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Crystal Structures and Cation Sites of the Rock-Forming Minerals

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ALLEN & UNWIN

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Acknowledgement

This work was supported in part by the U.S Department of Energy, Office of Basic Energy Sciences, through several grants to Los Alamos National Laboratory which is operated by the University of California under contract number W-7405-ENG-6. The author s particularly thank Dr. George Kolstadt (OBES Chemistry, Earth and Life Sciences) and Dr. Ryszard Gajewski (OBES Advanced Energy Projects) for generous support of the project. The autyhords thank Drs. Y. Ohashi (ARCO, Plano, TX), R. X. Fischer (Johannes Gutenberg Universitaet, Mainz) and L.W. Finger (Carnegie Institution, Washington, DC) for providing computer codes and discussions, and Drs. George Zweig, Klaus Lackner, and Wes Myers (Los Alamos National Laboratory) for discussions, support and encouragement throughout the project. Theoretical Division Office of Los Alamos National Laboratory is also thanked for its support. Tamsin C. McCormick is gratefully acknowledged for tireless proofreading, technical assistanc and moral support.

Introduction

This is the first installment of a free version of the first edition of the book. The data presented here are identical to those of the first edition and so may be cited as:

Smyth, J.R. and D.L. Bish (1988) Crystal Structures and Cation Sites of the Rock-Forming Minerals. Boston, Allen and Unwin, 332pp.

Chapter 1. Single Oxide Minerals

1.1. Hemioxides

Table 1.1.1. Cuprite and Ag_2O Unit Cells

End Member	Cuprite	Ag_2O
Formula	Cu_2O	Ag_2O
Form. Wt. (g)	143.079	231.739
Density (g/cm^3)	6.104	7.318
Mol. Vol. (cm^3)\	23.439	31.667
Z	2	2
Cryst. Sys.	Isometric	Isometric
Laue Class	*m*3*m*	*m*3*m*
Space Group	*Pn*3*m*	*Pn*3*m*
Cell Parameters		
a (Å)	4.2696	4.720
Vol.	77.833	105.15
Ref.	Borie (1974)	Borie (1974)

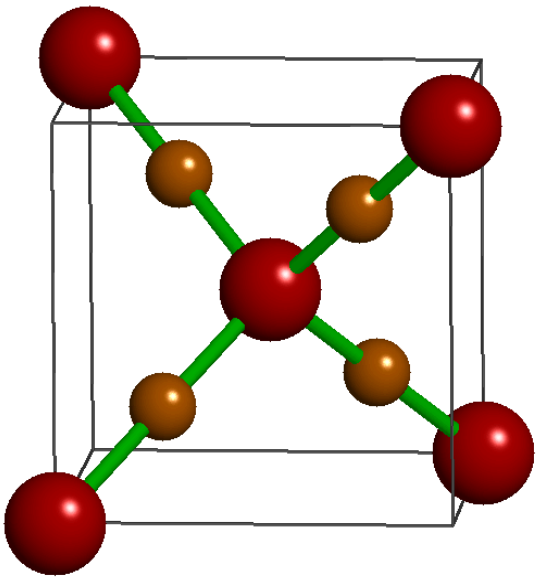

Figure 1.1. The crystal structure of cuprite. This structure is not ionic. The Cu and Ag atoms are in two-coordination which could not be sustained without the *sp* or *sd* hybrid orbitals of the Cu and Ag atoms. So Na_2O and K_2O synthetic compounds have the anti-fluorite structure and do not exist as minerals as the oxygen atoms readily hydrate to form hydroxides.

Table 1.1.2. Cuprite and Ag_2O Cation Sites

End Member	Cuprite	Ag_2O
C.N.	2	2
Cation	Cu	Ag
Point Sym.	$\bar{3}m$	$\bar{3}m$
Wyckoff Not.	4*b*	4*b*
Frac. Coords.		
x	0	0
y	0	0
z	0	0
Distances		
O (2)	1.849	2.044
Elect.Energy	-294.	-266.

1.2. Monoxides

The monoxides are those minerals that are oxides of a single divalent cation. The simplest are those of the periclase group that all have the cubic rocksalt (halite) or B1 structure. The monoxides of Be and Zn have an acentric, piezoelectric structure with the cation in tetrahedral coordination. In addition, monoxides of Cu (tenorite, CuO), and Hg (montroydite, HgO) have covalent structures with irregular coordination of the metal atoms.

1.2.1. The Periclase Group

The periclase group consists of monoxides of divalent metal cations, MgO (periclase), FeO (wüstite), CaO (lime), NiO (bunsenite), and MnO (manganosite). Of these, MgO-FeO solid solutions (ferro-periclase) are believed to compose a significant portion of the lower mantle. This structure is also adopted by NaCl (halite), KCl (sylvite), and PbS (galena), as well as numerous compounds that are not known to occur naturally as minerals.

1.2. Periclase Group

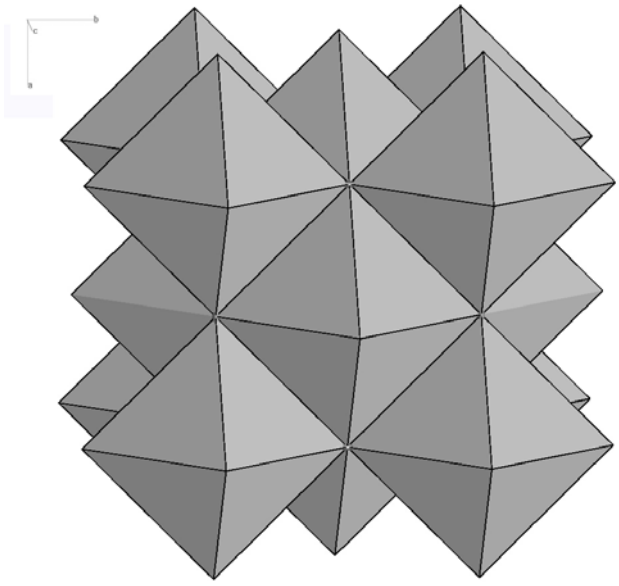

Figure 1.2.1. The crystal structure of periclase (MgO) and the other minerals of the periclase group. Both the cation and anion are in perfectly regular octahedral coordination with each other.

Table 1.2.1. The Periclase Group Unit Cells

	Periclase	Wüstite	Lime	Bunsenite	Manganosite
Formula	MgO	FeO	CaO	NiO	MnO
Form.Wt.	40.312	71.848	56.079	74.709	70.937
Z	4	4	4	4	4
CrystalSystem	Cub	Cub	Cub	Cub	Cub
PointGroup	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$
SpaceGroup	$Fm\bar{3}m$	$Fm\bar{3}m$	$Fm\bar{3}m$	$Fm\bar{3}m$	$Fm\bar{3}m$
UnitCell					
a(Å)	4.211	4.3108	4.8105	4.1684	4.446
Vol	74.67	80.11	111.32	72.43	87.88
MolarVol	11.244	12.062	16.762	10.906	13.223
Density	3.585	5.956	3.346	6.850	5.365
Thermal Expansion (Volumetric)					
alpha	31.6	33.9		33.	34.5
a0	0.3768	0.3203		0.3032	0.3317
a1	0.7404	1.4836		1.0463	1.2055
a2	-0.7446	-0.0000		0.0000	-0.2094
Elastic Properties					
Ks(GPa)	162.7	181.		114.7	153.0
G(Gpa)	131.1	46.1		81.2	68.1

Table 1.2.2. Cation Sites in the Periclase Group.

End Member	Periclase	Wüstite	Lime	Bunsenite	Manganosite
Formula	MgO	FeO	CaO	NiO	MnO
C.N.	6	6	6	6	6
Cation	Mg	Fe	Ca	Ni	Mn
Point Sym.	$m\bar{3}m$	$m\bar{3}\,m$	$m\bar{3}\,m$	$m\bar{3}\,m$	$m\bar{3}\,m$
Wyckoff Not.	4a	4a	4a	4a	4a
Frac. Coords.					
x	0	0	0	0	0
y	0	0	0	0	0
z	0	0	0	0	0
Distances					
O (6)	2.1055	2.1554	2.4053	2.0842	2.2230
Poly.Vol.	12.445	13.351	18.553	12.071	14.647
O.Q.E.	1.0000	1.0000	1.0000	1.0000	1.0000
O.A.V.	0.0	0.0	0.0	0.0	0.0
Site. Energy	-551.	-539.	-483.	-557.	-522.

1.3.2. Zincite Group

Table 1.3.1. Zincite Group Unit Cells

End Member	Zincite	Bromellite
Formula	ZnO	BeO
Form.Wt.	81.369	25.012
Density	5.712	3.080
Mol. Vol.	14.246	8.122
Z	2	2
Cryst.Sys.	Hexagonal	Hexagonal
Laue Grp.	6*mm*	6*mm*
Space Group	$P6_3mc$	$P6_3mc$
Cell Parameters		
a	3.2427	2.6984
c	5.1948	4.2770
Vol.	47.306	26.970

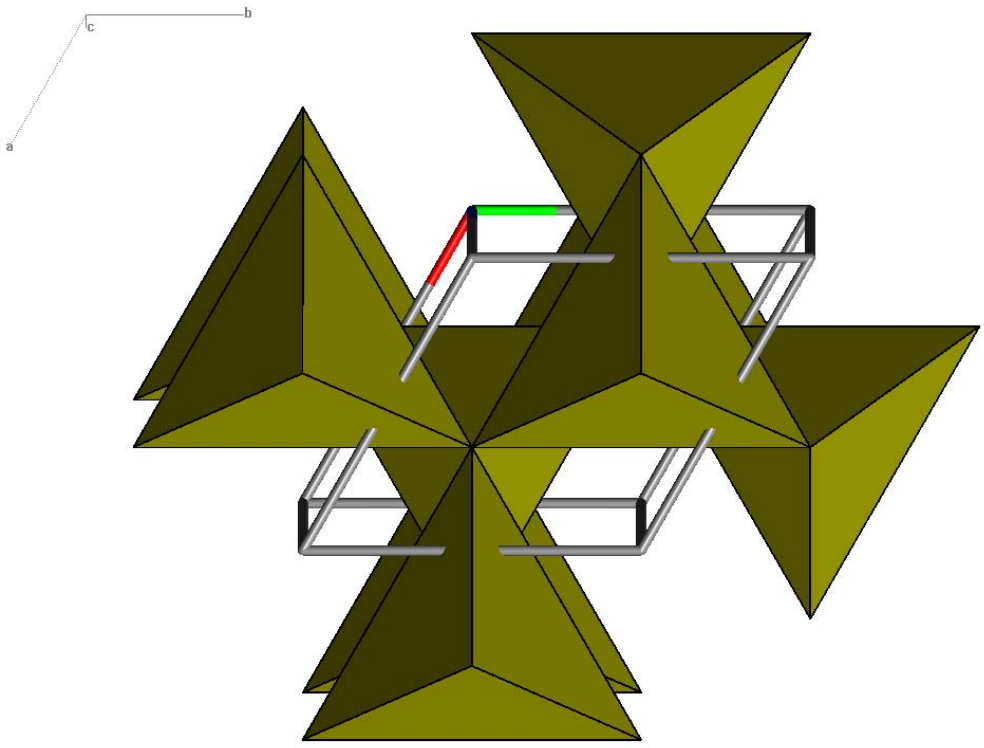

Figure 1.3. Zincite ZnO. The structure has Zn in regular tetrahedral coordination with oxygen and is strongly acentric (chiral) and piezoelectric. Also oxygen is in tetrahedral coordination with Zn. Bromellite (BeO) is isostructural.

