Appendix 3

Lattice Geometry

A1 PLANE SPACINGS

The value of d, the distance between adjacent planes in the set (hkl), may be found from the following equations.

Cubic:
$$\frac{1}{d^2} = \frac{h^2 + k^2 + l^2}{a^2}$$

Tetragonal:
$$\frac{1}{d^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

Hexagonal:
$$\frac{1}{d^2} = \frac{4}{3}\left(\frac{h^2 + hk + k^2}{a^2}\right) + \frac{l^2}{c^2}$$

Rhombohedral:
$$\frac{1}{d^2} = \frac{(h^2 + k^2 + l^2)\sin^2\alpha + 2(hk + kl + hl)\cos^2\alpha - \cos\alpha)}{a^2(1 - 3\cos^2\alpha + 2\cos^3\alpha)}$$

Orthorhombic:
$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}$$

Monoclinic:
$$\frac{1}{d^2} = \frac{1}{\sin^2\beta}\left(\frac{h^2}{a^2} + \frac{k^2\sin^2\beta}{b^2} + \frac{l^2}{c^2} - \frac{2hl\cos\beta}{ac}\right)$$

Triclinic:
$$\frac{1}{d^2} = \frac{1}{V^2}(S_{11}h^2 + S_{22}k^2 + S_{33}l^2 + 2S_{12}hk + 2S_{23}kl + 2S_{13}hl)$$

In the equation for triclinic crystals,

V = volume of unit cell (see below),

$S_{11} = b^2c^2\sin^2\alpha$,

$S_{22} = a^2c^2\sin^2\beta$,

$S_{33} = a^2b^2\sin^2\gamma$,

$S_{12} = abc^2(\cos\alpha\cos\beta - \cos\gamma)$,

$S_{23} = a^2bc(\cos\beta\cos\gamma - \cos\alpha)$,

$S_{13} = ab^2c(\cos\gamma\cos\alpha - \cos\beta)$.

A2 CELL VOLUMES

The following equations give the volume V of the unit cell.

Cubic: $V = a^3$

Tetragonal: $V = a^2c$

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

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

Orthorhombic: $V = abc$

Monoclinic: $V = abc\sin\beta$

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

A3 INTERPLANAR ANGLES

The angle ϕ between the plane $(h_1k_1l_1)$, of spacing d_1, and the plane $(h_2k_2l_2)$, of spacing d_2, may be found from the following equations. (V is the volume of the unit cell.)

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

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

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

Rhombohedral:

$$\cos\ \phi = \frac{a^4 d_1 d_2}{V^2}\left[\sin^2\alpha(h_1h_2 + k_1k_2 + l_1l_2)\right.$$
$$\left.+(\cos^2\alpha - \cos\alpha)(k_1l_2 + k_2l_1 + l_1h_2 + l_2h_1 + h_1k_2 + h_2k_1)\right]$$

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

Monoclinic:

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

Triclinic:

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

Appendix 4

The Rhombohedral-Hexagonal Transformation

The lattice of points shown in Fig. A1 is rhombohedral, that is, it possesses the symmetry elements characteristic of the rhombohedral system. The primitive rhombohedral cell has axes $\mathbf{a}_1(\mathbf{R})$, $\mathbf{a}_2(\mathbf{R})$, and $\mathbf{a}_3(\mathbf{R})$. The same lattice of points, however, may be referred to a hexagonal cell having axes $\mathbf{a}_1(\mathbf{H})$, $\mathbf{a}_2(\mathbf{H})$, and $\mathbf{c}(\mathbf{H})$. The hexagonal cell is no longer primitive, since it contains three lattice points per unit cell (at 0 0 0, $\frac{211}{333}$, and $\frac{122}{333}$), and it has three times the volume of the rhombohedral cell.

If one wishes to know the indices $(HK \cdot L)$, referred to hexagonal axes, of a plane whose indices (hkl), referred to rhombohedral axes, are known, the following equations may be used:

$$H = h - k,$$

$$K = k - l,$$

$$L = h + k + l.$$

Thus, the (001) face of the rhombohedral cell (shown shaded in the figure) has indices$(0\bar{1} \cdot 1)$. when referred to hexagonal axes.

Since a rhombohedral lattice may be referred to hexagonal axes, it follows that the powder pattern of a rhombohedral substance can be indexed as a hexagonal substance. How then can the true nature of the lattice be recognised? From the equations given above, it follows that

$$-H + K + L = 3k.$$

If the lattice is really rhombohedral, then k is an integer and the only lines appearing in the pattern will have hexagonal indices $(HK \cdot L)$ such that the sum $(-H + K + L)$ is always an integral multiple of 3. If this condition is not satisfied, the lattice is hexagonal.

When the pattern of a rhombohedral substance has been so indexed, i.e., with reference to hexagonal axes, and the true nature of the lattice determined, the indices (hkl) of the diffraction peeks referred to rhombohedral axes often are required. The transformation equations are

$$h = \tfrac{1}{3}(2H + K + L),$$

$$k = \tfrac{1}{3}(-H + K + L),$$

$$l = \tfrac{1}{3}(-H - 2K + L).$$

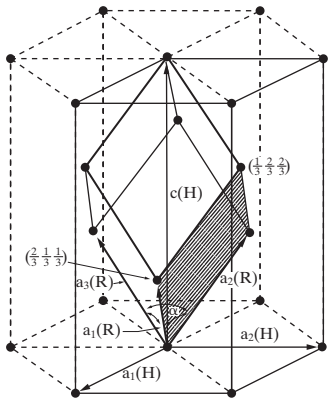

Figure A1 Rhombohedral and hexagonal unit cell in a rhombohedral lattice.

There is then the problem of determining the lattice parameters a_R and α of the rhombohedral unit cell. But the dimensions of the rhombohedral cell can be determined from the dimensions of the hexagonal cell, and this is an easier process than solving the rather complicated plane-spacing equation for the rhombohedral system. The first step is to index the pattern on the basis of hexagonal axes. Then the parameters a_H and c of the hexagonal cell are calculated in the usual way. Finally, the parameters of the rhombohedral cell are determined from the following equations:

$$a_R = \frac{1}{3}\sqrt{3a_H^2 + c^2}\,,$$

$$\sin\frac{\alpha}{2} = \frac{3}{2\sqrt{3 + (c/a_H)^2}}$$

Finally, it should be noted that, if the *c/a* ratio of the hexagonal cell in Fig. A1 takes on the special value of 2.45, then the angle α of the rhombohedral cell will equal 60° and the lattice of points will be face-centered cubic.

Further information on the rhombohedral-hexagonal relationship and on unit cell transformations in general may be obtained from the *International Tables for X-Ray Crystallography* [G1].

APPENDIX 5
CRYSTAL STRUCTURES OF SOME ELEMENTS

Most of the following data are from Pearson [G.16, Vol. 2], who should be consulted for data on certain high-temperature or high-pressure crystal forms not given below. The data on carbon and iodine, and the distance of closest approach in samarium, are from Barrett and Massalski [G.25]. Lattice parameters in both of these sources are given in Å units; they have been multiplied by 1.002056/1.00202, and rounded off to the same number of significant figures, in order to convert them to Å* units. See note on wavelength tables in Appendix 7.

