Crystallographic Data For Minerals

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With the advent of modern X–ray diffraction instruments and the improving availability of neutron diffraction instrument time, there has been a substantial improvement in the number and quality of structural characterizations of minerals. Also, the past 25 years has seen great advances in high pressure mineral synthesis technology so that many new high pressure silicate and oxide phases of potential geophysical significance have been synthesized in crystals of sufficient size for complete structural characterization by X–ray methods. The object of this work is to compile and present a summary of these data on a selected group of the more abundant, rock–forming minerals in an internally consistent format for use in geophysical and geochemical studies.

Using mostly primary references on crystal structure determinations of these minerals, we have compiled basic crystallographic property information for some 300 minerals. These data are presented in Table 1. The minerals were selected to represent the most abundant minerals composing the crust of the Earth as well as high pressure synthetic phases that are believed to compose the bulk of the solid Earth. The data include mineral name, ideal formula, ideal formula weight, crystal system, space group, structure type, Z (number of formula units per cell), unit cell edges, a, b, and c in Ångstrom units (10^{-10} m) and inter–axial angles α, β, γ in degrees, unit cell volume in Å^3, molar volume in cm^3, calculated density in Mg/m^3, and a reference to the complete crystal structure data.

To facilitate geochemical and geophysical modeling, data for pure synthetic end members are presented when available. Otherwise, data are for near end–member natural samples. For many minerals, structure data (or samples) for pure end members are not available, and in these cases, indicated by an asterisk after the mineral name, data for an impure, natural sample are presented together with an approximate ideal formula and formula weight and density calculated from the ideal formula.

In order to conserve space we have omitted the precision given by the original workers in the unit cell parameter determination. However, we have quoted the data such that the stated precision is less than 5 in the last decimal place given. The cell volumes, molar volumes and densities are calculated by us given so that the precision in the last given place is less than 5. The formula weights presented are calculated by us and given to one part in approximately 20,000 for pure phases and one part in 1000 for impure natural samples.

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Table 1. Crystallographic Properties of Minerals.

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Single Oxides																
Hemi–oxide																
Cuprite	Cu_2O	143.079	Cub.	$Pn\bar{3}m$	Cuprite	2	4.2696						77.833	23.439	6.104	25
Monoxides Group																
Periclase	MgO	40.312	Cub.	$Fm\bar{3}m$	Halite	4	4.211						74.67	11.244	3.585	93
Wustite	FeO	71.848	Cub.	$Fm\bar{3}m$	Halite	4	4.3108						80.11	12.062	5.956	67
Lime	CaO	56.079	Cub.	$Fm\bar{3}m$	Halite	4	4.1684						111.32	16.762.	3.346	235
Bunsenite	NiO	74.709	Cub.	$Fm\bar{3}m$	Halite	4	4.446						72.43	10.906	6.850	235
Manganosite	MnO	70.937	Cub.	$Fm\bar{3}m$	Halite	4	4.8105						87.88	13.223	5.365	195
Tenorite	CuO	79.539	Mono.	$C2/c$	Tenorite	4	4.6837	3.4226	5.1288		99.54		81.080	12.209	6.515	11
Montroydite	HgO	216.589	Orth.	$Pnma$	Montroydite	4	6.612	5.20	3.531				128.51	19.350	11.193	12
Zincite	ZnO	81.369	Hex.	$P6_3mc$	Wurtzite	2	3.2427		5.1948				47.306	14.246	5.712	189
Bromellite	BeO	25.012	Hex.	$P6_3mc$	Wurtzite	2	2.6984		4.2770				26.970	8.122	3.080	189
Sesquioxide Group																
Corundum	Al_2O_3	101.961	Trig.	$R\bar{3}c$	Corundum	6	4.7589		12.9912				254.80	25.577	3.986	157
Hematite	Fe_2O_3	159.692	Trig.	$R\bar{3}c$	Corundum	6	5.038		13.772				302.72	30.388	5.255	23
Eskolaite	Cr_2O_3	151.990	Trig.	$R\bar{3}c$	Corundum	6	4.9607		13.599				289.92	29.093	5.224	157
Karelianite	V_2O_3	149.882	Trig.	$R\bar{3}c$	Corundum	6	4.952		14.002				297.36	29.850	5.021	157
Bixbyite	Mn_2O_3	157.905	Cub.	$Ia\bar{3}$	Bixbyite	16	9.4146						834.46	31.412	5.027	75
Avicennite	Tl_2O_3	456.738	Cub.	$Ia\bar{3}$	Bixbyite	16	10.543						1171.9	44.115	10.353	167
Claudetite	As_2O_3	197.841	Mono.	$P2_1/n$	Claudetite	4	7.99	4.65	9.12		78.3		331.8	49.961	3.960	176
Arsenolite	As_2O_3	197.841	Cub.	$Fd\bar{3}m$	Arsenolite	16	11.0744						1358.19	51.127	3.870	177
Senarmontite	Sb_2O_3	291.498	Cub.	$Fd\bar{3}m$	Arsenolite	16	11.1519						1386.9	52.208	5.583	217
Valentinite	Sb_2O_3	291.498	Orth.	$Pccn$	Valentinite	4	4.911	12.464	5.412				331.27	49.881	5.844	216
Dioxide Group																
Brookite	TiO_2	79.890	Orth.	$Pbca$	Brookite	8	9.184	5.447	5.145				257.38	19.377	4.123	17
Anatase	TiO_2	79.890	Tetr.	$I4_1/amd$	Anatase	4	3.7842		9.5146				136.25	20.156	3.895	105
Rutile	TiO_2	79.890	Tetr.	$P4_2/mnm$	Rutile	2	4.5845		2.9533				62.07	18.693	4.2743	204
Cassiterite	SnO_2	150.69	Tetr.	$P4_2/mnm$	Rutile	2	4.737		3.185				71.47	21.523	7.001	15
Stishovite	SiO_2	60.086	Tetr.	$P4_2/mnm$	Rutile	2	4.1790		2.6651				46.54	14.017	4.287	20
Pyrolusite	MnO_2	86.94	Tetr.	$P4_2/mnm$	Rutile	2	4.396		2.871				55.48	86.937	5.203	121
Baddeleyite	ZrO_2	123.22	Mono.	$P2_1/c$	Baddeleyite	4	5.1454	5.2075	5.3107		99.23		140.45	21.149	5.826	208
Uraninite	UO_2	270.03	Cub.	$Fm\bar{3}m$	Fluorite	4	5.4682						163.51	24.620	10.968	126
Thorianite	ThO_2	264.04	Cub.	$Fm\bar{3}m$	Fluorite	4	5.5997						175.59	26.439	9.987	227
Multiple Oxides																
Chrysoberyl	$BeAl_2O_4$	126.97	Orth.	$Pnmb$	Olivine	4	4.424	9.396	5.471				227.42	34.244	3.708	96
Spinel Group																
Spinel	$MgAl_2O_4$	142.27	Cub.	$Fd\bar{3}m$	Spinel	8	8.0832						528.14	39.762	3.578	61
Hercynite	$FeAl_2O_4$	173.81	Cub.	$Fd\bar{3}m$	Spinel	8	8.1558						542.50	40.843	4.256	99
Magnesioferrite	$MgFe_2O_4$	200.00	Cub.	$Fd\bar{3}m$	Spinel	8	8.360						584.28	43.989	4.547	100
Magnesiochromite	$MgCr_2O_4$	192.30	Cub.	$Fd\bar{3}m$	Spinel	8	8.333						578.63	43.564	4.414	100
Magnetite	$FeFe_2O_4$	231.54	Cub.	$Fd\bar{3}m$	Spinel	8	8.394						591.43	44.528	5.200	100
Jacobsite	$MnFe_2O_4$	230.63	Cub.	$Fd\bar{3}m$	Spinel	8	8.5110						616.51	46.416	4.969	100
Chromite	$FeCr_2O_4$	223.84	Cub.	$Fd\bar{3}m$	Spinel	8	8.3794						588.31	44.293	5.054	100
Ulvoespinel	$TiFe_2O_4$	223.59	Cub.	$Fd\bar{3}m$	Spinel	8	8.536						621.96	46.826	4.775	106

