.	n. a.
Tl	649	303	1000	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	A	A	n. a.	n. a.	n. a.
Th-Mg	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	850	1000	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.
U	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	1400	1450	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.	n. a.
Zn	A	n. a.	n. a.	750	A	A	450	500	n. a.	n. a.	A	A	n. a.	n. a.	A

A attacked, *n. a.* not available

Table H.2 Maximum operating temperature (°C) of ceramics for handling liquid metals under an inert atmosphere

Molten metal or alloy	**Ceramic material**								
	Pyrex	**Fused silica (SiO_2)**	**Mullite ($Al_6Si_2O_{13}$)**	**Alumina (Al_2O_3)**	**Magnesia (MgO)**	**Spinel ($MgAl_2O_4$)**	**Zirconia (ZrO_2)**	**Beryllia (BeO)**	**Graphite (C)**
Ag									1300
Al								1200	
Au						1897			1300
Bi									850
Ca									900
Cd	540								
Fe				1600	1550		1550	1550	
Ga	560	1100							
In	530	820							
K	335								
Mg									1300
Mn						1710			
Na									
Ni				1470			1470	1800	
Pb	520			1100		1400			800
Sb		850							850
Si				1890	1450				
Sn	285	590	1300	1830					910
Tl									
Ti			A	A	1660	A	A	A	A (TiC)
Zn	510		1300						800

A attacked

Table H.3 Container material for handling molten salts, slags, and fluxes

Molten salts	Material class	Resistant materials	Remarks
chlorides	Pure metals	Gold	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere until 850 °C. Creep behavior for thin-walled crucibles
		Steel (Fe-0.8C)	Reducing or inert atmosphere (Ar, He) until 1200 °C
		Platinum	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (H_2) atmosphere until 1400 °C. Avoid carbon
		Molybdenum	Vacuum, reducing or inert atmosphere (Ar, He) until 1600 °C. Becomes brittle
		Iridium	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere until 1800 °C
	Glass	Borosilicate glass (Pyrex)	Dry and inert atmosphere (N_2, Ar, He) until 500 °C
	Refractory and advanced ceramics	Fused silica (SiO_2)	Dry and inert atmosphere (N_2, Ar, He) until 1200 °C
		Mullite ($Al_6Si_2O_{13}$)	Dry and inert atmosphere (N_2, Ar, He) until 1200 °C
		Electrofused alumina (Al_2O_3)	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere even with water vapor until 1500 °C
		Zirconia (ZrO_2, stabilized)	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere even with water vapor until 1600 °C
		Boron nitride (hexagonal)	Dry and inert (CO_2, N_2, Ar, He) or oxidizing (air, O_2) atmosphere until 1500 °C
	Carbon-based materials	Graphite	Reducing or inert atmosphere until 2000 °C
		Vitreous carbon	Reducing or inert atmosphere until 1500 °C. Oxidizing atmosphere until 600 °C
borates	Lithium metaborate	Platinum (max. 1100 °C)	Oxidizing melts
	Sodium borate	Platinum (max. 1100 °C)	Oxidizing melts
fluorides	Pure metals	Gold	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere until 850 °C. Creep behavior for thin-walled crucibles
		Nickel	Reducing or inert atmosphere (Ar, He) until 1000 °C
		Steel (Fe-0.8C)	Reducing or inert atmosphere (Ar, He) until 1200 °C

Table H.3 (*continued*)

Molten salts	Material class	Resistant materials	Remarks
fluorides	Pure metals	Platinum	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (H_2) atmosphere until 1400 °C. Avoid carbon
		Molybdenum	Reducing, vacuum, or inert atmosphere (Ar, He) until 1600 °C. Becomes brittle
		Iridium	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere until 1800 °C
	Refractory and advanced ceramics	Boron nitride (hexagonal)	Dry and inert (CO_2, N_2, Ar, He) or oxidizing (air, O_2) atmosphere until 1500 °C
	Carbon-based materials	Graphite	Reducing or inert atmosphere until 2000 °C
		Vitreous carbon	Reducing or inert atmosphere until 1500 °C. Oxidizing atmosphere until 600 °C
chloro-aluminates	Refractory metals	Molybdenum, tungsten, and zirconium	Inert atmosphere until 600 °C
	Ceramics and glasses	Borosilicate glass (Pyrex)	Up to 230 °C
		Vycor and fused silica	Until 600 °C
		Vitreous carbon	Inert atmosphere until 600 °C
hydroxides	Noble and precious metals	Pure silver, gold, and platinum	Reducing atmosphere; usually corroded if oxidizing impurities are present such as nitrates. Melt resistance: Ag > Au (990 °C) > Pt (1100 °C)
	Nickel	Grade Ni 200	Reducing atmosphere and anhydrous melts. Protected by its passivation layer of NiO_2, which is insoluble
	Pure zirconium and hafnium metals	Zircadyne grade 702	Oxidizing melts (max. 650 °C)
hydroxides	Refractory and advanced ceramics	Magnesia (MgO), beryllia (BeO), ceria (CeO_2), and zinc oxide (ZnO)	Suitable for basic melts only
		Electrofused alumina (Al_2O_3)	Suitable for acidic melts only
		Zirconia (ZrO_2)	Stable over the entire acidity range but sensitive to thermal shocks
		Glassy and impervious carbon	High-temperature capabilities over the entire acidic range but damaged by liquid sodium; sensitive to mechanical stress on cooling

Table H.3 (*continued*)

Molten salts	Material class	Resistant materials	Remarks
hydroxides	Polymers	Polytetrafluoroethylene	Suitable below 280 °C but avoid the presence or formation of any trace of free alkali metal. Perfect for the low melting point eutectic NaOH-KOH (170 °C)
sodium peroxide (Na_2O_2)	Metals	Nickel, iron	
titanates	Refractory metals	Molybdenum	Vacuum, reducing, or inert atmosphere (Ar, He) until 1800 °C. Becomes brittle
		Niobium	Vacuum, reducing, or inert atmosphere (Ar, He) until 1800 °C
		Iridium	Inert (CO_2, N_2, Ar, He), oxidizing (air, O_2), or reducing (CO) atmosphere until 2000 °C
		Tantalum	Vacuum, reducing, or inert atmosphere (Ar, He) until 2500 °C
		Tungsten	Vacuum, reducing, or inert atmosphere (Ar, He) until 2800 °C
carbonates	Metals and alloys	Pure gold	Oxidizing atmosphere until 850 °C. Completely immune toward molten alkali carbonates
		Pure aluminum	Can be used under an oxidizing atmosphere until 600 °C because it is protected by an $MAlO_2$ scale
		Gold-platinum	Oxidizing atmosphere until 700 °C
		Austenitic stainless steel 304L	Oxidizing atmosphere until 500 °C
carbonates	Metals and alloys	Austenitic stainless steel 310	Oxidizing atmosphere until 680 °C
		Nickel-based alloys	Oxidizing atmosphere until 600 °C
		High-chromium alloys	Oxidizing atmosphere until 700 °C
	Ceramics	Electrofused alumina	Oxidizing atmosphere until 1000 °C
		Graphite	Oxidizing atmosphere until 450 °C
nitrates	Metals	Platinum	Below 400 °C avoid the presence of peroxide anions
	Ceramics	Electrofused alumina (Al_2O_3)	Below 400 °C
	Polymers	Polytetrafluoroethylene	Suitable below 280 °C with eutectic mixtures

Table H.3 (*continued*)

Molten salts	Material class	Resistant materials	Remarks
sulfates	Metals	Pure iron	
		Platinum	
	Ceramics	Fused silica (SiO_2)	
alkali metal bisulfates ($MHSO_4$) and pyrosulfates ($M_2S_2O_7$)	Metals	Platinum	
	Ceramics	Fused	
Cryolite melts with dissolved aluminum metal	Advanced ceramics	Alumina (Al_2O_3)	Only in contact with alumina-saturated melts (12 wt% dissolved Al_2O_3). Inert or oxidizing atmospheres until 1000 °C
		Boron nitride (hexagonal)	Inert atmosphere until 1000 °C
	Carbon-based materials	Graphite SGL grade R8710	Inert atmosphere until 1000 °C. A layer of Al_4C_3 forms on the inner surface. Becomes fragile
		Impervious carbon	Inert atmosphere until 1000 °C. A layer of Al_4C_3 forms on the inner surface. Becomes fragile

Table H.4 Corrosion properties of materials in hydrochloric acid and hydrogen chloride. (Corrosion in the CPI: Corrosion by Hydrogen Chloride and Hydrochloric Acid. ASM International, Materials Park (1994), page 191–196 and 220–224)

Material class	Materials	Concentration and temperature range
Metals and alloys	Carbon and low alloy steels	Readily corroded
	Austenitic stainless steels (AISI 304, 316L)	Readily corroded
	Nickel grade 200 and Monel® 400	Resistant to dilute HCl below10 wt%
	High-silicon cast iron (Durichlor®, 14.4 wt% Si-3 wt% Mo) (not suitable with Fe^{3+}, Cu^{2+})	Resistant to all concentrations up to 95 °C
	Duplex austenitic-ferritic stainless steel SAF 2540	Resistant to dilute HCl below 3 wt% up to 100 °C
	Titanium alloy Ti-Pd (grades 7, 11) and Ti-Ru (grade 26, 28)	Resistant with Fe(III) or Cu(II) acting as corrosion inhibitors
	Zircadyne® 702 (not suitable with Fe^{3+}, Cu^{2+})	Resistant to all concentrations up to the boiling point

Table H.4 (*continued*)

Material class	Materials	Concentration and temperature range
Metals and alloys	Hastelloy® B2 (not suitable with Fe^{3+}, Cu^{2+})	Resistant to all concentrations up to the boiling point
	Pure tantalum	Resistant to 25 wt% up to 190 °C; resistant to 37 wt% up to 150 °C
	Niobium and niobium zirconium	Resistant to all concentrations at room temperature
	Gold and platinum	Resistant to all concentrations up to the boiling point
Polymers and elastomers	PE	Resistant at room temperature
	PP	Resistant to all concentrations up to 110 °C
	PVC	Resistant to all concentrations up to 110 °C
	PVDC	Resistant to all concentrations up to 80 °C
	PVDF (Kynar)	Resistant to all concentrations up to 135 °C
	ECTFE (Halar)	Resistant to 18 wt% at 90 °C
	Chlorobutyl elastomer	Resistant to 20 wt% at 90 °C
	PTFE (Teflon)	Resistant to all concentrations up to 260 °C
	Bromobutyl elastomer	Resistant to 20 wt% at 90 °C
	NR	Resistant to all concentrations up to 40 °C
	NBR	Permeable to HCl
Ceramics and glasses	Impervious graphite (Karbate®)	Resistant to all concentrations up to 165 °C
	Borosilicate glasses (Pyrex®)	Resistant to all concentrations up to 190 °C
	Fused silica and quartz	Resistant to all concentrations up to 200 °C
	Silicon carbide (Carborundum®)	Resistant to all concentrations up to 190 °C

A material is satisfactory for handling hydrofluoric acid if the corrosion rate is maintained below 50 µm/year (i.e., 2 mil/year)