Table 1.3.2. Zincite Group Cation Sites

End Member	Zincite	Bromellite
Formula	ZnO	BeO
C.N.	4	4
Cation	Zn	Be
Point Sym.	3*m*	3*m*
Wyckoff Not.	2*b*	2*b*
Frac. Coords.		
x	1/3	1/3
y	2/3	2/3
z	0	0
Distances		
O1(1)	1.988	1.619
O2(3)	1.969	1.642
Mean	1.974	1.636
σ	0.009	0.011
Poly.Vol.	3.942	2.247
TQE	1.0006	1.005
Ang.Var.	2.6	1.5
Site Energy	-1105.	-1333.

1.4. Tenorite (CuO) and Montroydite (HgO)

Table 1.4.1. Tenorite and Montroydite Unit Cells.

End Member	Tenorite	Montroydite
Formula	CuO	HgO
Form.Wt.	75.539	216.589
Density	6.515	11.193
Mol. Vol.	12.109	19.350
Z	4	4
Cryst.Sys.	Monoclinic	Orthorhombic
Laue Group	2/*m*	*mmm*
Space Group	*C*2/*c*	*Pnma*
Cell Parameters		
a	4.6837	6.612
b	3.4226	5.520
c	5.1288	3.521
β	99.54	
Vol.	81.080	128.51
Ref.	Asbrink & Norrby (1970)	Aurivilius (1956)

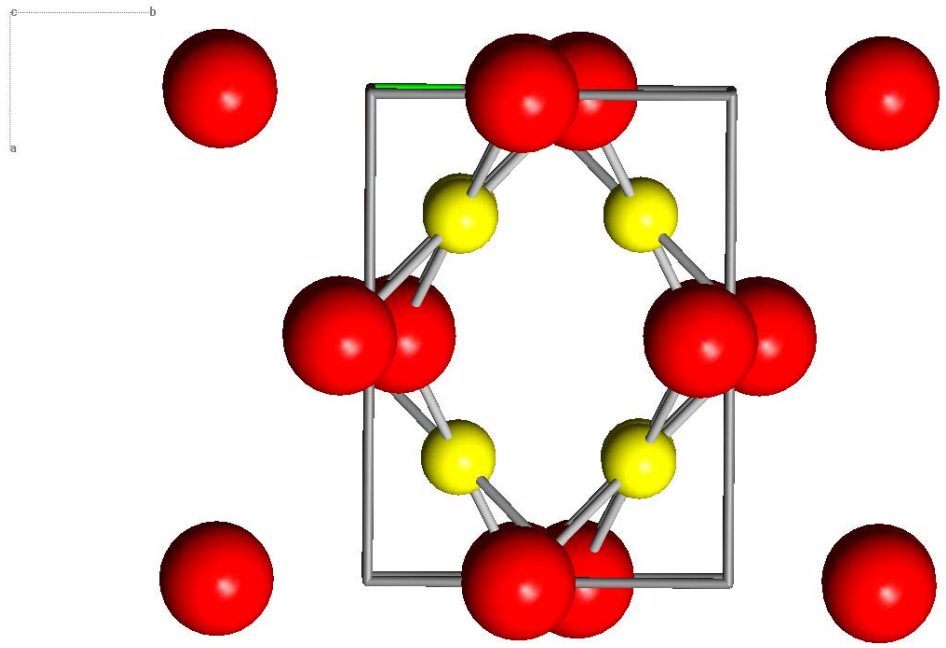

Figure 1.4a. Tenorite CuO. The structure has Cu^{2+} in 4-coordination with oxygen with two more oxygens further away.

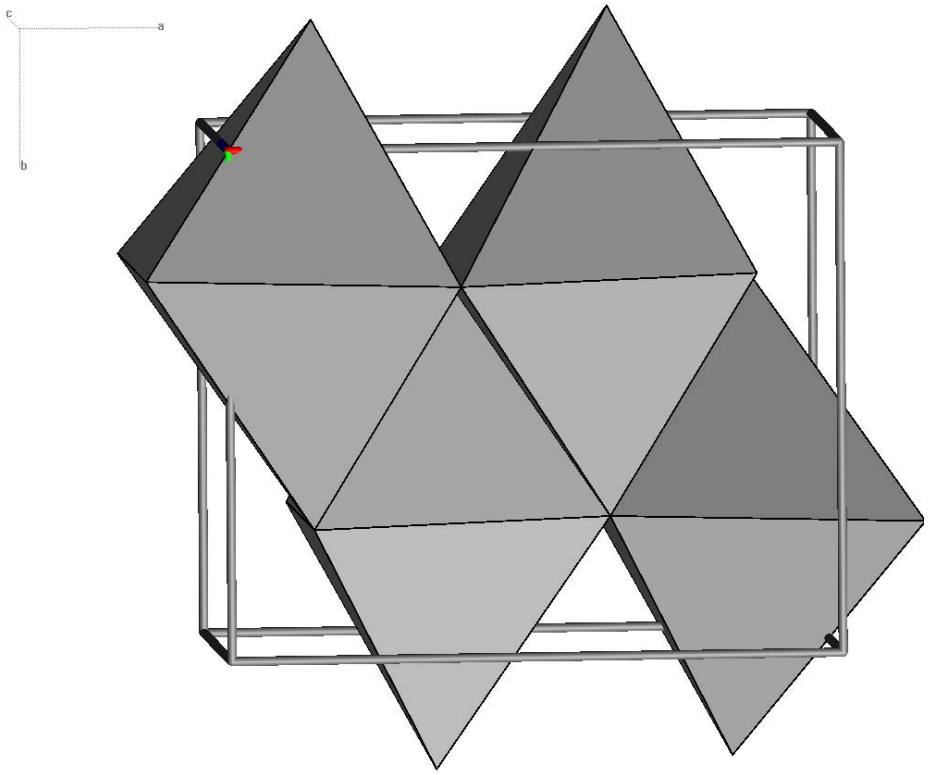

Figure 1.4b. Montroydite HgO. The structure is orthorhombic with Hg in irregular 6-coordination (four close and two further away).

Table 1.4.2. Tenorite and Montroydite Cation Sites

End Member	Tenorite	Montroydite
Formula	CuO	HgO
C.N.	4	5
Cation	Cu	Hg
Point Sym.	-1	*m*
Wyckoff Not.	4c	4c
Frac. Coords.		
x	1/4	0.1150
y	1/4	1/4
z	0	0.2450
Distances		
O1	(2)1.961	2.004
O2	(2)1.951	2.038
O3		2.847
O4		(2)2.825
Mean	1.956	2.508
σ	0.006	0.445
Poly.Vol.	planar	10.709
Site Energy	-1114.	-971.

1.5. Corundum Group

Table 1.5.1. Corundum Group Unit Cells.

End Member	Corundum	Hematite	Eskolaite	Karelianite
Formula	Al_2O_3	Fe_2O_3	Cr_2O_3	V_2O_3
Form.Wt.	101.961	159.692	151.990	149.882
Density	3.986	5.255	5.224	5.021
Mol. Vol.	25.577	30.388	29.093	29.850
Z	6	6	6	6
Cryst.Sys.	Trigonal	Trigonal	Trigonal	Trigonal
Laue Grp.	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$
Space Grp	$R\bar{3}c$	$R\bar{3}c$	$R\bar{3}c$	$R\bar{3}c$
Cell Parameters				
a	4.7589	5.038	4.9607	4.952
c	12.9912	13.772	13.599	14.002
Vol.	254.80	302.72	289.82	297.36
Ref.	Newnham & deHaan (1962)	Blake et al. (1966)	Newnham & deHaan (1962)	Newnham & deHaan (1962)

