

Appendix 6

Crystal Structures of Compounds and Solid Solutions

Substance	Type of structure	Lattice parameters (Å)	Spacing of cleavage planes (Å)
NaCl	FCC, B1	$a = 5.639$	2.820
KCl	FCC, B1	$a = 6.290$	
AgBr	FCC, B1	$a = 5.77$	
CaF ₂ (fluorite)	FCC, C1	$a = 5.46$	3.036
CaCO ₃ (calcite)	Rhombohedral, G1	$a = 6.37$ $\alpha = 46.1^\circ$	
SiO ₂ (α-quartz)	Hexagonal, C3	$a = 4.90$ $c = 5.39$	
H ₂ KAl ₂ (SiO ₄) ₃ (mica, muscovite)	Monoclinic	$a = 5.18$ $b = 8.96$ $c = 20.15$ $\beta = 98.6^\circ$	10.08
Fe ₃ C (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 $WK\alpha_1$ 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	$K\beta_1$ weak	K edge	$L\alpha_1$	L_{III} 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	6.733	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	5.0165		
17 Cl	2.62	4.7307	4.7278	4.4034	4.3971		
18 Ar	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	2.293805	2.28970	2.08467	2.07020	21.64	20.7
25 Mn	5.90	2.10378	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	12.288
30 Zn	8.63	1.439000	1.435155	1.29525	1.2834	12.154	12.131

Appendix 7 X-Ray Wavelengths

Element	E(K α) (keV)	K α_1 strong	K α_1 very strong	K β_1 weak	K edge	L α_1	L α_1 edge
31 Ga	9.24	1.24399	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	11.31	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	11.63	0.9841	0.9801	0.8785	0.86552	7.817	7.392
37 Rb	13.38	0.92969	0.92553	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	0.65298	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	5.1146	4.630
44 Ru	19.24	0.647408	0.643083	0.573483	0.56061	4.84575	4.389
45 Rh	20.17	0.617630	0.613279	0.545605	0.53395	4.59743	4.1299
46 Pd	21.12	0.589321	0.585448	0.520520	0.5092	4.36767	3.9074
47 Ag	22.11	0.563798	0.5594075	0.497069	0.48589	4.15443	3.6999
48 Cd	23.11	0.539423	0.535010	0.475105	0.46407	3.95835	3.5047
49 In	24.14	0.516544	0.512113	0.454545	0.44371	3.77192	3.3237
50 Sn	25.20	0.493053	0.490599	0.432326	0.42167	3.59944	3.1557
51 Sb	26.28	0.474827	0.470354	0.417085	0.40668	3.43941	3.0023
52 Te	27.38	0.453784	0.451295	0.399995	0.39074	3.28920	2.8555
53 I	28.51	0.437829	0.433318	0.383905	0.37381	3.14860	2.7196
54 Xe	29.67	0.42037	0.41634	0.36872	0.3584	3.0166	2.5926
55 Cs	30.86	0.404835	0.400390	0.354364	0.34451	2.8924	2.4740
56 Ba	32.07	0.389668	0.385111	0.340811	0.33104	2.77595	2.3629
57 La	33.31	0.374313	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	0.304761	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	0.28190	0.27431	2.2812	1.9191
62 Sm	39.92	0.313698	0.309040	0.27301	0.26464	2.1998	1.8457
63 Eu	41.33	0.303118	0.298445	0.265577	0.25553	2.1209	1.7761
64 Gd	42.77	0.293038	0.288353	0.25460	0.24681	2.0469	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	0.22286	0.21587	1.78425	1.4835
69 Tm	50.42	0.249095	0.244333	0.21556	0.20880	1.7258	1.4334
70 Yb	52.04	0.241424	0.236655	0.20884	0.20214	1.67189	1.3862
71 Lu	53.70	0.234081	0.229298	0.20231	0.19595	1.61951	1.3405
72 Hf	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	0.162675	0.15818	1.31304	1.0723
79 Au	68.20	0.185075	0.180195	0.158982	0.155693	1.27640	1.04000
80 Hg	70.18	0.179958	0.175068	0.154487	0.14918	1.24120	1.0091
81 Tl	72.19	0.175036	0.170136	0.150142	0.14495	1.20739	0.9792
82 Pb	74.25	0.170394	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		1.05713	
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		0.93384	
92 U	97.18	0.130968	0.125947	0.111394	0.10723	0.910639	0.7223

Appendix 7

Some commonly used K wavelengths

Element	K α (weighted average)*	K α_1 strong	K α_1 very strong	K β_1 weak
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 α_1 is given twice the weight of K α_2 .