ECTFE ethylene chlorotrifluoroethylene, NBR nitrile butadiene rubber, NR natural rubber, PE polyethylene, PP polypropylene, PTFE polytetrafluoroethylene, PVC polyvinyl chloride, PVDC polyvinylidene dichloride

Table H.5 Corrosion properties of materials in nitric acid

Material class	Materials	Concentration and temperature range
Metals and alloys	Carbon and low-alloy steels	Readily corroded
	Austenitic stainless steels (AISI 304, 316L): use ELI carbon content (< 0.05 wt% C), add carbide stabilizers (e.g., Ti, Nb), solution annealing after welding, addition of Si for 100 wt% HNO_3	Resistant up to 90 °C to concentrated HNO_3 below 30 wt%; resistant at room temperature to concentrated HNO_3 until 100 wt%
	Aluminum alloy series 30003 and 1001	Resistant to 93–100 wt% until 30 °C
	High-silicon cast iron (Duriron®, 14.4 wt% Si)	Resistant
	Titanium CP ASTM grade 2	Resistant to all concentrations up to the boiling point
	Zircadyne® 702	Resistant to 65–90 wt% up to the boiling point
	Hastelloy® C-276, Incoloy® 825, Chlorimet 3, 20Cb-3	Resistant to all concentrations up to the boiling point
	Pure tantalum	Resistant to all concentrations up to the boiling point
	Gold and platinum	Resistant to all concentrations up to the boiling point without chlorides
Ceramics and glasses	Impervious graphite	Resistant
	Borosilicate glasses	Resistant to concentrated HNO_3 up to 70 wt% until 125 °C
	Carborundum®	Resistant

A material is satisfactory for handling nitric acid if the corrosion rate is maintained below 50 µm/year (i.e., 2 mil/year)

Table H.6 Corrosion properties of materials in hydrofluoric acid and hydrogen fluoride

Material class	Materials	Concentration and temperature range
Metals and alloys	Pure copper	Resistant to concentrated HF below 70 wt% from room temperature up to boiling point
	Red brass (Cu-15Zn)	Resistant to concentrated HF below 70 wt% from room temperature up to the boiling point
	Nickel grade 200 and Monel® 400	Resistant to all concentrations up to the boiling point
	Magnesium metal	Forms a passivating film
	Gold and platinum	Resistant to all concentrations up to the boiling point
Polymers and elastomers	PE	
	PP	
	PVC	
	PVDC	
	PVDF	
	PTFE	
	NR	
	NBR	
Ceramics and glasses	Impervious graphite	Resistant
	Sapphire	Resistant
	Fluorite	

A material is satisfactory for handling hydrofluoric acid if the corrosion rate is maintained below 50 µm/year (i.e., 2 mil/year)

NBR nitrile butadiene rubber, NR natural rubber, PE polyethylene, PP polypropylene, PTFE polytetrafluoroethylene, PVC polyvinyl chloride, PVDC polyvinylidene dichloride, PVDF polyvinylidene difluoride

Table H.7 Corrosion resistance of materials in sulfuric acid

Material class	Materials	Concentration and temperature range
Metals and alloys	Carbon and low-alloy steels, and gray cast iron	At room temperature only for concentrations between 65 and 100 wt% (other concentrations require cathodic protection)
	Austenitic stainless steels AISI 304	Above 93 wt% up to 40 °C
	Austenitic stainless steels AISI 316L	Above 90 wt% up to 40 °C
	High-silicon cast iron (Duriron®, 14.4 wt% Si)	All concentrations from room temperature up to the boiling point
	Zircadyne® 702	Up to 50 wt% up to the boiling point
	Hastelloy® C-276	All concentrations up to the boiling point
	Incoloy® 825	Below 40 wt% and above 93 wt%
	Monel® 400	Up to 85 wt% at 30 °C (air-free)
	Lead	Up to 90 wt% at room temperature
	Illium® B	Up to 98 wt% up to 100 °C
	Pure tantalum	Up to 98 wt% up to the boiling point (no free SO_3)
	Gold and platinum	
Polymers and elastomers	PE	Up to 98 wt% at room temperature
	PP	
	PVC	Up to 93 wt% at room temperature
	PVDC	
	PVDF	Up to 98 wt% at 65 °C
	PTFE	All concentrations up to 260 °C
	NR	Up to 75 wt% at room temperature
	NBR	
Ceramics and glasses	Silica brick and quartz	Up to 98 wt% up to the boiling point
	Borosilicate glasses	
	Carborundum®	

A material is satisfactory for handling sulfuric acid if the corrosion rate is maintained below 50 µm/year (i.e., 2 mil/year)

NBR nitrile butadiene rubber, NR natural rubber, PE polyethylene, PP polypropylene, PTFE polytetrafluoroethylene, PVC polyvinyl chloride, PVDC polyvinylidene dichloride, PVDF polyvinylidene difluoride

Table H.8 Heat- and oxidation-resistant alloys for high-temperature use

Heat- and oxidation-resistant commercial alloys	Maximum operating temperature in dry air (°C)	Practical melting range (°C)	Oxidation rate at 980 °C (μm/1000 h)	Yield strength 0.2% at 800 °C (σ_{YS}/MPa)	Allowable stress (MPa)[a]	Time to rupture (h)[b]
Stainless steel 316	816	1370–1400				
Inconel® 625	980	1290–1360	193	294		2400
Stainless steel 309	982	1399–1454				
Hastelloy® HX	1050	1260–1355	153	200		2100
Incoloy® 800HT	1095	1357–1385	389	90		920
Haynes® 230	1149	1301–1371	89	160	28	5000
Stainless steel 310	1150	1354–1402		138		1000
Inconel® 601	1200	1360–1411		150		1000
Haynes® HR-160	1205	1293–1370	150	160		

[a] According to ASME Vessel Section II, art D, Table 1B

[b] Measured at 982 °C under a constant stress of 14 MPa

Table H.9 Resistance of metals and alloys to chlorine gas

Metals and alloys	Maximum operating temperature		Ignition temperature in dry chlorine (°C)
	Dry chlorine (°C)	Wet chlorine (°C)	
Titanium	−18	175	−18
Silver	40		
Cast iron	90		
Gold	120		
Aluminum 1100	120	130	
Mild steel	150		250
Niobium	200	100	
Copper	205		260–300
Hastelloy D	205		
Tantalum	250	375	
Stainless steel 304	290	40	

Table H.9 (*continued*)

Metals and alloys	Maximum operating temperature		Ignition temperature in dry chlorine (°C)
	Dry chlorine (°C)	Wet chlorine (°C)	
Stainless steel 316	310		
Monel 400	420		
Nichrome	425		
Magnesium	450		
Platinum	480		
Nickel 201	500	525–540	
Inconel 600	510		
Hastelloy B	510		
Hastelloy C-276	510		
Inconel 600	540		
Hastelloy B2	540		

I Economic Data for Metals, Industrial Minerals, and Electricity

I.1 Prices of Pure Elements

See ◘ Table I.1.

◘ **Table I.1** Prices of pure elements, metals, and some alloys (2014). (From *Mining Journal*, *Metal Bulletin Weekly*, *Mineral Price Watch*, Roskill Information Services, US Geological Survey, and *Industrial Minerals*)

Metal or alloy	Purity (wt%)	Price (US$/troy ounce)	Price (US$/lb)	Price (US$/kg)
Aluminum	99.50	0.057	0.830	1.83
Aluminum powder	99.97	0.560–0.995	4.17–14.69	18–32
Aluminum powder	97.00	0.140–0.224	2.04–3.27	4.5–7.2
Antimony (ingot)	99.65	0.286	4.17	9.20
Arsenic	99.00	0.057	0.825	1.819
Barium	99.70	12.44	181.44	400.00
Beryllium	99.50	26.40	385.00	849.00
Beryllium-copper master	n. r.	11.66	170	375
Bismuth	99.99	0.754	11.00	24.25
Boron	99.00	155.52	2267.96	5000
Cadmium	99.99	0.059	0.860	1.897
Cesium	99.99	630.87	9200	20,283
Calcium	99.90	0.151	2.20	4.85
Cerium	99.00	0.311	4.54	10.00
Chromium	99.90	0.451	6.58	14.50
Cobalt	99.80	1.008	14.70	32.41
Copper	99.9990	0.199	2.896	6.385
Copper (mill products)	99.90	0.473	6.895	15.20
Dysprosium	99.00	14.62	213.19	470.00
Erbium	99.90	5.13	74.84	165.00
Europium	99.00	31.10	453.59	1000.00

Table I.1 (*continued*)

Metal or alloy	Purity (wt%)	Price (US$/troy ounce)	Price (US$/lb)	Price (US$/kg)
Ferrochromium[a]	68–70 Cr			1.090
Ferromanganese[a]	78 Mn	0.033	0.48	1.060
Ferromolybdenum[a]	65–70 Mo	0.671	9.80	21.60
Ferroniobium[a]	65–70 Nb	14.74	17.92	39.50
Ferrosilicon[a]	75 Si	0.042	0.61	1.350
Ferrotitanium[a]	70 Ti	0.176	2.56	5.65
Ferrotungsten[a]	75 W	0.102	15.42	34.00
Ferrovanadium[a]	70–80 V	0.62	9.07	20.00
Gadolinium	99.90	2.95	43.09	95.00
Gallium	99.99	7.93	115.67	255
Germanium	99.99	59.10	861.82	1900
Gold 10 Kt	41.67	417	6081	13,406
Gold 14 Kt	58.33	688	10,033	22,119
Gold 18 Kt	75.00	885	12,906	28,453
Gold 20 Kt	83.33	985	14,365	32,265
Gold 24 Kt	99.995	1180	17,208	37,938
Hafnium	97.00	50.20	732.09	1614
Holmium	99.00	311.03	4535.92	10,000
Indium	99.99	22.24	324.32	715
Iridium	99.999	520	7583	16,718
Iron and steel (plate)	99.99	0.030	0.45	1.00
Iron (3 wt% C)	97 wt%	0.011	0.159	0.350
Lanthanum	99.00	0.299	4.35	9.60
Lead	99.90	0.058	0.842	1.856
Lithium	99.80	2.97	43.27	95.40
Lutetium	99.00	233	3402	7500
Magnesium	99.9	0.074	1.075	2.370
Manganese (flakes)	99.7	0.065	0.953	2.100
Mercury (flask 76 lb)	99.99	2.35	34.21	75.42

Table I.1 *(continued)*

Metal or alloy	Purity (wt%)	Price (US$/troy ounce)	Price (US$/lb)	Price (US$/kg)
Molybdenum (HIP)	99.95	4.06	59.26	130.65
Molybdenum (VAR)	99.9	6.857	100	220.46
Neodymium	99.50	2.58	37.65	83.00
Nickel (ingot)	99.00	0.481	7.015	15.47
Nickel (plate, rod)	99.80	3.204	46.72	103
Niobium	99.90	7.54	110.00	242.51
Niobium-1 wt% zirconium	99.00	7.95	116.00	255.74
Osmium	99.999	450	6563	14,468
Palladium	99.999	815.00	11,885	26,203
Platinum	99.999	1202	17,529	38,645
Potassium	99.90	2.80	40.82	90.00
Praseodymium	99.00	5.44	79.4	175.00
Rhenium (pellets)	99.90	89.14	1300	2866
Rhodium	99.9	1245	18,156	40,028
Rubidium	99.80	2479	36,151	79,700
Ruthenium	99.999	58.00	846	1865
Samarium	99.99	0.778	11.34	25.00
Selenium	99.50	1.650	24.00	52.91
Silicon (EG)	99.5–99.9	0.070	1.02	2.25
Silicon (MG)	98–98.5	0.063	0.92	2.02
Silicon (SG)	99.99	97.198	1417.48	3125
Silver	99.99	15.60	227.50	501.55
Sodium	99.90	2.05	29.94	66.00
Stainless steel 304 (ingot)	n. r.	0.106	1.542	3.400
Stainless steel 304 (plate)	n. r.	0.298	4.341	9.570
Stainless steel 316L (plate)	n. r.	0.420	6.124	13.50
Strontium	99.95	311	4536	10,000
Tantalum	99.80	12.44	181.44	400