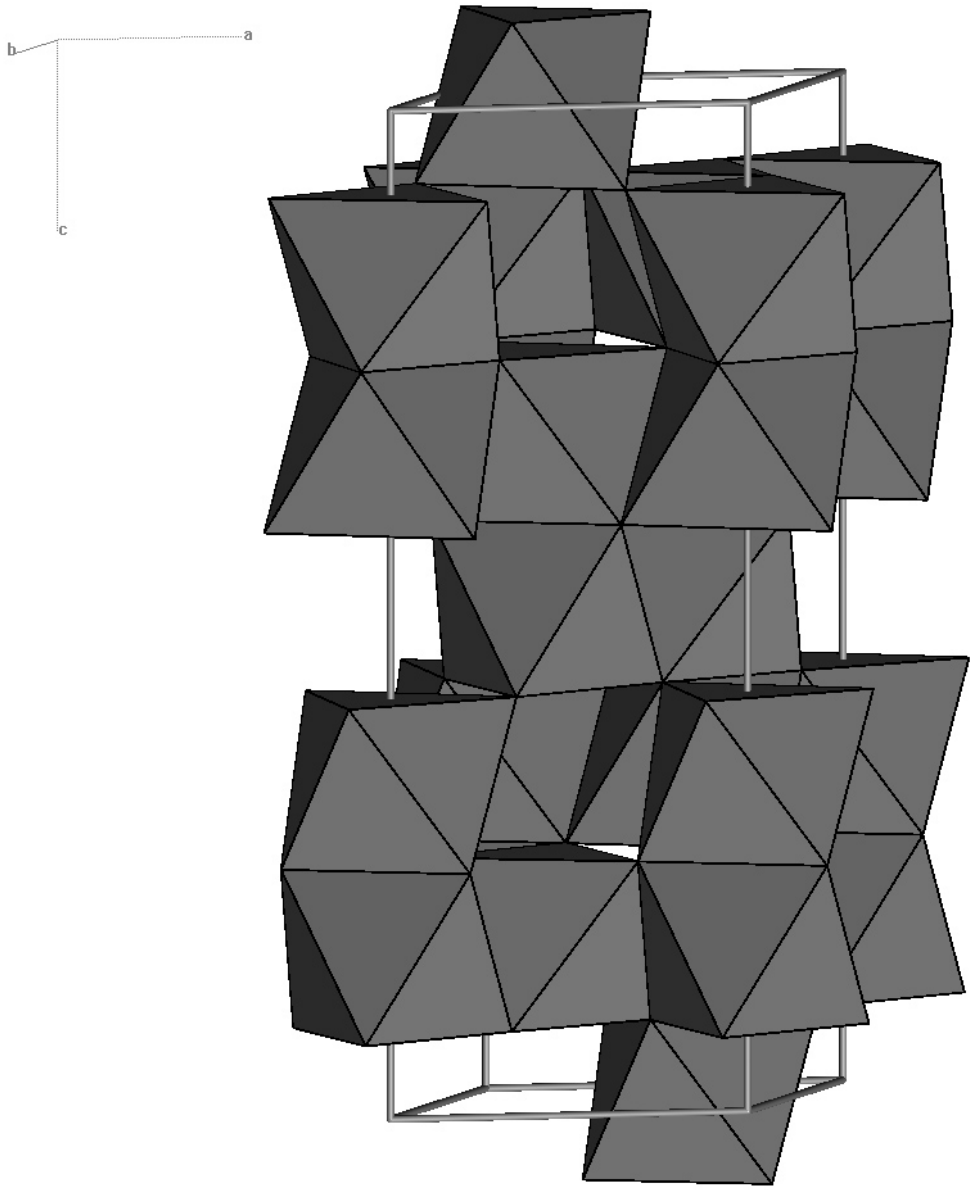

Figure 1.5. Corundum Al_2O_3. The structure has Al in octahedral coordination with oxygen. The structure is relatively dense with face-sharing octahedral. Hematite (Fe_2O_3), eskolaite(Cr_2O_3), and karelianite (V_2O_3) are isostructural.

Table 1.5.2. Corundum Group Cation Sites.

End Member	Corundum	Hematite	Eskolaite	Karelianite
C.N.	6	6	6	6
Cation	Al	Fe	Cr	V
Point Sym.	3	3	3	3
Wyckoff Not.	12*c*	12*c*	12*c*	12c
Frac. Coords.				
X	0	0	0	0
y	0	0	0	0
z	0.3520	0.3553	0.3475	0.3463
Distances				
O(3)	1.969	2.115	2.016	2.062
O(3)	1.856	1.945	1.965	2.062
Mean	1.913	2.030	1.990	2.012
σ	0.062	0.093	0.028	0.054
Poly.Vol.	9.066	10.754	10.312	10.719
O.Q.E.	1.0200	1.0264	1.0131	1.0098
Ang.Var.	66.6	85.0	45.2	32.7
Site Potential	-2529.	-2401.	-2416.	-2309.

1.6. Bixbyite Group

Table 1.6.1. Bixbyite Group Unit Cells.

End Member	Bixbyite	Avicennite
Formula	$(Mn_{.983}Fe_{.017})_2O_3$	Tl_2O_3
Form.Wt.	157.905	456.738
Density	5.027	10.353
Mol. Vol.	31.412	44.115
Z	16	16
Cryst.Sys.	Isometric	Isometric
Laue Grp.	*m*3	*m*3
Space Grp	*Ia*3	*Ia*3
Cell Parameters		
a	9.4146	10.543
Vol.	834.46	1171.91
Ref.	Geller (1971) (1971)	Papamantellos (1968)

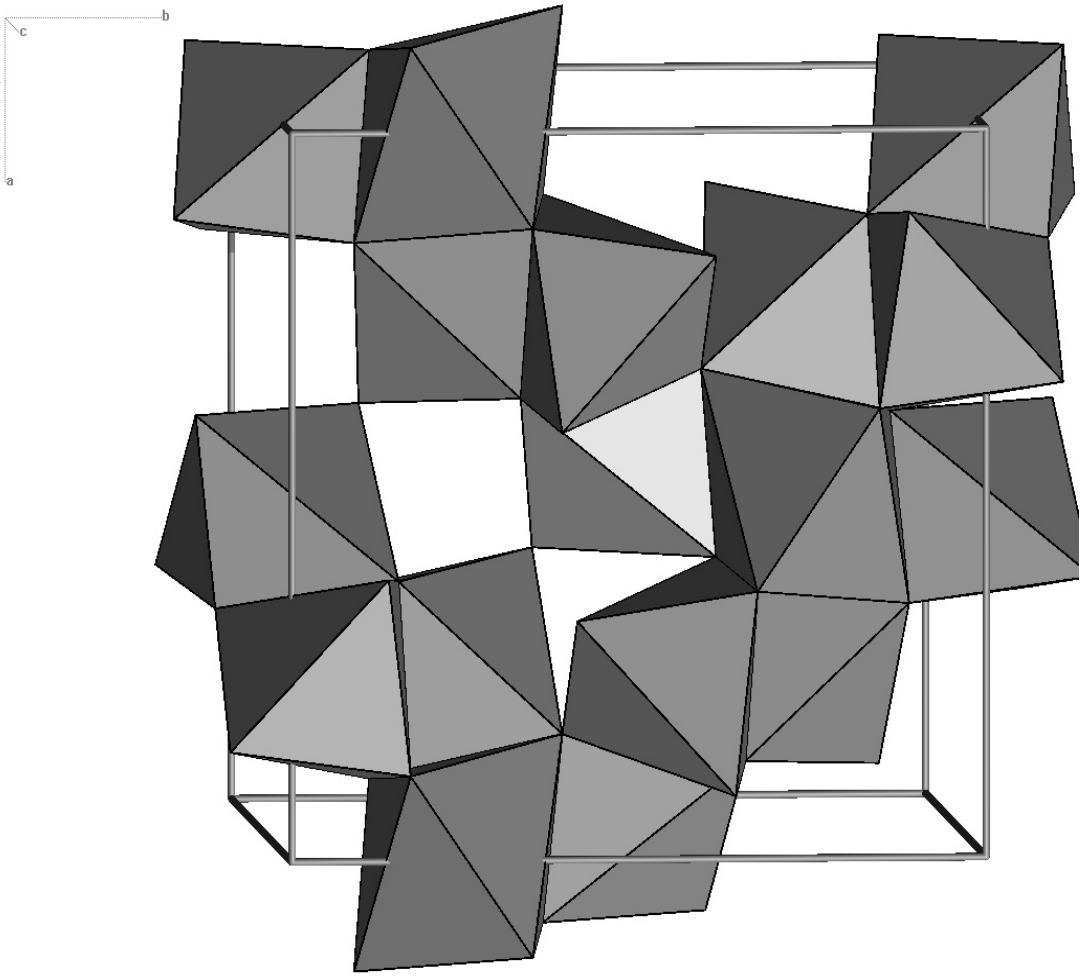

Figure 1.6. Bixbyite Mn_2O_3. There are two distinct Mn3+ sites, both in octahedral coordination. Mn1 is the more regular with point symmetry $\bar{3}$, whereas Mn2 is more distorted. Avicennite (Tl_2O_3), is isostructural, as are several of the pure rare earth sesquioxides.

Table 1.6.2. Bixbyite Group Cation Sites

End Member	Bixbyite		Avicennite	
Site	M1	M2	M1	M2
C.N.	6	6	6	6
Cation	Mn	Mn	Tl	Tl
Point Sym.	$\bar{3}$	2	$\bar{3}$	2
Wyckoff Not.	8b	24d	8b	24d
Frac. Coords.				
X	¼	-0.030	¼	-0.029
y	¼	0	¼	0
z	¼	¼	¼	¼
Distances				
O	(6)2.003	(2)1.927	(6)2.271	(2)2.140
O		(2)2.084		(2)2.140
O		(2)2.178		(2)2.475
Mean	2.003	2.063	2.271	2.268
σ	0.000	0.114	0.000	0.162
Poly.Vol.	10.580	10.759	15.046	13.764
O.Q.E.	1.0087	1.0605	1.0249	1.0895
Ang.Var.	28.9	181.8	77.8	224.3
Site Potential	-2468.	-2349.	-2160.	-2173.

1.7. Arsenic and Antimony Sesquioxides

Table 1.7.1. Arsenic and Antimony Sesquioxide Unit Cells.

End Member	Arsenolite	Senarmontite	Claudetite	Valentinite
Formula	As_2O_3	Sb_2O_3	As_2O_3	Sb_2O_3
Form.Wt.	197.841	291.498	197.841	291.498
Density	3.870	5.583	3.960	5.844
Mol. Vol.	51.127	52.208	49.961	49.887
Z	16	16	4	4
Cryst.Sys.	Isometric	Isometric	Monoclinic	Orthorhombic
Laue Grp.	*m*3*m*	*m*3*m*	2/*m*	*mmm*
Space Grp	$Fd\bar{3}m$	$Fd\bar{3}m$	$P2_1/n$	*Pccn*
Cell Parameters				
a	11.0744	11.1519	7.99	4.911
b			4.65	12.464
c			9.12	5.412
β			78.3	
Vol.	1358.19	1386.9	331.8	331.27
Ref.	Pertlik (1978)	Svensson (1975)	Pertlik (1975)	Svensson (1974)

Table 1.7.2. Arsenic and Antimony Sesquioxide Cation Sites.

End Member	Arsenolite	Senarmontite	Claudetite		Valentinite
C.N	3	3	3	3	5
Cation	As	Sb	As	As	Sb
Point Sym.	3m	3m	1	1	1
Wyckoff Not.	32e	32e	4e	4e	8e
Frac. Coords.					
x	0.0221	0.01027	0.6163	0.1841	0.04149
y	0.0221	0.01027	0.8311	0.2910	0.12745
z	0.0221	0.01027	0.3013	0.3717	0.17845
Distances					
O1	(3)1.787	(3)1.9774	1.794	1.821	2.022
O2			1.796	1.771	2.619
O3			1.790	1.772	2.019
O4					2.519
O5					1.977
Mean	1.787	1.974	1.794	1.788	2.231
σ	0.000	0.000	0.003	0.0298	0.311
Poly.Vol.	-	-	-	-	5.468
Site Potential	-2419.	-2217.	-2267.	-2356.	-2184.