Element	Type of Structure	Temp. (°C)	Lattice parameters (Å*)			Distance of closest approach (Å*)
			a	*b*	*c* or axial angle	
Ac Actinium	FCC, A1		5.311			3.755
Al Aluminum	FCC, A1	25	4.0497			2.8636
Am Americium, α*	Hex., La type	20	3.4681		11.240	3.4505
Sb Antimony	Rhomb., A7	25	4.5069		$\alpha = 57° 6'27''$	2.906
As Arsenic	Rhomb., A7	22.5	4.1319		$\alpha = 54° 8'$	2.507
Ba Barium	BCC, A2	25	5.013			4.341
Be Beryllium, α*	HCP, A3	R.T.	2.286		3.584	2.2257
Bi Bismuth	Rhomb., A7	25	4.736		$\alpha = 57° 14'$	3.071
B Boron*	Tetrag.	R.T.	8.80		5.05	
Cd Cadmium	HCP, A3	21	2.9789		5.6169	2.9789
Ca Calcium, α*	FCC, A1	26	5.5886			3.9517
C Carbon, diamond	Cubic, A4	20	3 5671			1.544
Carbon, graphite*	Hex., A9	20	2.4613		6.7080	1.421
Ce Cerium*	FCC, A1	23	5.1603			3.6488
Cs Cesium	BCC, A2	173°K	6.0797			5.265
Cr Chromium	BCC, A2	20	2.8847			2.498
Co Cobalt, α*	HCP, A3	R.T.	2.507		4.070	2.497
Cobalt, β	FCC, A1	R.T.	3.544			2.506
Cu Copper	FCC, A1	20	3.6148			2.5561
Dy Dysprosium, α*	HCP, A3	R.T.	3.5904		5.6477	3.5030
Er Erbium, α*	HCP, A3	R.T.	3.5589		5.5876	3.4681
Eu Europium	BCC, A2	25	4.5822			3.9682
Gd Gadolinium, α*	HCP, A3	20	3.6361		5.7828	3.5731
Ga Gallium	Orthorh.	R.T.	4.523	7.661	4.524	2.484
Ge Germanium	Cubic, A4	25	5.6577			2.4498
Au Gold	FCC, A1	25	4.0786			2.8840
Hf Hafnium, α*	HCP, A3	24	3.1947		5.0513	3.1274
Ho Holmium, α*	HCP, A3	R.T.	3.5774		5.6160	3.4858
In Indium	Tetrag., A6	R.T.	4.5981		4.9469	3.2513
I Iodine	Orthorh.	26	4.79	7.25	9.78	3.54
Ir Iridium	FCC, A1	R.T.	3.8390			2.7146
Fe Iron, α*	BCC, A2	20	2.8665			2.4824
Iron, γ	FCC, A1	916	3.6469			2.5787
Iron, δ	BCC, A2	1394	2.9323			2.5394
La Lanthanum, α*	Hex.	R.T.	3.770		12.159	3.739
Pb Lead	FCC, A1	25	4.9504			3.5004

Element	Type of Structure	Temp. (°C)	Lattice parameters (Å*)			Distance of closest approach (Å*)
			a	*b*	*c* or axial angle	
Li Lithium*	BCC, A2	25	3.5101			3.0398
Lu Lutetium*	HCP, A3	R.T.	3.5032		5.5511	3.4345
Mg Magnesium	HCP, A3	25	3.2095		5.2107	3.1971
Mn Manganese, α*	Cubic, A12	R.T.	8.9142			
Hg Mercury	Rhomb., A10	227°K	3.005		α = 70° 32′	3.005
Mo Molybdenum	BCC, A2	20	3.1469			2.7253
Nd Neodynium, α*	Hex., La type	R.T.	3.6580		11.7996	3.6280
Np Neptunium, α*	Orthorh.	20	6.663	4.723	4.887	2.60
Ni Nickel	FCC, A1		3.5239			2.4920
Nb Niobium	BCC, A2	25	3.3067			2.8637
Os Osmium	HCP, A3	20	2.7354		4.3193	2.6755
Pd Palladium	FCC, A1	22	3.8908			2.7511
P Phosphorous, black*	Orthorh.	22	3.3137	10.478	4.3765	2.224
Pt Platinum	FCC, A1	20	3.9240			2.7747
Pu Plutonium, α*	Monocl.	21	6.183	4.822	10.963 β = 101.79°	2.57
Po Polonium, α*	Cubic	~10	3.345			3.345
K Potassium	BCC, A2	78°K	5.247			4.524
Pr Praseodymium, α*	Hex., La type	R.T.	3.6726		11.8358	3.6402
Pa Protactinium	Tetrag.		3 925		3.238	3.212
Re Rhenium	HCP, A3	R.T.	2.760		4.458	2.741
Rh Rhodium	FCC, A1	20	3.8045			2.6902
Rb Rubidium	BCC, A2	20	5.70			4.94
Ru Ruthenium	HCP, A3	25	2.7059		4.2818	2.6503
Sm Samarium	Rhomb.		8.996		α = 23° 13′	3.588
Sc Scandium, α*	HCP, A3	R.T.	3.3091		5.2735	3.2561
Se Selenium*	Hex., A8	25	4.3658		4.9592	2.321
Si Silicon	Cubic, A4	25	5.4309			2.3517
Ag Silver	FCC, A1	25	4.0863			2.8895
Na Sodium	BCC, A2	20	4.2908			3.7159
Sr Strontium, α*	FCC, A1	25	6.0851			4.3029
S Sulphur*	Orthorh.	24.8	10.4650	12.8665	24.4869	2.037 (mean)
Ta Tantalum	BCC, A2	R.T.	3.298			2.856
Tc Technetium	HCP, A3	R.T.	2.735		4.388	2.703
Te Tellurium	Hex., A8	25	4.4568		5.9270	2.864
Tb Terbium, α*	HCP, A3	R.T.	3.6011		5.6938	3.5253
Tl Thallium, α*	HCP, A3	18	3.4567		5.5250	3.4077
Th Thorium, α*	FCC, A1	R.T.	5.0847			3.5951
Tm Thulium, α*	HCP, A3	R.T.	3.5376		5.5548	3.4474
Sn Tin (white), β*	Tetrag., A5	25	5.8317		3.1815	3.022
Tin (grey), α	Cubic, A4	20	6.4894			2.8100
Ti Titanium, α*	HCP, A3	25	2.9512		4.6845	2.8964
Titanium, β	BCC, A2	900	3.3066			2.8636
W Tungsten	BCC, A2	25	3.1653			2.7412
U Uranium, α*	Orthorh., A20	25	2.8538	5.8697	4.9550	2.7540
Uranium, β	Tetrag.	720	10.759		5.656	
Uranium, γ	BCC, A2	805	3.524			3.052
V Vanadium	BCC, A2	R.T.	3.0232			2.6182
Yb Ytterbium*	FCC, A1	R.T.	5.4864			3.8794
Y Yttrium*	HCP, A3	R.T.	3.6475		5.7308	3.5509
Zn Zinc	HCP, A3	25	2.6650		4.9470	2.6650
Zr Zirconium, α*	HCP, A3	25	3.2313		5.1479	3.1790
Zirconium, β	BCC, A2	862	3.6091			3.1256

* Ordinary form of an element that exists, or is thought to exist, in more than one form.

APPENDIX 6
CRYSTAL STRUCTURES OF SOME COMPOUNDS AND SOLID SOLUTIONS

Substance	Type of structure	Lattice parameters (Å)	Spacing of cleavage planes (Å)
NaCl KCl AgBr	FCC, B1 FCC, B1 FCC, B1	$a = 5.639$ $a = 6.290$ $a = 5.77$	2.820
CaF_2 (fluorite)	FCC, C1	$a = 5.46$	
$CaCO_3$ (calcite)	Rhombohedral, G1	$a = 6.37$ $\alpha = 46.1^\circ$	3.036
SiO_2 (α-quartz)	Hexagonal, C8	$a = 4.90$ $c = 5.39$	
$H_2KAl_2(SiO_4)_3$ (mica, muscovite)	Monoclinic	$a = 5.18$ $b = 8.96$ $c = 20.15$ $\beta = 98.6^\circ$	10.08
Fe_3C (cementite)	Orthorhombic	$a = 4.525$ $b = 5.088$ $c = 6.740$	
Austenite	FCC, A1	$a = 3.555 + 0.044x$ (x = weight percent carbon)	
Martensite	BC Tetragonal	$a = 2.867 - 0.013x$ $c = 2.867 + 0.116x$ (x = weight percent carbon)	

Appendix 7

X-Ray Wavelengths

All the following values are extracted from much longer tables on pp. 6-43 of Vol. 4 of the *International Tables for X-Ray Crystallography* [G.1], which are in turn taken from J. A. Bearden, *Rev. Mod. Phys.*, **39**, 78 (1967).

E($K\alpha$) is the energy $h\nu$ of the unresolved $K\alpha$ line to the nearest 0.01 keV. (The values in [G.1] are of higher accuracy.) In computing E($K\alpha$), $K\alpha_1$ is given twice the weight of $K\alpha_2$.

The wavelengths are given in Å* units. This unit is *defined* by the wavelength of the W$K\alpha_1$ line = 0.2090100 Å*. The Å* unit is believed to be equal to the angstrom Å to within 5 parts per million and involves a conversion factor of 1.002056 ± 0.000005 Å/kX. Because of the still remaining uncertainty in this conversion factor, it was decided to introduce the Å* unit. The distinction between Å and Å* is negligible except in work of the very highest accuracy.