Table I.1 (*continued*)

Metal or alloy	Purity (wt%)	Price (US$/troy ounce)	Price (US$/lb)	Price (US$/kg)
Tantalum-2.5 wt% tungsten	n. r.	20.839	304	670
Tellurium	99.99	3.98	58.00	128
Terbium	99.90	25.66	374.21	825.00
Thallium	99.00	39.8	580	1279
Thorium	99.90	150.00	2187.57	4822.76
Tin	99.90	0.544	7.94	17.50
Titanium (high purity)	99.99	3.51	51.26	113.00
Titanium alloy Ti-0.15Pd	n. r.	6.27	91.37	201.43
Titanium alloy Ti-6Al-4V	n. r.	2.18	31.75	70.00
Titanium (grade 2)	99.80	1.92	28.00	61.73
Titanium ingot	99.00	0.280	4.08	9.00
Titanium sponge	99.70	0.311	4.54	10.00
Tungsten	99.90	22.95	335	750
Uranium	99.00	0.542	7.90	17.42
Vanadium	99.00	50.00	729.17	1607.54
Ytterbium	99.90	49.8	725.7	1600
Yttrium	99.90	2.39	34.93	77.00
Zinc	99.995	0.067	0.978	2.156
Zircadyne® 702	99.00	6.17	90.00	198.42
Zirconium (sponge)	99.40	0.933	13.61	30.00

HIP hot isostatic pressing, n. r. not relevant, VAR vacuum arc remelting

[a] Prices of most ferroalloys are reported per unit mass of metal contained

I.2 World Annual Production of Commodities

See ▣ Table I.2.

▣ **Table I.2** World annual production of commodities in decreasing order (2014)

Commodity	World annual production (tonne)
Coal	7,824,000,000
Cement	4,000,000,000
Crude oil	3,980,000,000 (25,000,000,000 bbl)
Iron ore (hematite)	3,012,000,000
Natural gas	3,110,000,000 (4,359,000,000,000 m^3; 154,000,000,000,000 ft^3; 154 EJ)
Crude steel	1,500,000,000
Pig iron, sponge iron, direct reduced iron	1,100,000,000
Quicklime	350,000,000
Sulfuric acid (96 wt%)	284,000,000
Rock salt	250,000,000
Bauxite (metallurgical and refractory grades)	248,000,000
Phosphate rock	205,000,000
Gypsum	141,000,000
Alumina	108,000,000
Aluminum (primary)	53,000,000
Manganese ore	48,000,000
Stainless steels	38,600,000
Potash (potassium muriate)	36,000,000
Chromite ore	29,400,000
Kaolin	25,000,000
Magnesite	24,000,000
Feldspar	21,000,000
Copper	17,930,000
Bentonite	15,500,000
Zinc	13,513,000
Ferrochrome	11,400,000
Lead	11,274,000
Ilmenite concentrates	11,000,000
Barite	9,000,000

Table I.2 (*continued*)

Commodity	World annual production (tonne)
Talc	7,850,000
Ferrosilicon	7,800,000
TiO_2 feedstocks	6,500,000
Fluorite (fluorspar)	6,000,000
Borates	5,500,000
Nepheline syenite	5,400,000
Native sulfur	5,000,000
Ferromanganese	4,500,000
Fuller's earth	3,300,000
Silicomanganese	3,000,000
Diatomite	2,680,000
Asbestos	2,000,000
Silicon metal	2,000,000
Nickel	1,832,000
Zircon and baddeleyite	1,640,000
Magnesium	950,000
Rutile	800,000
Bromine	675,000
Tin	375,000
Flake mica	310,000
Molybdenum	269,100
Titanium metal	223,000
Antimony	180,000
Cobalt concentrates	150,000
Lithium carbonate	110,000
Sodium	108,000
Ferroniobium	95,000
Tungsten	80,000
Cobalt	77,000
Vanadium	76,000
Uranium	60,000
Chromium	45,000
Arsenic trioxide (white arsenic)	39,250

Table I.2 (*continued*)

Commodity	World annual production (tonne)
Silver	25,474 (819,000,000 troy ounces)
Cadmium	21,800
Bismuth	8100
Beryl	5000
Selenium	2800
Gold	2770 (89,000,000 troy ounces)
Tantalum	2200
Graphite	2100
Mercury	2000 (58,000 flasks)
Zirconium (metal)	1000
Lithium (metal)	1000
Indium	700
Gallium	280
Palladium	200
Beryllium	260
Platinum	158
Tellurium	125
Iodine	28
Diamonds	25 (124,000,000 Kt)

Conversion factors: 1 US barrel (bbl; oil) = 42 gal (liquid, US) (E) = 0.158987 m^3; 1 MMBtu = 10^6 Btu (E) = 1000 ft^3 (E) = 1.056 GJ; 1 mercury flask (US) = 76 lb (avoirdupois) (E) = 34.473 kg; 1 troy ounce = 1/12 pound (troy) (E) = 31.1035 g; 1 Kt (metric) = 200 mg (E)

I.3 Economic Data for Industrial Minerals

See ◘ Table I.3.

◘ **Table I.3** Economic data for industrial minerals, ores, fuels, and commodities (2014). (From *USGS Mineral Yearbook*, Roskill Information Services Ltd, Industrial Minerals Information Ltd, *Minerals Price Watch*, *Mining Journal, Mineral Sands Report*, and *Metal Bulletin Weekly*)

Industrial mineral or rock	Major producing countries/regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Alumina (nonmetallurgical grade)	China (34,100), Australia (18,000), USA (4600), Russia (2900), Jamaica (2000), Ukraine (1600), Suriname (1400), Canada (1400), Spain (1300), Venezuela (1200), Germany (1000), Greece (550)	85,000,000	Calcined alumina (99 wt% Al_2O_3): 675–850 Tabular alumina: 700–800 White fused alumina (94 wt% Al_2O_3): 1100–1300 Brown fused alumina (94 wt% Al_2O_3): 990–1020
Alumina trihydrate	USA		Alumina trihydrate (58 wt% Al_2O_3): 290–350
Andalusite	South Africa (295), France (65)	390,000	Andalusite (55–59 wt% Al_2O_3): 310–550
Anthracite	China (500,000), Russia (50,000), Indonesia (50,000), Vietnam (45,800), Turkey (5600), Spain (2600), South Africa (2600), USA (2100), Korea (2000)	800,000,000	Anthracite: 200–220
Antimony trioxide	China, USA, Mexico, Japan, South Africa	130,000	Antimony trioxide (99.5 wt% Sb_2O_3): 6950–8300
Apatite (see also phosphate rock)	USA (42,000), Morocco (25,000), China (20,000), Russia (Kola Peninsula)	70,000,000	Bone phosphate of lime: 45–50
Asbestos (i.e., chrysotile, crocidolite, amosite, anthophyllite, tremolite, and actinolite)	Russia (1000), China (440), Brazil (310), Kazakhstan (223), Canada (50), Greece (35), Swaziland (25), South Africa (20)	2,000,000	Chrysotile: 150–1200 Crocidolite: 650–920
Attapulgite and sepiolite (i.e., palygorskite or Fuller's earth)	USA (725), Senegal (103), Spain (94), Australia (19), South Africa (9)	950,000	Attapulgite: 110

Table I.3 (*continued*)

Industrial mineral or rock	Major producing countries/ regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Baddeleyite	South Africa, Russia, USA		Baddeleyite 98 wt% $(Zr,Hf)O_2$: 2500–3300
Ball clay	China, USA, UK (1100)		Kaolinitic clay (43 wt% Al_2O_3): 110–125
Barite (heavy spar)	China (4300), India (1700), USA (640), Morocco (770), Iran (330), Turkey (225), Kazakhstan (200), Mexico (134)	9,000,000	Lump ore: 150–180 Ground ore: 150–160 Drilling grade: 140–170 Chemical grade: 160–180 Paint grade (350 mesh, 98 wt%): 315–400
Bauxite (i.e., gibbsite, boehmite, and diaspore)	Australia (70,000), Indonesia (41,000), China (37,000), Brazil (34,000), Guinea (17,000), India (13,000), Jamaica (11,000), Kazakhstan (5500), Russia (5300), USA (5100), Suriname (3000), Greece (2350)	248,000,000	Refractory grade: 350–365 Calcined: 330–415 Abrasive grade: 100–120
Bentonite (montmorillonite clay)	USA (4900), China (3400), Greece (1250), Russia (920), India (998), Mexico (565), Japan (430), Germany (375), Turkey (380), Iran (350), Ukraine (211), Italy (102)	15,000,000	Foundry grade: 90–100 Litter grade: 40–65 API grade: 95–140
Beryl and bertrandite	USA (4.50), Russia (1.00), China (0.50), Kazakhstan (0.10), Mozambique (0.045), Madagascar (0.012), Portugal (0.005)	5500	Beryl ore (10 wt% BeO): 75–90
Borax and borates (kernite, tincal, colemanite, and ulexite)	Turkey (2280), USA (1250), Argentina (600), Russia (400), Chile (500), China (300), Bolivia (150)	5,496,000	Colemanite (40–42 wt% B_2O_3): 630–690 Ulexite (40 wt% B_2O_3): 620–650 Boric acid (H_3BO_3): 620–1000 Borax decahydrate: 910–1050
Bromine	USA (225), Israel (204), China (150), Jordan (70), Japan (20)	674,000	Bromine (purified, 99.95 wt% Br_2)
Brucite	China, USA	50,000	Brucite $Mg(OH)_2$: 160–300

Table I.3 (*continued*)