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Titanate Group																
Ilmenite	$FeTiO_3$	151.75	Trig.	$R\bar{3}$	Ilmenite	6	5.0884		14.0855				315.84	31.705	4.786	229
Pyrophanite	$MnTiO_3$	150.84	Trig.	$R\bar{3}$	Ilmenite	6	5.137		14.283				326.41	32.766	4.603	235
Perovskite	$CaTiO_3$	135.98	Orth.	*Pbnm*	Perovskite	4	5.3670	5.4439	7.6438				223.33	33.63	4.044	113
Armalcolite	$Mg_{.5}Fe_{.5}Ti_2O_5$	215.88	Orth.	*Bbmm*	Pseudobrookite	4	9.7762	10.0214	3.7485				367.25	55.298	3.904	230
Pseudobrookite	Fe_2TiO_5	239.59	Orth.	*Bbmm*	Pseudobrookite	4	9.767	9.947	3.717				361.12	54.375	4.406	3
Tungstates and Molybdates																
Ferberite	$FeWO_4$	303.70	Mono.	*P2/c*	Ferberite	2	4.730	5.703	4.952		90.0		133.58	40.228	7.549	225
Huebnerite	$MnWO_4$	302.79	Mono.	*P2/c*	Ferberite	2	4.8238	5.7504	4.9901		91.18		138.39	41.676	7.265	231
Scheelite	$CaWO_4$	287.93	Tetr.	$I4_1/a$	Scheelite	4	5.243		11.376				312.72	47.087	6.115	114
Powellite	$CaMoO_4$	200.02	Tetr.	$I4_1/a$	Scheelite	4	5.23		11.44				301.07	45.333	4.412	101
Stolzite	$PbWO_4$	455.04	Tetr.	$I4_1/a$	Scheelite	4	5.46		12.05				359.23	54.091	8.412	101
Wulfenite	$PbMoO_4$	367.12	Tetr.	$I4_1/a$	Scheelite	4	5.435		12.11				357.72	53.864	6.816	101
Hydroxides																
Gibbsite	$Al(OH)_3$	78.00	Mono.	$P2_1/n$	Gibbsite	8	8.684	5.078	9.736		94.54		427.98	32.222	2.421	188
Diaspore	AlO(OH)	59.99	Orth.	*Pbnm*	Goethite	4	4.401	9.421	2.845				117.96	17.862	3.377	34
Boehmite	AlO(OH)	59.99	Orth.	*Amam*	Boehmite	4	3.693	12.221	2.865				129.30	19.507	3.075	98
Brucite	$Mg(OH)_2$	58.33	Trig.	$P\bar{3}m1$	Brucite	1	3.124		4.766				40.75	24.524	2.377	243
Goethite	FeO(OH)	88.85	Orth.	*Pbnm*	Goethite	4	4.587	9.937	3.015				137.43	20.693	4.294	65
Lepidochrosite	FeO(OH)	88.85	Orth.	$Cmc2_1$	Boehmite	4	3.08	12.50	3.87				148.99	22.435	3.961	43
Carbonates																
Magnesite	$MgCO_3$	84.32	Trig.	$R\bar{3}c$	Calcite	6	4.6328		15.0129				279.05	28.012	3.010	54
Smithsonite	$ZnCO_3$	125.38	Trig.	$R\bar{3}c$	Calcite	6	4.6526		15.0257				281.68	28.276	4.434	54
Siderite	$FeCO_3$	115.86	Trig.	$R\bar{3}c$	Calcite	6	4.6916		15.3796				293.17	29.429	3.937	54
Rhodochrosite	$MnCO_3$	114.95	Trig.	$R\bar{3}c$	Calcite	6	4.7682		15.6354				307.86	30.904	3.720	54
Otavite	$CdCO_3$	172.41	Trig.	$R\bar{3}c$	Calcite	6	4.923		16.287				341.85	34.316	5.024	26
Calcite	$CaCO_3$	100.09	Trig.	$R\bar{3}c$	Calcite	6	4.9896		17.0610				367.85	36.9257	2.7106	54
Vaterite	$CaCO_3$	100.09	Hex.	$P6_3/mmc$	Vaterite	12	7.151		16.937				750.07	37.647	2.659	146
Dolomite	$CaMg(CO_3)_2$	184.41	Trig.	$R\bar{3}$	Dolomite	3	4.8069		16.0034				320.24	64.293	2.868	182
Ankerite	$CaFe(CO_3)_2$	215.95	Trig.	$R\bar{3}$	Dolomite	3	4.830		16.167				326.63	65.576	3.293	21
Aragonite	$CaCO_3$	100.09	Orth.	*Pmcn*	Aragonite	4	4.9614	7.9671	5.7404				226.91	34.166	2.930	51
Strontianite	$SrCO_3$	147.63	Orth.	*Pmcn*	Aragonite	4	5.090	8.358	5.997				255.13	38.416	3.843	51
Cerussite	$PbCO_3$	267.20	Orth.	*Pmcn*	Aragonite	4	5.180	8.492	6.134				269.83	40.629	6.577	191
Witherite	$BaCO_3$	197.39	Orth.	*Pmcn*	Aragonite	4	5.3126	8.8958	6.4284				303.81	45.745	4.314	51
Azurite	$Cu_3(OH)_2(CO_3)_2$	344.65	Mono.	$P2_1/c$	Azurite	2	5.0109	5.8485	10.345		92.43		302.90	91.219	3.778	245
Malachite	$Cu_2(OH)_2CO_3$	221.10	Mono.	$P2_1/a$	Malachite	4	9.502	11.974	3.240		98.75		364.35	54.862	4.030	244
Nitrates																
Soda Niter	$NaNO_3$	85.00	Trig.	$R\bar{3}c$	Calcite	6	5.0708		16.818				374.51	37.594	2.261	198
Niter	KNO_3	101.11	Orth.	*Pmcn*	Aragonite	4	5.4119	9.1567	6.5189				323.05	48.643	2.079	159
Borates																
Borax	$Na_2B_4O_5(OH)_4.8H_2O$	381.37	Mono.	*C2/c*	Borax		11.885	10.654	12.206		106.62		1480.97	223.00	1.710	128