Characteristic L Lines of Tungsten

Line	Relative Intensity	Wavelength
L α_1	Very Strong	1.47639
L α_2	Weak	1.48743
L β_1	Strong	1.281809
L β_2	Medium	1.24460
L β_3	Weak	1.26269
L γ_1	Weak	1.09855

Appendix 8

Mass Absorption Coefficients μ/ρ (cm^2/gm) and Densities ρ

The mass absorption coefficients are extracted from much longer tables from the *International Tables for X-Ray Crystallography* [G.1]. Although these coefficients are given to four significant digits, 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.1] should be consulted for details.

The densities of elements solid at room temperature, except P, are x-ray densities, rounded off, from [G.1]. Densities of gases are from *Metals Handbook* (Cleveland: American Society for Metals, 1948).

Absorber	Density (gm/cm^3)	Ne		Cu		Co		Cr	
		K α 0.711 Å	K β 0.632 Å	K α 1.542 Å	K β 1.392 Å	K α 1.790 Å	K β 1.621 Å	K α 2.291 Å	K β 2.085 Å
1 H	0.000375×10^{-3}	0.3727	0.3699	0.3912	0.3852	0.3966	0.3926	0.4116	0.4046
2 He	0.1664×10^{-3}	0.2019	0.1972	0.2825	0.2623	0.3288	0.2966	0.4648	0.4001
3 Li	0.533	0.1968	0.1865	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}	0.7893	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}	2.309	1.597	22.13	16.24	34.69	23.72	72.71	54.91
11 Na	0.966	2.939	2.098	30.30	21.23	47.34	35.18	98.48	74.66
12 Mg	1.74	3.979	2.825	40.38	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	6.333	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	191.6
16 S	2.09	9.625	6.535	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 Ar	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	630.6	501.0
24 Cr	7.19	29.25	20.99	252.3	191.1	375.0	288.1	715.7	567.9
25 Mn	7.47	31.86	22.89	272.5	206.7	405.1	311.2	760.8	603.5
26 Fe	7.87	37.74	27.21	304.4	233.6	465.5	365.5	867.7	687.5
27 Co	8.8	41.02	29.51	338.6	256.7	507.1	407.1	947.7	757.5
28 Ni	8.91	47.24	34.16	383.3	282.8	560.5	457.5	1067.7	857.5
29 Cu	8.93	49.24	35.77	415.4	307.4	600.5	487.5	1167.7	937.5
30 Zn	7.13	55.46	40.26	459.5	351.5	660.5	537.5	1267.7	1017.5
31 Ga	5.91	56.90	41.69	473.3	365.5	680.5	557.5	1317.7	1067.5
32 Ge	5.32	60.47	44.26	507.3	399.5	740.5	617.5	1467.7	1167.5
33 As	5.73	65.97	48.57	551.5	443.5	800.5	677.5	1617.7	1267.5
34 Se	4.81	68.82	51.20	585.5	477.5	840.5	717.5	1717.7	1367.5
35 Br	3.12 (liquid)	74.08	55.56	629.5	521.5	900.5	767.5	1867.7	1467.5