Industrial mineral or rock	Major producing countries/ regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Chromite (i.e., stratiform, podiform)	South Africa (10,700), Kazakhstan (5000), India (3800), Turkey (2290), Finland (695), Oman (616), Zimbabwe (600), Brazil (567), Pakistan (450), Russia (400), Iran (330), Australia (325)	27,300,000	Chemical grade (46 wt% Cr_2O_3): 185–250 Metallurgical grade (46 wt% Cr_2O_3): 150–180 Foundry grade: 300–380 Refractory grade: 300–330
Celestite	China (700), Spain (97), Mexico (42), Iran (15), Argentina (8), Morocco (2.5)	800,000	Celestite (94 wt% $SrSO_4$): 90–100
Coal (thermal) (see also anthracite)	China (3,000,000), USA (1,000,000), India (500,000), Australia (400,000), Russia (300,000), Indonesia (300,000), South Africa (250,000), Germany (180,000), Poland (140,000), Kazakhstan (100,000), Turkey (90,000), Colombia (85,000), Ukraine (70,000)	7,740,000,000	Thermal coal: 65–110
Diamond	Botswana (22 Mct), Democratic Republic of the Congo (20 Mct), Canada (10.8 Mct), Zimbabwe (8.5 Mct), Angola (8 Mct), Australia (7.6 Mct), South Africa (7 Mct), Namibia (1.2 Mct), China (1.1 Mct)	123,000,000 Kt	$ 200 per Kt
Diatomite (Kieselgur)	Argentina, (1000), USA (600), China (440), Japan (100), Mexico (84), Spain (83), Denmark (81), and France (75)	2,700,000	Diatomite filter aids: 605–865
Emery (corundum, magnetite, and spinel)	China[a] (1000), Australia[a] (50), Turkey (24.7), Greece (10), USA (3), Kazakhstan, Russia, Uruguay, Germany	37,000 1,050,000[a]	Coarse grain emery: 296–388 Medium grain emery: 374 Fine grain emery: 416
Feldspars (orthoclases and plagioclases)	Italy (4700), Turkey (4500), China (2400), Thailand (1100), USA (690), Iran (655), France (650), Spain (650), Japan (600), Poland (550)	20,875,000	Brightness (> 90): 170–210 Ceramic grade (325 mesh): 150–180 Glass grade low Fe (30 mesh): 70 Glass grade high Fe (30 mesh): 50 Crude: 22–23

Table I.3 (*continued*)

Industrial mineral or rock	**Major producing countries/regions and annual production (10^3 tonne)**	**World annual production (tonne)**	**Grade and price range (US$/tonne)**
Fluorspar (fluorite)	China (3300), Mexico (1300), Mongolia (405), Russia (250), South Africa (140), Spain (120)	6,000,000	HF acid grade: 330–360 Metallurgical grade (85 wt% CaF_2): 290–310 Metallurgical grade (90 wt% CaF_2): 250–275
Fused silica (high-purity silica sand 99.9 wt% SiO_2 melted in a carbon electrode arc furnace)	USA (100), China, Singapore, South Korea, and Japan	200,000	High-purity grade (99.9 wt%): 285–360 Lower-purity grade (99.5 wt%): 260–340
Garnet (pyrope, almamdine, spessartine, uvarovite, grossular, andradite)	India (700), Australia (150), China (470), USA (55)	335,000	Almandine (8–250 mesh): 170–240
Graphite (crystalline, flake, microcrystalline, amorphous)	China (1800), India (145), Brazil (90), Canada (20), Russia (14), Ukraine (8)	2,100,000	Synthetic powder (99.95 wt%): 7000–20,000 Crystalline flakes (94–97 wt% C): 1200–1300 Amorphous powder (80–85 wt% C): 430–480 Crude concentrate (85 wt% C): 500–550
Gypsum and anhydrite	China (37,000), Thailand (12,000), Iran (12,000), USA (9500), Spain (7100), Mexico (6500), Slovakia (7000), Brazil (4000), Australia (3100), Russia (2900), Canada (2500)	145,000,000	Crude gypsum: 7 Calcined gypsum: 17
Ilmenite	Canada (2500), Australia (1300), Norway (870), South Africa (1370), China (1000), India (700), Mozambique (640), Ukraine (600), Madagascar (520), USA (300), Brazil (120), Sri Lanka (63), Malaysia (30)	10,900,000	Ilmenite (54 wt% TiO_2): 130–140
Iodine crystals (sublimed)	Chile (16), Japan (9.8), USA (1.3), China (0.55)	28,000	Iodine crystal (99.5 wt% I_2): 33,000–37,000

Table I.3 (*continued*)

Industrial mineral or rock	Major producing countries/ regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Iron ore (hematite, magnetite)	China (1,350,000), Australia (490,000), Brazil (460,000), Russia (105,000), India (170,000), Ukraine (80,000), South Africa (60,000), Kazakhstan (51,000), USA (54,000), Iran (48,000), Canada (34,000), Sweden (28,000)	3,035,000,000	Iron ore (65 wt% Fe_2O_3): 65–70
Iron oxide (pigments)	India (500), USA (70), Spain (8)	1,100,000	Iron oxide, brown: 1015–1080 Iron oxide, red: 1440–1650
Kaolin (china clay)	USA (5500), Germany (4900), Bangladesh (3000), Brazil (2200), Iran (1500), UK (1000), Indonesia (1500), South Korea (1100), Czech Republic (660), Turkey (650), Vietnam (650)	39,000,000	Filler grade: 120–190 Paper grade: 240–300 Sanitary grade: 180–190
Kyanite	USA (95), India (5), China (3), Zimbabwe (4), Australia (1), Brazil (0.2)	110,000	Calcined (54–60 wt% Al_2O_3): 375–440 Raw (54–60 wt% Al_2O_3): 225–320
Leucoxene	Australia (225)	225,000	Leucoxene (91 wt% TiO_2): 1400–1465
Lithium chemicals	Chile, Argentina, China, USA		Lithium carbonate: 6048–7000 Lithium hydroxide (56% LiOH): 16,128–19,040
Lithium minerals	Australia (450), Chile (70), China (58), Argentina (17), USA (1.5)	25,000 (lithium content)	Petalite (4.2 wt% Li_2O): 170–265 Spodumene (5.0 wt% Li_2O): 310–400 Spodumene (7.5 wt% Li_2O): 725–790
Magnesite	China (14,500), Russia (2600), Slovakia (750), Turkey (1000), Austria (870), Australia (670), Spain (575), Brazil (500), Greece (400), Netherlands (280), India (215), Canada (150)	23,200,000	Caustic magnesia: 200 Dead burned magnesia: 450–550 Electrofused magnesia: 690–710
Manganese dioxide and rhodocrosite	Africa (167), Europe (58), Australia (35), South America (8), North America (3)	271,000	Electrolytic manganese dioxide: 1750–1800 Chemical manganese dioxide:1400–1600 Natural manganese dioxide: 950–1000

Table I.3 *(continued)*

Industrial mineral or rock	Major producing countries/ regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Mica (muscovite ground)	China (132), USA (50), Korea (32), France (20), Canada (15), Finland (12), Argentina (10), Russia (9), Turkey (5), Brazil (4), Malaysia (4), Iran (3)	305,000	Dry ground: 300–400 Wet ground: 700–1250
Mica (muscovite sheet)	India (4), China, Argentina, Brazil, South Africa, Madagascar	5000	Low quality: 200–430 Highest quality: 600–1200
Microsilica	USA, China, Spain, Brazil	350,000	100–160
Mullite (synthetic)	Germany, Italy, Japan, USA, UK	60,000	Fused mullite: 1000–1500 Fused zirconia mullite: 1200–1500 Sintered mullite: 750–1350
Natural gas (STP)	Russia (669,000 m^3), USA (651,000 m^3), Iran (151,000 m^3), Qatar (146,000 m^3), Canada (145,000 m^3), China (102,000 m^3), Norway (101,000 m^3), Saudi Arabia (100,000 m^3), Algeria (78,000 m^3), Netherlands (76,000 m^3), Malaysia (62,000 m^3), Egypt (61,000 m^3), Turkmenistan (60,000 m^3), Mexico (53,000 m^3), United Arab Emirates (52,000 m^3), UK (48,000 m^3), Argentina (45,000 m^3), Nigeria (40,000 m^3), Trinidad and Tobago (43,000 m^3), Venezuela (31,000 m^3), Ukraine (21,000 m^3), Brazil (18,000 m^3), Azerbaijan (16,200 m^3), Germany (13,000 m^3), Peru (12,000 m^3), Romania (11,000 m^3), Colombia (10,000 m^3), Democratic Republic of the Congo (10,000 m^3)	3,450,000 m^3	Natural gas (USA): US$ 2.70 per 1 MMBtu (GJ) Natural gas (European Union): US$ 6.80 per 1 MMBtu (GJ)
Nepheline syenite	Russia (4620), Canada (610), Norway (330)	5,500,000	Norway: 165–210 Canada: 57–60
Nitrates (soda niter and Saltpeter)	Chile (980), Israel (520), USA (180), Denmark (70), Norway (30), Russia (22), Poland (10), Ukraine (5)	1,817,000	Soda niter ($NaNO_3$): 215 Saltpeter (KNO_3)

Table I.3 (*continued*)

Industrial mineral or rock	**Major producing countries/regions and annual production (10^3 tonne)**	**World annual production (tonne)**	**Grade and price range (US$/tonne)**
Olivine (fayalite and forsterite, synthetic by calcining chrysotile asbestos mining tailing)	Norway (3500), USA, Japan, South Korea, Taiwan, Spain, Italy, Brazil, Mexico	4,000,000	Concentrate: 15–20 Refractory grade: 85–95 Foundry grade: 90–140 Tundish spray: 115–150 EBT filler: 85–95
Perlite	Greece (720), China (700), Iran (750), Turkey (440), USA (400), Japan (300), Hungary (70)	3,500,000	Expanded perlite: 210–410 Graded perlite: 30–60 Raw perlite: 100–110
Petalite	Australia (100), Canada, Zimbabwe	200,000	Petalite (4.2 wt% Li_2O): 165–260
Petroleum (crude)	Saudi Arabia (525,000), Russia (509,000), USA (360,000), China (210,000), Iran (205,000), Mexico (151,000), United Arab Emirates (150,000), Canada (145,000), Venezuela (140,000), Kuwait (140,000), Iraq (136,000), Nigeria (120,000), Brazil (113,000), Russia (100,000), Norway (100,000), UK (65,000)	3,980,000,000	Crude oil (Brent): 65.00 US$/bbl Crude oil (West Texas Intermediate): 58.00 US$/bbl Heating oil (New York Mercantile Exchange): 184.38 US$/gal Gasoline: 2.00 US$/gal
Phosphate rock (i.e., apatite, fluoroapatite, hydroxyfluoroapatite)	China (85,000), USA (30,000), Morocco (28,000), Russia (11,000), Colombia (8900), Jordan (7600), Brazil (6000), Syria (3400), Israel (3000), Vietnam (2600), Tunisia (2600), Australia (2400), India (2300), Kazakhstan (2200)	203,000,000	Phosphate rock (65–72% bpl): 32–46 Monoammonium phosphate: 180 Diammonium phosphate: 145 Triple superphosphate: 120
Potash	Canada (11,000), Russia (6500), Belarus (5300), Germany (3200), Israel (1800), Jordan (1400), USA (1100), Chile (890)	35,000,000	Muriate of potash (60 wt% K_2O): 340–360
Pumice and pozzolan	Italy (5600), Greece (900), Turkey (812), USA (580), Germany (580), Spain (580), France (464), Chile (464)	11,600,000	Abrasive: 164 Stone washing: 121 Landscaping: 29 Concrete block: 15
Pyrite	China (7.0), Finland (340), Russia (71), Brazil (25)	7,500,000	200–400
Pyrophyllite (roseki)	South Korea (900), Japan (30), China (20)	923,000	Pyrophyllite ore: 10 Processed pyrophyllite: 150–400

Table I.3 (*continued*)