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Kernite	$Na_2B_4O_6(OH)_2.3H_2O$	273.28	Mono.	$P2_1/c$	Kernite	4	7.0172	9.1582	15.6774		108.86		953.41	143.560	1.904	48
Colemanite	$CaB_3O_4(OH)_3.H_2O$	205.55	Mono.	$P2_1/a$	Colemanite	4	8.743	11.264	6.102		110.12		564.30	84.869	2.419	42
Sulfates																
Barite	$BaSO_4$	233.40	Orth.	$Pbnm$	Barite	4	7.157	8.884	5.457				346.97	52.245	4.467	147
Celestite	$SrSO_4$	183.68	Orth.	$Pbnm$	Barite	4	6.870	8.371	5.355				307.96	46.371	3.961	147
Anglesite	$PbSO_4$	303.25	Orth.	$Pbnm$	Barite	4	6.959	8.482	5.398				318.62	47.977	6.321	147
Anhydrite	$CaSO_4$	136.14	Orth.	$Amma$	Anhydrite	4	7.006	6.998	6.245				306.18	46.103	2.953	118
Gypsum	$CaSO_42H_2O$	172.17	Mono.	$I2/a$	Gypsum	4	5.670	15.201	6.533		118.60		494.37	74.440	2.313	46
Alunite*	$KAl_3(SO_4)_2(OH)_6$	414.21	Trig.	$R\bar{3}m$	Alunite	3	7.020		17.223				735.04	147.572	2.807	145
Jarosite*	$KFe_3(SO_4)_2(OH)_6$	500.81	Trig.	$R\bar{3}m$	Alunite	3	7.304		17.268				797.80	160.172	3.127	112
Antlerite	$Cu_3(SO_4)(OH)_4$	354.71	Orth.	$Pnma$	Antlerite	4	8.244	6.043	11.987				597.19	89.920	2.959	91
Thenardite	Na_2SO_4	142.04	Orth.	$Fddd$	Thenardite	8	9.829	12.302	5.868				709.54	53.419	2.659	90
Arcanite	K_2SO_4	174.27	Orth.	$Pmcn$	Arcanite	4	5.763	10.071	7.476				433.90	65.335	2.667	142
Epsomite	$MgSO_47H_2O$	246.48	Orth.	$P2_12_12_1$	Epsomite	4	11.846	12.002	6.859				975.18	146.838	1.678	36
Phosphates																
Hydroxyapatite	$Ca_5(PO_4)_3OH$	502.32	Hex.	$P6_3/m$	Apatite	2	9.424		6.879				529.09	159.334	3.153	214
Fluorapatite	$Ca_5(PO_4)_3F$	504.31	Hex.	$P6_3/m$	Apatite	2	9.367		6.884				523.09	157.527	3.201	215
Chlorapatite	$Ca_5(PO_4)_3Cl$	520.77	Hex.	$P6_3/m$	Apatite	2	9.628		6.764				543.01	163.527	3.185	137
Monazite	$CePO_4$	235.09	Mono.	$P2_1/n$	Monazite	4	6.77	7.04	6.46		104.0		298.7	44.98	5.23	76
Xenotime	YPO_4	183.88	Tetr.	$I4_1/amd$	Zircon	4	6.878		6.036				285.54	43.00	4.277	123
Whitlockite	$MgFeCa_{18}H_2(PO_4)_{14}$	2133.	Trig.	$R3c$	Whitlockite	3	10.330		37.103				3428.8	688.386	3.099	38
Triphylite	$LiFePO_4$	157.76	Orth.	$Pmnb$	Olivine	4	10.334	6.010	4.693				291.47	43.888	3.595	237
Lithiophyllite	$LiMnPO_4$	156.85	Orth.	$Pmnb$	Olivine	4	6.05	10.32	4.71				294.07	44.280	3.542	101
Amblygonite*	$LiAl(F,OH)PO_4$	146.9	Tric.	$P\bar{1}$	Amblygonite	2	5.18	7.15	5.04	112.11	97.78	67.88	160.20	48.242	3.045	16
Augelite*	$Al_2(OH)_3PO_4$	199.9	Mono.	$C2/m$	Augelite	4	13.124	7.988	5.066		112.42		490.95	73.924	2.705	101
Berlinite	$AlPO_4$	121.95	Trig.	$P3_121$	Quartz	3	4.943		10.974				232.21	46.620	2.616	206
Orthosilicates																
Garnet Group																
Pyrope	$Mg_3Al_2Si_3O_{12}$	403.15	Cub.	$Ia\bar{3}d$	Garnet	8	11.452						1501.9	113.08	3.565	8
Almandine	$Fe_3Al_2Si_3O_{12}$	497.76	Cub.	$Ia\bar{3}d$	Garnet	8	11.531						1533.2	115.43	4.312	8
Spessartine	$Mn_3Al_2Si_3O_{12}$	495.03	Cub.	$Ia\bar{3}d$	Garnet	8	11.612						1565.7	117.88	4.199	161
Grossular	$Ca_3Al_2Si_3O_{12}$	403.15	Cub.	$Ia\bar{3}d$	Garnet	8	11.845						1661.9	125.12	3.600	161
Andradite	$Ca_3Fe_2Si_3O_{12}$	508.19	Cub.	$Ia\bar{3}d$	Garnet	8	12.058						1753.2	131.99	3.850	161
Uvarovite	$Ca_3Cr_2Si_3O_{12}$	500.48	Cub.	$Ia\bar{3}d$	Garnet	8	11.988						1722.8	129.71	3.859	161
Olivine Group																
Forsterite	Mg_2SiO_4	140.70	Orth.	$Pbnm$	Olivine	4	4.7534	10.1902	5.9783				289.58	43.603	3.227	69
Fayalite	Fe_2SiO_4	203.77	Orth.	$Pbnm$	Olivine	4	4.8195	10.4788	6.0873				307.42	46.290	4.402	69
Tephroite	Mn_2SiO_4	201.96	Orth.	$Pbnm$	Olivine	4	4.9023	10.5964	6.2567				325.02	48.939	4.127	69
Liebenbergite	Ni_2SiO_4	209.50	Orth.	$Pbnm$	Olivine	4	4.726	10.118	5.913				282.75	42.574	4.921	124
Ca–olivine	Ca_2SiO_4	172.24	Orth.	$Pbnm$	Olivine	4	5.078	11.225	6.760				385.32	58.020	2.969	50
Co–olivine	Co_2SiO_4	209.95	Orth.	$Pbnm$	Olivine	4	4.7811	10.2998	6.0004				295.49	44.493	4.719	32
Monticellite	$CaMgSiO_4$	156.48	Orth.	$Pbnm$	Olivine	4	4.822	11.108	6.382				341.84	51.472	3.040	165
Kirschsteinite	$CaFeSiO_4$	188.01	Orth.	$Pbnm$	Olivine	4	4.844	10.577	6.146				314.89	47.415	3.965	32