1.8. Rutile Group

Table 1.8.1. Rutile Group Unit Cells

End Member	Rutile	Pyrolusite	Cassiterite	Stishovite
Formula	TiO_2	MnO_2	SnO_2	SiO_2
Form.Wt.	79.899	86.937	150.689	60.085
Density	4.2743	5.203	7.001	4.287
Mol. Vol.	18.693	16.708	21.523	14.017
Z	2	2	2	2
Cryst.Sys.	Tetragonal	Tetragonal	Tetragonal	Tetragonal
Laue Grp.	4/*mmm*	4/*mmm*	4/*mmm*	4/*mmm*
Space Group	$P4_2/mnm$	$P4_2/mnm$	$P4_2/mnm$	$P4_2/mnm$
Cell Parameters				
a	4.5845	4.396	4.737	4.1790
c	2.9533	2.871	3.185	2.6651
Vol.	62.07	55.48	71.47	46.54
Ref.	Shintani et al. (1975)	Kondrasev & Zaslevskij (1951)	Baur (1956)	Baur & Khan (1971)

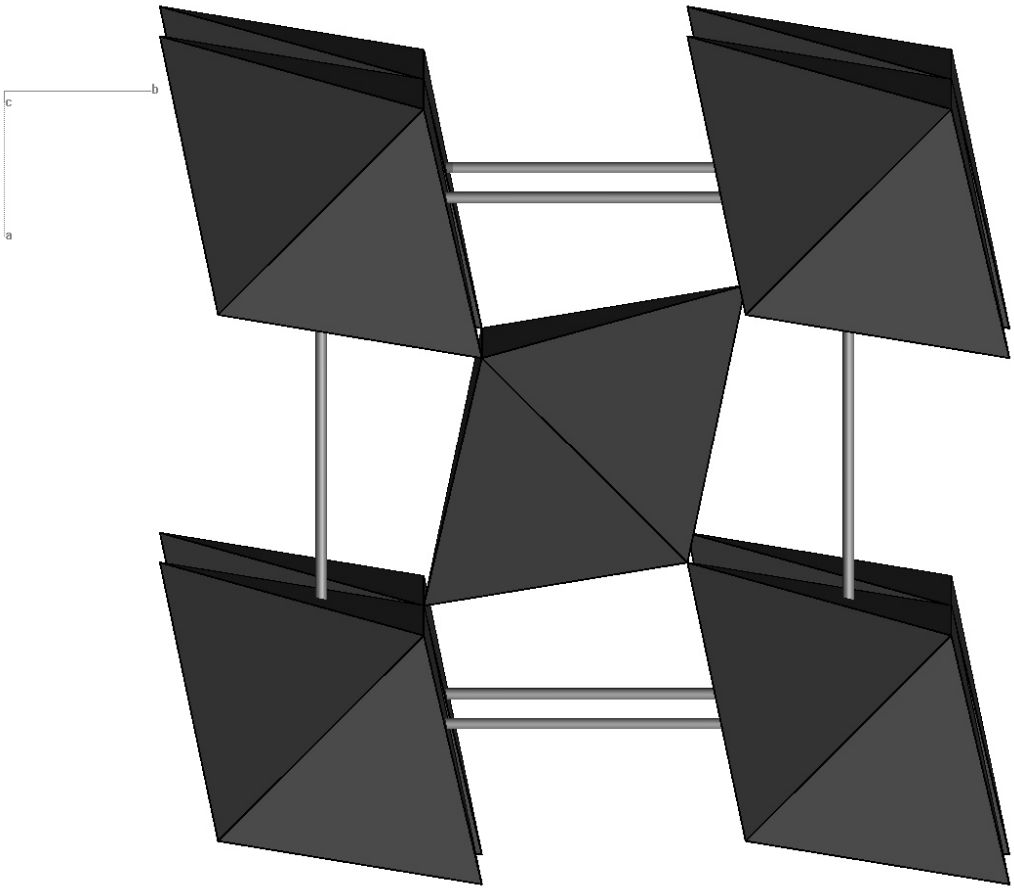

Figure 1.8. Rutile TiO_2. All Ti atoms are in identical octahedral coordination. Octahedra share edges, but not faces. Each oxygen id bonded to three Ti atoms. Several tetravalent metal oxides have this structure of which pyrolusite (MnO_2), cassiterite (SnO_2), and stishovite (high pressure SiO_2) occur as minerals.

Table 1.8.2. Rutile Group Cation Sites

End Member	Rutile	Pyrolusite	Cassiterite	Stishovite
C.N.	6	6	6	6
Cation	Ti	Mn	Sn	Si
Point Sym.	*mmm*	*mmm*	*mmm*	*mmm*
Wyckoff Not.	2a	2a	2a	2a
Frac. Coords.				
X	0	0	0	0
y	0	0	0	0
z	0	0	0	0
Distances				
O(2)	1.977	1.878	2.057	1.810
O(4)	1.944	1.891	2.051	1.757
Mean	1.955	1.887	2.053	1.775
σ	0.017	0.007	0.003	0.027
Poly.Vol.	9.846	8.847	11.292	7.365
O.Q.E.	1.0081	1.0079	1.0145	1.0080
Ang.Var.	28.4	28.0	51.1	27.1
Site Potential	-4133.	-4289	-3953.	-4550.

1.9. TiO_2 Polymorphs and Baddeleyite

Table 1.9.1. Polymorphs and Baddeleyite Unit Cells

End Member	Rutile	Anatase	Brookite	Baddeleyite
Formula	TiO_2	TiO_2	TiO_2	ZrO_2
Form.Wt.	79.899	79.899	79.899	123.219
Density	4.2743	3.895	4.123	5.826
Mol. Vol.	18.693	20.516	19.377	21.149
Z	2	4	8	4
Cryst.Sys.	Tetragonal	Tetragonal	Orthorhombic	Monoclinic
Laue Grp.	4/*mmm*	4/*mmm*	*mmm*	2/*m*
Space Group	$P4_2/mnm$	$I4_1/amd$	*Pbca*	$P2_1/c$
Cell Parameters				
a	4.5845	3.7842	9.184	5.1454
b	4.5845	3.7842	5.447	5.2075
c	2.9533	9.5146	5.145	5.3107
β				99.23
Vol.	62.07	136.25	257.38	140.45
Ref.	Shintani et al. (1975)	Horn et al. (1972)	Baur (1961)	Smith & Newkirk (1965)

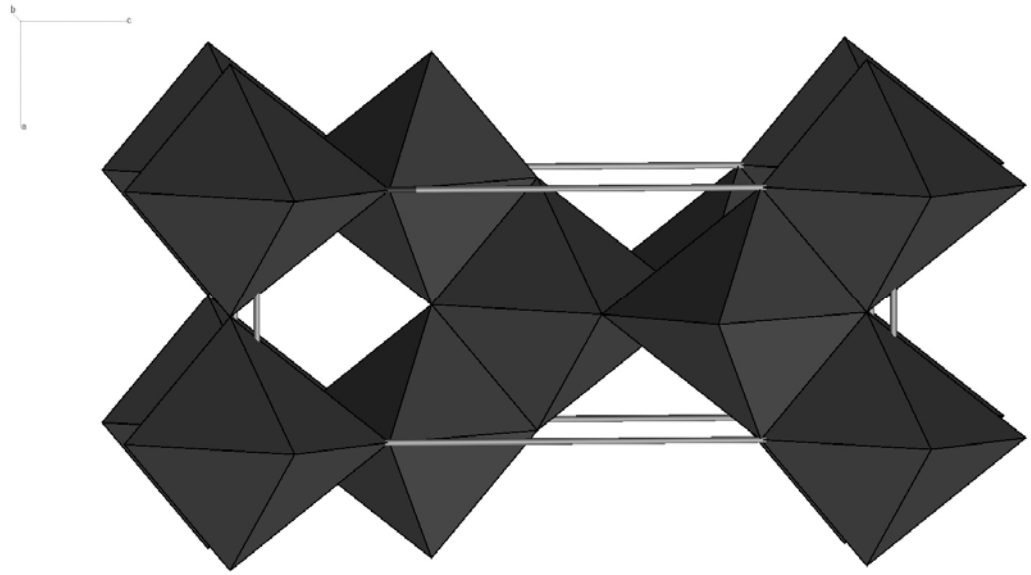

Figure 1.9a. Anatase TiO_2. All Ti atoms are in identical octahedral coordination with point symmetry $\bar{4}2m$. Octahedra share edges, but not faces. Each oxygen is bonded to three Ti atoms.