Industrial mineral or rock	**Major producing countries/ regions and annual production (10^3 tonne)**	**World annual production (tonne)**	**Grade and price range (US$/tonne)**
Quartz crystals (i.e., lascas)	Brazil (1594), Commonwealth of Independent States, USA, Madagascar, Namibia, Angola, South Africa, Venezuela	2168	780
Rutile (natural and synthetic)	Australia (480), South Africa (130), Ukraine (100), Sierra Leone (68), India (30), Kazakhstan (17), Madagascar (10), Malaysia (10)	800,000	Natural (91–95 wt% TiO_2): 820–1000 Synthetic (95 wt% TiO_2): 410
Salt (halite, rock salt)	China (65,000), USA (55,000), India (22,000), Germany (18,000), Canada (13,000), Australia (11,000), Mexico (10,000), Chile (9900), Brazil (7000), Netherlands (7000), UK (6700), France (6000), Ukraine (5950), Spain (4500), Italy (3000), Egypt (2500), Russia (2000)	290,000,000	Rock salt (vacuum salt): 50–60 Solar salt: 45–60
Silica sand	USA, Canada		Container glass: 25–30 Foundry grade: 30–35 Silica flour (–20 µm): 300–375 Silica flour (–45 µm): 180–215
Silicon carbide	Norway, USA, Netherlands, Ukraine, Brazil, Japan	400,000	Black grade (99%): 3100–3400 Refractory grade (97.5 wt%): 1600–2000 Refractory grade (95 wt%): 1400–1500 Metallurgical (88–92 wt%): 1050–1120
Soda ash (see also trona and macholite)	USA (10,700), Kenya (500), Botswana (260), Ethiopia (5)	14,000,000	Soda ash (natural): 150–200 Soda ash (synthetic): 195–300
Sodium sulfate	USA, Russia, Canada, Spain, Germany, China		75–170
Spinel	USA (25), Brazil, Japan	30,000	
Spodumene and lepidolite	Australia, Canada	100,000	Concentrate (7.25 wt% Li_2O): 460–490 Glass grade (7.25 wt% Li_2O): 270–310

Table I.3 (*continued*)

Industrial mineral or rock	Major producing countries/ regions and annual production (10^3 tonne)	World annual production (tonne)	Grade and price range (US$/tonne)
Sulfur	China (12,000), USA (9000), Canada (7000), Russia (7000)	70,000,000	Canadian solid state: 140–155
Talc	China (2200), Brazil (650), USA (615), India (450), France (420), Finland (430), Russia (150), Canada (147), Italy (110), Australia (9)	7,800,000	Plastic grade: 200–210 Ceramic grade: 100 Micronized: 450–590
Titanium dioxide pigment	USA, Finland, Germany, UK, China	6,500,000	2900–3000
Titanium slag (sulfate and chloride)	Canada (1000), South Africa (800), Norway (150)	2,150,000	80 wt% TiO_2: 338 85 wt% TiO_2: 385 95 wt% TiO_2: 520
Trona and nacholite (sodium carbonate and bicarbonate)	USA (15,700), Kenya (220)	16,000,000	Soda ash: 215–340
Vanadium pentoxide	South Africa, Australia, USA		98 wt% V_2O_5: 3000–5000
Vermiculite	South Africa (170), China (130), USA (100), Brazil (50), Russia (30), Australia (11), India (10)	523,000	Raw: 160–260
Wollastonite	China (300), India (180), USA (70), Mexico (48), Finland (12), Spain (8)	620,000	Acicular grade (–200 mesh): 210–250
Zeolites	China (2500), Cuba (600), Japan (160), USA (43), Hungary (20), Slovakia (12), Georgia (6)	3500	
Zirconia	USA, Russia, China	100,000	Electrofused zirconia (pigment grade): 3600–4800 Electrofused zirconia (refractory): 6000–7000
Zircon sand	Australia (762), South Africa (385), Indonesia (127), USA (115), Senegal (85), Mozambique (44), Madagascar (20)	1,700,000	Zircon, standard grade (66.5 wt% ZrO_2): 950–1100 Zircon, flour (0.045 mm): 1500–2000

bpl bone phosphate of lime, EBT elliptical bottom taphole [a]Synthetic corundum

I.4 Prices of Electricity in Various Countries

See ◘ Table I.4.

◘ **Table I.4** Prices of electricity for selected countries (2004)

Country	**Electricity price[a] (US$/kWh)**
Australia	0.056
Brazil	0.083
Canada	0.030
India	0.059
Japan	0.128
Norway	0.052
Russia	0.432
South Africa	0.021
USA	0.043

[a] UK Electricity Association; prices include local taxes but exclude recoverable VAT

J Astronomical Data

Table J.1 Astronomical data for solar planets and Pluto. (From Collective (2012) *The Astronomical Almanac for the Year 2012*. US Government Printing Office, Washington, DC; Seidelmann, P.K. (ed.) (1992) *Explanatory Supplement to the Astronomical Almanac*. University Science Books, Mill Valley, CA.; Lang, K.R. (1992) *Astrophysical Data: Planets and Stars*. Springer, New York; Allen, C.W. (1976) *Astrophysical Quantities, 3rd. edn*. Athlone Press, London)

Solar planet	Mass ($M/10^{24}$ kg)	Equatorial radius (R_e/km)	Flattening (α)	Mean density (ρ/ $\mathrm{kg \cdot m^{-3}}$)	Sidereal rotation period (T_{ROT})	Mean acceleration gravity ($g/\mathrm{m \cdot s^{-2}}$)	Sidereal orbiting period (T_{ORB})	Semimajor axis of elliptical orbit (a/AU)	Eccentricity of orbit (e)	Inclination (tilting angle)	Ecliptic angle (i)	Albedo	Satellites
Mercury	0.330	2440	None	5430	58.6 days	3.70	87.97 days	0.387	0.206	None	7°	0.11	0
Venus	4.869	6052	None	5240	233 days	8.87	244.7 days	0.723	0.007	177.3°	3.39°	0.65	0
Earth	5.974	6378	0.00335	5520	23 h 56 min 4 s	9.80	365.25 days	1.000	0.017	23.45°	None	0.37	1
Mars	0.642	3396	0.00648	3940	24 h 37 min 23 s	3.71	686.98 days	1.524	0.093	25.19°	1.85°	0.15	2
Jupiter	1899	71,492	0.06476	1330	9 h 55 min 30 s	23.12	11.863 years	5.203	0.048	3.12°	1.31°	0.52	67
Saturn	568.5	60,268	0.09796	700	10 h 30 min	8.96	29.41 years	9.539	0.056	26.73°	2.49°	0.47	62
Uranus	86.6	25,559	0.02293	1300	17 h 14 min	7.77	84.02 years	19.191	0.046	97.86°	0.77°	0.51	27
Neptune	102.8	24,764	0.01710	1760	18 h	11.00	164.79 years	30.061	0.010	29.56°	1.77°	0.41	14
Pluto[a]	0.015	1195	None	1100	6 days 9 h 17 min	0.72	248.4 years	39.529	0.246	118°	17.15°	0.30	5

Conversion factors and fundamental constants: $c = 2.99792458 \times 10^8$ m/s (E); $G = 6.67408 \times 10^{-11}\ \mathrm{m^3 \cdot kg^{-1} \cdot s^{-2}}$; 1 AU = $149.597870700 \times 10^6$ km;
1 light year = 9.46073×10^{15} m; 1 parsec = $30.85677581 \times 10^{15}$ m

[a] Pluto has not been considered a solar planet since 2011, and is now considered to be an object from the Kuiper belt

Table J.2 Earth and Moon astronomical data

Earth–Sun system	Earth distance from Sun at aphelion	1.0167 AU
	Earth distance from Sun at perihelion	0.9833 AU
	Earth date of aphelion passage	July 4, 5 h 5 min
	Earth date of perihelion passage	January 2, 4 h 52 min
	Earth sidereal orbiting period around sun (T_{ORB})	365.25636 days
Earth dimensions, area, and volume	Major orbital semiaxis (a_E)	1 AU = 149.59787×10^6 km
	Mean equatorial radius (R_e)	6378.1366 km
	Mean polar radius (R_p)	6356.755 km
	Difference in equatorial and polar semiaxes	21.385 km
	Mean flattening factor $a = [(R_e - R_p)/R_e]$	1/298.25642
	Surface area (A_E)	5.10×10^8 km^2
	Volume (V_E)	1.0832×10^{12} km^3
Earth mass-related properties	Average mass (M_E)	5.9722×10^{24} kg
	Average mass density (ρ_E)	5515 kg/m^3
	Moment of inertia (I_E)	8.070×10^{37} kg · m^2
	Rotational angular momentum (L_E)	5.861×10^{33} J · s
	Mean acceleration of gravity at equator (g_e)	9.78036 m/s^2
	Mean acceleration of gravity at poles (g_p)	9.83208 m/s^2
	Mean acceleration of gravity of ellipsoid	9.79780 m/s^2
Earth rotation	Mean rotational velocity (u_{ORB})	29.78 km/s
	Rotational angular velocity (ω_E)	7.292116×10^{-5} rad/s
	Sidereal rotational period (T_{ROT})	86,164.09 s About 23 h 56 min 4 s
	Inclination (tilting) angle	23.45°
Moon characteristics	Mean distance to Earth (semimajor axis)	384,400 km
	Eccentricity	0.0549
	Mean radius	1737.1 km
	Flattening	0.0012
	Mass	7.342×10^{22} kg
	Mass density	3344 kg/m^3
	Mean acceleration of gravity	1.622 m/s^2
	Orbital period	27.321661 days
	Ecliptic angle	5.145°

K Materials Societies

Table K.1 Materials-related professional societies

Acronym	Professional society	Address
AA	Aluminum Association Inc.	1525 Wilson Boulevard, Suite 600, Arlington, VA 22209, USA Tel.: +1-703-3582960 Fax: +1-703-3582961 URL: ▸ http://www.aluminum.org/
ABM	Brazilian Association for Materials and Metallurgy	R. Antonio Comparato 218, Campo Belo, São Paulo-SP, CEP 04605-030, Brazil Tel.: +55-11-55364333 Fax: +55-11-50444273 E-mail: abm@abmbrasil.com.br URL: ▸ http://www.abmbrasil.com.br/
ACA	American Crystallographics Association	PO Box 96, Ellicott Station, Buffalo, NY 14205-0096, USA URL: ▸ http://www.hwi.buffalo.edu/ACA/
ACarS	American Carbon Society	URL: ▸ http://www.americancarbonsociety.org/
ACerS	American Ceramic Society	735 Ceramic Place, Suite 100, Westerville, OH 43081, USA Tel.: +1-866-7213322 Fax: +1-614-8996109 E-mail: info@ceramics.org URL: ▸ http://www.ceramics.org/
ACI	American Concrete Institute	PO Box 19150, Detroit, MI 48219, USA Tel.: +1-313-9309277 Fax: +1-313-9309088 E-mail: service@cssinfo.com URL: ▸ http://www.cssinfo/info/aci.html
ACMA	American Composites Manufacturers Association	3033 Wilson Boulevard, Suite 420, Arlington, VA 22201, USA Tel.: +1-703-5250511 Fax: +1-703-5250743 E-mail: info@acmanet.org URL: ▸ http://www.acmanet.org/
ACPS	Australian Coal Preparation Society	76 Broadmeadow Road, Broadmeadow, NSW 2292, Australia Tel.: +61-2-49264870 Fax: +61-2-49264902 E-mail: acpsnsw@acps.com.au URL: ▸ http://www.acps.com.au/
ACS	American Chemical Society	1155 16th Street, NW, Washington, DC 20036, USA Tel.: +1-202-8724600 URL: ▸ https://www.acs.org/
ADA	American Dental Association	211 East Chicago Avenue, Chicago, IL 60611, USA Tel.: +1-312-4402500 Fax: +1-312-4402800 URL: ▸ http://www.ada.org/

