

Appendix A

A.1 Fundamental Units and Some Physical Constants

SI: LeSystème International d'Unités

Seven SI base units

Length	meter	m
Mass	kilogram	kg
Time	second	s
Electric current	ampere	A
Thermodynamic temperature	kelvin	K
Amounts of substance	mole	mol
Luminous intensity	candera	cd

Derived SI units with a specific name

Quantity	Term · Symbol	Relevance to other units
Frequency	Hertz Hz	s^{-1}
Force	Newton N	$m \cdot kg \cdot s^{-2}$
Pressure, Stress	Pascal Pa	N/m^2 $m^{-1} \cdot kg \cdot s^{-2}$
Energy Work, Calorific value	Joule J	$N \cdot m$ $m^2 \cdot kg \cdot s^{-2}$
Power	Watt W	J/s $m^2 \cdot kg \cdot s^{-3}$
Electric charge	Coulomb C	$A \cdot s$ $s \cdot A$
Voltage, Potential	Volt V	W/A $m^2 \cdot kg \cdot s^{-3} \cdot A^{-1}$
Electric capacity	Farad F	C/V $m^{-2} \cdot kg^{-1} \cdot s^2 \cdot A^2$
Electrical resistivity	Ohm Ω	V/A $m^2 \cdot kg \cdot s^{-3} \cdot A^{-2}$
Radioactivity	Becquerel Bq	s^{-1}
Absorbed dose	Gray Gy	J/kg $m^2 \cdot s^{-2}$
Dose equivalent	Sievert Sv	J/kg $m^2 \cdot s^{-2}$
Plane angle	Radian rad	
Solid angle	Steradian sr	

Time: minute and hour, Plane angle: degree, minute, second, Volume: liter and Mass: metric ton. These units are non-SI units, but they are accepted for use with the SI units.

Physical constants

Quantity	Symbol	Value	Unit	
			SI	CGS
Velocity of light in vacuum	c	2.997925	10^8 m/s	10^{10} cm/s
Planck's constant	h	6.6260	10^{-34} J·s	10^{-27} erg·s
Avogadro's number	N_A	6.02217	10^{23} /mol	10^{23} /mol
Atomic mass unit ^a	amu	1.66053	10^{-27} kg	10^{-24} g
Universal gravitation constant	G	6.67259	10^{-11} m ³ /s ² ·kg	10^{-8} cm ³ /s ² ·g
Permeability of vacuum free space	μ_0	$4\pi=12.56637$	10^{-7} H/m	—
Permittivity of vacuum free space	ϵ_0	8.854188	10^{-12} F/m	—
Charge of electron	e	1.60219	10^{-19} C	10^{-20} emu
		4.80320	—	10^{-10} esu
Faraday's constant	F	9.64853	10^4 C/mol	10^3 emu/mol
Electron rest mass	m_e	9.10956	10^{-31} g	10^{-28} g
Electron specific charge	e/m_e	1.7588	10^{11} C/kg	10^7 emu/g
Electron radius	r_e	2.81794	10^{-15} m	10^{-13} cm
Electron Compton wavelength	λ_e	2.42631	10^{-12} m	10^{-10} cm
Proton rest mass	m_p	1.67262	10^{-27} kg	10^{-24} g
	m_p/m_e	1836.15	1	1
Fine structure constant	α	7.29735	10^{-3}	10^{-3}
	α^{-1}	137.036	1	1
Rydberg constant	R_∞	1.09737	10^7 /m	10^5 /cm
Bohr radius	a_0	5.29177	10^{-11} m	10^{-9} cm
Gas constant	R	8.31451	J/mol·K	10^7 erg/mol·K
Molar volume of ideal gas at N.T.P. ^b	V_m	22.414	10^{-3} m ³ /mol	10^3 cm ³ /mol
Boltzmann constant	k_B	1.38062	10^{-23} J/K	10^{-16} erg/K
Stefan-Boltzmann constant	σ	5.67051	10^{-8} W/m ² ·K ⁴	10^{-5} erg/s·cm ² ·K ⁴

^aOne twelfth of mass of ¹²C.

^bTemperature 273.15 K, Pressure 101325 Pa(1 atm).

Units frequently used with SI units

Quantity	Symbol	Value	Unit	
			SI	CGS
electron volt	eV	1.60219	10^{19} J	10^{-12} erg
angstrom	Å^a		0.1nm= 10^{-10} m	10^{-8} cm
barn	b		10^{-28} m ²	

^a Å is also used in comparison to the electric current A.

A.2 Atomic Weight, Density, Debye Temperature and Mass Absorption Coefficients (cm²/g) for Elements