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Zircon Group																
Zircon	$ZrSiO_4$	183.30	Tetr.	$I4_1/amd$	Zircon	4	6.6042		5.9796				260.80	39.270	4.668	95
Hafnon	$HfSiO_4$	270.57	Tetr.	$I4_1/amd$	Zircon	4	6.5725		5.9632				257.60	38.787	6.976	212
Thorite*	$ThSiO_4$	324.1	Tetr.	$I4_1/amd$	Zircon	4	7.1328		6.3188				321.48	48.407	6.696	222
Coffinite*	$USiO_4$	330.2	Tetr.	$I4_1/amd$	Zircon	4	6.995		6.236				305.13	45.945	7.185	115
Willemite Group																
Phenacite	Be_2SiO_4	110.10	Trig.	$R\bar{3}$	Willemite	18	12.472		8.252				1111.6	37.197	2.960	241
Willemite	Zn_2SiO_4	222.82	Trig.	$R\bar{3}$	Willemite	18	13.971		9.334				1577.8	52.795	4.221	207
Eucryptite	$LiAlSIO_4$	126.00	Trig.	$R\bar{3}$	Willemite	18	13.473		9.001				1415.0	47.347	2.661	97
Aluminosilicate Group																
Andalusite	Al_2SiO_5	162.05	Orth.	*Pnnm*	Andalusite	4	7.7980	7.9031	5.5566				342.44	51.564	3.1426	233
Sillimanite	Al_2SiO_5	162.05	Orth.	*Pbnm*	Sillimanite	4	7.4883	7.6808	5.7774				332.29	50.035	3.2386	233
Kyanite	Al_2SiO_5	162.05	Tric.	$P\bar{1}$	Kyanite	4	7.1262	7.8520	5.5747	89.99	101.11	106.03	293.72	44.227	3.6640	233
Topaz	$Al_2SiO_4(OH,F)_2$	182.0	Orth.	*Pbnm*	Topaz	4	4.6651	8.8381	8.3984				346.27	52.140	3.492	242
Humite Group																
Norbergite*	$Mg_3SiO_4F_2$	203.0	Orth.	*Pbnm*	Norbergite	4	4.7104	10.2718	8.7476				423.25	63.73	3.186	73
Chondrodite*	$Mg_5(SiO_4)_2F_2$	343.7	Mono.	$P2_1/b$	Chondrodite	2	4.7284	10.2539	7.8404		109.06		359.30	108.20	3.158	74
Humite*	$Mg_7(SiO_4)_3F_2$	484.4	Orth.	*Pbnm*	Humite	4	4.7408	10.2580	20.8526				1014.09	152.70	3.159	183
Clinohumite*	$Mg_9(SiO_4)_4F_2$	624.1	Mono.	$P2_1/b$	Clinohumite	2	4.7441	10.2501	13.6635		100.786		652.68	196.55	3.259	186
Staurolite*	$Fe_4Al_{18}Si_8O_{46}(OH)_2$	1704.	Mono.	$C2/m$	Staurolite	1	7.8713	16.6204	5.6560		90.0		739.94	445.67	3.823	209
Other Orthosilicates																
Titanite	$CaTiSiO_5$	196.06	Mono.	$P2_1/a$	Titanite	4	7.069	8.722	6.566				370.23	55.748	3.517	213
Datolite	$CaBSiO_4(OH)$	159.94	Mono.	$P2_1/c$	Datolite	4	4.832	7.608	9.636		90.40		354.23	53.338	2.999	63
Gadolinite*	$RE_2FeB_2Si_2O_{10}$	604.5	Mono	$P2_1/a$	Datolite	2	10.000	7.565	4.786		90.31		360.69	108.62	5.565	148
Chloritoid*	$FeAl_2SiO_5(OH)_2$	251.9	Tric.	$P\bar{1}$	Chloritoid	4	9.46	5.50	9.15	97.05	101.56	90.10	462.72	69.674	3.616	88
Sapphirine*	$Mg_{3.5}Al_9Si_{1.5}O_{20}$	690.0	Mono.	$P2_1/a$	Sapphirine	4	11.266	14.401	9.929		125.46		1312.11	197.57	3.493	149
Prehnite*	$Ca_2Al(Al,Si_3)O_{10}(OH)_2$	412.391	Orth.	*Pncm*	Prehnite	2	4.646	5.483	18.486				470.91	141.82	2.908	170
Pumpelleyite	$Ca_8(Mg_2FeAl)Al_8Si_{12}O_{42}(OH)_{14}$	1915.1	Mono.	$C2/m$	Pumpelleyite	1	8.831	5.894	19.10		97.53		985.6	593.6	3.226	172
Axinite	$HFeCa_2Al_2BSi_4O_{16}$	570.12	Tric.	$P\bar{1}$	Axinite	2	7.157	9.199	8.959	91.8	98.14	77.30	569.61	171.54	3.324	220
Sorosilicates & Cyclosilicates																
Epidote Group																
Zoisite	$Ca_2Al_3Si_3O_{12}(OH)$	454.36	Orth.	*Pnma*	Zoisite	4	16.212	5.559	10.036				904.47	136.19	3.336	52
Clinozoisite	$Ca_2Al_3Si_3O_{12}(OH)$	454.36	Mono.	$P2_1/m$	Epidote	2	8.879	5.583	10.155		115.50		454.36	136.83	3.321	52
Hancockite*	$Ca(Pb,Sr)FeAl_2Si_3O_{12}(OH)$	590.6	Mono.	$P2_1/m$	Epidote	2	8.96	5.67	10.30		114.4		476.5	143.5	4.12	53
Allanite*	$CaRE(Al,Fe)_3Si_3O_{12}(OH)$	565.2	Mono.	$P2_1/m$	Epidote	2	8.927	5.761	10.150		114.77		473.97	142.74	3.96	53
Epidote*	$Ca_2FeAl_2Si_3O_{12}(OH)$	454.4	Mono.	$P2_1/m$	Epidote	2	8.8877	5.6275	10.1517		115.383		458.73	138.15	3.465	70
Melilite Group																
Melilite*	$CaNaAlSi_2O_7$	258.2	Tetr.	$P\bar{4}2_1m$	Melilite	2	7.6344		5.0513				294.41	88.662	2.912	134
Gehlenite*	$Ca_2AlAlSiO_7$	274.2	Tetr.	$P\bar{4}2_1m$	Melilite	2	7.7173		5.0860				302.91	91.220	3.006	135
Akermanite	$Ca_2MgSi_2O_7$	272.64	Tetr.	$P\bar{4}2_1m$	Melilite	2	7.835		5.010				307.55	92.619	2.944	116
Other Sorosilicates and Cyclosilictaes																
Lawsonite	$CaAl_2Si_2O_7(OH)_2H_2O$	314.24	Orth.	*Ccmm*	Lawsonite	4	8.795	5.847	13.142				675.82	101.76	3.088	19
Beryl	$Be_3Al_2Si_6O_{18}$	537.51	Hex.	P6/mmc	Beryl	2	9.2086		9.1900				674.89	203.24	2.645	152
Cordierite*	$Mg_2Al_4Si_5O_{18}$	584.97	Orth.	*Ccmm*	Beryl	4	17.079	9.730	9.356				1554.77	234.11	2.499	45