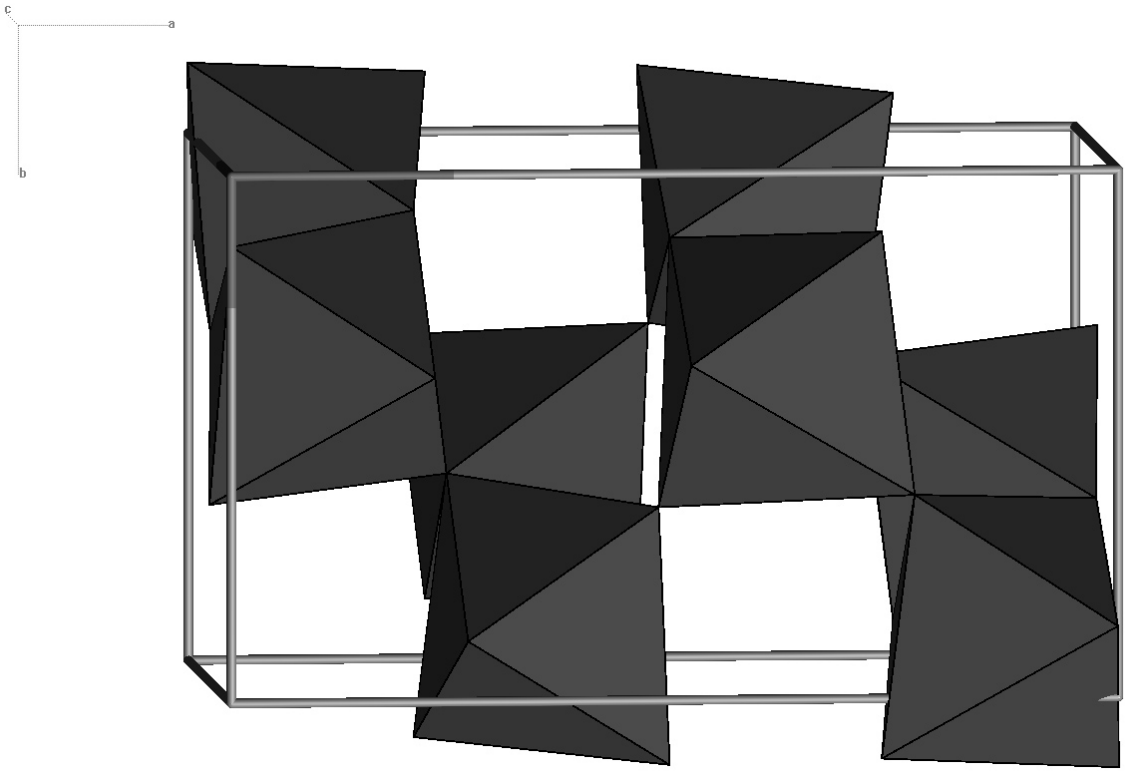

Figure 1.9b. Brookite TiO_2. All Ti atoms are in identical octahedral coordination with point symmetry 1. Octahedra share edges, but not faces. Each oxygen is bonded to three Ti atoms.

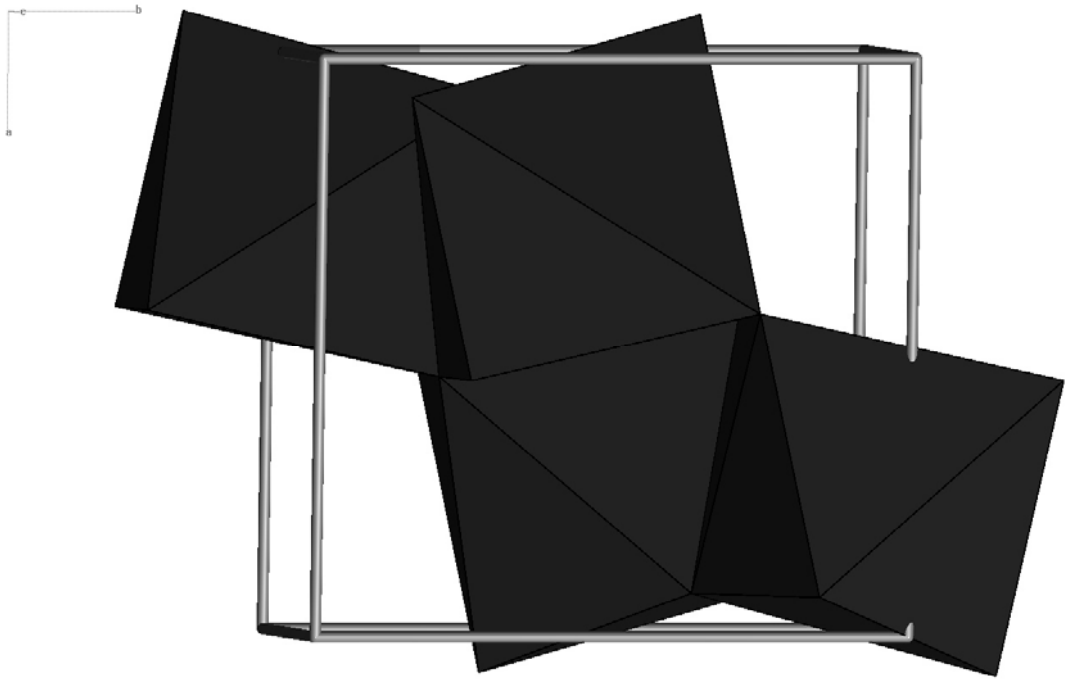

Figure 1.6. Baddeleyite ZrO_2. The structure is a distorted anti-fluorite structure with Zr in irregular 7-coordination with point symmetry 1.

Table 1.9.2. TiO_2 Polymorphs and Baddeleyite Cation Sites

End Member	Rutile	Anatase	Brookite	Baddeleyite
C.N.	6	6	6	7
Cation	Ti	Ti	Ti	Zr
Point Sym.	*mmm*	$\bar{4}2m$	1	1
Wyckoff Not.	2a	4a	8c	4e
Frac. Coords.				
x	0	0	0.1290	0.2758
y	0	3/4	0.0972	0.0411
z	0	1/8	-0.1371	0.2082
Distances				
O1	(2)1.977	(2)1.964	1.993	2.051
O1	(4)1.944	(4)1.937	1.865	2.163
O1			1.993	2.057
O2			1.919	2.151
O2			2.046	2.285
O2				2.189
Mean	1.955	1.946	1.959	2.159
σ	0.017	0.014	0.062	0.084
Poly.Vol.	9.846	9.374	9.741	14.533
O.Q.E.	1.0081	1.0319	1.0204	-
Ang.Var.	28.4	113.7	68.6	
Site Energy	-4133.	-4094.	-4107.	-3893.

1.10. MnO_2 Polymorphs

Table 1.10.1. MnO_2 Polymorph Unit Cells

End Member	Pyrolusite	Ramsdellite
Formula	MnO_2	MnO_2
Form.Wt.	86.937	86.937
Density	5.203	4.874
Mol. Vol.	16.708	17.838
Z	2	4
Cryst.Sys.	Tetragonal	Orthorhombic
Laue Grp.	4/*mmm*	*mmm*
Space Group	$P4_2/mnm$	*Pnam*
Cell Parameters		
a	4.396	9.32
b	4.396	4.46
c	2.871	2.850
Vol.	55.48	118.47
Ref.	Kondrasev & Zaslevskij (1951)	Kondrasev & Zaslevskij (1951)

Figure 1.10. Ramsdellite MnO_2. All Mn4+ atoms are in identical octahedral coordination with point symmetry m.

Table 1.10.2. MnO_2 Polymorph Cation Sites.

End Member	Pyrolusite	Ramsdellite
C.N.	6	6
Cation	Mn	Mn
Point Sym.	*mmm*	*m*
Wyckoff Not.	2*a*	4*c*
Frac. Coords.		
x	0	0.140
y	0	0.020
z	0	¼
Distances		
O1	(2)1.878	(2)1.949
O1	(4)1.890	(1)1.887
O2		(2)1.861
O2		(1)1.837
Mean	1.887	1.891
σ	0.007	0.048
Poly.Vol.	8.847	8.798
O.Q.E.	1.0079	1.0169
Ang.Var.	28.0	54.1
Site Energy	-4289.	-4127.

1.11.4 Uraninite Group

Table 1.11.1. Uraninite Group Unit Cells.

End Member	Uraninite	Thorianite
Formula	UO_2	ThO_2
Form.Wt.	270.029	264.039
Density	10.968	9.987
Mol. Vol.	24.620	26.439
Z	4	4
Cryst.Sys.	Isometric	Isometric
Laue Grp.	*m*3*m*	*m*3*m*
Space Group	*Fm*3*m*	*Fm*3*m*
Cell Parameters		
a	5.4682	5.5997
Vol.	163.51	175.59
Ref.	Leonova (1959)	Vogel & Kempter (1959)

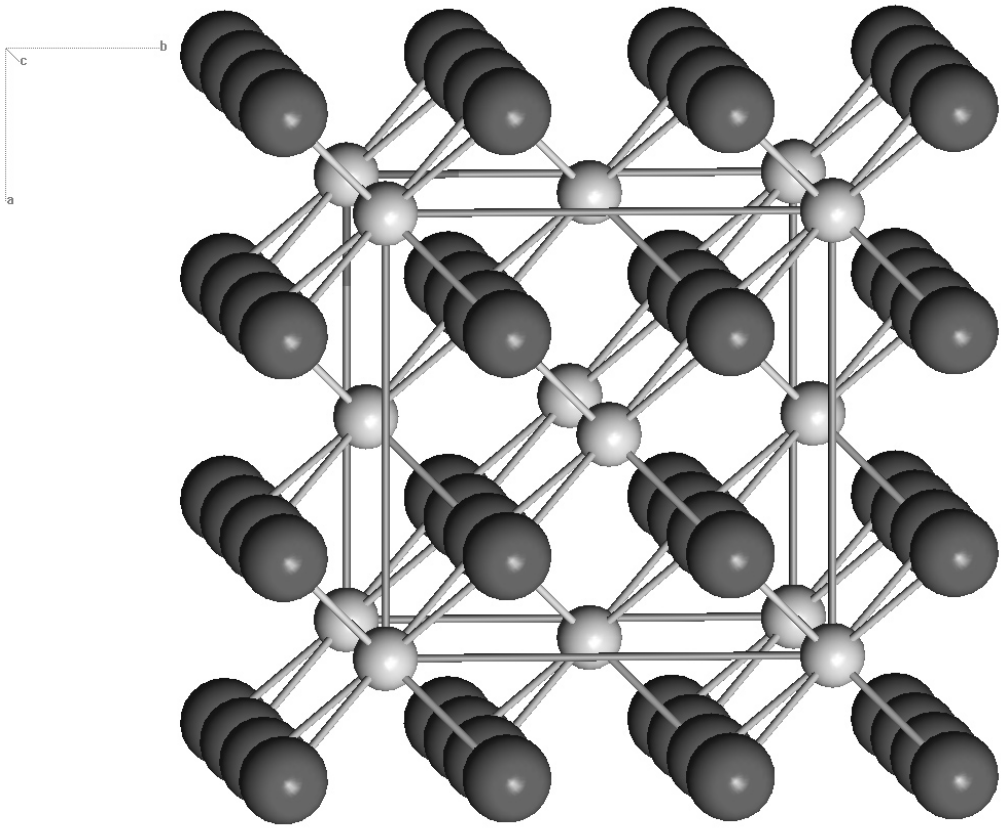

Figure 1.11. Uraninite UO_2. All U^{4+} atoms are in identical eight-fold cubic coordination with point symmetry m3m. Thorianite (ThO_2), cerianite (CeO_2), and fluorite (CaF_2) are isostructural.