Characteristic radiation	Wavelength (Å)	1	2	3	4	5	6	7	8
		Hydrogen	Helium	Lithium	Beryllium	Boron	Carbon	Nitrogen	Oxygen
	Atomic weight	1.0079	4.0026	6.941	9.0122	10.811	12.011	14.0067	15.9994
	Density	8.375E-05	1.664E-04	0.533	1.86	2.47	2.27	1.165E-03	1.332E-03
	ϑ (K)	344		1440					
Cr Ka	2.2910	4.12E-01	4.98E-01	1.30E+00	3.44E+00	7.59E+00	1.50E+01	2.47E+01	3.78E+01
Cr Kb ₁	2.0849	4.05E-01	4.25E-01	1.01E+00	2.59E+00	5.69E+00	1.12E+01	1.86E+01	2.84E+01
Fe Ka	1.9374	4.00E-01	3.81E-01	8.39E-01	2.09E+00	4.55E+00	8.99E+00	1.49E+01	2.28E+01
Fe Kb ₁	1.7566	3.96E-01	3.35E-01	6.63E-01	1.58E+00	3.39E+00	6.68E+00	1.10E+01	1.70E+01
Co Ka	1.7903	3.97E-01	3.43E-01	6.93E-01	1.67E+00	3.59E+00	7.07E+00	1.17E+01	1.80E+01
Co Kb ₁	1.6208	3.93E-01	3.07E-01	5.55E-01	1.27E+00	2.67E+00	5.24E+00	8.66E+00	1.33E+01
Cu Ka	1.5418	3.91E-01	2.92E-01	5.00E-01	1.11E+00	2.31E+00	4.51E+00	7.44E+00	1.15E+01
Cu Kb ₁	1.3922	3.88E-01	2.68E-01	4.12E-01	8.53E-01	1.73E+00	3.33E+00	5.48E+00	8.42E+00
Mo Ka	0.7107	3.73E-01	2.02E-01	1.98E-01	2.56E-01	3.68E-01	5.76E-01	8.45E-01	1.22E+00
Mo Kb ₁	0.6323	3.70E-01	1.97E-01	1.87E-01	2.29E-01	3.09E-01	4.58E-01	6.45E-01	9.08E-01
Characteristic radiation	Wavelength (Å)	9	10	11	12	13	14	15	16
		Fluorine	Neon	Sodium	Magnesium	Aluminium	Silicon	Phosphorus	Sulfur
	Atomic weight	18.9984	20.1797	22.9898	24.305	26.9815	28.0855	30.9738	32.066
	Density	1.696E-03	8.387E-04	0.966	1.74	2.70	2.33	1.82(yellow)	2.09
	ϑ (K)	75		158	400	428	645		
Cr Ka	2.2910	5.15E+01	7.41E+01	9.49E+01	1.26E+02	1.55E+02	1.96E+02	2.30E+02	2.81E+02
Cr Kb ₁	2.0849	3.89E+01	5.61E+01	7.21E+01	9.62E+01	1.18E+02	1.51E+02	1.77E+02	2.17E+02
Fe Ka	1.9374	3.13E+01	4.52E+01	5.82E+01	7.78E+01	9.59E+01	1.22E+02	1.44E+02	1.77E+02
Fe Kb ₁	1.7566	2.33E+01	3.38E+01	4.37E+01	5.85E+01	7.23E+01	9.27E+01	1.09E+02	1.35E+02
Co Ka	1.7903	2.47E+01	3.58E+01	4.62E+01	6.19E+01	7.64E+01	9.78E+01	1.15E+02	1.42E+02
Co Kb ₁	1.6208	1.83E+01	2.66E+01	3.45E+01	4.63E+01	5.73E+01	7.36E+01	8.70E+01	1.07E+02
Cu Ka	1.5418	1.58E+01	2.29E+01	2.97E+01	4.00E+01	4.96E+01	6.37E+01	7.55E+01	9.33E+01
Cu Kb ₁	1.3922	1.16E+01	1.69E+01	2.20E+01	2.96E+01	3.68E+01	4.75E+01	5.64E+01	6.98E+01
Mo Ka	0.7107	1.63E+00	2.35E+00	3.03E+00	4.09E+00	5.11E+00	6.64E+00	7.97E+00	9.99E+00
Mo Kb ₁	0.6323	1.19E+00	1.69E+00	2.17E+00	2.92E+00	3.64E+00	4.73E+00	5.67E+00	7.11E+00
Characteristic radiation	Wavelength (Å)	17	18	19	20	21	22	23	24
		Chlorine	Argon	Potassium	Calcium	Scandium	Titanium	Vanadium	Chromium
	Atomic weight	35.4527	39.948	39.0983	40.078	44.9559	47.867	50.9415	51.9961
	Density	3.214E-03	1.663E-03	0.862	1.53	2.99	4.51	6.09	7.19
	ϑ (K)	92		91	230	360	420	380	630
Cr Ka	2.2910	3.16E+02	3.42E+02	4.21E+02	4.90E+02	5.16E+02	5.90E+02	7.47E+01	8.68E+01
Cr Kb ₁	2.0849	2.44E+02	2.66E+02	3.28E+02	3.82E+02	4.03E+02	4.44E+02	4.79E+02	6.70E+01
Fe Ka	1.9374	2.00E+02	2.18E+02	2.70E+02	3.14E+02	3.32E+02	3.58E+02	3.99E+02	4.92E+02
Fe Kb ₁	1.7566	1.52E+02	1.67E+02	2.07E+02	2.42E+02	2.56E+02	2.77E+02	3.09E+02	3.85E+02
Co Ka	1.7903	1.61E+02	1.76E+02	2.18E+02	2.55E+02	2.69E+02	2.91E+02	3.25E+02	4.08E+02
Co Kb ₁	1.6208	1.22E+02	1.34E+02	1.66E+02	1.95E+02	2.06E+02	2.27E+02	2.50E+02	2.93E+02
Cu Ka	1.5418	1.06E+02	1.16E+02	1.45E+02	1.70E+02	1.80E+02	2.00E+02	2.19E+02	2.47E+02
Cu Kb ₁	1.3922	7.95E+01	8.75E+01	1.09E+02	1.29E+02	1.37E+02	1.52E+02	1.66E+02	1.85E+02
Mo Ka	0.7107	1.15E+01	1.28E+01	1.62E+01	1.93E+01	2.08E+01	2.34E+01	2.60E+01	2.99E+01
Mo Kb ₁	0.6323	8.20E+00	9.14E+00	1.16E+01	1.38E+01	1.49E+01	1.68E+01	1.87E+01	2.15E+01

ϑ : Debye temperature, Unit of density: Mg/m³.

Characteristic radiation	Wavelength (Å)	25	26	27	28	29	30	31	32
		Manganese	Iron	Cobalt	Nickel	Copper	Zinc	Gallium	Germanium
	Atomic weight	54.9381	55.845	58.9332	58.6934	63.546	65.39	69.723	72.61
	Density	7.47	7.87	8.8	8.91	8.93	7.13	5.91	5.32
ϑ (K)	410	470	445	450	343	327	320	374	
Cr Ka	2.2910	9.75E+01	1.13E+02	1.24E+02	1.44E+02	1.53E+02	1.71E+02	1.83E+02	1.99E+02
Cr Kb ₁	2.0849	7.53E+01	8.69E+01	9.60E+01	1.12E+02	1.18E+02	1.32E+02	1.42E+02	1.55E+02
Fe Ka	1.9374	6.16E+01	7.10E+01	7.85E+01	9.13E+01	9.68E+01	1.08E+02	1.16E+02	1.27E+02
Fe Kb ₁	1.7566	3.75E+02	5.43E+01	6.00E+01	6.98E+01	7.40E+01	8.27E+01	8.86E+01	9.69E+01
Co Ka	1.7903	3.93E+02	5.72E+01	6.32E+01	7.35E+01	7.80E+01	8.71E+01	9.34E+01	1.02E+02
Co Kb ₁	1.6208	3.06E+02	3.42E+02	4.81E+01	5.60E+01	5.94E+01	6.64E+01	7.12E+01	7.78E+01
Cu Ka	1.5418	2.70E+02	3.02E+02	3.21E+02	4.88E+01	5.18E+01	5.79E+01	6.21E+01	6.79E+01
Cu Kb ₁	1.3922	2.07E+02	2.32E+02	2.48E+02	2.79E+02	3.92E+01	4.38E+01	4.70E+01	5.14E+01
Mo Ka	0.7107	3.31E+01	3.76E+01	4.10E+01	4.69E+01	4.91E+01	5.40E+01	5.70E+01	6.12E+01
Mo Kb ₁	0.6323	2.38E+01	2.71E+01	2.96E+01	3.40E+01	3.57E+01	3.93E+01	4.15E+01	4.46E+01