Wavelengths (in Å* units) and Energies (in keV) of Some Characteristic Emission Lines and Absorption Edges

Element	E($K\alpha$) (keV)	$K\alpha_2$ strong	$K\alpha_1$ very strong	$K\beta_1$ week	K edge	$L\alpha_1$	L_{111} edge
1 H							
2 He							
3 Li	0.05		228		226.5		
4 Be	0.11		114		111		
5 B	0.18		67.6				
6 C	0.28		44.7		43.68		
7 N	0.39		31.6		30.99		
8 O	0.52		23.62		23.32		
9 F	0.68		18.32				
10 Ne	0.85		14.610	14.452	14.3018		
11 Na	1.04		11.9101	11.575	11.569		405
12 Mg	1.25		9.8900	9.521	9.5122		250.7
13 Al	1.49	8.34173	8.33834	7.960	7.94813		170.4
14 Si	1.74	7.12791	7.12542	6.753	6.738		123
15 P	2.01	6.160	6.157	5.796	5.784		94
16 S	2.31	5.37496	5.37216	5.0316	5.0185		
17 Cl	2.62	4.7307	4.7278	4.4034	4.3971		
18 A	2.96	4.19474	4.19180	3.8860	3.87090		
19 K	3.31	3.7445	3.7414	3.4539	3.4365		42.1
20 Ca	3.69	3.36166	3.35839	3.0897	3.0703	36.33	35.49
21 Sc	4.09	3.0342	3.0309	2.7796	2.762	31.35	
22 Ti	4.51	2.75216	2.74851	2.51391	2.49734	27.42	27.29
23 V	4.95	2.50738	2.50356	2.28440	2.2691	24.25	
24 Cr	5.41	2.293806	2.28970	2.08487	2.07020	21.64	20.7
25 Mn	5.90	2.10578	2.101820	1.91021	1.89643	19.45	
26 Fe	6.40	1.939980	1.936042	1.75661	1.74346	17.59	17.525
27 Co	6.93	1.792850	1.788965	1.62079	1.60815	15.972	15.915
28 Ni	7.47	1.661747	1.657910	1.500135	1.48807	14.561	14.525
29 Cu	8.04	1.544390	1.540562	1.392218	1.38059	12.336	13.288
30 Zn	8.63	1.439000	1.435155	1.29525	1.2834	12.254	12.131

Element	E($K\alpha$) (keV)	$K\alpha_2$ strong	$K\alpha_1$ very strong	$K\beta_1$ week	K edge	$L\alpha_1$	L_{111} edge
31 Ga	9.24	1.34399	1.340083	1.20789	1.1958	11.292	11.100
32 Ge	9.88	1.258011	1.254054	1.12894	1.11658	10.4361	10.187
33 As	10.53	1.17987	1.17588	1.05730	1.0450	9.6709	9.367
34 Se	11.21	1.10882	1.10477	0.99218	0.97974	8.9900	8.646
35 Br	11.91	1.04382	1.03974	0.93279	0.9204	8.3746	7.984
36 Kr	12.63	0.9841	0.9801	0.8785	0.86552	7.817	7.392
37 Rb	13.38	0.92969	0.925553	0.82868	0.81554	7.3183	6.862
38 Sr	14.14	0.87943	0.87526	0.78292	0.76973	6.8628	6.387
39 Y	14.93	0.83305	0.82884	0.74072	0.72766	6.4488	5.962
40 Zr	15.75	0.79015	0.78593	0.70173	0.68883	6.0705	5.579
41 Nb	16.58	0.75044	0.74620	0.66576	0.06298	5.7243	5.230
42 Mo	17.44	0.713590	0.709300	0.632288	0.61978	5.40655	4.913
43 Tc	18.33	0.67932	0.67502	0.60130	0.58906	5.1148	4.630
44 Ru	19.24	0.647408	0.643083	0.572482	0.58061	4.84575	4.389
45 Rh	20.17	0.617630	0.613279	0.545605	0.53395	4.59743	4.1299
46 Pd	21.12	0.589821	0.585448	0.520520	0.6092	4.36767	3.9074
47 Ag	22.11	0.563798	0.5594075	0.497069	0.48589	4.15443	3.6999
48 Cd	23.11	0.539422	0.535010	0.475105	0.48407	3.95635	3.5047
49 In	24.14	0.516544	0.512113	0.454545	0.44371	3.77192	3.3237
50 Sn	25.20	0.495053	0.490599	0.435236	0.42467	3.59994	3.1557
51 Sb	26.28	0.474827	0.470354	0.417085	0.40868	3.43941	3.0003
52 Te	27.38	0.455784	0.451295	0.399995	0.30074	3.28920	2.8555
53 I	28.51	0.437829	0.433318	0.383905	0.37381	3.14860	2.7196
54 Xe	29.67	0.42087	0.41634	0.36872	0.3584	3.0166	2.5926
55 Cs	30.86	0.404835	0.400290	0.354364	0.36451	2.8924	2.4740
56 Ba	32.07	0.389668	0.385111	0.340811	0.33104	2.77595	2.3629
57 La	33.31	0.375313	0.370737	0.327983	0.31844	2.66570	2.261
58 Ce	34.57	0.361683	0.357092	0.315816	0.30643	2.5615	2.166
59 Pr	35.87	0.348749	0.344140	0.304261	0.29518	2.4630	2.0791
60 Nd	37.19	0.336472	0.331846	0.293299	0.28453	2.3704	1.9967
61 Pm	38.54	0.324803	0.320160	0.28290	0.27431	2.2822	1.9191
62 Sm	39.92	0.313698	0.309040	0.27301	0.26464	2.1998	1.8457
63 Eu	41.33	0.303118	0.298446	0.263577	0.25553	2.1209	1.7761
64 Gd	42.77	0.293038	0.288353	0.25460	0.24681	2.0468	1.7117
65 Tb	44.24	0.283423	0.278724	0.24608	0.23841	1.9765	1.6497
66 Dy	45.73	0.274247	0.269533	0.23788	0.23048	1.90881	1.5916
67 Ho	47.26	0.265486	0.260756	0.23012	0.22291	1.8450	1.5368
68 Er	48.83	0.257110	0.252365	0.22266	0.21567	1.78425	1.4835
69 Tm	50.42	0.249095	0.244338	0.21556	0.20880	1.7268	1.4334
70 Yb	52.04	0.241424	0.236655	0.20884	0.20224	1.67189	1.3862
71 Lu	53.70	0.234081	0.229298	0.20231	0.19595	1.61951	1.3405
72 Ht	55.40	0.227024	0.222227	0.19607	0.18982	1.56958	1.2972
73 Ta	57.11	0.220305	0.215497	0.190089	0.18394	1.52197	1.2553
74 W	58.87	0.213828	0.2090100	0.184374	0.17837	1.47639	1.2155
75 Re	60.67	0.207611	0.202781	0.178880	0.17302	1.43230	1.1773
76 Os	62.50	0.201639	0.196794	0.173611	0.16787	1.39121	1.1408
77 Ir	64.36	0.195904	0.191047	0.168542	0.16292	1.35128	1.1058
78 Pt	66.26	0.190381	0.185511	0.163675	0.15818	1.31304	1.0723
79 Au	68.20	0.185075	0.180195	0.158982	0.153693	1.27640	1.04000
80 Hg	70.18	0.179958	0.175068	0.154487	0.14918	1.24120	1.0091
81 Ti	72.19	0.175036	0.170136	0.150142	0.14495	1.20739	0.9793
82 Pb	74.25	0.170294	0.165376	0.145970	0.140880	1.17501	0.95073
83 Bi	76.34	0.165717	0.160789	0.141948	0.13694	1.14386	0.9234
84 Po	78.48	0.16130	0.15636	0.13807		1.11386	
85 At	80.66	0.15705	0.15210	0.13432		1.08500	
86 Rn	82.88	0.15294	0.14798	0.13069		1.05723	
87 Fr	85.14	0.14896	0.14399	0.12719		1.03049	
88 Ra	87.46	0.14512	0.14014	0.12382		1.00473	0.8028
89 Ac	89.81	0.14141	0.136417	0.12055		0.97993	
90 Th	92.22	0.137829	0.132813	0.117396	0.11307	0.95600	0.7607
91 Pa	94.67	0.134343	0.129325	0.114345		0.93284	
92 U	97.18	0.130968	0.125947	0.111394	0.10723	0.910639	0.7223

Appendix: X-Ray Wavelengths

Some commonly used K wavelengths

Element	$K\alpha$ (weighted average)*	$K\alpha_2$ strong	$K\alpha_1$ very strong	$K\beta_1$ week
Cr	2.29100	2.293606	2.28970	2.08487
Fe	1.937355	1.939980	1.936042	1.75661
Co	1.790260	1.792850	1.788965	1.62079
Cu	1.541838	1.544390	1.540562	1.392218
Mo	0.710730	0.713590	0.709300	0.632288

*$K\alpha_1$ is given twice the weight of Ka_2.