Table 1.11.2. Uraninite Group Cation Sites

End Member	Uraninite	Thorianite
C.N.	8	8
Cation	U^{4+}	Th^{4+}
Point Sym.	*m*3*m*	*m*3*m*
Wyckoff Not.	4*b*	4*b*
Frac. Coords.		
x	0	0
y	0	0
z	0	0
Distances		
O(8)	2.368	2.425
Poly.Vol.	40.876	43.807
Site Energy	-3396.	-3316.
Ref.	Leonova (1959)	Vogel & Kempter (1959)

1.12. TeO_2 Polymorphs

Table 1.12.1. TeO_2 Polymorph Unit Cells

End Member	Tellurite	Paratellurite
Formula	TeO_2	TeO_2
Form.Wt.	159.599	159.599
Density	5.749	6.043
Mol. Vol.	27.759	26.412
Z	8	4
Cryst.Sys.	Orthorhombic	Tetragonal
Laue Grp.	*mmm*	422
Space Group	*Pbca*	$P4_12_12$
Cell Parameters		
a	12.035	4.796
b	5.464	4.796
c	5.607	7.626
Vol.	368.71	175.41
Ref.	Beyer (1967)	Leciejewicz (1961)

Table 1.12.2. TeO_2 Polymorph Cation Sites

End Member	Tellurite	Paratellurite
C.N.	4	4
Cation	Te	Te
Point Sym.	1	2
Wyckoff Not.	8d	4a
Frac. Coords.		
X	0.1182	0.0200
y	0.0255	0.0200
z	0.3781	0
Distances		
O1	1.877	(2)1.919
O2	2.196	(2)2.087
O3	1.927	
O4	2.070	
Mean	2.018	2.003
σ	0.144	0.097
Poly.Vol.	2.494	2.508
T.Q.E.	1.424	1.395
Ang.Var.	544.	651.
Site Energy	-3758.	-3784.

2.1.1. Ilmenite Group

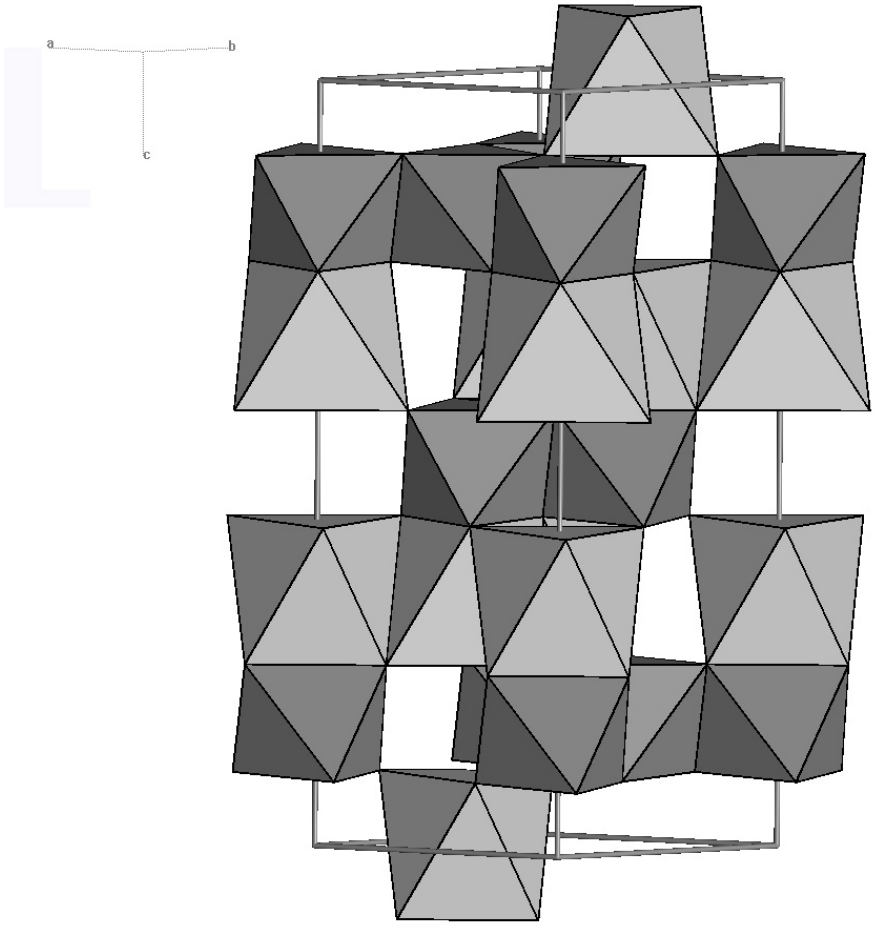

Figure 2.1. The crystal structure of ilmenite ($FeTiO_3$), [1 1 0] projection, *c* vertical. The structure is an ordered derivative of the corundum structure with Fe and Ti both in octahedral coordination but ordered into alternate layers in the *c*-direction. The structure is dense with face-sharing octahedra.

Table 2.1.1. Ilmenite Group Unit Cells

End Member	Ilmenite	Pyrophanite	Akimotoite
Formula	$FeTiO_3$	$MnTiO_3$	$MgSiO_3$
Form.Wt.	151.745	150.836	100.396
Density	4.786	4.603	3.810
Mol. Vol.	31.705	32.766	26.354
Z	6	6	6
Cryst.Sys.	Trigonal	Trigonal	Trigonal
Laue Grp.	$\bar{3}$	$\bar{3}$	$\bar{3}$
Space Group	$R\bar{3}$	$R\bar{3}$	$R\bar{3}$
Cell Parameters			
a	5.0884	5.137	4.7286
c	14.0855	14.283	13.5591
Vol.	315.84	326.41	262.54
Ref.	Wechsler & Prewitt (1984)	Wyckoff (1963)	Horiuchi et al. (1982)

Table 2.1.1.2. Ilmenite Group Tetravalent Metal Sites

End Member	Ilmenite	Pyrophanite	Akimotoite
C.N.	6	6	6
Cation	Ti	Ti	Si
Point Sym.	3	3	3
Wyckoff Not.	6c	6c	6c
Frac. Coords.			
X	0	0	0
y	0	0	0
z	0.14640	0.1430	0.15768
Distances			
O(2)	2.089	2.190	1.830
O(4)	1.874	1.912	1.768
Mean	1.982	2.051	1.799
σ	0.117	0.152	0.034
Poly.Vol.	10.001	11.067	7.592
O.Q.E.	1.0277	1.0310	1.0152
Ang.Var.	86.0	91.4	52.8
Site Potential	-3959.	-3809.	-4352.

Table 2.1.1.2. Ilmenite Group Divalent Metal Sites.

End Member	Ilmenite	Pyrophanite	Akimotoite
C.N.	6	6	6
Cation	Fe	Mn	Mg
Point Sym.	3	3	3
Wyckoff Not.	6c	6c	6c
Frac. Coords.			
X	0	0	0
y	0	0	0
z	0.35537	0.3570	0.3597
Distances			
O(3)	2.201	2.230	2.163
O(3)	2.078	2.024	1.990
Mean	2.081	2.230	2.076
σ	0.068	0.113	0.095
Poly.Vol.	12.562	12.336	11.238
O.Q.E.	1.0271	1.0289	1.0429
Ang.Var.	91.8	91.8	143.4
Site Potential	-1179.	-1220.	-1183.

2.2. Perovskite Group

There are numerous compounds with this structure or derivatives. The mineral perovskite is $CaTiO_3$, but $MgSiO_3$ adopts this structure at pressures above 23 GPa and likely constitutes about 40% of the total mass of the Earth.

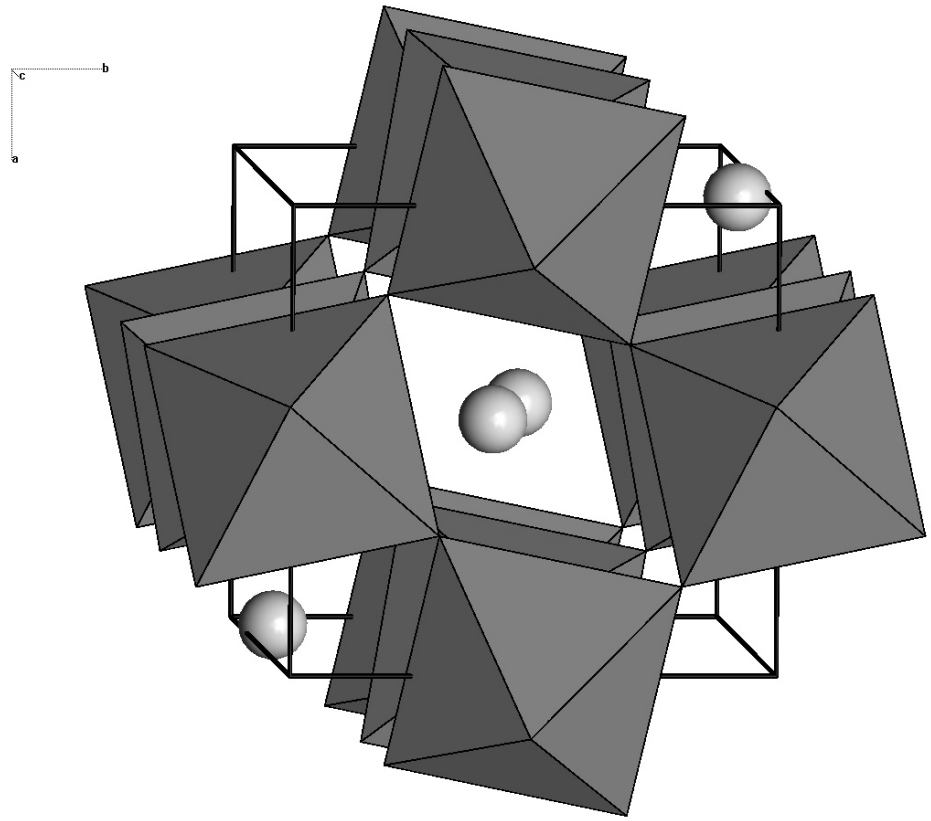

Figure 2.2. Perovskite, $CaTiO_3$, perspective c-axis projection, a vertical

Table 2.2.1. Perovskite Group Unit Cells.