Characteristic radiation	Wavelength (Å)	33	34	35	36	37	38	39	40
		Arsenic	Selenium	Bromine	Krypton	Rubidium	Strontium	Yttrium	Zirconium
	Atomic weight	74.9216	78.96	79.904	83.8	85.4678	87.62	88.9059	91.224
	Density	5.78	4.81	3.12 (liq.)	3.488E-03	1.53	2.58	4.48	6.51
ϑ (K)	282	90		72	56	147	280	291	
Cr Ka	2.2910	2.19E+02	2.34E+02	2.60E+02	2.77E+02	3.03E+02	3.28E+02	3.58E+02	3.86E+02
Cr Kb ₁	2.0849	1.70E+02	1.82E+02	2.02E+02	2.15E+02	2.36E+02	2.56E+02	2.79E+02	3.00E+02
Fe Ka	1.9374	1.39E+02	1.49E+02	1.65E+02	1.76E+02	1.93E+02	2.10E+02	2.29E+02	2.47E+02
Fe Kb ₁	1.7566	1.06E+02	1.14E+02	1.27E+02	1.35E+02	1.48E+02	1.61E+02	1.76E+02	1.91E+02
Co Ka	1.7903	1.12E+02	1.20E+02	1.33E+02	1.42E+02	1.56E+02	1.70E+02	1.85E+02	2.00E+02
Co Kb ₁	1.6208	8.55E+01	9.16E+01	1.02E+02	1.09E+02	1.19E+02	1.30E+02	1.42E+02	1.54E+02
Cu Ka	1.5418	7.47E+01	8.00E+01	8.90E+01	9.52E+01	1.04E+02	1.13E+02	1.24E+02	1.39E+02
Cu Kb ₁	1.3922	5.65E+01	6.05E+01	6.74E+01	7.21E+01	7.90E+01	8.59E+01	9.40E+01	1.01E+02
Mo Ka	0.7107	6.61E+01	6.95E+01	7.56E+01	7.93E+01	8.51E+01	9.06E+01	9.70E+01	1.63E+01
Mo Kb ₁	0.6323	4.82E+01	5.08E+01	5.55E+01	5.84E+01	6.30E+01	6.72E+01	7.21E+01	7.61E+01

Characteristic radiation	Wavelength (Å)	41	42	43	44	45	46	47	48
		Niobium	Molybdenum	Technetium	Ruthenium	Rhodium	Palladium	Silver	Cadmium
	Atomic weight	92.9064	95.94	[99]	101.07	102.9055	106.42	107.8682	112.411
	Density	8.58	10.22	11.50	12.36	12.42	12.00	10.50	8.65
ϑ (K)	275	450		600	480	274	225	209	
Cr Ka	2.2910	4.16E+02	4.42E+02	4.74E+02	5.01E+02	5.36E+02	5.63E+02	6.02E+02	6.26E+02
Cr Kb ₁	2.0849	3.25E+02	3.45E+02	3.70E+02	3.92E+02	4.20E+02	4.41E+02	4.72E+02	4.90E+02
Fe Ka	1.9374	2.67E+02	2.84E+02	3.05E+02	3.23E+02	3.46E+02	3.63E+02	3.89E+02	4.05E+02
Fe Kb ₁	1.7566	2.05E+02	2.19E+02	2.35E+02	2.49E+02	2.67E+02	2.81E+02	3.01E+02	3.13E+02
Co Ka	1.7903	2.16E+02	2.30E+02	2.47E+02	2.62E+02	2.80E+02	2.95E+02	3.16E+02	3.29E+02
Co Kb ₁	1.6208	1.66E+02	1.76E+02	1.90E+02	2.01E+02	2.16E+02	2.27E+02	2.43E+02	2.53E+02
Cu Ka	1.5418	1.45E+02	1.54E+02	1.66E+02	1.76E+02	1.89E+02	1.99E+02	2.13E+02	2.22E+02
Cu Kb ₁	1.3922	1.10E+02	1.17E+02	1.26E+02	1.34E+02	1.44E+02	1.51E+02	1.63E+02	1.69E+02
Mo Ka	0.7107	1.77E+01	1.88E+01	2.04E+01	2.17E+01	2.33E+01	2.47E+01	2.65E+01	2.78E+01
Mo Kb ₁	0.6323	8.10E+01	1.38E+01	1.49E+01	1.58E+01	1.70E+01	1.80E+01	1.94E+01	2.02E+01

ϑ : Debye temperature, Unit of density: Mg/m³.