Characteristic L Lines of Tungsten

Line	Relative Intensity	Wavelength
$L\alpha_1$	Very Strong	1.47639
$L\alpha_2$	Weak	1.48743
$L\beta_1$	Strong	1.281809
$L\beta_2$	Medium	1.24460
$L\beta_3$	Weak	1.26269
$L\gamma_1$	Weak	1.09855

REFERENCES

The following books are listed more or less in the order they are encountered in the text

G.1 *International Tables for Crystallography*, Ed. A.J.C Wilson, Vol. A-C (Dordrecht Kluwer Academic Pub. for International Union of Crystallography, 1995). The reference ''book" for crystallography and diffraction.

APPENDIX 8
MASS ABSORPTION COEFFICIENTS μ/ρ (cm^2/gm) AND DENSITIES ρ

The mass absorption coefficients are extracted from much longer tables on pp. 61–66 of Vol. 4 of the *International Tables for X-Ray Crystallography* [G.11]. Although these coefficients are given to four significant figures, the actual accuracy is much less; the uncertainty ranges from less than 2 percent to more than 15 percent, depending on absorber and wavelength. [G.11] should be consulted for details.

The densities of elements solid at room temperature, except *P*, are x-ray densities, rounded off, from pp. 46–56 of Vol. 3 of [G.11]. Densities of gases are from *Metals Handbook* (Cleveland: American Society for Metals, 1948).

Absorber	Density (gm/cm^3)	Mo		Cu		Co		Cr	
		$K\alpha$ 0.711 Å	$K\beta$ 0.632 Å	$K\alpha$ 1.542 Å	$K\beta$ 1.392 Å	$K\alpha$ 1.790 Å	$K\beta$ 1.621 Å	$K\alpha$ 2.291 Å	$K\beta$ 2.085 Å
1 H	0.08375×10^{-3}	0.3727	0.3699	0.3912	0.3882	0.3966	0.3928	0.4116	0.4046
2 He	0.1664×10^{-3}	0.2019	0.1972	0.2835	0.2623	0.3288	0.2966	0.4648	0.4001
3 Li	0.533	0.1968	0.1866	0.4770	0.3939	0.6590	0.5283	1.243	0.9639
4 Be	1.85	0.2451	0.2216	1.007	0.7742	1.522	1.152	3.183	2.388
5 B	2.47	0.3451	0.2928	2.142	1.590	3.357	2.485	7.232	5.385
6 C	2.27 (graphite)	0.5348	0.4285	4.219	3.093	6.683	4.916	14.46	10.76
7 N	1.165×10^{-3}	0.7898	0.6054	7.142	5.215	11.33	8.330	24.42	18.23
8 O	1.332×10^{-3}	1.147	0.8545	11.03	8.062	17.44	12.85	37.19	27.88
9 F	1.696×10^{-3}	1.584	1.154	15.95	11.66	25.12	18.57	53.14	39.99
10 Ne	0.8387×10^{-3}	2.209	1.597	22.13	16.24	34.69	25.72	72.71	54.91
11 Na	0.966	2.939	2.098	30.30	22.23	47.34	35.18	98.48	74.66
12 Mg	1.74	3.979	2.825	40.88	30.08	63.54	47.38	130.8	99.62
13 Al	2.70	5.043	3.585	50.23	37.14	77.54	58.08	158.0	120.7
14 Si	2.33	6.533	4.624	65.32	48.37	100.4	75.44	202.7	155.6
15 P	1.82 (yellow)	7.870	5.569	77.28	57.44	118.0	89.05	235.5	181.6
16 S	2.09	9.625	6.835	92.53	68.90	141.2	106.6	281.9	217.2
17 Cl	3.214×10^{-3}	11.64	8.261	109.2	81.79	164.7	125.3	321.5	250.2
18 A	1.663×10^{-3}	12.62	8.949	119.5	89.34	180.9	137.3	355.5	275.8
19 K	0.862	16.20	11.51	148.4	111.7	222.0	169.9	426.8	334.2
20 Ca	1.53	19.00	13.56	171.4	129.0	257.4	196.4	499.6	389.3
21 Sc	2.99	21.04	15.00	186.0	140.8	275.5	212.2	520.9	410.7
22 Ti	4.51	23.25	16.65	202.4	153.2	300.5	231.0	571.4	449.0
23 V	6.09	25.24	18.07	222.6	168.0	332.7	254.7	75.06	501.0
24 Cr	7.19	29.25	20.99	252.3	191.1	375.0	288.1	85.71	65.79
25 Mn	7.47	31.86	22.89	272.5	206.7	405.1	311.2	96.08	73.75
26 Fe	7.87	37.74	27.21	304.4	233.6	56.25	345.5	113.1	86.77
27 Co	8.8	41.02	29.51	338.6	258.7	62.86	47.71	124.6	96.06
28 Ni	8.91	47.24	34.18	48.83	282.8	73.75	56.05	145.7	112.5
29 Cu	8.93	49.34	35.77	51.54	38.74	78.11	59.22	155.2	119.5
30 Zn	7.13	55.46	40.26	59.51	45.30	88.71	68.00	171.7	133.5
31 Ga	5.91	56.90	41.69	62.13	46.65	94.15	71.39	186.9	144.0
32 Ge	5.32	60.47	44.26	67.92	51.44	102.0	77.79	199.9	154.5
33 As	5.78	65.97	48.57	75.65	57.01	114.0	86.76	224.0	173.3
34 Se	4.81	68.82	51.20	82.89	62.32	125.1	95.11	246.1	190.4
35 Br	3.12 (liquid)	74.68	55.56	90.29	68.07	135.8	103.5	266.2	206.2

Absorber	Density (gm/cm³)	Mo		Cu		Co		Cr	
		$K\alpha$ 0.711 Å	$K\beta$ 0.632 Å	$K\alpha$ 1.542 Å	$K\beta$ 1.392 Å	$K\alpha$ 1.790 Å	$K\beta$ 1.621 Å	$K\alpha$ 2.291 Å	$K\beta$ 2.085 Å
36 Kr	3.488×10^{-3}	79.10	58.64	97.02	73.22	145.7	111.2	284.6	220.7
37 Rb	1.53	83.00	62.07	106.3	80.16	159.6	121.8	311.7	241.8
38 Sr	2.58	88.04	65.59	115.3	86.77	173.5	132.2	339.3	263.4
39 Y	4.48	97.56	72.57	127.1	96.19	190.2	145.4	368.9	286.9
40 Zr	6.51	16.10	75.20	136.8	103.3	204.9	156.6	398.6	309.7
41 Nb	8.58	16.96	81.22	148.8	112.3	222.9	170.4	431.9	336.4
42 Mo	10.22	18.44	13.29	158.3	119.7	236.6	181.0	457.4	356.5
43 Tc	11.50	19.78	14.30	167.7	126.9	250.8	191.9	485.5	378.0
44 Ru	12.36	21.33	15.40	180.8	137.0	269.4	206.6	517.9	404.4
45 Rh	12.42	23.05	16.65	194.1	147.1	289.0	221.8	555.2	433.7
46 Pd	12.00	24.42	17.63	205.0	155.6	304.3	234.0	580.9	455.1
47 Ag	10.50	26.38	19.10	218.1	165.8	323.5	248.9	617.4	483.5
48 Cd	8.65	27.73	20.13	229.3	174.0	341.8	262.1	658.8	513.5
49 In	7.29	29.13	21.18	242.1	183.3	362.7	277.1	705.8	548.0
50 Sn	7.29	31.18	22.62	253.3	193.1	374.1	288.7	708.8	556.6
51 Sb	6.69	33.01	23.91	266.5	203.6	391.3	303.1	733.4	578.8
52 Te	6.25	33.92	24 67	273.4	208.4	404.4	311.7	768.9	602.7
53 I	4.95	36.33	26.53	291.7	221.9	434.0	333.2	835.2	650.8
54 Xe	5.495×10^{-3}	38.31	27.86	309.8	235.9	459.0	353.4	755.4	685.2
55 Cs	1.91 (−10°C)	40.44	29.51	325.4	247.5	483.8	371.5	802.7	725.1
56 Ba	3.59	42.37	31.00	336.1	256.0	499.0	383.6	587.3	644.6
57 La	6.17	45.34	33.10	353.5	270.8	519.0	401.9	222.9	661.5
58 Ce	6.77	48.56	35.54	378.8	289.6	559.1	431.5	240.4	509.4
59 Pr	6.78	50.78	37.09	402.2	306.8	596.2	458.8	260.5	205.3
60 Nd	7.00	53.28	38.88	417.9	319.8	531.7	475.9	271.3	213.4
61 Pm		55.52	40.52	441.1	336.4	401.4	503.2	284.7	223.8
62 Sm	7.54	57.96	42.40	453.5	346.6	411.8	446.3	295.0	231.5
63 Eu	5.25	61.18	44.74	417.9	369.0	165.2	476.9	312.7	244.9
64 Gd	7.87	62.79	45.95	426.7	377.2	169.5	346.7	318.9	250.3
65 Tb	8.27	66.77	48.88	321.9	399.9	178.7	367.1	338.9	265.2
66 Dy	8.53	68.89	50.38	336.6	360.2	184.9	142.9	351.7	275.0
67 Ho	8.80	72.14	52.76	128.4	272.4	189.8	146.3	363.3	283.4
68 Er	9.04	75.61	55.07	134.3	291.7	198.4	153.0	379.7	296.1
69 Tm	9.33	78.98	57.94	140.2	288.5	207.4	159.8	397.0	309.6
70 Yb	6.97	80.23	59.22	144.7	110.9	214.0	164.9	409.6	319.4
71 Lu	9.84	84.18	62.04	152.0	116.5	224.6	173.2	429.5	335.1
72 Hf	13.28	86.33	64.15	157.7	121.0	232.9	179.6	445.0	347.2
73 Ta	16.67	89.51	66.07	161.5	123.9	238.3	183.9	454.7	355.0
74 W	19.25	95.76	70.57	170.5	131.5	249.7	193.7	470.4	369.1
75 Re	21.02	98.74	72.47	178.3	137.3	261.8	202.7	495.5	388.0
76 Os	22.58	100.2	74.13	183.8	141.3	270.3	209.0	512.4	401.1
77 Ir	22.55	103.4	77.20	192.2	147.6	283.4	218.8	539.6	421.6
78 Pt	21.44	108.6	80.23	198.2	151.2	295.2	226.4	571.6	443.9
79 Au	19.28	111.3	82.33	207.8	160.6	303.3	235.7	568.0	446.7
80 Hg	13.55	114.7	85.30	216.2	166.6	317.0	245.7	597.9	468.9
81 Tl	11.87	119.4	88.25	222.2	171.1	326.3	252.7	616.9	483.3
82 Pb	11.34	122.8	90.55	232.1	178.6	340.8	263.8	644.5	504.9
83 Bi	9.80	125.9	93.50	242.9	187.5	355.3	275.8	667.2	524.2
86 Rn	4.40 (liq., −62°C)	117.2	100.7	263.7	203.0	387.1	299.7	731.4	573.2
90 Th	11.72	99.46	73.34	306.8	236.6	449.0	348.4	844.1	663.0
92 U	19.05	96.67	72.63	305.7	236.2	446.3	346.9	774.0	657.1
94 Pu	19.81	48.84	78.99	352.9	271.2	519.6	401.6	803.2	771.6