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Tourmaline*	$NaFe_3Al_6B_3Si_6O_{27}(OH)_4$	1043.3	Trig.	*R3m*	Tourmaline	3	15.992		7.190				1592.5	319.7	3.263	66
Vesuvianite*	$Ca_{19}Fe_2MgAl_{10}Si_{18}O_{70}(OH,F)_8$	2935.	Tetr.	P4/nnc	Vesuvianite	2	15.533		11.778				2841.8	427.9	3.429	6
Chain Silicates																
Enstatite/Ferrosilite Group																
Enstatite	$Mg_2Si_2O_6$	200.79	Orth.	*Pbca*	Orthopyroxene	8	18.227	8.819	5.179				832.49	62.676	3.204	197
Ferrosilite	$Fe_2Si_2O_6$	263.86	Orth.	*Pbca*	Orthopyroxene	8	18.427	9.076	5.237				875.85	65.941	4.002	197
Clinoenstatite	$Mg_2Si_2O_6$	200.79	Mono.	$P2_1/c$	Clinoenstatite	4	9.626	8.825	5.188		108.33		418.36	62.994	3.188	150
Clinoferrosilite	$Fe_2Si_2O_6$	263.86	Mono.	$P2_1/c$	Clinoenstatite	4	9.7085	9.0872	5.2284		108.43		437.60	65.892	4.005	33
Clinopyroxene Group																
Diopside	$CaMgSi_2O_6$	216.56	Mono.	*C2/c*	Clinopyroxene	4	9.746	8.899	5.251		105.63		438.58	66.039	3.279	39
Hedenbergite	$CaFeSi_2O_6$	248.10	Mono.	*C2/c*	Clinopyroxene	4	9.845	9.024	5.245		104.70		450.72	67.867	3.656	39
Jadeite	$NaAlSi_2O_6$	202.14	Mono.	*C2/c*	Clinopyroxene	4	9.423	8.564	5.223		107.56		401.85	60.508	3.341	39
Acmite	$NaFeSi_2O_6$	231.08	Mono.	*C2/c*	Clinopyroxene	4	9.658	8.795	5.294		107.42		429.06	64.606	3.576	44
Cosmochlor	$NaCrSi_2O_6$	227.15	Mono.	*C2/c*	Clinopyroxene	4	9.579	8.722	5.267		107.37		419.98	63.239	3.592	39
Spodumene	$LiAlSi_2O_6$	186.09	Mono.	*C2/c*	Clinopyroxene	4	9.461	8.395	5.218		110.09		389.15	58.596	3.176	39
Ca–Tschermaks	$CaAlAlSiO_6$	218.20	Mono.	*C2/c*	Clinopyroxene	4	9.609	8.652	5.274		106.06		421.35	63.445	3.438	164
Pyroxenoid Group																
Wollastonite	$Ca_3Si_3O_9$	348.49	Tric.	$C\bar{1}$	Wollastonite	4	10.104	11.054	7.305	99.53	100.56	83.44	788.04	118.66	2.937	163
Bustamite*	$(Ca_{2.4}Fe_{.6})Si_3O_9$	358.6	Tric.	$I\bar{1}$	Bustamite	4	9.994	10.946	7.231	99.30	100.56	83.29	764.30	115.09	3.116	163
Rhodonite	$Mn_5Si_5O_{15}$	655.11	Tric.	$P\bar{1}$	Rhodonite	2	7.616	11.851	6.707	92.55	94.35	105.67	579.84	174.62	3.752	155
Pyroxmangite	$Mn_7Si_7O_{21}$	917.16	Tric.	$P\bar{1}$	Pyroxmangite	2	6.721	7.603	17.455	113.18	82.27	94.13	812.31	244.63	3.749	155
Aenigmatite*	$Na_2Fe_5TiSi_6O_{20}$	867.5	Tric.	$P\bar{1}$	Aenigmatite	2	10.406	10.813	8.926	104.93	96.87	125.32	744.52	224.21	3.869	40
Pectolite*	$HNaCa_2Si_3O_9$	332.4	Tric.	$P\bar{1}$	Pectolite	2	7.980	7.023	7.018	90.54	95.14	102.55	382.20	115.10	2.888	163
Petalite	$LiAlSi_4O_{10}$	306.26	Mono.	P2/a	Petalite	2	11.737	5.171	7.630		112.54		427.71	128.80	2.378	219
Amphibole Group																
Gedrite*	$Na_{.5}(Mg_5Fe_2)Al_2Si_6O_{22}(OH)_2$	853.23	Orth.	*Pnma*	Orthoamphibole	4	18.531	17.741	5.249				1725.65	259.8	3.184	169
Anthophyllite*	$(Mg_5Fe_2)Si_8O_{22}(OH)_2$	843.94	Orth.	*Pnma*	Orthoamphibole	4	18.560	18.013	5.2818				1765.8	265.9	3.111	58
Cummingtonite*	$(Mg_5Fe_2)Si_8O_{22}(OH)_2$	843.94	Mono.	*C2/m*	Amphibole	2	9.51	18.19	5.33		101.92		902.14	271.7	3.14	60
Tremolite*	$Na_{.5}Ca_2Mg_5Si_8O_{22}(OH)_2$	823.90	Mono	*C2/m*	Amphibole	2	9.863	18.048	5.285		104.79		909.60	273.9	3.01	92
Pargasite*	$NaCa_2FeMg_4Al_2Si_6O_{22}(OH)_2$	864.72	Mono.	*C2/m*	Amphibole	2	9.910	18.022	5.312		105.78		912.96	274.9	3.165	185
Glaucophane*	$Na_2(FeMg_3Al)Si_8O_{22}(OH)_2$	789.44	Mono.	*C2/m*	Amphibole	2	9.541	17.740	5.295		103.67		870.8	262.2	3.135	168
Sheet Silictaes																
Talc and Pyrophyllite																
Talc	$Mg_3Si_4O_{10}(OH)_2$	379.65	Tric.	$C\bar{1}$	Talc	2	5.290	9.173	9.460	90.46	98.68	90.09	453.77	136.654	2.776	175
Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$	360.31	Tric.	$C\bar{1}$	Talc	2	5.160	8.966	9.347	91.18	100.46	89.64	425.16	128.036	2.814	125
Trioctahedral Mica Group																
Annite*	$KFe_3(AlSi_3)O_{10}(OH)_2$	511.9	Mono.	*C2/m*	1M	2	5.386	9.324	10.268		100.63		506.82	152.63	3.215	94
Phlogopite*	$KMg_3AlSi_3O_{10}(OH)_2$	417.3	Mono.	*C2/m*	1M	2	5.308	9.190	10.155		100.08		487.69	146.87	2.872	94
Lepidolite*	$KAlLi_2AlSi_3O_{10}(OH)_2$	385.2	Mono.	*C2/c*	$2M_1$	4	5.209	9.053	20.185		99.125		939.82	141.52	2.724	192
Lepidolite*	$KAlLi_2AlSi_3O_{10}(OH)_2$	385.2	Mono.	*C2/c*	$2M_2$	4	9.04	5.22	20.21		99.58		940.38	141.60	2.791	193
Lepidolite*	$KAlLi_2AlSi_3O_{10}(OH)_2$	385.2	Mono.	*C2/m*	1M	2	5.20	9.01	10.09		99.28		466.6	140.5	2.825	194
Zinnwaldite*	$K(AlFeLi)AlSi_3O_{10}(OH)_2$	434.1	Mono.	*C2/m*	1M	2	5.296	9.140	10.096		100.83		480.0	144.55	2.986	82

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Dioctahedral Mica Group																
Muscovite*	$KAl_2AlSi_3O_{10}(OH)_2$	398.3	Mono.	*C2/c*	$2M_1$	4	5.1918	9.0153	20.0457		95.74		933.56	140.57	2.834	187
Paragonite*	$NaAl_2AlSi_3O_{10}(OH)_2$	384.3	Mono.	*C2/c*	$2M_1$	4	5.128	8.898	19.287		94.35		877.51	132.13	2.909	129
Margarite*	$CaAl_2AlSi_3O_{10}(OH)_2$	399.3	Mono.	*C2/c*	$2M_2$	4	5.1038	8.8287	19.148		95.46		858.89	129.33	3.061	83
Bityite*	$Ca(LiAl)_2(AlBeSi_2)O_{10}(OH)_2$	387.2	Mono.	*C2/c*	$2M_1$	4	5.058	8.763	19.111		95.39		843.32	126.98	3.049	130
Chlorite Group																
Chlorite*	$(Mg_5Al)(AlSi_3)O_{10}(OH)_2$	555.8	Mono.	*C2/m*	Chlorite–II*b*2	2	5.327	9.227	14.327		96.81		699.24	210.57	2.640	109
Chlorite*	$(Mg_5Al)(AlSi_3)O_{10}(OH)_2$	555.8	Tric.	$C\bar{1}$	Chlorite–II*b*4	2	5.325	9.234	14.358	90.33	97.38	90.00	700.14	210.85	2.636	108
Clay Group																
Nacrite	$Al_2Si_2O_5(OH)_4$	258.16	Mono.	*Cc*	Nacrite	4	8.909	5.156	15.697		113.70		658.95	99.221	2.602	24
Dickite	$Al_2Si_2O_5(OH)_4$	258.16	Mono.	*Cc*	Dickite	4	5.178	8.937	14.738		103.82		662.27	99.721	2.588	22
Kaolinite	$Al_2Si_2O_5(OH)_4$	258.16	Tric.	*P*1	Kaolinite	2	5.1554	8.9448	7.4048	91.700	104.862	89.822	329.89	99.347	2.599	22
Amesite*	$(Mg_2Al)(AlSi)O_5(OH)_4$	278.7	Tric.	*C*1	Amesite	4	5.319	9.208	14.060	90.01	90.27	89.96	688.61	103.69	2.778	86
Lizardite*	$Mg_3Si_2O_5(OH)_4$	277.1	Trig.	*P*31*m*	Lizardite 1T	1	5.332		7.233				178.09	107.26	2.625	144
Tektosilicates																
Silica Group																
Quartz	SiO_2	60.085	Trig.	$P3_221$	Quartz	3	4.1934		5.4052				113.01	22.688	2.648	127
Coesite	SiO_2	60.085	Mono.	*C2/c*	Coesite	16	7.1464	12.3796	7.1829		120.283		548.76	20.657	2.909	210
Tridymite	SiO_2	60.085	Mono.	*Cc*	Tridymite	48	18.494	4.991	25.832		117.75		2110.2	26.478	2.269	111
Cristobalite	SiO_2	60.085	Tetr.	$P4_12_12$	Cristobalite	4	4.978		6.948				172.17	25.925	2.318	173
Stishovite	SiO_2	60.085	Tetr.	$P4_2/mnm$	Rutile	2	4.1790		2.6651				46.54	14.017	4.287	20
Feldspar Group																
Sanidine	$KAlSi_3O_8$	278.33	Mono.	*C2/m*	Sanidine	4	8.595	13.028	7.179		115.94		722.48	108.788	2.558	199
Orthoclase	$KAlSi_3O_8$	278.33	Mono.	*C2/m*	Sanidine	4	8.561	12.996	7.192		116.01		719.13	108.283	2.571	47
Microcline	$KAlSi_3O_8$	278.33	Tric.	$C\bar{1}$	Sanidine	4	8.560	12.964	7.215	90.65	115.83	87.70	720.07	108.425	2.567	31
High Albite	$NaAlSi_3O_8$	262.23	Tric.	$C\bar{1}$	Albite	4	8.161	12.875	7.110	93.53	116.46	90.24	667.12	100.452	2.610	234
Low Albite	$NaAlSi_3O_8$	262.23	Tric.	$C\bar{1}$	Albite	4	8.142	12.785	7.159	94.19	116.61	87.68	664.48	100.054	2.621	89
Anorthite	$CaAl_2Si_2O_8$	278.36	Tric.	$P\bar{1}$	Anorthite	8	8.173	12.869	14.165	93.11	115.91	91.261	1336.35	100.610	2.765	228
Celsian	$BaAl_2Si_2O_8$	375.47	Mono.	*I2/c*	Anorthite	8	8.627	13.045	14.408		115.22		1466.90	110.440	3.400	158
Feldspathoid Group																
Leucite	$KAlSi_2O_6$	218.25	Tetr.	$I4_1/a$	Leucite	16	13.09		13.75				2356.	88.69	2.461	139
Kalsilite	$KAlSiO_4$	158.17	Hex.	$P6_3$	Nepheline	2	5.16		8.69				200.4	60.34	2.621	178
Nepheline	$KNa_3Al_4Si_4O_{16}$	584.33	Hex.	$P6_3$	Nepheline	2	9.993		8.374				724.19	218.09	2.679	64
Meionite*	$Ca_4Al_6Si_6O_{24}CO_3$	932.9	Tetr.	$P4_2/n$	Scapolite	2	12.194		7.557				1123.7	338.40	2.757	131
Marialite*	$Na_4Al_6Si_6O_{24}Cl$	863.5	Tetr.	$P4_2/n$	Scapolite	2	12.059		7.587				1103.3	332.26	2.599	132
Zeolite Group																
Analcime*	$Na_{16}Al_{16}Si_{32}O_{96}{\cdot}16H_2O$	3526.1	Tetr.	$I4_1/acd$	Analcime	1	13.721		13.735				2585.8	1557.4	2.264	138
Chabazite*	$Ca_2Al_4Si_8O_{24}{\cdot}13H_2O$	1030.9	Trig.	$R\bar{3}m$	Chabazite	1	13.803		15.075				2487.2	499.4	2.065	37
Mordenite*	$K_8Al_8Si_{40}O_{96}{\cdot}24H_2O$	3620.4	Orth.	*Cmcm*	Mordenite	1	18.167	20.611	7.529				2819.2	1698.0	2.132	153
Clinoptilolite*	$KNa_2CaAl_6Si_{30}O_{72}{\cdot}24H_2O$	2750.0	Mono.	*C2/m*	Heulandite	1	17.633	17.941	7.400		116.39		2097.1	1263.0	2.177	211
Heulandite*	$Ca_4K_{1.2}Al_{10}Si_{26}O_{72}{\cdot}26H_2O$	2827.7	Mono.	*C2/m*	Heulandite	1	17.715	17.831	7.430		115.93		2132.2	1284.3	2.221	4
Thomsonite*	$NaCa_2Al_5Si_5O_{20}{\cdot}6H_2O$	671.8	Orth	*Pncn*	Thomsonite	4	13.089	13.047	13.218				2257.3	339.9	2.373	5