Characteristic radiation	Wavelength (Å)	49	50	51	52	53	54	55	56
		Indium	Tin	Antimony	Tellurium	Iodine	Xenon	Caesium	Barium
	Atomic weight	114.818	118.71	121.76	127.6	126.9045	131.29	132.9054	137.327
	Density	7.29	7.29	6.69	6.25	4.95	5.495E-03	1.91(263K)	3.59
	ϑ (K)	108	200	211	153		64	38	110
Cr Ka	2.2910	6.63E+02	6.91E+02	7.23E+02	7.40E+02	7.96E+02	7.21E+02	7.60E+02	5.70E+02
Cr Kb ₁	2.0849	5.19E+02	5.42E+02	5.70E+02	5.85E+02	6.31E+02	6.52E+02	6.86E+02	6.45E+02
Fe Ka	1.9374	4.28E+02	4.47E+02	4.71E+02	4.83E+02	5.22E+02	5.40E+02	5.69E+02	5.86E+02
Fe Kb ₁	1.7566	3.32E+02	3.47E+02	3.65E+02	3.74E+02	4.08E+02	4.22E+02	4.46E+02	4.61E+02
Co Ka	1.7903	3.49E+02	3.64E+02	3.83E+02	3.94E+02	4.25E+02	4.40E+02	4.65E+02	4.80E+02
Co Kb ₁	1.6208	2.69E+02	2.81E+02	2.96E+02	3.04E+02	3.30E+02	3.43E+02	3.63E+02	3.76E+02
Cu Ka	1.5418	2.36E+02	2.47E+02	2.59E+02	2.67E+02	2.88E+02	2.99E+02	3.17E+02	3.25E+02
Cu Kb ₁	1.3922	1.80E+02	1.88E+02	1.98E+02	2.04E+02	2.20E+02	2.29E+02	2.43E+02	2.52E+02
Mo Ka	0.7107	2.95E+01	3.10E+01	3.27E+01	3.38E+01	3.67E+01	3.82E+01	4.07E+01	4.23E+01
Mo Kb ₁	0.6323	2.16E+01	2.26E+01	2.39E+01	2.47E+01	2.68E+01	2.80E+01	2.98E+01	3.10E+01
Characteristic radiation	Wavelength (Å)	57	58	59	60	61	62	63	64
		Lanthanum	Cerium	Praseodymium	Neodymium	Promethium	Samarium	Europium	Gadolinium
	Atomic weight	138.9055	140.115	140.9077	144.24	[145]	150.36	151.965	157.25
	Density	6.17	6.77	6.78	7.00		7.54	5.25	7.87
	ϑ (K)	142							200
Cr Ka	2.2910	2.25E+02	2.38E+02	2.38E+02	2.51E+02	2.94E+02	2.79E+02	3.09E+02	2.98E+02
Cr Kb ₁	2.0849	7.44E+02	4.94E+02	1.88E+02	1.98E+02	2.32E+02	2.21E+02	2.44E+02	2.35E+02
Fe Ka	1.9374	6.18E+02	5.61E+02	4.48E+02	4.55E+02	1.94E+02	2.04E+02	2.03E+02	1.95E+02
Fe Kb ₁	1.7566	4.83E+02	5.10E+02	5.39E+02	4.92E+02	5.88E+02	1.63E+02	4.08E+02	1.53E+02
Co Ka	1.7903	5.07E+02	5.35E+02	5.65E+02	5.05E+02	4.00E+02	1.76E+02	4.19E+02	1.61E+02
Co Kb ₁	1.6208	3.95E+02	4.17E+02	4.41E+02	4.57E+02	4.82E+02	3.54E+02	4.80E+02	3.35E+02
Cu Ka	1.5418	3.48E+02	3.68E+02	3.90E+02	4.04E+02	4.26E+02	4.34E+02	4.34E+02	4.03E+02
Cu Kb ₁	1.3922	2.66E+02	2.82E+02	2.99E+02	3.10E+02	3.28E+02	3.35E+02	3.52E+02	3.60E+02
Mo Ka	0.7107	4.49E+01	4.77E+01	5.07E+01	5.30E+01	5.63E+01	5.78E+01	6.09E+01	6.26E+01
Mo Kb ₁	0.6323	3.29E+01	3.49E+01	3.72E+01	3.88E+01	4.13E+01	4.24E+01	4.47E+01	4.60E+01
Characteristic radiation	Wavelength (Å)	65	66	67	68	69	70	71	72
		Terbium	Dysprosium	Holmium	Erbium	Thulium	Ytterbium	Lutetium	Hafnium
	Atomic weight	158.9253	162.5	164.9303	167.26	168.9342	173.04	174.967	178.49
	Density	8.27	8.53	8.80	9.04	9.33	6.97	9.84	13.28
	ϑ (K)		210				120	210	252
Cr Ka	2.2910	3.32E+02	3.25E+02	3.47E+02	3.52E+02	3.86E+02	3.87E+02	4.31E+02	4.25E+02
Cr Kb ₁	2.0849	2.63E+02	2.57E+02	2.72E+02	2.78E+02	3.05E+02	3.04E+02	3.39E+02	3.34E+02
Fe Ka	1.9374	2.19E+02	2.14E+02	2.28E+02	2.32E+02	2.53E+02	2.51E+02	2.80E+02	2.77E+02
Fe Kb ₁	1.7566	1.71E+02	1.68E+02	1.78E+02	1.82E+02	1.96E+02	1.96E+02	2.18E+02	2.16E+02
Co Ka	1.7903	1.80E+02	1.76E+02	1.87E+02	1.91E+02	2.06E+02	2.06E+02	2.29E+02	2.27E+02
Co Kb ₁	1.6208	3.60E+02	1.38E+02	1.46E+02	1.49E+02	1.59E+02	1.59E+02	1.78E+02	1.76E+02
Cu Ka	1.5418	3.21E+02	3.62E+02	1.29E+02	1.32E+02	1.40E+02	1.42E+02	1.56E+02	1.55E+02
Cu Kb ₁	1.3922	3.76E+02	3.87E+02	4.02E+02	4.17E+02	1.08E+02	1.08E+02	1.21E+02	1.20E+02
Mo Ka	0.7107	6.58E+01	6.83E+01	7.13E+01	7.44E+01	7.79E+01	8.04E+01	8.40E+01	8.69E+01
Mo Kb ₁	0.6323	4.83E+01	5.02E+01	5.24E+01	5.48E+01	5.74E+01	5.93E+01	6.19E+01	6.41E+01

ϑ : Debye temperature, Unit of density: Mg/m³.

Characteristic radiation	Wavelength (Å)	73	74	75	76	77	78	79	80
		Tantalum	Tungsten	Rhenium	Osmium	Iridium	Platinum	Gold	Mercury
	Atomic weight	180.9479	183.84	186.207	190.23	192.217	195.08	196.9665	200.59
	Density	16.67	19.25	21.02	22.58	22.55	21.44	19.28	13.55
	ϑ (K)	240	400	430	500	420	240	165	71.9
Cr Ka	2.2910	4.32E+02	4.57E+02	5.01E+02	4.99E+02	5.20E+02	5.41E+02	5.51E+02	5.41E+02
Cr Kb ₁	2.0849	3.39E+02	3.61E+02	3.94E+02	3.92E+02	4.11E+02	4.23E+02	4.34E+02	4.16E+02
Fe Ka	1.9374	2.83E+02	3.01E+02	3.27E+02	3.27E+02	3.40E+02	3.57E+02	3.61E+02	3.39E+02
Fe Kb ₁	1.7566	2.20E+02	2.34E+02	2.57E+02	2.55E+02	2.65E+02	2.61E+02	2.79E+02	2.60E+02
Co Ka	1.7903	2.31E+02	2.46E+02	2.68E+02	2.68E+02	2.78E+02	2.76E+02	2.95E+02	2.73E+02
Co Kb ₁	1.6208	1.79E+02	1.91E+02	2.09E+02	2.09E+02	2.16E+02	2.14E+02	2.29E+02	2.16E+02
Cu Ka	1.5418	1.58E+02	1.68E+02	1.87E+02	1.84E+02	1.91E+02	1.88E+02	2.01E+02	1.88E+02
Cu Kb ₁	1.3922	1.22E+02	1.30E+02	1.43E+02	1.42E+02	1.48E+02	1.45E+02	1.55E+02	1.41E+02
Mo Ka	0.7107	9.04E+01	9.38E+01	9.74E+01	1.00E+02	1.04E+02	1.07E+02	1.12E+02	1.15E+02
Mo Kb ₁	0.6323	6.67E+01	6.92E+01	7.19E+01	7.41E+01	7.70E+01	7.97E+01	8.29E+01	8.54E+01