Appendix 9

Quadratic Forms of Miller Indices

Cubic					Hexagonal	
$h^2 + k^2 + l^2$	hkl				$h^2 + hk + k^2$	hk
	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

Appendix: Quadratic Forms of Miller Indices

	Cubic				Hexagonal	
$h^2 + k^2 + l^2$	*hkl*				$h^2 + hk + k^2$	*hk*
	Simple	Face-centered	Body-centered	Diamond		
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	

Appendix 10

Atomic Scattering Factors

$\frac{\sin\theta}{\lambda}$ (Å^{-1})	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
H	1	0.81	0.48	0.25	0.13	0.07	0.04	0.03	0.02	0.01	0.00	0.00	
He	2	1.88	1.46	1.05	0.75	0.52	0.35	0.24	0.18	0.14	0.11	0.09	
Li^{+}	2	1.96	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Li	3	2.2	1.8	1.5	1.3	1.0	0.8	0.6	0.5	0.4	0.3	0.3	
Be^{+2}	2	2.0	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
Be	4	2.9	1.9	1.7	1.6	1.4	1.2	1.0	0.9	0.7	0.6	0.5	
B^{+3}	2	1.99	1.9	1.8	1.7	1.6	1.4	1.3	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	0.9	0.7	
C	6	4.6	3.0	2.2	1.9	1.7	1.6	1.4	1.3	1.16	1.0	0.9	
N^{+5}	2	2.0	2.0	1.9	1.9	1.8	1.7	1.6	1.5	1.4	1.3	1.16	
N^{+3}	4	3.7	3.0	2.4	2.0	1.8	1.66	1.56	1.49	1.39	1.28	1.17	
N	7	5.8	4.2	3.0	2.3	1.9	1.65	1.54	1.49	1.39	1.29	1.17	
O	8	7.1	5.3	3.9	2.9	2.2	1.8	1.6	1.5	1.4	1.35	1.26	
O^{-2}	10	8.0	5.5	3.8	2.7	2.1	1.8	1.5	1.5	1.4	1.35	1.26	
F	9	7.8	6.2	4.45	3.35	2.65	2.15	1.9	1.7	1.6	1.5	1.35	
F^{-}	10	8.7	6.7	4.8	3.5	2.8	2.2	1.9	1.7	1.55	1.5	1.35	
Ne	10	9.3	7.5	5.8	4.4	3.4	2.65	2.2	1.9	1.65	1.55	1.5	
Na^{+}	10	9.5	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Na	11	9.65	8.2	6.7	5.25	4.05	3.2	2.65	2.25	1.95	1.75	1.6	
Mg^{+2}	10	9.75	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Mg	12	10.5	8.6	7.25	5.95	4.8	3.85	3.15	2.55	2.2	2.0	1.8	
Al^{+3}	10	9.7	8.9	7.8	6.65	5.5	4.45	3.65	3.1	2.65	2.3	2.0	
Al	13	11.0	8.95	7.75	6.6	5.5	4.5	3.7	3.1	2.65	2.3	2.0	
Si^{+4}	10	9.75	9.15	8.25	7.15	6.05	5.05	4.2	3.4	2.95	2.6	2.3	
Si	14	11.35	9.4	8.2	7.15	6.1	5.1	4.2	3.4	2.95	2.6	2.3	
P^{+5}	10	9.8	9.25	8.45	7.5	6.55	5.65	4.8	4.05	3.4	3.0	2.6	
P	15	12.4	10.0	8.45	7.45	6.5	5.65	4.8	4.05	3.4	3.0	2.6	
P^{-3}	18	12.7	9.8	8.4	7.45	6.5	5.65	4.85	4.05	3.4	3.0	2.6	
S^{+6}	10	9.85	9.4	8.7	7.85	6.85	6.05	5.25	4.5	3.9	3.35	2.9	
S	16	13.6	10.7	8.95	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	
S^{-2}	18	14.3	10.7	8.9	7.85	6.85	6.0	5.25	4.5	3.9	3.35	2.9	
Cl	17	14.6	11.3	9.25	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	
Cl^{-}	18	15.2	11.5	9.3	8.05	7.25	6.5	5.75	5.05	4.4	3.85	3.35	
A	18	15.9	12.6	10.4	8.7	7.8	7.0	6.2	5.4	4.7	4.1	3.6	
K^{+}	18	16.5	13.3	10.8	8.85	7.75	7.05	6.44	5.9	5.3	4.8	4.2	
K	19	16.5	13.3	10.8	9.2	7.9	6.7	5.9	5.2	4.6	4.2	3.7	3.3
Ca^{+2}	18	16.8	14.0	11.5	9.3	8.1	7.35	6.7	6.2	5.7	5.1	4.6	
Ca	20	17.5	14.1	11.4	9.7	8.4	7.3	6.3	5.6	4.9	4.5	4.0	3.6
Sc^{+3}	18	16.7	14.0	11.4	9.4	8.3	7.6	6.9	6.4	5.8	5.35	4.85	
Sc	21	18.4	14.9	12.1	10.3	8.9	7.7	6.7	5.9	5.3	4.7	4.3	3.9
Ti^{+4}	18	17.0	14.4	11.9	9.9	8.5	7.85	7.3	6.7	6.15	5.65	5.05	
Ti	22	19.3	15.7	12.8	10.9	9.5	8.2	7.2	6.3	5.6	5.0	4.6	4.2
V	23	20.2	16.6	13.5	11.5	10.1	8.7	7.6	6.7	5.9	5.3	4.9	4.4
Cr	24	21.1	17.4	14.2	12.1	10.6	9.2	8.0	7.1	6.3	5.7	5.1	4.6
Mn	25	22.1	18.2	14.9	12.7	11.1	9.7	8.4	7.5	6.6	6.0	5.4	4.9