Table K.1 (*continued*)

Acronym	Professional society	Address
AESF	American Electroplaters and Surface Finishers Society	12644 Research Parkway, Orlando, FL 32826-3298, USA Tel.: +1-407-2816441 Fax: +1-407-2816446 URL: ▸ http://www.aesf.org/
AGA	American Gas Association	400 North Capitol Street, Washington, DC 20001, USA Tel.: +1-202-8247000 Fax: +1-202-8247115 URL: ▸ http://www.aga.org/
AGU	American Geophysical Union	2000 Florida Avenue NW, Washington, DC 20009-1277, USA Tel.: +1-202-4626900 Fax: +1-202-3280566 E-mail: service@kosmos.agu.org URL: ▸ http://www.agu.org/
AIAA	American Institute of Aeronautics and Astronautics	1801 Alexander Bell Drive, Suite 500, Reston, VA 20191-4344, USA Tel.: +1-703-2647500 Fax: +1-703-2647551 URL: ▸ http://www.aiaa.org/
AIChE	American Institute of Chemical Engineers	Three Park Avenue, New York, NY, 10016-5901, USA Tel.: +1-212-5917338 URL: ▸ http://www.aiche.org/
AIE	American Institute of Engineers	5420 San Martin Way, Antioch, CA 94531-8506, USA Tel.: +1-510-7586240 Fax: +1-510-7586240 E-mail: aie@members-aie.org URL: ▸ http://www.members-aie.org/
AIGS	Asian Institute of Gemmological Sciences	919/1 Jewelry Trade Center, North Tower 33rd Floor, Silom Road, Bangrak, Bangkok 10500, Thailand Tel.: +66-2-2674315 Fax: +66-2-2674320 E-mail: info@aigsthailand.com URL: ▸ http://www.aigsthailand.com
AIM	Associazione Italiana di Metallurgia	Piazza R. Morandi, 2, 20121 Milan, Italy Tel.: +39-02-76021132 Fax: +39-02-76020551 E-mail: aim@aimnet.it URL: ▸ http://www.metallurgia-italiana.net/
AIME	American Institute of Mining, Metallurgical, and Petroleum Engineers	Three Park Avenue, New York, NY 10016, USA Tel.: +1-212-4197676 Fax: +1-212-4197671 URL: ▸ http://www.aimeny.org/
AIP	American Institute of Physics	One Physics Ellipse, College Park, MD 20740-3843, USA Tel.: +1-301-2093100 Fax: +1-301-2090843 URL: ▸ http://www.aip.org/

Table K.1 (*continued*)

Acronym	Professional society	Address
AISI	American Iron and Steel Institute	1101 17th Street NW, Washington, DC 20036, USA Tel.: +1-202-4527100 URL: ► http://www.steel.org/
AIST	Association for Iron and Steel Technology	186 Thorn Hill Road, Warrendale, PA 15086, USA Tel.: +1-724-7766040 Fax: +1-724-7761880 E-mail: info@aist.org URL: ► http://www.aist.org/
ANS	American Nuclear Society	555 North Kennington Avenue, La Grange Park, IL 60526, USA Tel.: +1-708-3526611 Fax: +1-708-5790499 E-mail: nucleus@ans.org URL: ► http://www.ans.org/
API	American Petroleum Institute	1220 L Street NW, Washington, DC, 20005, USA Tel.: +1-202-6828000 URL: ► http://www.api.org/
APS	American Physical Society	One Physics Ellipse, College Park, MD 20740-3844, USA Tel.: +1-301-2093200 Fax: +1-301-2090865 E-mail: opa@aps.org URL: ► http://www.aps.org/
ASCE	American Society of Civil Engineers	1015 15th Street, Suite 600, Washington, DC 20005, USA Tel.: +1-202-7892200 Fax: +1-202-2896797 URL: ► http://www.asce.org/
ASM	American Society for Metals	9639 Kinsman Road, Materials Park, OH 44073-0002, USA Tel.: +1-440-3385151 Fax: +1-440-3384634 URL: ► http://www.asm-intl.org/
ASME	American Society of Mechanical Engineers	3 Park Avenue, New York, NY 10016-5990, USA Tel.: +1-212-7057722 URL: ► http://www.asme.org/
ASNDT	American Society for Nondestructive Testing	PO Box 28518, 1711 Arlingate Lane, Columbus, OH 43228-0518, USA URL: ► http://www.asnt.org/
ASNE	American Society of Naval Engineers	1452 Duke Street, Alexandria, VA 22314-3458, USA Tel.: +1-703-836-6727 Fax: +1-703-836-7491 URL: ► http://www.navalengineers.org/
ASTM	ASTM International	100 Barr Harbor Drive, West Conshohocken, PA 19428-2959, USA Tel.: +1-202-8625100 URL: ► http://www.astm.org/

Table K.1 (*continued*)

Acronym	Professional society	Address
ATITAN	Association Titane	Centre des Salorges, 16 Quai E. Renaud, BP 90517, 44105 Nantes Cedex 4, France Tel.: +33-2-40446057 Fax: +33-2-40446380 E-mail: m.brau@nantes.cci.fr URL: ▸ http://www.titane.asso.fr/
AuGS	Australian Geological Survey	GPO Box 378, Canberra, ACT 2601, Australia Tel.: +61-2-62499111 Fax: +61-2-62499999 URL: ▸ http://www.ga.gov.au/
AVS	American Vacuum Society	120 Wall Street, 32 Floor, New York, NY 10005, USA Tel.: +1-212-2480200 Fax: +1-212-2480245 URL: ▸ http://www.vacuum.org/
AWS	American Welding Society	550 NW LeJeune Road, PO Box 351040, Miami, FL 33126, USA Tel.: +1-305-4439353 Fax: +1-305-4437559 URL: ▸ http://www.amweld.org/
AZA	American Zinc Association	2025 M Street NW, Suite 800, Washington, DC 20036, USA Tel.: +1-202-3671151 Fax: +1-202-3672232 URL: ▸ http://www.zinc.org/
BGS	British Geological Survey	Kingsley Dunham Centre, Keyworth, Nottingham NG12 5GG, UK Tel.: +44-115-9363100 Fax: +44-115-9363200 URL: ▸ http://www.bgs.ac.uk/
BIR	Bureau of International Recycling	Avenue Franklin Roosevelt 24, 1050 Brussels, Belgium Tel.: +32-2-6275770 Fax: +32-2-6275773 URL: ▸ http://www.bir.org/
BRGM	Bureau de Recherches Géologiques et Minières	3 Avenue Claude-Guillemin, BP 36009, 45060 Orléans Cedex 2, France Tel.: +33-2-38643434 URL: ▸ http://www.brgm.fr/
CAEF	European Foundry Association	c/o Bundesverband der Deutschen Gießerei-Industrie, Sohnstraße 70, 40237 Düsseldorf, Germany Tel.: +49-211-6871217 Fax: +49-211-6871205 URL: ▸ http://www.caef.org/
CAFA	Canadian Foundry Association	1 Nicholas Street, Suite 1500, Ottawa, ON K1N 7B7, Canada Tel.: +1-613-7894894 Fax: +1-613-7895957 URL: ▸ http://www.foundryassociation.ca/

■ **Table K.1** (*continued*)

Acronym	Professional society	Address
CCDC	Cambridge Crystallographic Data Centre	12 Union Road, Cambridge CB2 1EZ, UK Tel.:+44-1223336408 Fax:+44-1223336033 E-mail: admin@ccdc.cam.ac.uk URL: ▸ http://www.ccdc.cam.ac.uk/
CDA	Copper Development Association	260 Madison Avenue, New York, NY 10016, USA Tel.: +1-212-2517200 Fax: +1-212-2517234 E-mail: questions@cda.copper.org URL: ▸ http://www.cda.org/
CDI	Cobalt Development Institute	167 High Street, Guildford GU1 3AJ, UK Tel.: +44-1483-578877 Fax: +44-1483-573873 URL: ▸ http://www.thecdi.com/
CEFIC	European Chemical Industry Council	URL: ▸ http://www.cefic.org/
CerSJ	Ceramic Society of Japan	2-22-17 Hyakunincho, Shinjuku, Tokyo 169-0073, Japan Fax: +81-3-33625714 E-mail: information@cersj.org URL: ▸ http://www.ceramic.or.jp/i
CGA	Canadian Gemmological Association	1767 Avenue Road, Toronto, ON M5M 3Y8 Canada Tel.: +1-416-7850962 Fax: +1-416-7859043 E-mail: info@canadiangemmological.com URL: ▸ http://www.canadiangemmological.com/
CIM	Canadian Institute of Mining, Metallurgy and Petroleum	3400 de Maisonneuve Blvd W, Suite 855, Montreal, QC H3Z 3B8, Canada Tel.: +1-514-9392710 Fax: +1-514-9392714 E-mail: cim@cim.org URL: ▸ http://www.cim.org/
DIS	Ductile Iron Society	28938 Lorain Road, Suite 202, North Olmsted, OH 44070, USA Tel.: +1-440-7348040 Fax: +1-440-7348182 E-mail: jhall@ductile.org URL: ▸ http://www.ductile.org/
ECerS	European Ceramic Society	Avenue Gouverneur Cornez, 4, 7000 Mons, Belgium Tel.: +32-65-403421 Fax: +32-65-403458 E-mail: ecers@bcrc.be URL: ▸ http://www.ecers.org/
ECHA	European Chemical Agency	Annankatu 18, 00120 Helsinki, Finland URL: ▸ http://echa.europa.eu/

Table K.1 (*continued*)

Acronym	Professional society	Address
ECS	Electrochemical Society	10 South Main Street, Pennington NJ 08534-2896, USA Tel.: +1-609-7371902 Fax: +1-609-7372743 E-mail: ecs@electrochem.org URL: ▸ http://www.electrochem.org/
EPMF	European Precious Metals Federation	Avenue de Broqueville 12, 1150 Brussels, Belgium Tel.: +32-2-7756386 Fax: +32-2-7790523 URL: ▸ http://www.epmf.be/
EPMS	European Powder Metallurgy Society	2nd Floor, Talbot House, Market Street, Shrewsbury SY1 1LG, UK Tel.: +44-1743-248899 Fax: +44-1743-362968 E-mail: info@epma.com URL: ▸ http://www.epma.com/
EPRI	Electric Power Research Institute	3412 Hillview Avenue, Palo Alto, CA 94304-1395, USA Tel.: +1-650-8552000 URL: ▸ http://www.epri.com/
EUROALLIAGES	Association of European Ferro-alloy Producers	Avenue de Broqueville 12, 1150 Brussels, Belgium Tel.: +32-2-7756301 E-mail: euroalliages@euroalliages.be URL: ▸ http://www.euroalliages.com/
EuroChlor	EuroChlor	Avenue E. Van Nieuwenhuyse 4, Box 2, 1160 Brussels, Belgium Tel.: +32-2-6767211 Fax: +32-2-6767241 E-mail: eurochlor@cefic.be URL: ▸ http://www.eurochlor.org/
EURO-METAUX	European Association of Metals	Avenue de Broqueville 12, 1150 Brussels, Belgium Tel. +32-2-775-6311 Fax: +32-2-779-0523 E-mail: eurometaux@eurometaux.be URL: ▸ http://www.eurometaux.org/
EUROMINES	European Association of Mining Industries, Metal Ores & Industrial Minerals	Avenue de Broqueville 12, 1150 Brussels, Belgium Tel.: +32-2-7756331 Fax: +32-2-7706303 E-mail: secretariat@euromines.be URL: ▸ http://www.euromines.org/
EUROROC	European & International Federation of Natural Stone Industries	Tel.: +49-611-9771211 Fax: +49-611-9771248 E-mail: office@euroroc.net URL: ▸ http://www.euroroc.net/
EUROSURVEYS	The Geological Surveys of Europe	URL: ▸ http://www.eurogeosurveys.org/
GAA	Gemmological Association of Australia	URL: ▸ http://www.gem.org.au/