Characteristic radiation	Wavelength (Å)	81	82	83	84	85	86	87	88
		Thallium	Lead	Bismuth	Polonium	Astatine	Radon	Francium	Radium
	Atomic weight	204.3833	207.2	208.9804	[210]	[210]	[222]	[223]	[226]
	Density	11.87	11.34	9.80	4.40 (liq. , 211K)				
	ϑ (K)	78.5	105	119					
Cr Ka	2.2910	5.97E+02	6.43E+02	6.66E+02	6.91E+02	6.80E+02	7.34E+02	7.58E+02	7.43E+02
Cr Kb ₁	2.0849	4.87E+02	5.07E+02	5.24E+02	5.44E+02	5.33E+02	5.76E+02	5.97E+02	5.85E+02
Fe Ka	1.9374	4.03E+02	4.20E+02	4.34E+02	4.52E+02	4.44E+02	4.77E+02	4.93E+02	4.87E+02
Fe Kb ₁	1.7566	3.14E+02	3.27E+02	3.39E+02	3.54E+02	3.45E+02	3.73E+02	3.84E+02	3.80E+02
Co Ka	1.7903	3.31E+02	3.43E+02	3.55E+02	3.70E+02	3.63E+02	3.92E+02	4.03E+02	3.98E+02
Co Kb ₁	1.6208	2.57E+02	2.67E+02	2.76E+02	2.88E+02	2.82E+02	3.04E+02	3.12E+02	3.10E+02
Cu Ka	1.5418	2.26E+02	2.35E+02	2.44E+02	2.54E+02	2.48E+02	2.67E+02	2.77E+02	2.73E+02
Cu Kb ₁	1.3922	1.75E+02	1.81E+02	1.88E+02	1.96E+02	1.86E+02	2.05E+02	2.13E+02	2.10E+02
Mo Ka	0.7107	1.18E+02	1.22E+02	1.26E+02	1.32E+02	1.17E+02	1.08E+02	8.70E+01	8.80E+01
Mo Kb ₁	0.6323	8.79E+01	9.08E+01	9.41E+01	9.83E+01	1.02E+02	1.01E+02	1.04E+02	1.08E+01

Characteristic radiation	Wavelength (Å)	89	90	91	92	93	94	95	96
		Actinium	Thorium	Protactinium	Uranium	Neptunium	Plutonium	Americium	Curium
	Atomic weight	[227]	232.0381	231.0359	238.0289	[237]	[239]	[243]	[247]
	Density	11.72			19.05	19.81			
	ϑ (K)	163			207				
Cr Ka	2.2910	7.39E+02	7.68E+02	7.38E+02	7.66E+02	8.00E+02	7.60E+02	7.95E+02	8.12E+02
Cr Kb ₁	2.0849	6.18E+02	5.09E+02	5.82E+02	6.17E+02	6.30E+02	6.00E+02	6.27E+02	6.40E+02
Fe Ka	1.9374	5.30E+02	4.85E+02	4.82E+02	5.28E+02	5.52E+02	4.98E+02	5.81E+02	5.90E+02
Fe Kb ₁	1.7566	4.44E+02	3.89E+02	3.75E+02	4.00E+02	4.10E+02	3.89E+02	4.07E+02	4.21E+02
Co Ka	1.7903	4.61E+02	4.06E+02	3.94E+02	4.20E+02	4.30E+02	4.08E+02	4.26E+02	4.37E+02
Co Kb ₁	1.6208	3.81E+02	3.48E+02	3.06E+02	3.26E+02	3.35E+02	3.17E+02	3.33E+02	3.43E+02
Cu Ka	1.5418	3.17E+02	3.06E+02	2.71E+02	2.88E+02	3.14E+02	2.80E+02	3.22E+02	3.38E+02
Cu Kb ₁	1.3922	2.85E+02	2.19E+02	2.08E+02	2.22E+02	2.27E+02	2.16E+02	2.27E+02	2.32E+02
Mo Ka	0.7107	9.08E+01	9.65E+01	1.01E+02	1.02E+02	4.22E+01	3.99E+01	4.81E+01	4.90E+01
Mo Kb ₁	0.6323	1.10E+02	9.87E+01	1.19E+02	7.49E+01	1.25E+02	1.29E+02	1.31E+02	1.34E+02

ϑ : Debye temperature, Unit of density: Mg/m³.

A.3 Atomic Scattering Factors as a Function of $\sin \theta/\lambda$

$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
H	1	0.81	0.48	0.25	0.13	0.07	0.04	0.03	0.02	0.01
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14
Li	3	2.2	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4
Be	4	2.9	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7
B	5	3.5	2.4	1.9	1.7	1.5	1.4	1.2	1.2	1.0
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16
N	7	5.8	4.2	3.0	2.3	1.9	1.65	1.54	1.49	1.39
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4
F	9	7.8	6.2	4.45	3.35	2.65	2.15	1.9	1.7	1.6
Ne	10	9.3	7.5	5.8	4.4	3.4	2.65	2.2	1.9	1.65
Na	11	9.65	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95
Mg	12	10.5	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2
Al	13	11.0	8.95	7.75	6.6	5.5	4.5	3.7	3.1	2.65
Si	14	11.35	9.4	8.2	7.15	6.1	5.1	4.2	3.4	2.95
P	15	12.4	10.0	8.45	7.45	6.5	5.65	4.8	4.05	3.4
S	16	13.6	10.7	8.95	7.85	6.85	6.0	5.25	4.5	3.9
Cl	17	14.6	11.3	9.25	8.05	7.25	6.5	5.75	5.05	4.4
A	18	15.9	12.6	10.4	8.7	7.8	7.0	6.2	5.4	4.7
K	19	16.5	13.3	10.8	9.2	7.9	6.7	5.9	5.2	4.6
Ca	20	17.5	14.1	11.4	9.7	8.4	7.3	6.3	5.6	4.9
Sc	21	18.4	14.9	12.1	10.3	8.9	7.7	6.7	5.9	5.3
Ti	22	19.3	15.7	12.8	10.9	9.5	8.2	7.2	6.3	5.6
V	23	20.2	16.6	13.5	11.5	10.1	8.7	7.6	6.7	5.9
Cr	24	21.1	17.4	14.2	12.1	10.6	9.2	8.0	7.1	6.3
Mn	25	22.1	18.2	14.9	12.7	11.1	9.7	8.4	7.5	6.6
Fe	26	23.1	18.9	15.6	13.3	11.6	10.2	8.9	7.9	7.0
Co	27	24.1	19.8	16.4	14.0	12.4	10.7	9.3	8.3	7.3
Ni	28	25.0	20.7	17.2	14.6	12.7	11.2	9.8	8.7	7.7
Cu	29	25.9	21.6	17.9	15.2	13.3	11.7	10.2	9.1	8.1
Zn	30	26.8	22.4	18.6	15.8	13.9	12.2	10.7	9.6	8.5

(Continued)