$\frac{\sin\theta}{\lambda}$ (Å^{-1})	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
Fe	26	23.1	18.9	15.6	13.3	11.6	10.2	8.9	7.9	7.0	6.3	5.7	5.2
Co	27	24.1	19.8	16.4	14.0	12.1	10.7	9.3	8.3	7.3	6.7	6.0	5.5
Ni	28	25.0	20.7	17.2	14.6	12.7	11.2	9.8	8.7	7.7	7.0	6.3	5.8
Cu	29	25.9	21.6	17.9	15.2	13.3	11.7	10.2	9.1	8.1	7.3	6.6	6.0
Zn	30	26.8	22.4	18.6	15.8	13.9	12.2	10.7	9.6	8.5	7.6	6.9	6.3
Ga	31	27.8	23.3	19.3	16.5	14.5	12.7	11.2	10.0	8.9	7.9	7.3	6.7
Ge	32	28.8	24.1	20.0	17.1	15.0	13.2	11.6	10.4	9.3	8.3	7.6	7.0
As	33	29.7	25.0	20.8	17.7	15.6	13.8	12.1	10.8	9.7	8.7	7.9	7.3
Se	34	30.6	25.8	21.5	18.3	16.1	14.3	12.6	11.2	10.0	9.0	8.2	7.5
Br	35	31.6	26.6	22.3	18.9	16.7	14.8	13.1	11.7	10.4	9.4	8.6	7.8
Kr	36	32.5	27.4	23.0	19.5	17.3	15.3	13.6	12.1	10.8	9.8	8.9	8.1
Rb^+	36	33.6	28.7	24.6	21.4	18.9	16.7	14.6	12.8	11.2	9.9	8.9	
Rb	37	33.5	28.2	23.8	20.2	17.9	15.9	14.1	12.5	11.2	10.2	9.2	8.4
Sr	38	34.4	29.0	24.5	20.8	18.4	16.4	14.6	12.9	11.6	10.5	9.5	8.7
Y	39	35.4	29.9	25.3	21.5	19.0	17.0	15.1	13.4	12.0	10.9	9.9	9.0
Zr	40	36.3	30.8	26.0	22.1	19.7	17.5	15.6	13.8	12.4	11.2	10.2	9.3
Nb	41	37.3	31.7	26.8	22.8	20.2	18.1	16.0	14.3	12.8	11.6	10.6	9.7
Mo	42	38.2	32.6	27.6	23.5	20.8	18.6	16.5	14.8	13.2	12.0	10.9	10.0
Tc	43	39.1	33.4	28.3	24.1	21.3	19.1	17.0	15.2	13.6	12.3	11.3	10.3
Ru	44	40.0	34.3	29.1	24.7	21.9	19.6	17.5	15.6	14.1	12.7	11.6	10.6
Rh	45	41.0	35.1	29.9	25.4	22.5	20.2	18.0	16.1	14.5	13.1	12.0	11.0
Pd	46	41.9	36.0	30.7	26.2	23.1	20.8	18.5	16.6	14.9	13.6	12.3	11.3
Ag	47	42.8	36.9	31.5	26.9	23.8	21.3	19.0	17.1	15.3	14.0	12.7	11.7
Cd	48	43.7	37.7	32.2	27.5	24.4	21.8	19.6	17.6	15.7	14.3	13.0	12.0
In	49	44.7	38.6	33.0	28.1	25.0	22.4	20.1	18.0	16.2	14.7	13.4	12.3
Sn	50	45.7	39.5	33.8	28.7	25.6	22.9	20.6	18.5	16.6	15.1	13.7	12.7
Sb	51	46.7	40.4	34.6	29.5	26.3	23.5	21.1	19.0	17.0	15.5	14.1	13.0
Te	52	47.7	41.3	35.4	30.3	26.9	24.0	21.7	19.5	17.5	16.0	14.5	13.3
I	53	48.6	42.1	36.1	31.0	27.5	24.6	22.2	20.0	17.9	16.4	14.8	13.6
Xe	54	49.6	43.0	36.8	31.6	28.0	25.2	22.7	20.4	18.4	16.7	15.2	13.9
Cs	55	50.7	43.8	37.6	32.4	28.7	25.8	23.2	20.8	18.8	17.0	15.6	14.5
Ba	56	51.7	44.7	38.4	33.1	29.3	26.4	23.7	21.3	19.2	17.4	16.0	14.7
La	57	52.6	45.6	39.3	33.8	29.8	26.9	24.3	21.9	19.7	17.9	16.4	15.0
Pr	59	54.5	47.4	40.9	35.2	31.1	28.0	25.4	22.9	20.6	18.8	17.1	15.7
Nd	60	55.4	48.3	41.6	35.9	31.8	28.6	25.9	23.4	21.1	19.2	17.5	16.1
Pm	61	56.4	49.1	42.4	36.6	32.4	29.2	26.4	23.9	21.5	19.6	17.9	16.4
Sm	62	57.3	50.0	43.2	37.3	32.9	29.8	26.9	24.4	22.0	20.0	18.3	16.8
Eu	63	58.3	50.9	44.0	38.1	33.5	30.4	27.5	24.9	22.4	20.4	18.7	17.1
Gd	64	59.3	51.7	44.8	38.8	34.1	31.0	28.1	25.4	22.9	20.8	19.1	17.5
Tb	65	60.2	52.6	45.7	39.6	34.7	31.6	28.6	25.9	23.4	21.2	19.5	17.9
Dy	66	61.1	53.6	46.5	40.4	35.4	32.2	29.2	26.3	23.9	21.6	19.9	18.3
Ho	67	62.1	54.5	47.3	41.1	36.1	32.7	29.7	26.8	24.3	22.0	20.3	18.6
Er	68	63.0	55.3	48.1	41.7	36.7	33.3	30.2	27.3	24.7	22.4	20.7	18.9
Tm	69	64.0	56.2	48.9	42.4	37.4	33.9	30.8	27.9	25.2	22.9	21.0	19.3

$\frac{\sin\theta}{\lambda}$ ($\mathrm{A}^{\circ -1}$)	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.1	1.2
Yb	70	64.9	57.0	49.7	43.2	38.0	34.4	31.3	28.4	25.7	23.3	21.4	19.7
Lu	71	65.9	57.8	50.4	43.9	38.7	35.0	31.8	28.9	26.2	23.8	21.8	20.0
Hf	72	66.8	58.6	51.2	44.5	39.3	35.6	32.3	29.3	26.7	24.2	22.3	20.4
Ta	73	67.8	59.5	52.0	45.3	39.9	36.2	32.9	29.8	27.1	24.7	22.6	20.9
W	74	68.8	60.4	52.8	46.1	40.5	36.8	33.5	30.4	27.6	25.2	23.0	21.3
Re	75	69.8	61.3	53.6	46.8	41.1	37.4	34.0	30.9	28.1	25.6	23.4	21.6
Os	76	70.8	62.2	54.4	47.5	41.7	38.0	34.6	31.4	28.6	26.0	23.9	22.0
Ir	77	71.7	63.1	55.3	48.2	42.4	38.6	35.1	32.0	29.0	26.5	24.3	22.3
Pt	78	72.6	64.0	56.2	48.9	43.1	39.2	35.6	32.5	29.5	27.0	24.7	22.7
Au	79	73.6	65.0	57.0	49.7	43.8	39.8	36.2	33.1	30.0	27.4	25.1	23.1
Hg	80	74.6	65.9	57.9	50.5	44.4	40.5	36.8	33.6	30.6	27.8	25.6	23.6
Ti	81	75.5	66.7	58.7	51.2	45.0	41.1	37.4	34.1	31.1	28.3	26.0	24.1
Pb	82	76.5	67.5	59.5	51.9	45.7	41.6	37.9	34.6	31.5	28.8	26.4	24.5
Bi	83	77.5	68.4	60.4	52.7	46.4	42.2	38.5	35.1	32.0	29.2	26.8	24.8
Po	84	78.4	69.4	61.3	53.5	47.1	42.8	39.1	35.6	32.6	29.7	27.2	25.2
At	85	79.4	70.3	62.1	54.2	47.7	43.4	39.6	36.2	33.1	30.1	27.6	25.6
Rn	86	80.3	71.3	63.0	55.1	48.4	44.0	40.2	36.8	33.5	30.5	28.0	26.0
Fr	87	81.3	72.2	63.8	55.8	49.1	44.5	40.7	37.3	34.0	31.0	28.4	26.4
Ra	88	82.2	73.2	64.6	56.5	49.8	45.1	41.3	37.8	34.6	31.5	28.8	26.7
Ac	89	83.2	74.1	65.5	57.3	50.4	45.8	41.8	38.3	35.1	32.0	29.2	27.1
Th	90	84.1	75.1	66.3	58.1	51.1	46.5	42.4	38.8	35.5	32.4	29.6	27.5
Pa	91	85.1	76.0	67.1	58.8	51.7	47.1	43.0	39.3	36.0	32.8	30.1	27.9
U	92	86.0	76.9	67.9	59.6	52.4	47.7	43.5	39.8	36.5	33.3	30.6	28.3
Np	93	87	78	69	60	53	48	44	40	37	34	31	29
Pu	94	88	79	69	61	54	49	44	41	38	34	31	29
Am	95	89	79	70	62	55	50	45	42	38	35	32	30
Cm	96	90	80	71	62	55	50	46	42	39	35	32	30
Bk	97	91	81	72	63	56	51	46	43	39	36	33	30
Cf	98	92	82	73	64	57	52	47	43	40	36	33	31
	99	93	83	74	65	57	52	48	44	40	37	34	31
	100	94	84	75	66	58	53	48	44	41	37	34	31

From Peiser, Rooksby, and Wilson (see [10]). More extensive tables, at smaller intervals of $(\sin\theta)/\lambda$, are given in [G.1].