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Harmotome*	$Ba_2Ca_5Al_5Si_{11}O_{32}\cdot12H_2O$	1466.7	Mono.	$P2_1/m$	Phillipsite	1	9.879	14.139	8.693		124.8		996.9	600.5	2.443	184
Phillipsite*	$K_{2.5}Ca_{1.5}Al_5Si_{10}O_{32}\cdot12H_2O$	1291.5	Mono.	$P2_1/m$	Phillipsite	1	9.865	14.300	8.668		124.2		1011.3	609.1	2.120	184
Laumontite*	$CaAl_2Si_4O_{12}\cdot4H_2O$	470.44	Mono	Am	Laumontite	4	7.549	14.740	13.072	90.	90.	111.9	1349.6	203.2	2.315	202
Natrolite*	$Na_2Al_2Si_3O_{10}\cdot2H_2O$	380.23	Orth.	$Fdd2$	Natrolite	8	18.326	18.652	6.601				2256.3	169.87	2.238	174
Sodalite*	$Na_4Al_3Si_3O_{12}\cdot Cl$	484.6	Cub.	$P\bar{4}3n$	Sodalite	2	8.870						697.86	210.16	2.306	133
Stilbite*	$Na_{1.3}Ca_{4.2}Al_{10}Si_{26}O_{72}\cdot34H_2O$	2968.	Mono.	$C2/m$	Stilbite	1	13.64	18.24	11.27		128.0		2210.	1331.	2.23	71
Scolecite*	$CaAl_2Si_3O_{10}\cdot3H_2O$	392.34	Mono	Fd	Natrolite	8	18.508	18.981	6.527		90.64		2292.8	172.62	2.273	107
Gonnardite*	$Na_6Ca_2Al_9Si_{11}O_{40}\cdot12H_2O$	1626.04	Tetr.	$I\bar{4}2d$	Natrolite	1	13.21		6.622				1155.6	696.00	2.336	141
Edingtonite*	$Ba_2Al_4Si_6O_{20}\cdot8H_2O$	997.22	Tetr.	$P\bar{4}2_1m$	Edingtonite	1	9.581		6.526				599.06	360.81	2.764	140
Gismondine*	$Ca_4Al_8Si_8O_{32}\cdot16H_2O$	1401.09	Mono.	$P2_1/a$	Gismondine	1	10.024	10.626	9.832		92.40		1024.3	630.21	2.223	226
Garronite*	$NaCa_{2.5}Al_6Si_{10}O_{32}\cdot13H_2O$	1312.12	Tetr.	$I\bar{4}m2$	Gismondine	1	9.9266		10.3031				1015.24	611.48	2.146	9
Merlinoite*	$K_5Ca_2Al_9Si_{23}O_{64}\cdot24H_2O$	2620.81	Orth.	$Immm$	Merlinoite	1	14.116	14.229	9.946				1982.28	1193.92	2.195	72
Ferrierite*	$Na_3KMgAl_5Si_{31}O_{72}\cdot18H_2O$	2614.2	Mono.	$P2_1/a$	Ferrierite	1	18.886	14.182	7.470		90.0		2000.8	1205.1	2.169	79
Ferrierite*	$NaKMg_2Al_7Si_{29}O_{72}\cdot18H_2O$	2590.3	Orth.	$Immm$	Ferrierite	1	19.236	14.162	7.527		90.0		2050.5	1235.0	2.097	80
Faujasite*	$Na_2CaAl_4Si_8O_{24}\cdot16H_2O$	1090.9	Cub.	$Fd\bar{3}m$	Sodalite	16	24.74						15142.	570.02	1.914	18
Erionite*	$MgNaK_2Ca_2Al_9Si_{27}O_{72}\cdot18H_2O$	2683.1	Hex.	$P6_3/mmc$	Erionite	1	13.252		14.810				2252.4	1356.6	1.978	201
Cancrinite*	$Ca_{1.5}Na_6Al_6Si_6O_{24}\cdot1.6CO_2$	1008.5	Hex.	$P6_3$	Cancrinite	1	12.590		5.117				702.4	423.05	2.383	81
Pollucite*	$CsAlSi_2O_6$	312.06	Cub.	$Ia\bar{3}d$	Analcime	16	13.682						2561.2	96.41	3.237	156
Brewsterite*	$SrAl_2Si_6O_{16}\cdot5H_2O$	656.17	Mono.	$P2_1/m$	Brewsterite	2	6.767	17.455	7.729		94.40		910.2	274.12	2.394	10
High Pressure Silicates																
Phase B Group																
Phase B	$Mg_{12}Si_4O_{19}(OH)_2$	741.09	Mono.	$P2_1/c$	PhsB	4	10.588	14.097	10.073		104.10		1458.4	219.567	3.380	59
Anhydrous B	$Mg_{14}Si_5O_{24}$	864.78	Orth.	$Pmcb$	AnhB	2	5.868	14.178	10.048				835.96	251.749	3.435	59
Superhydrous B	$Mg_{10}Si_3O_{14}(OH)_4$	619.40	Orth.	$Pnnm$	PhsB	2	5.0894	13.968	8.6956				618.16	186.159	3.327	166
$MgSiO_3$–Group																
$MgSiO_3$–perovskite	$MgSiO_3$	100.40	Orth.	$Pbnm$	Perovskite	4	4.7754	4.9292	6.8969				162.35	24.445	4.107	103
$MgSiO_3$–ilmenite	$MgSiO_3$	100.40	Trig.	$R\bar{3}$	Ilmenite	6	4.7284		13.5591				262.54	26.354	3.810	102
$MgSiO_3$–garnet	$MgSiO_3$	100.40	Tetr.	$I4_1/a$	Garnet	32	11.501		11.480				1518.5	28.581	3.513	7
Wadsleyite Group																
Wadsleyite	Mg_2SiO_4	140.71	Orth.	$Imma$	Wadsleyite	8	5.6983	11.4380	8.2566				538.14	40.515	3.4729	104
β–Co_2SiO_4	Co_2SiO_4	209.95	Orth.	$Imma$	Wadsleyite	8	5.753	11.524	8.340				552.92	41.628	5.044	151
Silicate Spinel Group																
γ–Mg_2SiO_4	Mg_2SiO_4	140.71	Cub.	$Fd\bar{3}m$	Spinel	8	8.0449						524.56	39.493	3.563	196
γ–Fe_2SiO_4	Fe_2SiO_4	203.78	Cub.	$Fd\bar{3}m$	Spinel	8	8.234						558.26	42.030	4.848	236
γ–Ni_2SiO_4	Ni_2SiO_4	209.95	Cub.	$Fd\bar{3}m$	Spinel	8	8.138						538.96	40.577	5.174	236
γ–Co_2SiO_4	Co_2SiO_4	209.50	Cub.	$Fd\bar{3}m$	Spinel	8	8.044						520.49	39.187	5.346	151
Silica Group																
Coesite	SiO_2	60.085	Mono.	$C2/c$	Coesite	16	7.1464	12.3796	7.1829		120.283		548.76	20.657	2.909	210
Stishovite	SiO_2	60.085	Tetr.	$P4_2/mnm$	Rutile	2	4.1790		2.6651				46.54	14.017	4.287	20
Halides																
Halite	NaCl	58.443	Cub.	$Fm\bar{3}m$	Halite	4	5.638						179.22	26.985	2.166	235
Sylvite	KCl	74.555	Cub.	$Fm\bar{3}m$	Halite	4	6.291						248.98	37.490	1.989	235
Villiaumite	NaF	41.988	Cub.	$Fm\bar{3}m$	Halite	4	4.614						98.23	14.791	2.839	235
Carobbiite	KF	58.100	Cub.	$Fm\bar{3}m$	Halite	4	5.34						152.3	22.93	2.53	235