End Member	Perovskite	$MgSiO_3$
Formula	$CaTiO_3$	$MgSiO_3$
Form.Wt.	135.98	100.396
Density	4.044	4.107
Mol. Vol.	33.63	24.445
Z	4	4
Cryst.Sys.	Orthorhombic	Orthorhombic
Laue Grp.	*mmm*	*mmm*
Space Group	*Pbnm*	*Pbnm*
Cell Parameters		
a	5.3670	4.7754
b	5.4439	4.9292
c	7.6438	6.8969
Vol.	223.33	162.35
Ref.	Kay & Bailey (1957)	Horiuchi etal. (1987)

Table 2.2.2. Perovskite Group Cation Sites.

End Member	Perovskite		$MgSiO_3$	
C.N.	10	6	8	6
Cation	Ca	Ti	Mg	Si
Point Sym.	m	$\bar{1}$	m	$\bar{1}$
Wyckoff Not.	4c	4b	4c	4b
Frac. Coords.				
x	0	0	0.974	0
y	0.030	½	0.063	½
z	¼	0	¼	0
Distances				
O1	(1)2.794	(2)1.924	(1)2.014	(2)1.801
O1	(1)2.664		(1)2.097	
O1	(1)2.883			
O1	(1)2.486			
O2	(2)2.584	(2)1.924	(2)2.278	(2)1.782
O2	(2)2.553	(2)1.928	(2)2.052	(2)1.796
O2	(2)2.685		(2)2.427	
Mean	2.647	1.926	2.203	1.793
σ	0.121	0.002	0.171	0.008
Poly.Vol.	37.112	9.492	20.100	7.681
O.Q.E.		1.0019		1.0005
Ang.Var.		6.7		1.6
Site Energy	-950.	-4256.	-1143.	-4518.

2.3. Oxide Spinel Group

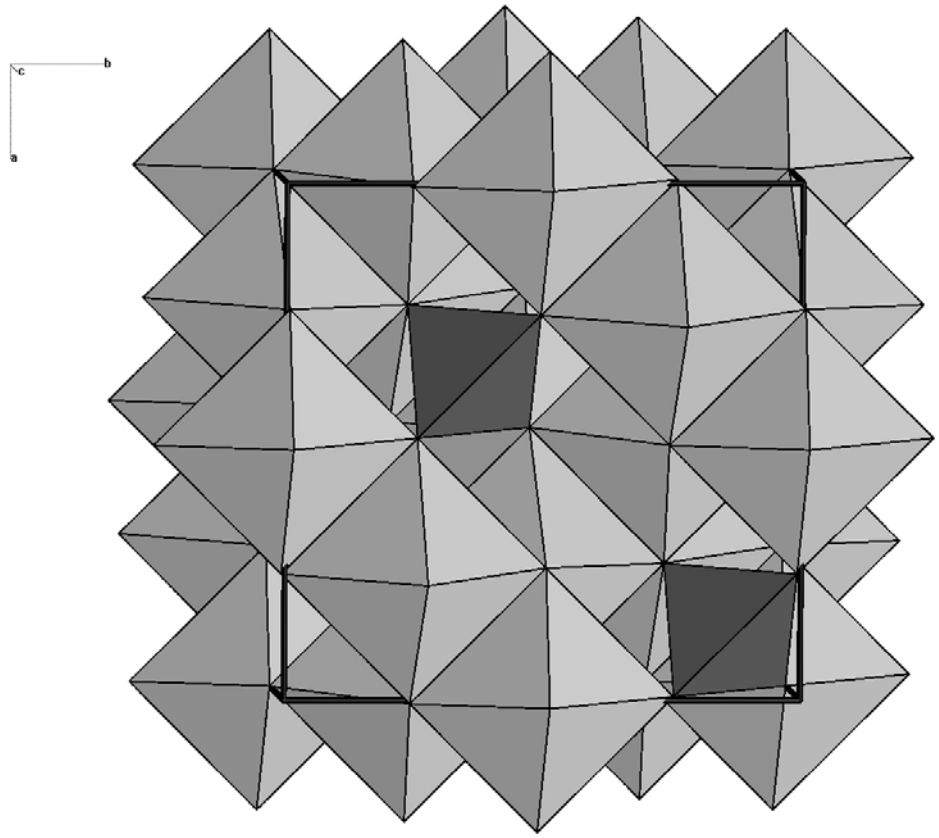

Figure 2.3. Spinel, $MgAl_2O_4$, perspective *a*-axis projection. Oxygen is in an approximately cubic close-packed arrangement, and there are twice as many octahedral as tetrahedral sites. The octahedron has point symmetry $\bar{3}m$, and the tetrahedron $\bar{4}3m$. All oxygen atoms are in identical environments bonded to three octahedral and a single tetrahedral cation.

Table 2.3.1. Oxide Spinel Group Unit Cells.

End Member	Spinel	Hercynite	Magnesio-Ferrite	Magnetite	Jacobsite	Magnesio-chromite	Chromite	Ulvospinel
Formula	$MgAl_2O_4$	$FeAl_2O_4$	$MgFe_2O_4$	$FeFe_2O_4$	$MnFe_2O_4$	$MgCr_2O_4$	$FeCr_2O_4$	$TiFe_2O_4$
Form.Wt.	142.273	173.808	200.004	231.539	230.630	192.302	223.837	223.592
Density	3.578	4.256	4.547	5.200	4.969	4.414	5.054	4.775
Mol. Vol.	39.762	40.843	43.989	44.528	46.416	43.564	44.293	46.826
Z	8	8	8	8	8	8	8	8
Cryst.Sys.	Isometric	Isometric	Isometric	Isometric	Isometric	Isometric	Isometric	Isometric
Laue Grp.	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$	$m\bar{3}m$
Space Group	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$
Cell Parameters								
a	8.0832	8.1558	8.360	8.394	8.5110	8.333	8.3792	8.536
Vol.	528.14	542.50	584.28	591.43	616.51	578.63	588.31	621.96
Ref.	Fischer (1967)	Hill (1984)	Hill et al. (1979)	Hill et al. (1979)	Hill et al. (1979)	Hill et al. 1979)	Hill et al. (1979)	Ishikawa et al. (1972)

Table 2.3.2. Oxide Spinel Group Octahedral Sites.

End Member	Spinel	Hercynite	Magnesio-Ferrite	Magnetite	Jacobsite	Magnesio-chromite	Chromite	Ulvospinel
C.N.	6	6	6	6	6	6	6	6
Occupant	$Al_{.96}Mg_{.04}$	Al	$Mg_{.45}Fe_{.55}$	$Fe_{.5}Fe_{.5}$	$Fe_{.93}Mn_{.07}$	Cr	Cr	$Fe_{.5}Ti_{.5}$
Point Sym	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$
Wyckoff Not.	16*d*	16*d*	16*d*	16*d*	16*d*	16*d*	16*d*	16*d*
Frac.Coord.								
x	½	½	½	½	½	½	½	½
y	½	½	½	½	½	½	½	½
z	½	½	½	½	½	½	½	½
Distances								
O(6)	1.926	1.937	2.033	2.059	2.035	1.994	1.990	2.044
Poly.Vol.	9.371	9.505	11.151	11.612	11.074	10.440	10.322	11.252
O.Q.E.	1.0108	1.0125	1.0033	1.0015	1.0092	1.0087	1.0123	1.0084
Ang.Var.	40.8	47.4	12.2	5.6	34.7	32.8	46.7	31.6
Site Energy	-2407.	-2444.	-1791.	-1701.	-2226.	-2353.	-2377.	-2293.
Model Chg.	2.96	3.0	2.55	2.5	2.925	3.0	3.0	3.0

Table 2.3.3. Oxide Spinel Group Tetrahedral Sites.

End Member	Spinel	Hercynite	Magnesio-Ferrite	Magnetite	Jacobsite	Magnesio-chromite	Chromite	Ulvospinel
C.N.	4	4	4	4	4	4	4	4
Occupant	$Mg_{.93}Al_{.07}$	Fe	$Mg_{.10}Fe_{.90}$	Fe^{3+}	$Mn_{.85}Fe_{.15}$	Mg	Fe	Fe^{+2}
Point Sym	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$
Wyckoff Not.	8a	8a	8a	8a	8a	8a	8a	8a
Frac.Coord								
x	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
y	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
z	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
Distances								
O(4)	1.924	1.954	1.911	1.887	2.012	1.966	2.006	2.011
Poly.Vol.	3.653	3.827	3.584	3.449	4.181	3.899	4.141	4.172
T.Q.E.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Ang.Var.	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Site Energy	-1269.	-1179.	-2211.	-2384.	-1293.	-1189.	-1149.	-1164.
Model Chg.	2.07	2.00	2.90	3.0	2.15	2.0	2.0	2.0

2.4. Pseudobrookite Group

Table 2.4.1. Pseudobrookite Group Unit Cells

End Member	Pseudobrookote	Tialite	Armalcolite
Formula	Fe_2TiO_5	Al_2TiO_5	$(Mg_{.5}Fe_{.5})TiO_5$
Form.Wt.	239.591	181.860	215.876
Density	4.406	3.702	3.904
Mol. Vol.	54.375	49.128	55.298
Z	4	4	4
Cryst.Sys.	Orthorhombic	Orthorhombic	Orthorhombic
Laue Grp.	*mmm*	*mmm*	*mmm*
Space Group	*Bbmm*	*Bbmm*	*Bbmm*
Cell Parameters			
a	9.767	9.429	9.7762
b	9.947	9.636	10.0214
c	3.717	3.591	3.7485
Vol.	361.12	326.27	367.25
Ref.	Akimoto (1957)	Morosin & Lynch (1972)	Wechsler et al. (1976)