REFERENCES

The following books are listed more or less in the order they are encountered in the text

G.1 *International Tables for Crystallography*, Ed. A.J.C Wilson, Vol. A-C (Dordrecht Kluwer Academic Pub. for International Union of Crystallography, 1995). The reference ''book" for crystallography and diffraction.

Appendix 11

Multiplicity Factors for the Powder Method

Cubic:	$\frac{hkl}{48^*}$	$\frac{hhl}{24}$	$\frac{0kl}{24^*}$	$\frac{0kk}{12}$	$\frac{hhh}{8}$	$\frac{00l}{6}$	
Hexagonal and Rhombohedral:	$\frac{hk \cdot l}{24^*}$	$\frac{hh \cdot l}{12^*}$	$\frac{0k \cdot l}{12^*}$	$\frac{hk \cdot 0}{12^*}$	$\frac{hh \cdot 0}{6}$	$\frac{0k \cdot 0}{6}$	$\frac{00 \cdot l}{2}$
Tetragonal:	$\frac{hkl}{16^*}$	$\frac{hhl}{8}$	$\frac{0kl}{8}$	$\frac{hk0}{8^*}$	$\frac{hh0}{4}$	$\frac{0k0}{4}$	$\frac{00l}{2}$
Orthorhombic:	$\frac{hkl}{8}$	$\frac{0kl}{4}$	$\frac{h0l}{4}$	$\frac{hk0}{4}$	$\frac{h00}{2}$	$\frac{0k0}{2}$	$\frac{00l}{2}$
Monoclinic:	$\frac{hkl}{4}$	$\frac{h0l}{2}$	$\frac{0k0}{2}$				
Triclinic:	$\frac{hkl}{2}$						

Note that, in cubic crystals, for example, *hhl* stands for such indices as 112 (or 211), 0*kl* for such indices as 012 (or 210), 0*kk* for such indices as 011 (or 110), etc.

* These are the usual multiplicity factors. In some crystals, planes having these indices comprise two forms with the same spacing but different structure factor, and the multiplicity factor for each form is half the value given above. In the cubic system, for example, there are some crystals in which permutations of the indices (*hkl*) produce planes which are not structurally equivalent; in such crystals (AuBe is an example), the plane (123), for example, belongs to one form and has a certain structure factor, while the plane (321) belongs to another form and has a different structure factor. These are 48/2 = 24 planes in the first form and 24 planes in the second. This question is discussed more fully by Henry, Lipson, and Wooster [G.15].

Appendix 12
Lorentz-Polarization Factor $\left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}\right)$

Θ°	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
2	1639	1486	1354	1239	1138	1048	968.9	898.3	835.1	778.4
3	727.2	680.9	638.8	600.5	565.6	533.6	504.3	477.3	452.3	429.3
4	408.0	388.2	369.9	352.7	336.8	321.9	308.0	294.9	282.6	271.1
5	260.3	250.1	240.5	231.4	222.9	214.7	207.1	199.8	192.9	186.3
6	180.1	174.2	168.5	163.1	158.0	153.1	148.4	144.0	139.7	135.6
7	131.7	128.0	124.4	120.9	117.6	114.4	111.4	108.5	105.6	102.9
8	100.3	97.80	95.37	93.03	90.78	88.60	86.51	84.48	82.52	80.63
9	78.79	77.02	75.31	73.66	72.05	70.49	68.99	67.53	66.12	64.74
10	63.41	62.12	60.87	59.65	58.46	57.32	56.20	55.11	54.06	53.03
11	52.04	51.06	50.12	49.19	48.30	47.43	46.58	45.75	44.94	44.16
12	43.39	42.64	41.91	41.20	40.50	39.82	39.16	38.51	37.88	37.27
13	36.67	36.08	35.50	34.94	34.39	33.85	33.33	32.81	32.31	31.82
14	31.34	30.87	30.41	29.96	29.51	29.08	28.66	28.24	27.83	27.44
15	27.05	26.66	26.29	25.92	25.56	25.21	24.86	24.52	24.19	23.86
16	23.54	23.23	22.92	22.61	22.32	22.02	21.74	21.46	21.18	20.91
17	20.64	20.38	20.12	19.87	19.62	19.38	19.14	18.90	18.67	18.44
18	18.22	18.00	17.78	17.57	17.36	17.15	16.95	16.75	16.56	16.36
19	16.17	15.99	15.80	15.62	15.45	15.27	15.10	14.93	14.76	14.60
20	14.44	14.28	14.12	13.97	13.81	13.66	13.52	13.37	13.23	13.09
21	12.95	12.81	12.68	12.54	12.41	12.28	12.15	12.03	11.91	11.78
22	11.66	11.54	11.43	11.31	11.20	11.09	10.98	10.87	10.76	10.65
23	10.55	10.45	10.35	10.24	10.15	10.05	9.951	9.857	9.763	9.671
24	9.579	9.489	9.400	9.313	9.226	9.141	9.057	8.973	8.891	8.810
25	8.730	8.651	8.573	8.496	8.420	8.345	8.271	8.198	8.126	8.054
26	7.984	7.915	7.846	7.778	7.711	7.645	7.580	7.515	7.452	7.389
27	7.327	7.266	7.205	7.145	7.086	7.027	6.969	6.912	6.856	6.800
28	6.745	6.692	6.637	6.584	6.532	6.480	6.429	6.379	6.329	6.279
29	6.230	6.183	6.135	6.088	6.042	5.995	5.950	5.905	5.861	5.817
30	5.774	5.731	5.688	5.647	5.605	5.564	5.524	5.484	5.445	5.406
31	5.367	5.329	5.292	5.254	5.218	5.181	5.145	5.110	5.075	5.040
32	5.006	4.972	4.939	4.906	4.873	4.841	4.809	4.777	4.746	4.715
33	4.685	4.655	4.625	4.595	4.566	4.538	4.509	4.481	4.453	4.426
34	4.399	4.372	4.346	4.320	4.294	4.268	4.243	4.218	4.193	4.169
35	4.145	4.121	4.097	4.074	4.052	4.029	4.006	3.984	3.962	3.941
36	3.919	3.898	3.877	3.857	3.836	3.816	3.797	3.777	3.758	3.739
37	3.720	3.701	3.683	3.665	3.647	3.629	3.612	3.594	3.577	3.561
38	3.544	3.527	3.513	3.497	3.481	3.465	3.449	3.434	3.419	3.404
39	3.389	3.375	3.361	3.347	3.333	3.320	3.306	3.293	3.280	3.268
40	3.255	3.242	3.230	3.218	3.206	3.194	3.183	3.171	3.160	3.149
41	3.138	3.127	3.117	3.106	3.096	3.086	3.076	3.067	3.057	3.048
42	3.038	3.029	3.020	3.012	3.003	2.994	2.986	2.978	2.970	2.962
43	2.954	2.946	2.939	2.932	2.925	2.918	2.911	2.904	2.897	2.891
44	2.884	2.878	2.872	2.866	2.860	2.855	2.849	2.844	2.838	2.833