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Fluorite	CaF_2	78.077	Cub.	$Fm\bar{3}m$	Fluorite	4	5.460						162.77	24.509	3.186	232
Frankdicksonite	BaF_2	175.34	Cub.	$Fm\bar{3}m$	Fluorite	4	6.1964						237.91	35.824	4.894	180
Sellaite	MgF_2	62.309	Tetr.	$P4_2/mnm$	Rutile	2	4.660		3.078				66.84	20.129	3.096	101
Calomel	Hg_2Cl_2	472.09	Tetr.	$I4/mmm$	Calomel	2	4.45		10.89				215.65	64.94	7.269	101
Cryolite	Na_3AlF_6	209.95	Mono.	$P2_1/n$	Cryolite	2	5.40	5.60	7.78		90.18					101
Neighborite	$NaMgF_3$	104.30	Orth.	$Pcmn$	Perovskite	4	5.363	7.676	5.503				226.54	34.11	3.058	101
Chlorargyrite	AgCl	143.32	Cub.	$Fm\bar{3}m$	Halite	4	5.556						171.51	25.83	5.550	101
Iodyrite	AgI	234.77	Hex.	$P6_3mc$	Wurtzite	2	4.58		7.49				136.06	40.98	5.730	101
Nantokite	CuCl	98.99	Cub.	$F\bar{4}3m$		4	5.418						159.04	23.95	4.134	101
Sulfides																
Pyrrhotite	Fe_7S_8	647.44	Trig.	$P3_1$	Pyrrhotite	3	6.8673		17.062				696.84	139.90	4.628	62
Pyrite	FeS_2	119.98	Cub.	$Pa3$	Pyrite	4	5.418						159.04	23.95	5.010	29
Cattierite	CoS_2	123.06	Cub.	$Pa\bar{3}$	Pyrite	4	5.5385						169.89	25.582	4.811	162
Vaesite	NiS_2	122.84	Cub.	$Pa\bar{3}$	Pyrite	4	5.6865						183.88	27.688	4.437	162
Marcasite	FeS_2	119.98	Orth.	$Pnnm$	Marcasite	2	4.436	5.414	3.381				81.20	24.45	4.906	30
Troilite	FeS	89.911	Hex.	$P\bar{6}2c$	Troilite	12	5.963		11.754				361.95	18.167	4.839	117
Smythite	$(Fe,Ni)_9S_{11}$	855.3	Trig	$R\bar{3}m$	Smythite	1	3.4651		34.34				357.08	215.07	3.977	221
Chalcopyrite	$CuFeS_2$	183.51	Tetr.	$I\bar{4}2d$	Chalcopyrite	4	5.289		10.423				291.57	43.903	4.180	84
Cubanite	$CuFe_2S_3$	271.43	Orth.	$Pcmn$	Cubanite	4	6.467	11.117	6.231				447.97	67.453	4.024	218
Covelllite	CuS	95.60	Hex.	$P6_3/mmc$	Covellite	6	3.7938		16.341				203.68	20.447	4.676	56
Chalcocite	Cu_2S	159.14	Mono.	$P2_1/c$	Chalcocite	48	15.246	11.884	13.494		116.35		2190.9	27.491	5.789	57
Tetrahedrite	$Cu_{12}FeZnSb_4S_{13}$	1660.5	Cub.	$I\bar{4}3m$	Tetrahedrite	2	10.364						1113.2	335.25	4.953	179
Bornite	Cu_5FeS_4	501.80	Orth.	$Pbca$	Bornite	16	10.950	21.862	10.950				2521.3	98.676	5.085	122
Enargite	Cu_3AsS_4	393.80	Orth.	$Pmn2_1$	Enargite	2	7.407	6.436	6.154				296.63	89.329	4.408	2
Niccolite	NiAs	133.63	Hex.	$P6_3/mmc$	NiAs	2	3.619		5.035				57.11	17.199	7.770	240
Cobaltite	CoAsS	165.92	Orth.	$Pca2_1$	Cobaltite	4	5.582	5.582	5.582				173.93	26.189	6.335	77
Sphalerite	ZnS	97.434	Cub.	$F\bar{4}3m$	Sphalerite	4	5.4053						157.93	23.780	4.097	239
Wurtzite(2H)	ZnS	97.434	Hex	$P6_3mc$	Wurtzite	2	3.8227		6.2607				79.23	23.860	4.084	119
Greenockite	CdS	144.464	Hex	$P6_3mc$	Wurtzite	2	4.1348		6.7490				99.93	30.093	4.801	235
Pentlandite	$Ni_5Fe_4S_8$	773.5	Cub.	$Fm\bar{3}m$	Halite	4	10.044						1013.26	152.571	5.069	87
Alabandite	MnS	87.02	Cub.	$Fm\bar{3}m$	Halite	4	5.214						141.75	21.344	4.076	224
Galena	PbS	239.25	Cub.	$Fm\bar{3}m$	Halite	4	5.9315						208.69	31.423	7.614	160
Clausthalite	PbSe	286.15	Cub.	$Fm\bar{3}m$	Halite	4	6.1213						229.37	34.537	8.285	160
Altaite	PbTe	334.79	Cub.	$Fm\bar{3}m$	Halite	4	6.4541						268.85	40.482	8.270	160
Molybdenite(2H)	MoS_2	160.07	Hex	$P6_3/mmc$	Molybdenite	2	3.1602		12.294				106.33	32.021	4.999	28
Tungstenite	WS_2	247.92	Hex	$P6_3/mmc$	Molybdenite–2H2		3.1532		12.323				105.77	31.853	7.785	203
Acanthite	Ag_2S	247.80	Mono.	$P2_1/c$	Acanthite	4	4.231	6.930	9.526		125.48		227.45	34.248	7.236	190
Argentite	Ag_2S	247.80	Cub.	$Im3m$	Argentite	2	4.86						114.79	34.569	7.168	41
Proustite	Ag_3AsS_3	494.72	Trig.	$R3c$	Proustite	6	10.82		8.69				881.06	88.44	5.594	55
Pyrargyrite	Ag_3SbS_3	541.55	Trig.	$R3c$	Proustite	6	11.04		8.72				920.42	92.39	5.861	55
Cinnabar	HgS	232.65	Trig.	$P3_221$	Cinnabar	3	4.145		9.496				141.29	28.361	8.202	14
Metacinnabar	HgS	232.65	Cub.	$F\bar{4}3m$	Sphalerite	4	5.8717						202.44	30.482	7.633	13
Coloradoite	HgTe	328.19	Cub.	$F\bar{4}3m$	Sphalerite	4	6.440						267.09	40.217	8.161	223
Stibnite	Sb_2S_3	339.69	Orth.	$Pnma$	Stibnite	4	11.302	3.8341	11.222				486.28	73.222	4.639	143
Orpiment	As_2S_3	246.04	Mono.	$P2_1/n$	Orpiment	4	11.475	9.577	4.256		90.68		467.68	70.422	3.494	154