$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Ga	31	27.8	23.3	19.3	16.5	14.5	12.7	11.2	10.0	8.9
Ge	32	28.8	24.1	20.0	17.1	15.0	13.2	11.6	10.4	9.3
As	33	29.7	25.0	20.8	17.7	15.6	13.8	12.1	10.8	9.7
Se	34	30.6	25.8	21.5	18.3	16.1	14.3	12.6	11.2	10.0
Br	35	31.6	26.6	22.3	18.9	16.7	14.8	13.1	11.7	10.4
Kr	36	32.5	27.4	23.0	19.5	17.3	15.3	13.6	12.1	10.8
Rb	37	33.5	28.2	23.8	20.2	17.9	15.9	14.1	12.5	11.2
Sr	38	34.4	29.0	24.5	20.8	18.4	16.4	14.6	12.9	11.6
Y	39	35.4	29.9	25.3	21.5	19.0	17.0	15.1	13.4	12.0
Zr	40	36.3	30.8	26.0	22.1	19.7	17.5	15.6	13.8	12.4
Nb	41	37.3	31.7	26.8	22.8	20.2	18.1	16.0	14.3	12.8
Mo	42	38.2	32.6	27.6	23.5	20.8	18.6	16.5	14.8	13.2
Tc	43	39.1	33.4	28.3	24.1	21.3	19.1	17.0	15.2	13.6
Ru	44	40.0	34.3	29.1	24.7	21.9	19.6	17.5	15.6	14.1
Rh	45	41.0	35.1	29.9	25.4	22.5	20.2	18.0	16.1	14.5
Pd	46	41.9	36.0	30.7	26.2	23.1	20.8	18.5	16.6	14.9
Ag	47	42.8	36.9	31.5	26.9	23.8	21.3	19.0	17.1	15.3
Cd	48	43.7	37.7	32.2	27.5	24.4	21.8	19.6	17.6	15.7
In	49	44.7	38.6	33.0	28.1	25.0	22.4	20.1	18.0	16.2
Sn	50	45.7	39.5	33.8	28.7	25.6	22.9	20.6	18.5	16.6
Sb	51	46.7	40.4	34.6	29.5	26.3	23.5	21.1	19.0	17.0
Te	52	47.7	41.3	35.4	30.3	26.9	24.0	21.7	19.5	17.5
I	53	48.6	42.1	36.1	31.0	27.5	24.6	22.2	20.0	17.9
Xe	54	49.6	43.0	36.8	31.6	28.0	25.2	22.7	20.4	18.4
Cs	55	50.7	43.8	37.6	32.4	28.7	25.8	23.2	20.8	18.8
Ba	56	51.7	44.7	38.4	33.1	29.3	26.4	23.7	21.3	19.2
La	57	52.6	45.6	39.3	33.8	29.8	26.9	24.3	21.9	19.7
Ce	58	53.6	46.5	40.1	34.5	30.4	27.4	24.8	22.4	20.2
Pr	59	54.5	47.4	40.9	35.2	31.1	28.0	25.4	22.9	20.6
Nd	60	55.4	48.3	41.6	35.9	31.8	28.6	25.9	23.4	21.1
Pm	61	56.4	49.1	42.4	36.6	32.4	29.2	26.4	23.9	21.5
Sm	62	57.3	50.0	43.2	37.3	32.9	29.8	26.9	24.4	22.0
Eu	63	58.3	50.9	44.0	38.1	33.5	30.4	27.5	24.9	22.4
Gd	64	59.3	51.7	44.8	38.8	34.1	31.0	28.1	25.4	22.9
Tb	65	60.2	52.6	45.7	39.6	34.7	31.6	28.6	25.9	23.4

(Continued)

$\frac{\sin \theta}{\lambda} (\text{\AA}^{-1})$	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Dy	66	61.1	53.6	46.5	40.4	35.4	32.2	29.2	26.3	23.9
Ho	67	62.1	54.5	47.3	41.1	36.1	32.7	29.7	26.8	24.3
Er	68	63.0	55.3	48.1	41.7	36.7	33.3	30.2	27.3	24.7
Tm	69	64.0	56.2	48.9	42.4	37.4	33.9	30.8	27.9	25.2
Yb	70	64.9	57.0	49.7	43.2	38.0	34.4	31.3	28.4	25.7
Lu	71	65.9	57.8	50.4	43.9	38.7	35.0	31.8	28.9	26.2
Hf	72	66.8	58.6	51.2	44.5	39.3	35.6	32.3	29.3	26.7
Ta	73	67.8	59.5	52.0	45.3	39.9	36.2	32.9	29.8	27.1
W	74	68.8	60.4	52.8	46.1	40.5	36.8	33.5	30.4	27.6
Re	75	69.8	61.3	53.6	46.8	41.1	37.4	34.0	30.9	28.1
Os	76	70.8	62.2	54.4	47.5	41.7	38.0	34.6	31.4	28.6
Ir	77	71.7	63.1	55.3	48.2	42.4	38.6	35.1	32.0	29.0
Pt	78	72.6	64.0	56.2	48.9	43.1	39.2	35.6	32.5	29.5
Au	79	73.6	65.0	57.0	49.7	43.8	39.8	36.2	33.1	30.0
Hg	80	74.6	65.9	57.9	50.5	44.4	40.5	36.8	33.6	30.6
Tl	81	75.5	66.7	58.7	51.2	45.0	41.1	37.4	34.1	31.1
Pb	82	76.5	67.5	59.5	51.9	45.7	41.6	37.9	34.6	31.5
Bi	83	77.5	68.4	60.4	52.7	46.4	42.2	38.5	35.1	32.0
Po	84	78.4	69.4	61.3	53.5	47.1	42.8	39.1	35.6	32.6
At	85	79.4	70.3	62.1	54.2	47.7	43.4	39.6	36.2	33.1
Rn	86	80.3	71.3	63.0	55.1	48.4	44.0	40.2	36.8	33.5
Fr	87	81.3	72.2	63.8	55.8	49.1	44.5	40.7	37.3	34.0
Ra	88	82.2	73.2	64.6	56.5	49.8	45.1	41.3	37.8	34.6
Ac	89	83.2	74.1	65.5	57.3	50.4	45.8	41.8	38.3	35.1
Th	90	84.1	75.1	66.3	58.1	51.1	46.5	42.4	38.8	35.5
Pa	91	85.1	76.0	67.1	58.8	51.7	47.1	43.0	39.3	36.0
U	92	86.0	76.9	67.9	59.6	52.4	47.7	43.5	39.8	36.5
Np	93	87	78	69	60	53	48	44	40	37
Pu	94	88	79	69	61	54	49	44	41	38
Am	95	89	79	70	62	55	50	45	42	38
Cm	96	90	80	71	62	55	50	46	42	39
Bk	97	91	81	72	63	56	51	46	43	39
Cf	98	92	82	73	64	57	52	47	43	40