Θ°	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
45	2.828	2.824	2.819	2.814	2.810	2.805	2.801	2.797	2.793	2.789
46	2.785	2.782	2.778	2.775	2.772	2.769	2.766	2.763	2.760	2.757
47	2.755	2.752	2.750	2.748	2.746	2.744	2.742	2.740	2.738	2.737
48	2.736	2.735	2.733	2.732	2.731	2.730	2.730	2.729	2.729	2.728
49	2.728	2.728	2.728	2.728	2.728	2.728	2.729	2.729	2.730	2.730
50	2.731	2.732	2.733	2.734	2.735	2.737	2.738	2.740	2.741	2.743
51	2.745	2.747	2.749	2.751	2.753	2.755	2.758	2.760	2.763	2.766
52	2.769	2.772	2.775	2.778	2.782	2.785	2.788	2.792	2.795	2.799
53	2.803	2.807	2.811	2.815	2.820	2.824	2.828	2.833	2.838	2.843
54	2.848	2.853	2.858	2.863	2.868	2.874	2.879	2.885	2.890	2.896
55	2.902	2.908	2.914	2.921	2.927	2.933	2.940	2.946	2.953	2.960
56	2.967	2.974	2.981	2.988	2.996	3.004	3.011	3.019	3.026	3.034
57	3.042	3.050	3.059	3.067	3.075	3.084	3.092	3.101	3.110	3.119
58	3.128	3.137	3.147	3.156	3.166	3.175	3.185	3.195	3.205	3.215
59	3.225	3.235	3.246	3.256	3.267	3.278	3.289	3.300	3.311	3.322
60	3.333	3.345	3.356	3.368	3.380	3.392	3.404	3.416	3.429	3.441
61	3.454	3.466	3.479	3.492	3.505	3.518	3.532	3.545	3.559	3.573
62	3.587	3.601	3.615	3.629	3.643	3.658	3.673	3.688	3.703	3.718
63	3.733	3.749	3.764	3.780	3.796	3.812	3.828	3.844	3.861	3.878
64	3.894	3.911	3.928	3.946	3.963	3.980	3.998	4.016	4.034	4.052
65	4.071	4.090	4.108	4.127	4.147	4.166	4.185	4.205	4.225	4.245
66	4.265	4.285	4.306	4.327	4.348	4.369	4.390	4.412	4.434	4.456
67	4.478	4.500	4.523	4.546	4.569	4.592	4.616	4.640	4.664	4.688
68	4.712	4.737	4.762	4.787	4.812	4.838	4.864	4.890	4.916	4.943
69	4.970	4.997	5.024	5.052	5.080	5.109	5.137	5.166	5.195	5.224
70	5.254	5.284	5.315	5.345	5.376	5.408	5.440	5.471	5.504	5.536
71	5.569	5.602	5.636	5.670	5.705	5.740	5.775	5.810	5.846	5.883
72	5.919	5.956	5.994	6.032	6.071	6.109	6.149	6.189	6.229	6.270
73	6.311	6.352	6.394	6.437	6.480	6.524	6.568	6.613	6.658	6.703
74	6.750	6.797	6.844	6.892	6.941	6.991	7.041	7.091	7.142	7.194
75	7.247	7.300	7.354	7.409	7.465	7.521	7.578	7.636	7.694	7.753
76	7.813	7.874	7.936	7.999	8.063	8.128	8.193	8.259	8.327	8.395
77	8.465	8.536	8.607	8.680	8.754	8.829	8.905	8.982	9.061	9.142
78	9.223	9.305	9.389	9.474	9.561	9.649	9.739	9.831	9.924	10.02
79	10.12	10.21	10.31	10.41	10.52	10.62	10.73	10.84	10.95	11.06
80	11.18	11.30	11.42	11.54	11.67	11.80	11.93	12.06	12.20	12.34
81	12.48	12.63	12.78	12.93	13.08	13.24	13.40	13.57	13.74	13.92
82	14.10	14.28	14.47	14.66	14.86	15.07	15.28	15.49	15.71	15.94
83	16.17	16.41	16.66	16.91	17.17	17.44	17.72	18.01	18.31	18.61
84	18.93	19.25	19.59	19.94	20.30	20.68	21.07	21.47	21.89	22.32
85	22.77	23.24	23.73	24.24	24.78	25.34	25.92	26.52	27.16	27.83
86	28.53	29.27	30.04	30.86	31.73	32.64	33.60	34.63	35.72	36.88
87	38.11	39.43	40.84	42.36	44.00	45.76	47.68	49.76	52.02	54.50

From Henry, Lipson, and Wooster [G.15].

APPENDIX 14

ATOMIC WEIGHTS

Based on the assigned relative atomic mass of $^{12}C = 12$.

Element	Symbol	Atomic number	Atomic weight
Actinium	Ac	89	(227)
Aluminium	Al	13	26.9815
Americium	Am	95	(243)
Antimony	Sb	51	121.75
Argon	Ar	18	39.948
Arsenic	As	33	74.9216
Astatine	At	85	(210)
Barium	Ba	56	137.34
Berkelium	Bk	97	(247)
Beryllium	Be	4	9.01218
Bismuth	Bi	83	208.9806
Boron	B	5	10.81
Bromine	Br	35	79.904
Cadmium	Cd	48	112.40
Calcium	Ca	20	40.08
Californium	Cf	98	(248)
Carbon	C	6	12.011
Cerium	Ce	58	140.12
Cesium	Cs	55	132.9055
Chlorine	Cl	17	35.453
Chromium	Cr	24	51.996
Cobalt	Co	27	58.9332
Copper	Cu	29	63.546
Curium	Cm	96	(247)
Dysprosium	Dy	66	162.50
Einsteinium	Es	99	(254)
Erbium	Er	68	167.26
Europium	Eu	63	151.96
Fermium	Fm	100	(253)
Fluorine	F	9	18.9984
Francium	Fr	87	(223)
Gadolinium	Gd	64	157.25
Gallium	Ga	31	69.72
Germanium	Ge	32	72.59
Gold	Au	79	196.9665
Hafnium	Hf	72	178.49
Helium	He	2	4.00260
Holmium	Ho	67	164.9303
Hydrogen	H	1	1.0080
Indium	In	49	114.82
Iodine	I	53	126.9045
Iridium	Ir	77	192.22
Iron	Fe	26	55.847
Krypton	Kr	36	83.80
Lanthanum	La	57	138.9055
Lawrencium	Lr	103	(257)
Lead	Pb	82	207.2
Lithium	Li	3	6.941
Lutetium	Lu	71	174.97
Magnesium	Mg	12	24.305
Manganese	Mn	25	54.9380
Mendelevium	Md	101	(256)
Mercury	Hg	80	200.59
Molybdenum	Mo	42	95.94
Neodymium	Nd	60	144.24
Neon	Ne	10	20.179
Neptunium	Np	93	237.0482
Nickel	Ni	28	58.71
Niobium	Nb	41	92.9064
Nitrogen	N	7	14.0067
Nobelium	No	102	(254)
Osmium	Os	76	190.2
Oxygen	O	8	15.9994
Palladium	Pd	46	106.4
Phosphorus	P	15	30.9738
Platinum	Pt	78	195.09
Plutonium	Pu	94	(242)
Polonium	Po	84	(210)
Potassium	K	19	39.102
Praseodymium	Pr	59	140.9077
Promethium	Pm	61	(147)
Protactinium	Pa	91	231.0359
Radium	Ra	88	226.0254
Radon	Rn	86	(222)
Rhenium	Re	75	186.2
Rhodium	Rh	45	102.9055
Rubidium	Rb	37	85.4678
Ruthenium	Ru	44	101.07
Samarium	Sm	62	150.4
Scandium	Sc	21	44.9559
Selenium	Se	34	78.96
Silicon	Si	14	28.086
Silver	Ag	47	107.868
Sodium	Na	11	22.9898
Strontium	Sr	38	87.62
Sulfur	S	16	32.06
Tantalum	Ta	73	180.9479
Technetium	Tc	43	98.9062
Tellurium	Te	52	127.60
Terbium	Tb	65	158.9254
Thallium	Tl	81	204.37
Thorium	Th	90	232.0381
Thulium	Tm	69	168.9342
Tin	Sn	50	118.69
Titanium	Ti	22	47.90
Tungsten	W	74	183.85
Uranium	U	92	238.029
Vanadium	V	23	50.9414
Xenon	Xe	54	131.30
Ytterbium	Yb	70	173.04
Yttrium	Y	39	88.9059
Zinc	Zn	30	65.37
Zirconium	Zr	40	91.22

Values in parentheses represent the most stable known isotopes.

APPENDIX 15
PHYSICAL CONSTANTS

Charge on electron	e	1.602×10^{-19}	coulomb
Mass of electron	m	9.109×10^{-31}	kg
Mass of neutron		1.675×10^{-27}	kg
Velocity of light	c	2.998×10^{8}	m/sec
Planck's constant	h	6.626×10^{-34}	joule sec
Boltzmann's constant	k	1.381×10^{-23}	joule/deg K
Avogadro's number	N	6.023×10^{26}	per kg mol
Gas constant ($=Nk$)	R	8.314×10^{3}	joules/deg K, kg mol
		1.986×10^{3}	cal/deg K, kg mol

1 cal	=	4.186	joule
1 erg	=	10^{-7}	joule
1 eV	=	1.602×10^{-19}	joule