Table K.1 (*continued*)

Acronym	Professional society	Address
GAGB	Gemmological Association of Great Britain	Tel.: +44-20-7404-3334 Fax: +44-20-7404-8843 E-mail: information@gem-a.info URL: ▸ http://www.gagtl.ac.uk/
GCA	German Gemmological Association	Prof.-Schlossmacher-Str. 1, 55743 Idar-Oberstein, Germany Tel.: +49-678143011 Fax: +49-678141616 URL: ▸ http://www.gemcertificate.com/
GI	Gold Institute	1112 16th Street NW, Suite 240, Washington, DC 20036, USA Tel.: +1-202-8350185 Fax: +1-202-8350155 E-mail: info@goldinstitute.org URL: ▸ http://www.responsiblegold.org/
GIA	Gemological Institute of America	World Headquarters and Robert Mouawad Campus, 5345 Armada Drive, Carlsbad, CA 92008, USA Tel.: +1-760-6034000 URL: ▸ http://www.gia.edu/
GSA	Geological Society of America	3300 Penrose Place, Boulder, CO 80301, USA Tel.: +1-303-4472020 Fax: +1-303-4471133 E-mail: web@geosociety.org URL: ▸ http://www.geosociety.org/
GSC	Geological Survey of Canada	601 Booth Street, Ottawa, ON K1A 0E8, Canada Tel.: +1-613-9963919 Fax: +1-613-9438742 E-mail: info-ottawa@gsc.nrcan.gc.ca URL: ▸ http://gsc.nrcan.gc.ca/
I2a	International Antimony Association	Avenue de Broqueville 12, 1150 Brussels, Belgium Tel.: +32-2-7623093 Fax.: +32-2-7628229 URL: ▸ http://www.antimony.com/
ICA	International Cadmium Association	Avenue de Tervueren 168, Box 4, 1150 Brussels, Belgium Tel.: +32-2-7770560 Fax: +32-2-7770565 E-mail: info@cadmium.org URL: ▸ http://www.cadmium.org/
ICDA	International Chromium Development Association	45 Rue de Lisbonne, 75008 Paris, France Tel.: +33-1-40-76-0689 Fax: +33-1-40-76-0687 E-mail: info@icdachromium.com URL: ▸ http://www.icdachromium.com/
IEEE	Institute of Electrical and Electronics Engineers	445 Hoes Lane, PO Box 1331, Piscataway, NJ 08855-0459, USA Tel.: +1-732-9810060 Fax: +1-732-9810225 URL: ▸ http://www.ieee.org/

Table K.1 (*continued*)

Acronym	Professional society	Address
IISI	International Iron and Steel Institute	Rue Colonel Bourg 120, 1140 Brussels, Belgium Tel.:+32-2-7028900 Fax:+32-2-7028899 E-mail: info@iisi.be URL: ▸ http://www.worldsteel.org/
ILA	International Lime Association	Annastr. 67–71, 50968 Cologne, Germany Tel.: +49-221-93467440 Fax: +49-221-93467410 URL: ▸ http://www.internationallime.org/home
ILZRO	International Lead-Zinc Research organization Inc.	2525 Meridian Parkway, PO Box 12036, Research Triangle Park, NC 27709-2036, USA Tel.: +1-919-3614647 Fax: +1-919-3611957 E-mail: rputnam@ilzro.org URL: ▸ http://www.ilzro.org/
IMA	Industrial Minerals Association	Boulevard S. Dupuis 233, Box 124, 1070 Brussels, Belgium Tel.: +32-2-5245500 Fax: +32-2-5244575 E-mail: secretariat@ima-eu.org URL: ▸ http://www.ima-eu.org/
IMA	International Magnesium Association	1303 Vincent Place, Suite One, McLean, VA 22101, USA Tel.: +1-703-442888 Fax: +1-703-8211824 E-mail: ima@bellatlantic.net URL: ▸ http://www.intlmag.org/
IMA	International Mineralogical Association	15 Rue Notre Dame des Pauvres, BP 20, 54501 Vandoeuvre-les-Nancy Cedex, France Tel.: +33-3-83594246 Fax: +33-3-83511798 E-mail: mohnen@crpg.cnrs-nancy.fr URL: ▸ http://www.ima-mineralogy.org/
IMAM	Iron Mining Association of Minnesota	11 East Superior Street, Suite 514, Duluth, MN 55802, USA Tel.: +1-218-7227724 Fax: +1-218-7206707 URL: ▸ http://www.taconite.org/
IMI	International Manganese Institute	17 Avenue Hoche, 75008 Paris, France Tel.: +33-1-45630634 Fax: +33-1-42894292 E-mail: info@manganese.org URL: ▸ http://www.manganese.org/
IMnI	International Manganese Institute	17 Rue Duphot, 75001 Paris, France URL: ▸ http://www.manganese.org/

■ **Table K.1** (*continued*)

Acronym	Professional society	Address
IMOA	International Molybdenum Association	Unit 7, Hackford Walk, 119–123 Hackford Road, London SW9 0QT, UK Tel.: +44-171-5822777 Fax: +44-171-5820556 URL: ▸ http://www.imoa.org.uk
IOM3	Institute of Materials, Minerals and Mining	1 Carlton House Terrace, London, SW1Y 5DB, UK Tel.: +44-20-74517300 Fax: +44-20-78391702 URL: ▸ http://www.iom3.org/
IPA	International Platinum Groups Metals Association	Schiess-Staett-Strasse 30, 80339 Munich, Germany Tel.: +49-89-51996770 Fax: +49-89-51996719 E-mail: info@ipa-news.com URL: ▸ http://ipa-news.com/
IPI	International Potash Institute	Baumgärtlistrasse 17, PO Box 569, 8810 Horgen, Switzerland Tel.: +41-43-8104922 Fax: +41-43-8104925 E-mail: ipi@ipipotash.org URL: ▸ http://www.ipipotash.org/
IPMI	International Precious Metals Institute	4400 Bayou Blvd, Suite 18, Pensacola, FL 32503-1908, USA Tel.: +1-850-4761156 Fax: +1-850-4761548 E-mail: ipmi@pond.com URL: ▸ http://www.ipmi.org/
ITA	International Titanium Association	1871 Folsom Street, Suite 200, Boulder, CO 80302-5714, USA Tel.: +1-303-4437515 Fax: +1-303-4434406 E-mail: afitz@titanium.net URL: ▸ http://www.titanium.org/
ITIA	International Tungsten Industry Association	Unit 7, Hackford Walk, 119–123 Hackford Road, London SW9 0QT, UK Tel.: +44-171-582-2777 Fax: +44-171-582-0556 E-mail: info@itia.info URL: ▸ http://www.itia.org.uk
ITRI	International Tin Research Institute Ltd	Unit 3, Curo Park, Frogmore, St Albans AL2 2DD, UK Tel.: +44-1727-875-544 Fax: +44-1727-871-341 E-mail: info@itri.co.uk URL: ▸ http://www.itri.co.uk/
IZA	International Zinc Association	Avenue de Tervueren 168, Box 4, 1150 Brussels, Belgium Tel.: +32-2-7760070 Fax: +32-2-7760089 E-mail: info@iza.com URL: ▸ http://www.iza.com/

Table K.1 (*continued*)

Acronym	Professional society	Address
JTS	Japan Titanium Society	2–9, Kanda Nishiki-Cho, Chiyoda-Ku, Tokyo, ZIP 101, Japan Tel.: +81-3-32955958 Fax: +81-3-32936187 URL: ▸ http://www.titan-japan.com/
LDA	Lead Development Association International	42 Weymount Street, London W1N 3LQ, UK Tel.: +1-44-171-4998422 Fax: +1-44-171-4931555 URL: ▸ http://www.ldaint.org/
MAA	Marble Institute of America	28901 Clemens Road, Suite 100, Cleveland, OH 44145, USA Tel.: +1-440-2509222 Fax: +1-440-2509223 URL: ▸ http://www.marble-institute.com/
MAC	Mineralogical Association of Canada	90 Rue de la Couronne, Quebec, QC G1K 9A9, Canada Tel.: +1-418-6530333 Fax: +1-418-6530777 E-mail: office@mineralogicalassociation.ca URL: ▸ http://www.mineralogicalassociation.ca/
MES	Minerals Engineering Society	2 Ryton Close, Blyth, Worksop S81 8DN, UK Tel.: +44-1909-591787 E-mail: secretary@mineralsengineering.org URL: ▸ http://www.mineralsengineering.org/
MII	Minerals Information Institute	505 Violet Street, Golden, CO 80401, USA Tel.: +1-303-2779190 Fax: +1-303-2779198 E-mail: mii@mii.org URL: ▸ http://www.mii.org/
MMTA	Minor Metals Trade Association	Suite 53, 3 Whitehall Court, London SW1A 2EL, UK Tel.: +44-20-7830237 Fax: +44-20-78391386 E-mail: info@mmta.co.uk URL: ▸ http://www.mmta.co.uk/
MRS	Materials Research Society	506 Keystone Drive, Warrendale, PA 15086-7573, USA Tel.: +1-724-7793003 Fax: +1-724-7798313 URL: ▸ http://www.mrs.org/
MS	Mineralogical Society	41 Queen's Gate, London SW7 5HR, UK Tel.: +44-20-75847516 Fax: +44-20-78238021 E-mail: info@minersoc.org URL: ▸ http://www.minersoc.org/
MSA	Mineralogical Society of America	3635 Concorde Parkway, Suite 500, Chantilly, VA 20151-1125, USA Tel.: +1-703-6529950 Fax: +1-703-6529951 E-mail: business@minsocam.org URL: ▸ http://www.minsocam.org/

■ **Table K.1** (*continued*)