A.4 Quadratic Forms of Miller Indices for Cubic and Hexagonal Systems

$h^2+k^2+l^2$	Cubic				Hexagonal	
	$h k l$				h^2+hk+k^2	$h k$
	Simple	Face centered	Body centered	Diamond		
1	100				1	10
2	110		110		2	
3	111	111		111	3	11
4	200	200	200		4	20
5	210				5	
6	211		211		6	
7					7	21
8	220	220	220	220	8	
9	300,221				9	30
10	310		310		10	
11	311	311		311	11	
12	222	222	222		12	22
13	320				13	31
14	321		321		14	
15					15	
16	400	400	400	400	16	40
17	410,322				17	
18	411,330		411,330		18	
19	331	331		331	19	32
20	420	420	420		20	
21	421				21	41
22	332		332		22	
23					23	
24	422	422	422	422	24	
25	500,430				25	50
26	510,431		510,431		26	
27	511,333	511,333		511,333	27	33
28					28	42
29	520,432				29	
30	521		521		30	
31					31	51
32	440	440	440	440	32	
33	522,441				33	
34	530,433		530,433		34	
35	531	531		531	35	
36	600,442	600,442	600,442		36	60
37	610				37	43
38	611,532		611,532		38	
39					39	52
40	620	620	620	620	40	
41	621,540,443				41	
42	541		541		42	
43	533	533		533	43	61
44	622	622	622		44	
45	630,542				45	
46	631		631		46	
47					47	
48	444	444	444	444	48	44
49	700,632				49	70,53
50	710,550,543		710,550,543		50	
51	711,551	711,551		711,551	51	
52	640	640	640		52	62
53	720,641				53	
54	721,633,552		721,633,552		54	
55					55	
56	642	642	642	642	56	
57	722,544				57	71
58	730		730		58	
59	731,553	731,553		731,553	59	

A.5 Volume and Interplanar Angles of a Unit Cell

Cellvolumes

$$\text{Cubic : } V = a^3$$

$$\text{Tetragonal : } V = a^2c$$

$$\text{Hexagonal : } V = \frac{\sqrt{3}a^2c}{2} = 0.866a^2c$$

$$\text{Trigonal : } V = a^3\sqrt{1 - 3\cos^2\alpha + 2\cos^3\alpha}$$

$$\text{Orthorhombic : } V = abc$$

$$\text{Monoclinic : } V = abc \sin\beta$$

$$\text{Triclinic : } V = abc\sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$

Interplanar angles

The angle ϕ between the plane $(h_1k_1l_1)$ of spacing d_1 and the plane $(h_2k_2l_2)$ of d_2 is estimated from the following equation, where V is the volume of a unit cell:

$$\text{Cubic : } \cos\phi = \frac{h_1h_2 + k_1k_2 + l_1l_2}{\sqrt{(h_1^2 + k_1^2 + l_1^2)(h_2^2 + k_2^2 + l_2^2)}}$$

$$\text{Tetragonal : } \cos\phi = \frac{\frac{h_1h_2+k_1k_2}{a^2} + \frac{l_1l_2}{c^2}}{\sqrt{\left(\frac{h_1^2+k_1^2}{a^2} + \frac{l_1^2}{c^2}\right)\left(\frac{h_2^2+k_2^2}{a^2} + \frac{l_2^2}{c^2}\right)}}$$

$$\text{Hexagonal : } \cos\phi = \frac{h_1h_2 + k_1k_2 + \frac{1}{2}(h_1k_2 + h_2k_1) + \frac{3a^2}{4c^2}l_1l_2}{\sqrt{(h_1^2+k_1^2+h_1k_1+\frac{3a^2}{4c^2}l_1^2)(h_2^2+k_2^2+h_2k_2+\frac{3a^2}{4c^2}l_2^2)}}$$

$$\text{Trigonal : } \cos\phi = \frac{a^4d_1d_2}{V^2}[\sin^2\alpha(h_1h_2 + k_1k_2 + l_1l_2) + (\cos^2\alpha - \cos\alpha)(k_1l_2 + k_2l_1 + l_1h_2 + l_2h_1 + h_1k_2 + h_2k_1)]$$

$$\text{Orthorhombic : } \cos\phi = \frac{\frac{h_1h_2}{a^2} + \frac{k_1k_2}{b^2} + \frac{l_1l_2}{c^2}}{\sqrt{\left(\frac{h_1^2}{a^2} + \frac{k_1^2}{b^2} + \frac{l_1^2}{c^2}\right)\left(\frac{h_2^2}{a^2} + \frac{k_2^2}{b^2} + \frac{l_2^2}{c^2}\right)}}$$

$$\text{Monoclinic : } \cos\phi = \frac{d_1d_2}{\sin^2\beta} \left[\frac{h_1h_2}{a^2} + \frac{k_1k_2\sin^2\beta}{b^2} + \frac{l_1l_2}{c^2} - \frac{(l_1h_2 + l_2h_1)\cos\beta}{ac} \right]$$

$$\text{Triclinic : } \cos\phi = \frac{d_1d_2}{V^2} [S_{11}h_1h_2 + S_{22}k_1k_2 + S_{33}l_1l_2 + S_{23}(k_1l_2 + k_2l_1) + S_{13}(l_1h_2 + l_2h_1) + S_{12}(h_1k_2 + h_2k_1)]$$

$$S_{11} = b^2c^2 \sin^2\alpha \quad S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$$

$$S_{22} = a^2c^2 \sin^2\beta \quad S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$$

$$S_{33} = a^2b^2 \sin^2\gamma \quad S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$$

A.6 Numerical Values for Calculation of the Temperature Factor

Values of $\phi(x) = \frac{1}{x} \int_0^x \frac{\xi}{e^\xi - 1} d\xi$ $x = \frac{\Theta}{T}$, Θ : Debye temperature

x	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
0	1.000	0.975	0.951	0.928	0.904	0.882	0.860	0.839	0.818	0.797
1	0.778	0.758	0.739	0.721	0.703	0.686	0.669	0.653	0.637	0.622
2	0.607	0.592	0.578	0.565	0.552	0.539	0.526	0.514	0.503	0.491
3	0.480	0.470	0.460	0.450	0.440	0.431	0.422	0.413	0.404	0.396
4	0.388	0.380	0.373	0.366	0.359	0.352	0.345	0.339	0.333	0.327
5	0.321	0.315	0.310	0.304	0.299	0.294	0.289	0.285	0.280	0.276
6	0.271	0.267	0.263	0.259	0.255	0.251	0.248	0.244	0.241	0.237

For x larger than 7, $\phi(x)$ values are approximated by $(1.642/x)$.

Debye temperatures are compiled in Appendix A.2 using the following reference:
(C.Kittel: *Introduction to Solid State Physics*, 6th Edition, John Wiley & Sons, New York (1986), p.110.)