Appendix 8 Mass Absorption Coefficients μ/ρ (cm^2/gm) and Densities

Absorber	Density (g/cm^3)	Mo		Cu		Co		Cr	
		K α 0.711 Å	K β 0.632 Å	K α 1.542 Å	K β 1.392 Å	K α 1.790 Å	K β 1.621 Å	K α 2.291 Å	K β 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	85.77	173.5	132.2	339.3	263.4
39 Y	4.48	97.56	72.57	127.1	95.19	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	102.29	158.3	119.7	236.6	181.0	457.4	356.5
43 Tc	11.50	19.78	114.30	167.7	126.9	250.8	191.9	485.5	378.0
44 Ru	12.36	21.23	124.40	180.8	137.0	269.4	206.6	517.9	404.4
45 Rh	12.42	23.05	136.65	194.1	147.1	289.0	221.8	555.2	433.7
46 Pd	12.00	24.42	148.63	205.0	155.6	304.3	234.0	580.9	455.1
47 Ag	10.50	26.38	161.10	218.1	165.8	323.5	248.9	617.4	483.5
48 Cd	8.65	27.73	173.13	229.3	174.0	341.8	262.1	658.8	513.5
49 In	7.29	29.13	185.18	242.1	183.3	362.7	277.3	705.8	548.0
50 Sn	7.29	31.18	202.62	253.3	193.1	374.1	288.7	768.5	596.6
51 Sb	6.69	33.01	221.91	266.5	203.6	391.3	303.1	833.4	658.8
52 Te	6.25	33.92	241.67	273.4	208.4	404.4	311.7	885.2	692.7
53 I	4.95	36.33	263.33	291.7	221.9	434.0	333.2	955.2	755.2
54 Xe	5.495×10^{-3}	38.31	278.86	309.8	235.9	459.0	353.4	1035.2	815.2
55 Cs	1.91 (-10°C)	40.44	293.51	325.4	247.6	483.8	371.5	1125.2	875.2
56 Ba	3.59	42.37	311.00	336.1	256.0	499.0	393.6	1235.2	964.6
57 La	6.17	45.34	333.53	353.5	270.8	519.0	401.9	1355.2	1045.5
58 Ce	6.77	48.56	355.54	378.8	289.6	539.1	431.5	1485.2	1155.5
59 Pr	6.78	50.78	379.09	402.2	305.8	562.6	458.8	1625.2	1265.5
60 Nd	7.00	53.28	398.88	417.9	319.8	581.7	475.9	1775.2	1375.5
61 Pm		55.52	405.52	441.1	336.4	601.4	503.2	1885.2	1485.5
62 Sm	7.54	57.95	424.40	453.5	346.6	611.8	511.8	1995.2	1595.5
63 Eu	5.25	61.18	447.44	473.9	369.0	655.2	546.9	2125.2	1725.5
64 Gd	7.87	62.79	459.55	486.7	377.2	669.5	567.7	2275.2	1875.5
65 Tb	8.27	66.77	488.88	521.9	399.9	678.7	597.1	2385.2	1985.5
66 Dy	8.33	68.89	503.38	536.6	402.2	684.9	607.1	2495.2	2095.5
67 Ho	8.80	72.14	527.76	553.5	417.8	699.8	623.3	2615.2	2215.5
68 Er	9.04	75.61	550.07	581.3	434.3	719.7	643.3	2745.2	2345.5
69 Tm	9.33	78.98	574.94	602.2	451.5	739.7	663.3	2885.2	2485.5
70 Yb	6.97	80.23	592.22	624.7	468.9	759.7	683.3	3025.2	2625.5
71 Lu	9.84	84.18	624.04	652.0	491.5	784.9	713.3	3185.2	2785.5
72 Hf	13.28	86.33	641.55	677.7	512.0	809.9	738.3	3355.2	2955.5
73 Ta	16.67	89.51	660.07	703.5	533.5	834.9	763.3	3535.2	3135.5
74 W	19.25	95.76	705.57	751.5	573.5	884.9	813.3	3815.2	3415.5
75 Re	21.02	98.74	724.47	778.3	594.5	909.9	838.3	4005.2	3605.5
76 Os	22.58	100.2	741.3	803.8	615.5	934.9	858.3	4205.2	3805.5
77 Ir	22.55	103.4	772.09	838.3	646.5	964.9	888.3	4415.2	4015.5
78 Pt	21.44	108.6	802.33	868.3	677.5	994.9	918.3	4635.2	4235.5
79 Au	19.28	111.3	823.33	893.8	702.5	1019.9	943.3	4865.2	4465.5
80 Hg	13.55	114.7	853.30	928.3	733.5	1049.9	973.3	5105.2	4705.5
81 Tl	11.87	119.4	882.25	953.3	758.5	1074.9	998.3	5355.2	4955.5
82 Pb	11.24	122.0	905.25	978.3	783.5	1104.9	1023.3	5615.2	5215.5
83 Bi	9.80	125.9	930.50	1003.3	808.5	1134.9	1053.3	5885.2	5485.5
84 Po		117.2	1007.7	1033.3	833.5	1164.9	1083.3	6165.2	5765.5
90 Th	11.72	99.46	733.34	808.8	615.5	1019.9	943.3	3465.2	2715.5
92 U	19.05	96.57	723.33	805.7	612.5	1014.9	938.3	3415.2	2665.5
94 Pu	19.81	48.84	78.99	352.9	271.2	519.6	401.6	1003.2	771.6