Acronym	Professional society	Address
MTI	Materials Technology Institute	1215 Fern Ridge Parkway, Suite 206, St Louis, MO 63141-4405, USA Tel.: +1-314-5767712 Fax: +1-314-5766078 E-mail: mtiadmin@mti-global.org URL: ▸ http://www.mti-global.org/
NACE	National Association of Corrosion Engineers	1440 South Creek Drive, Houston, TX 77084-4906, USA Tel.: +1-281-2286200 Fax: +1-281-5796694 URL: ▸ http://www.nace.org/
NiDI	Nickel Development Institute	214 King Street West, Suite 510, Toronto, ON M5H 3S6, Canada Tel.: +1-416-5917999 Fax: +1-416-5917987 URL: ▸ http://www.nidi.org/
NIST	National Institute of Standards and Technology	100 Bureau Drive, Stop 1070, Gaithersburg, MD 20899-1070, USA Tel.: +1-301-9756478 E-mail: inquiries@nist.gov URL: ▸ http://www.nist.org/
OSA	Optical Society of America	2010 Massachusetts Avenue NW, Washington, DC 20036 USA Tel.: +1-202-2238130 Fax: +1-202-2231096 URL: ▸ http://www.osa.org/
PCA	Portland Cement Association	5420 Old Orchard Road, Skokie, IL 60077, USA Tel.: +1-847-9666200 Fax: +1-847-9668389 URL: ▸ http://www.cement.org/
PIA	Plastics Institute of America	University of Massachusetts Lowell, 333 Aiken Street, Lowell, MA 01854-3686, USA Tel.: +1-978-9343130 Fax: +1-978-4584141 E-mail: info@plasticsinstitute.org URL: ▸ http://www.plasticsinstitute.org/
SAE	SAE International	400 Commonwealth Drive, Warrendale, PA 15096-0001, USA Tel.: +1-724-7764841 Fax: +1-724-7765760 URL: ▸ http://www.sae.org/
SAIMM	South African Institute of Mining and Metallurgy	PO Box 61127, Marshalltown 2107, South Africa Tel.:+27-11-8341273/7 Fax: +27-11-8385923 URL: ▸ http://www.saimm.co.za/
SF2M	Société Française de Métallurgie et de Matériaux	250 Rue Saint-Jacques, 75005 Paris, France Tel.: +33-1-46330800 Fax: +33-1-46330880 URL: ▸ http://www.sf2m.asso.fr/

Table K.1 (*continued*)

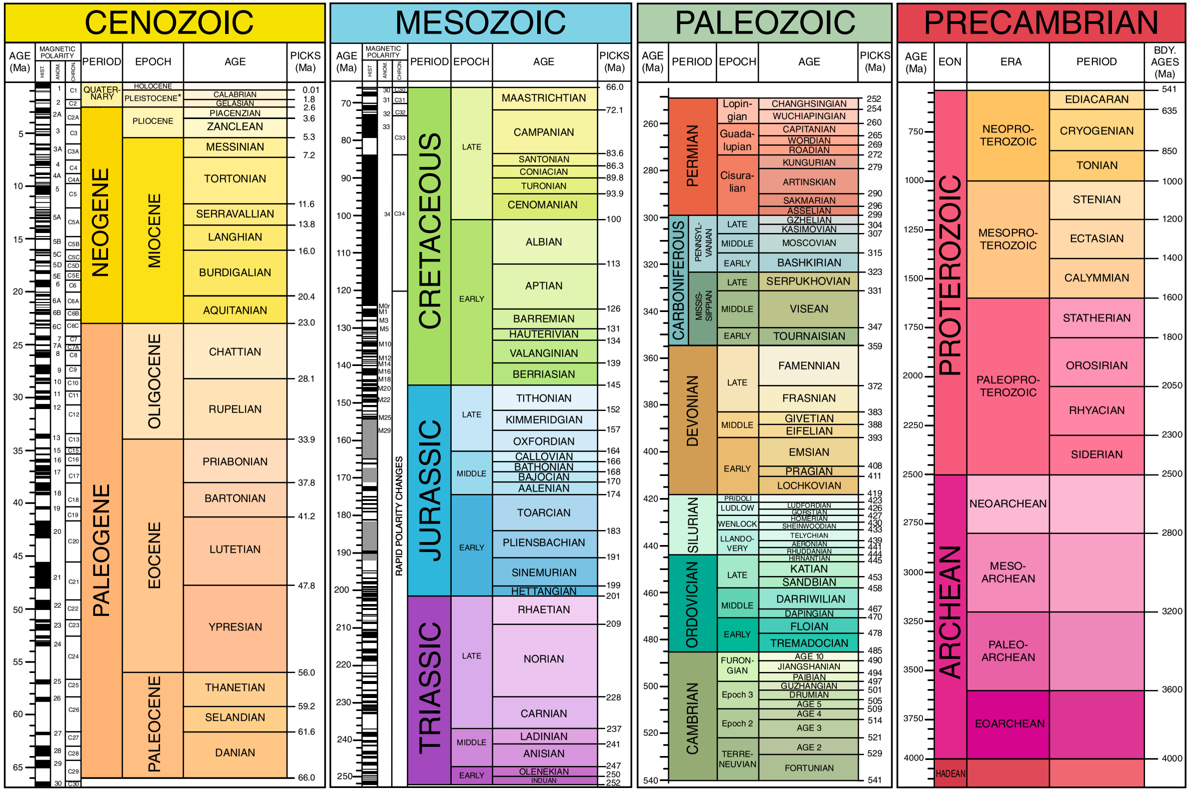
Acronym	Professional society	Address
SFMO	Société Française de Minéralogie et de Cristallographie	Campus Boucicaut, Bâtiment 7, 140 Rue de Lourmel, 75015 Paris, France Tel.: +33-1-44276024 E-mail: sfmc@ccr.jussieu.fr URL: ▸ http://wwwobs.univ-bpclermont.fr/
SI	Salt Institute	700 North Fairfax Street, Suite 600, Fairfax Plaza, Alexandria, VA 22314-2040, USA Tel.: +1-703-5494648 Fax: +1-703-5482194 URL: ▸ http://www.saltinstitute.org/
SIC	Scandium Information Center	URL: ▸ http://www.scandium.org/
SII	Silver Institute	The Silver Institute, 1200 G Street NW, Suite 800 Washington, DC 20005, USA Tel.: +1-202-8350185 Fax: +1-202-8350155 E-mail: info@silverinstitute.org URL: ▸ http://www.silverinstitute.org/
SME	Society of Manufacturing Engineers	One SME Drive, PO Box 930, Dearborn, MI 48121-0930, USA Tel.: +1-313-2711500 URL: ▸ http://www.sme.org/
SME	Society for Mining, Metallurgy, and Exploration	8307 Shaffer Parkway Littleton, CO 80127-4102, USA Tel.: +1-303-9739550 URL: ▸ http://www.smenet.org/
SNAME	Society of Naval Architects and Marine Engineers	601 Pavonia Avenue, Jersey City, NJ 07306, USA Tel.: +1-201-7984800 Fax: +1-201-7984975 URL: ▸ http://www.sname.org/
SPE	Society of Petroleum Engineers	PO Box 833836, Richardson, TX 75083-3836, USA Tel.: +1-972-9529393 Fax: +1-972-9529435 URL: ▸ http://www.spe.org/
SPI	Society of the Plastics Industry	1667 K Street NW, Suite 1000, Washington, DC 20006, USA Tel.: +1-202-745200 Fax: +1-202-2967005 URL: ▸ http://www.socplas.org/
SUI	Sulphur Institute	1140 Connecticut Avenue, NW, Suite 612, Washington, DC 20036, USA Tel.: +1-202-3319660 Fax: +1-202-2932940 E-mail: sulphur@sulphurinstitute.org URL: ▸ http://www.sulphurinstitute.org/

■ **Table K.1** (*continued*)

Acronym	**Professional society**	**Address**
SVC	Society of Vacuum Coaters	71 Pinon Hill Place NE, Albuquerque, NM 87122-1407, USA Tel.: +1-505-8567188 Fax: +1-505-8566716 E-mail: svcinfo@svc.org URL: ▸ http://www.svc.org/
TIC	Tantalum Niobium International Study Center	Washington Street 40, Brussels, 1050 Belgium Tel.: +32-2-6495158 Fax: +32-2-6496447 E-mail: tantniob@agoranet.be URL: ▸ http://www.tanb.org/
TIG	Titanium Information Group	URL: ▸ http://www.titaniuminfogroup.co.uk/
TMS	The Mineral, Metals, and Materials Society	4184 Thorn Hill Road, Warrendale, PA 15086, USA Tel.: +1-724-7769000 Fax: +1-724-7763770 E-mail: robinson@tms.org URL: ▸ http://www.tms.org/
UI	Uranium Institute	12th Floor, Bowater House West, 114 Knightsbridge, London SW1X 7LJ, UK Tel.: +44-171-2250303 Fax: +44-171-2250308 E-mail: ui@uilondon.org. URL: ▸ http://www.uilondon.org/
UIC	Uranium Information Centre	GPO Box 1649N, Melbourne, VIC 3001, Australia Tel.: +61-3-96297744 Fax: +61-3-96297207 URL: ▸ http://www.uic.com.au
USGS	US Geological Survey	807 National Center, Reston, VA 20192, USA URL: ▸ http://www.usgs.gov/
VANITEC	Vanadium International Technical Committee	Suite 5, 90 Calverley Road, Tunbridge Wells, TN1 2UN, UK Tel.: +44-1892-530448 Fax: +44-1892-458481 E-mail: info@vanitec.org URL: ▸ http://vanitec.org/
WNA	World Nuclear Association	Tower House, 10 Southampton Street, London WC2E 7HA, UK URL: ▸ http://www.world-nuclear.org/
WBMS	World Bureau of Metals Statistics	27a High Street, Ware SG12 9BA, UK Tel.: +44-1920461274 Fax: +44-1920464258 E-mail: enquiries@world-bureau.co.uk URL: ▸ http://www.world-bureau.com/
ZIA	Zircon Industry Association	URL: ▸ http://www.zircon-association.org

L Geological Time Scale

GSA GEOLOGIC TIME SCALE v. 4.0



THE GEOLOGICAL SOCIETY OF AMERICA®

*The Pleistocene is divided into four ages, but only two are shown here. What is shown as Calabrian is actually three ages—Calabrian from 1.8 to 0.78 Ma, Middle from 0.78 to 0.13 Ma, and Late from 0.13 to 0.01 Ma.

Walker, J.D., Geissman, J.W., Bowring, S.A., and Babcock, L.E., compilers, 2012, Geologic Time Scale v. 4.0: Geological Society of America, doi: 10.1130/2012.CTS004R3C. ©2012 The Geological Society of America.

The Cenozoic, Mesozoic, and Paleozoic are the Eras of the Phanerozoic Eon. Names of units and age boundaries follow the Gradstein et al. (2012) and Cohen et al. (2012) compilations. Age estimates and picks of boundaries are rounded to the nearest whole number (1 Ma) for the pre-Cenomanian, and rounded to one decimal place (100 ka) for the Cenomanian to Pleistocene interval. The numbered epochs and ages of the Cambrian are provisional.

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Gradstein, F.M, Ogg, J.G., Schmitz, M.D., et al., 2012, The Geologic Time Scale 2012: Boston, USA, Elsevier, DOI: 10.1016/B978-0-444-59425-9.00004-4.

Bibliography

Only general references not cited elsewhere in this book are listed here. For instance, references about semiconductors or superconductors are listed in the corresponding section entitled "Further Reading" in Chaps. 5 and 6 respectively, while general references about metallurgy or comprehensive series in materials science are listed here.

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