Table 1. Crystallographic Properties of Minerals (continued).

Mineral	Formula	Formula Weight	Crystal System	Space Group	Structure Type	Z	*a* (Å)	*b* (Å)	*c* (Å)	α (°)	β (°)	γ (°)	Unit Cell Vol (Å^3)	Molar Vol (cm^3)	Density (calc)(Mg/m^3)	Ref.
Realgar	AsS	106.99	Mono.	$P2_1/n$	Realgar	16	9.325	13.571	6.587		106.38		799.75	30.107	3.554	154
Bismuthinite	Bi_2S_3	514.15	Orth.	$Pmcn$	Stibnite	4	3.981	11.147	11.305				501.67	75.539	6.806	110
Hazelwoodite	Ni_3S_2	240.26	Trig.	$R32$	Hazelwoodite	1	4.0718			89.459	89.459	89.459	67.50	40.655	5.910	171
Cooperite	PtS	227.15	Tetr.	$P4_2/mmc$	Cooperite	2	3.465		6.104				73.29	22.070	10.292	35
Vysotskite	PdS	138.46	Tetr.	$P4_2/m$	Cooperite	8	6.429		6.611				273.25	20.572	6.731	27
Millerite	NiS	90.77	Trig.	$R3m$	Millerite	9	9.6190		3.1499				252.4	16.891	5.374	181
Linneaite	Co_3S_4	305.06	Cub.	$Fd\bar{3}m$	Spinel	8	9.406						832.2	62.652	4.869	120
Polydymite	Ni_3S_4	304.39	Cub.	$Fd\bar{3}m$	Spinel	8	9.489						854.4	64.326	4.732	49
Violarite	$FeNi_2S_4$	301.52	Cub.	$Fd\bar{3}m$	Spinel	8	9.465						847.93	63.839	4.723	49
Greigite	Fe_3S_4	295.80	Cub.	$Fd\bar{3}m$	Spinel	8	9.875						962.97	72.499	4.080	238
Daubreelite	$FeCr_2S_4$	288.10	Cub.	$Fd\bar{3}m$	Spinel	8	9.995						998.50	75.175	3.832	205
Loellingite	$FeAs_2$	205.69	Orth.	$Pnnm$	Loellingite	2	5.3001	5.9838	2.8821				91.41	27.527	7.472	136
Arsenopyrite	FeAsS	162.83	Mono.	$C2_1/d$	Arsenopyrite	8	6.546	9.451	5.649			89.94	349.48	26.312	6.189	68
Native Elements																
Diamond	C	12.011	Cub.	$Fd\bar{3}m$	Diamond	8	3.56679						45.38	3.4163	3.5158	235
Graphite	C	12.011	Hex.	$P6_3/mmc$	Graphite	4	2.456		6.696				34.98	5.267	2.281	235
Silicon	Si	28.086	Cub.	$Fd\bar{3}m$	Diamond	8	5.43070						160.16	12.058	2.329	235
Sulfur(α)	S	32.064	Orth.	$Fddd$	Sulfur	128	10.467	12.870	24.493				3299.5	15.443	2.076	235
Sulfur(β)	S	32.064	Mono.	$P2_1$	Sulfur	48	10.926	10.885	10.790		95.92		1276.41	16.016	2.002	78
Kamacite	Fe	55.847	Cub	$Im\bar{3}m$	α–Iron	2	2.8665						23.55	7.093	7.873	235
Taenite	FeNi	114.557	Cub	$Fm\bar{3}m$	Taenite	32	7.168						368.29	13.864	8.263	235
Nickel	Ni	58.710	Cub.	$Fm\bar{3}m$	FCC	4	3.52387						43.76	6.590	8.910	235
Copper	Cu	63.540	Cub.	$Fm\bar{3}m$	FCC	4	3.61496						47.24	7.113	8.932	235
Arsenic	As	74.922	Trig.	$R\bar{3}m$	Arsenic	18	3.7598		10.5475				129.12	4.321	17.340	200
Tin	Sn	118.690	Tetr.	$I4_1/amd$	Tin	4	5.8197		3.17488				107.54	16.194	7.329	235
Ruthenium	Ru	101.070	Hex.	$P6_3/mmc$	HCP	2	2.7056		4.2803				27.14	8.172	12.368	85
Rhodium	Rh	102.905	Cub.	$Fm\bar{3}m$	FCC	4	3.8031						55.01	8.283	12.424	235
Palladium	Pd	106.40	Cub.	$Fm\bar{3}m$	FCC	4	3.8898						60.16	9.059	11.746	235
Silver	Ag	107.87	Cub.	$Fm\bar{3}m$	FCC	4	4.0862						68.23	10.273	17.500	235
Antimony	Sb	121.75	Trig.	$R3m$	Arsenic	6	4.3083		11.2743				180.06	18.075	6.736	235
Tellurium	Te	127.60	Trig.	$P3_121$	Selenium	3	4.456		5.921				101.82	20.441	6.242	1
Iridium	Ir	192.20	Cub.	$Fm\bar{3}m$	FCC	4	3.8394						56.60	8.522	22.553	235
Osmium	Os	190.20	Hex.	$P6_3/mmc$	HCP	2	2.7352		4.3190				27.98	8.427	22.570	235
Platinum	Pt	195.09	Cub.	$Fm\bar{3}m$	FCC	4	3.9231						60.38	9.092	21.458	235
Gold	Au	196.967	Cub.	$Fm\bar{3}m$	FCC	4	4.07825						67.83	10.214	19.285	235
Lead	Pb	207.190	Cub.	$Fm\bar{3}m$	FCC	4	4.9505						121.32	18.268	11.342	235
Bismuth	Bi	208.980	Trig.	$R\bar{3}m$	Arsenic	6	4.54590		11.86225				212.29	21.311	9.806	235

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