A.7 Fundamentals of Least-Squares Analysis

Let us consider that the number of n -points have coordinates $(x_1, y_1), (x_2, y_2) \dots (x_n, y_n)$, and the x and y are related by a straight line with the form of $y = a + bx$. Our problem is to find the best value of a and b which makes the sum of the squared errors a minimum by using the least-squares method. In this case, we use the following two normal equations:

$$\sum y = \sum a + b \sum x, \tag{1}$$

$$\sum xy = a \sum x + b \sum x^2. \tag{2}$$

For given n -points, the following four steps are suggested:

- (i) Substitute the experimental data into $y = a + bx$ for obtaining n -equations.

$$\left. \begin{aligned} y_1 &= a + bx_1 \\ y_2 &= a + bx_2 \\ &\vdots \\ y_n &= a + bx_n \end{aligned} \right\}. \tag{3}$$

- (ii) Multiply each equation by the coefficient of a (1 in the present case) and add for obtaining the first normal equation.

$$\begin{aligned} y_1 &= a + bx_1, \\ y_2 &= a + bx_2, \\ &\vdots \\ y_n &= a + bx_n, \\ \hline \sum^n y &= \sum a + b \sum x. \end{aligned} \tag{4}$$

- (iii) Multiply each equation by the coefficient b and add for obtaining the second normal equation.

$$\begin{aligned} x_1 y_1 &= x_1 a + b x_1^2, \\ x_2 y_2 &= x_2 a + b x_2^2, \\ &\vdots \\ x_n y_n &= x_n a + b x_n^2 \\ \hline \sum^n x y &= a \sum x + b \sum x^2 \end{aligned} \tag{5}$$

- (iv) Simultaneous solution of the two equations of (4) and (5) yields the value of a and b .

A.8 Prefixes to Unit and Greek Alphabet

Notation	Symbol	Factor
exa	E	10^{18}
peta	P	10^{15}
tera	T	10^{12}
giga	G	10^9
mega	M	10^6
kilo	k	10^3
hecto	h	10^2
deca	da	10

Notation	Symbol	Factor
deci	d	10^{-1}
centi	c	10^{-2}
milli	m	10^{-3}
micro	μ	10^{-6}
nano	n	10^{-9}
pico	p	10^{-12}
femto	f	10^{-15}
atto	a	10^{-18}

Greek alphabet

<i>A, α</i>	Alpha	<i>N, ν</i>	Nu
<i>B, β</i>	Beta	<i>Ξ, ζ</i>	Xi
<i>Γ, γ</i>	Gamma	<i>O, o</i>	Omicron
<i>Δ, δ</i>	Delta	<i>Π, π</i>	Pi
<i>E, ε</i>	Epsilon	<i>P, ρ</i>	Rho
<i>Z, ζ</i>	Zeta	<i>Σ, σ</i>	Sigma
<i>H, η</i>	Eta	<i>T, τ</i>	Tau
<i>Θ, θ, θ</i>	Theta	<i>Y, υ</i>	Upsilon
<i>I, ι</i>	Iota	<i>Φ, φ, ϕ</i>	Phi
<i>K, κ</i>	Kappa	<i>X, χ</i>	Chi
<i>Λ, λ</i>	Lambda	<i>Ψ, ψ</i>	Psi
<i>M, μ</i>	Mu	<i>Ω, ω</i>	Omega

A.9 Crystal Structures of Some Elements and Compounds

Elements or compounds	Crystal systems	Lattice parameter	
Al	<i>fcc</i>	$a = 0.40497 \text{ nm}$	
$\alpha\text{-Al}_2\text{O}_3$	hexagonal (corundum structure)	$a = 0.4763 \text{ nm}$	$c = 0.13003 \text{ nm}$
Au	<i>fcc</i>	$a = 0.40786 \text{ nm}$	
CaO	NaCl	$a = 0.48105 \text{ nm}$	
CaF ₂	ZnS	$a = 0.5463 \text{ nm}$	
Cr	<i>bcc</i>	$a = 0.28847 \text{ nm}$	
CsCl	CsCl	$a = 0.4123 \text{ nm}$	
Cu	<i>fcc</i>	$a = 0.36148 \text{ nm}$	
CuCl	ZnS	$a = 0.54057 \text{ nm}$	
Cu ₂ O	CsCl(cuprite structure)	$a = 0.42696 \text{ nm}$	
Fe α	<i>bcc</i>	$a = 0.28665 \text{ nm}$	
γ	<i>fcc</i>	$a = 0.36469 \text{ nm}$	
δ	<i>bcc</i>	$a = 0.29323 \text{ nm}$	
FeS	NaCl(pyrite structure)	$a = 0.5408 \text{ nm}$	
K	<i>bcc</i>	$a = 0.5247 \text{ nm}$	
Mg	<i>hcp</i>	$a = 0.32095 \text{ nm}$	$c = 0.52107 \text{ nm}$
MgO	NaCl	$a = 0.42112 \text{ nm}$	
Mo	<i>bcc</i>	$a = 0.31469 \text{ nm}$	
NaCl	NaCl	$a = 0.56406 \text{ nm}$	
NaF	NaCl	$a = 0.4620 \text{ nm}$	
Ni	<i>fcc</i>	$a = 0.35239 \text{ nm}$	
NiO	NaCl	$a = 0.41769 \text{ nm}$	
Pt	<i>fcc</i>	$a = 0.39240 \text{ nm}$	
Si	diamond	$a = 0.54309 \text{ nm}$	
SiO ₂ α -quartz	(Rhombohedral)	$a = 0.4913 \text{ nm}$	$c = 0.5405 \text{ nm}$
β -quartz	(hexagonal)	$a = 0.501 \text{ nm}$	$c = 0.547 \text{ nm}$
Tridymite	(hexagonal)	$a = 0.503 \text{ nm}$	$c = 0.822 \text{ nm}$
α -cristobalite	(hexagonal)	$a = 0.4973 \text{ nm}$	$c = 0.6926 \text{ nm}$
Ti	<i>hcp</i>	$a = 0.29512 \text{ nm}$	$c = 0.46845 \text{ nm}$
TiC	NaCl	$a = 0.43186 \text{ nm}$	
TiO ₂	CsCl(rutile structure)	$a = 0.45929 \text{ nm}$	$c = 0.29591 \text{ nm}$
W	<i>bcc</i>	$a = 0.31653 \text{ nm}$	
Zn	<i>hcp</i>	$a = 0.26650 \text{ nm}$	$c = 0.49470 \text{ nm}$
β -ZnS	ZnS	$a = 0.54109 \text{ nm}$	

These data are taken from the following references.

B.D. Cullity: Elements of X-ray Diffraction (2nd Edition), Addison-Wesley (1978).

F.S. Galasso: Structure and Properties of Inorganic Solids, Pergamon Press (1970).