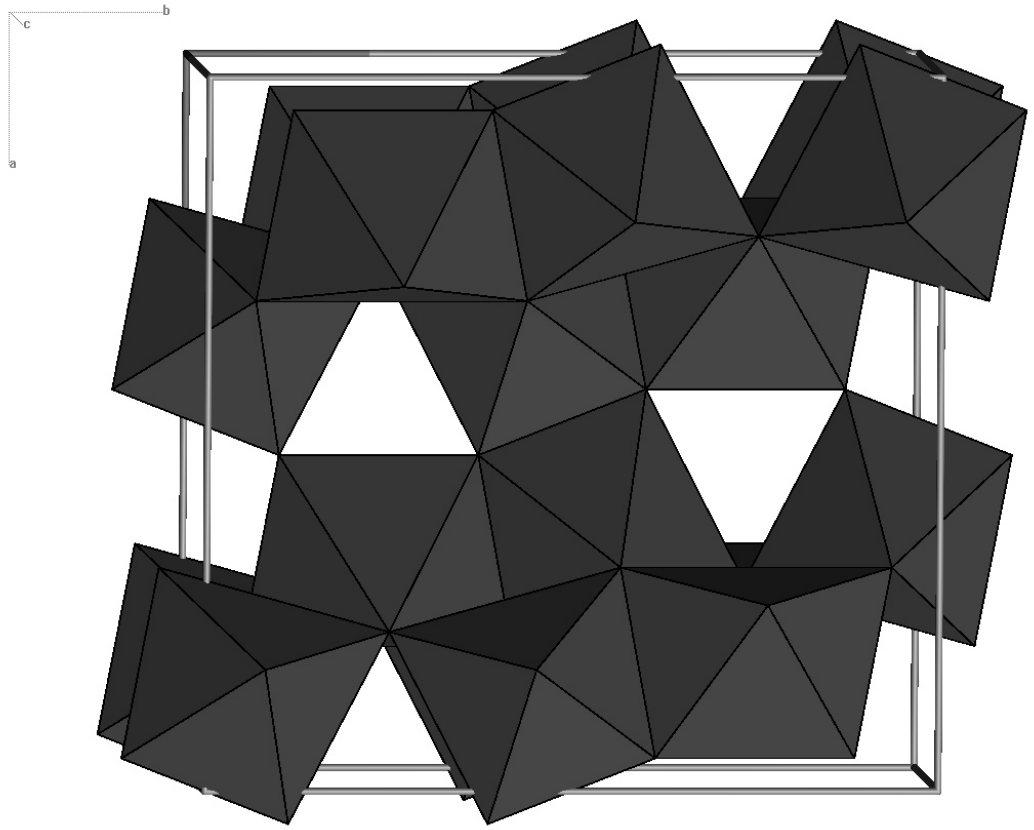

Figure 2.4. Pseudobrookite, Fe_2TiO_5. There are two distinct octahedral sites, M1 with point symmetry mm and M2 with point symmetry m. There are twice as many M2 sites as M1. In pseudobrookite and tialite (Al_2TiO_5), M2 is slight larger whereas in armalcolite ($(Mg,Fe)Ti_2O_5$) and ferropseudobrookite ($FeTi_2O_5$), M1 is slightly larger.

Table 2.4.2. Pseudobrookite Group M1 Sites

End Member	Pseudobrookote	Tialite	Armalcolite
C.N.	6	6	6
Cation	Ti	Ti	Fe.5Mg.5
Point Sym.	*mm*	*mm*	*mm*
Wyckoff Not.	4*c*	4*c*	4*c*
Frac. Coords.			
X	0.190	0.1854	0.19223
y	¼	¼	¼
z	0	0	0
Distances			
O1(2)	1.899	1.921	2.036
O2(2)	1.986	1.821	1.965
O3(2)	1.937	2.092	2.193
Mean	1.941	1.944	2.065
σ	0.039	0.122	0.104
Poly.Vol.	9.410	8.935	10.418
O.Q.E.	1.0239	1.0672	1.0848
Ang.Var.	76.1	181.8	230.9
Site Energy	-4093.	-4052.	-1248.
Model Chg.	4.0	4.0	2.0

Table 2.4.3. Pseudobrookite Group M2 Sites

End Member	Pseudobrookote	Tialite	Armalcolite
C.N.	6	6	6
Cation	Fe^{3+}	Al	Ti
Point Sym.	*m*	*m*	*m*
Wyckoff Not.	8*f*	8*f*	8*f*
Frac. Coords.			
X	0.135	0.13478	0.13479
y	0.560	0.56150	0.56447
z	0	0	0
Distances			
O1	2.304	2.080	2.064
O2	1.906	1.900	1.991
O2	1.827	1.808	1.845
O3	2.302	2.133	2.176
O3(2)	1.966	1.866	1.943
Mean	2.045	1.939	1.993
σ	0.206	0.126	0.114
Poly.Vol.	10.468	9.188	10.014
O.Q.E.	1.0678	1.0418	1.0391
Ang.Var.	207.0	128.1	121.5
Site Energy	-2395.	-2545.	-3941.
Model Chg.	3.0	3.0	4.0

2.5. Tungstate Group

2.5.1 Tungstate Group Unit Cells

End Member	Ferberite	Huebnerite	Scheelite
Formula	$FeWO_4$	$MnWO_4$	$CaWO_4$
Form.Wt.	303.695	302.786	287.928
Density	7.549	7.265	6.115
Mol. Vol.	40.228	41.676	47.087
Z	2	2	2
Cryst.Sys.	Monoclinic	Monoclinic	Tetragonal
Laue Grp.	2/*m*	2/*m*	4/*m*
Space Group	*P*2/*c*	*P*2/*c*	$I4_1/a$
Cell Parameters			
a	4.730	4.8238	5.243
b	5.703	5.7504	
c	4.952	4.9901	11.376
β	90.00	91.18	
Vol.	133.58	138.39	312.72
Ref.	Uelkue (1967)	Weitzel (1976)	Kay et al. (1964)

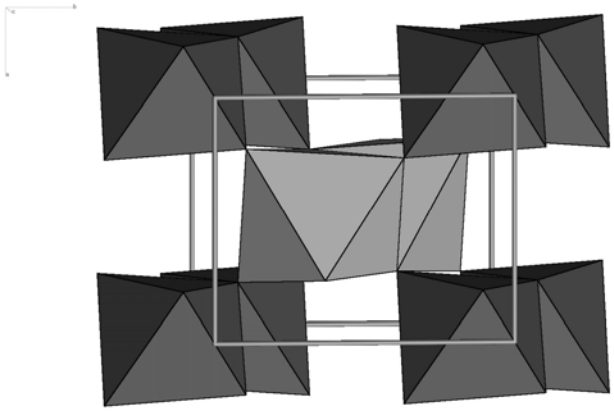

Figure 2.5. The crystal structure of ferberite, $FeWO_4$.

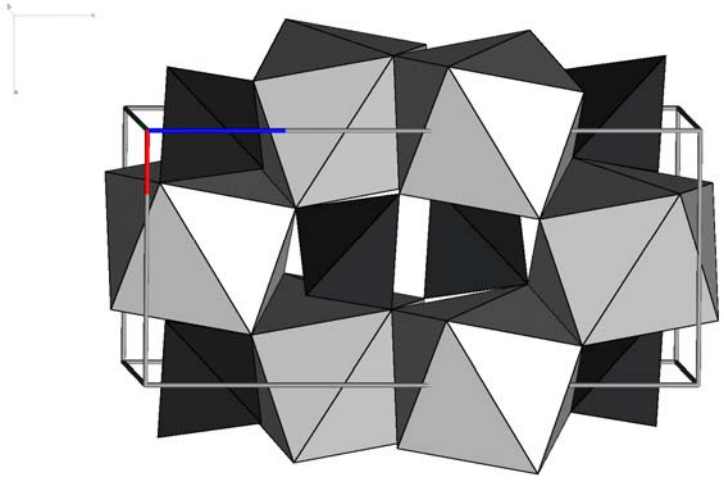

Figure 2.5. The crystal structure of scheelite, $CaWO_4$. Unlike ferberite and huebnerite, scheelite has tungsten in tetrahedral coordination.

Table 2.5.1. Tungstate Group Divalent Sites

End Member	Ferberite	Huebnerite	Scheelite
C.N.	6	6	6
Cation	Fe^{2+}	Mn2+	Ca
Point Sym.	2	2	2
Wyckoff Not.	2*f*	2*f*	4*b*
Frac. Coords.			
X	½	½	0
y	0.6744	0.6866	¼
z	¼	¼	$^5/_8$
Distances			
1	(2)2.057	(2)2.081	(4)2.479
2	(2)2.183	(2)2.294	(4)2.438
3	(2)2.146	(2)2.154	
Mean	2.129	2.176	2.458
σ	0.058	0.097	0.022
Poly.Vol.	12.559	13.286	26.376
O.Q.E.	1.0165	1.0246	
Ang.Var.	56.06	80.83	
Site Energy	-1297.	-1262.	-1144.

Table 2.5.3. Tungstate Group Tungsten Sites.

End Member	Ferberite	Huebnerite	Scheelite
C.N.	6	6	4
Cation	W	W	W
Point Sym.	2	2	-4
Wyckoff Not.	2*e*	2*e*	4*a*
Frac. Coords.			
X	0	0	0
y	0.1799	0.1853	¼
z	¼	¼	$^1/_8$
Distances			
1	(2)1.915	(2)1.936	(4)1.785
2	(2)2.122	(2)2.157	
3	(2)1.776	(2)1.756	
Mean	1.938	1.959	1.785
σ	0.156	0.179	0.000
Poly.Vol.	9.302	9.398	2.910
Q.E.	1.0339	1.0416	1.0024
Ang.Var.	95.94	115.87	9.65
Site Energy	-8255.	-8258.	-8225.

Table 4.1.1. Garnet Group Unit Cells.

End Member	Pyrope	Almandine	Spessartine	Grossular	Andradite	Uvarovite
Formula	$Mg_3Al_2Si_3O_{12}$	$Fe_3Al_2Si_3O_{12}$	$Mn_3Al_2Si_3O_{12}$	$Ca_3Al_2Si_3O_{12}$	$Ca_3Fe_2Si_3O_{12}$	$Ca_3Cr_2Si_3O_{12}$
Form. Wt. (g)	403.150	497.755	495.028	450.454	508.1858	500.483
Density (g/cm^3)	3.559	4.312	4.199	3.600	3.850	3.859
Mol. Vol. (cm^3)	113.28	115.43	117.88	125.12	131.99	129.71
Z	8	8	8	8	8	8
Cryst. Sys.	Isometric	Isometric	Isometric	Isometric	Isometric	Isometric
Laue Class	*m*3*m*	*m*3*m*	*m*3*m*	*m*3*m*	*m*3*m*	*m*3*m*
Space Group	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$	$Ia\bar{3}d$
Cell Parameters						
a (Å)	11.459	11.531	11.612	11.845	12.058	11.988
Vol.	1504.7	1533.2	1565.7	1661.9	1753.2	1722.8
Ref.	Novak & Gibbs (1971)	Novak & Gibbs (1971)	Novak & Gibbs (1971)	Novak & Gibbs (1971)	Novak & Gibbs (1971)	Novak & Gibbs (1971)

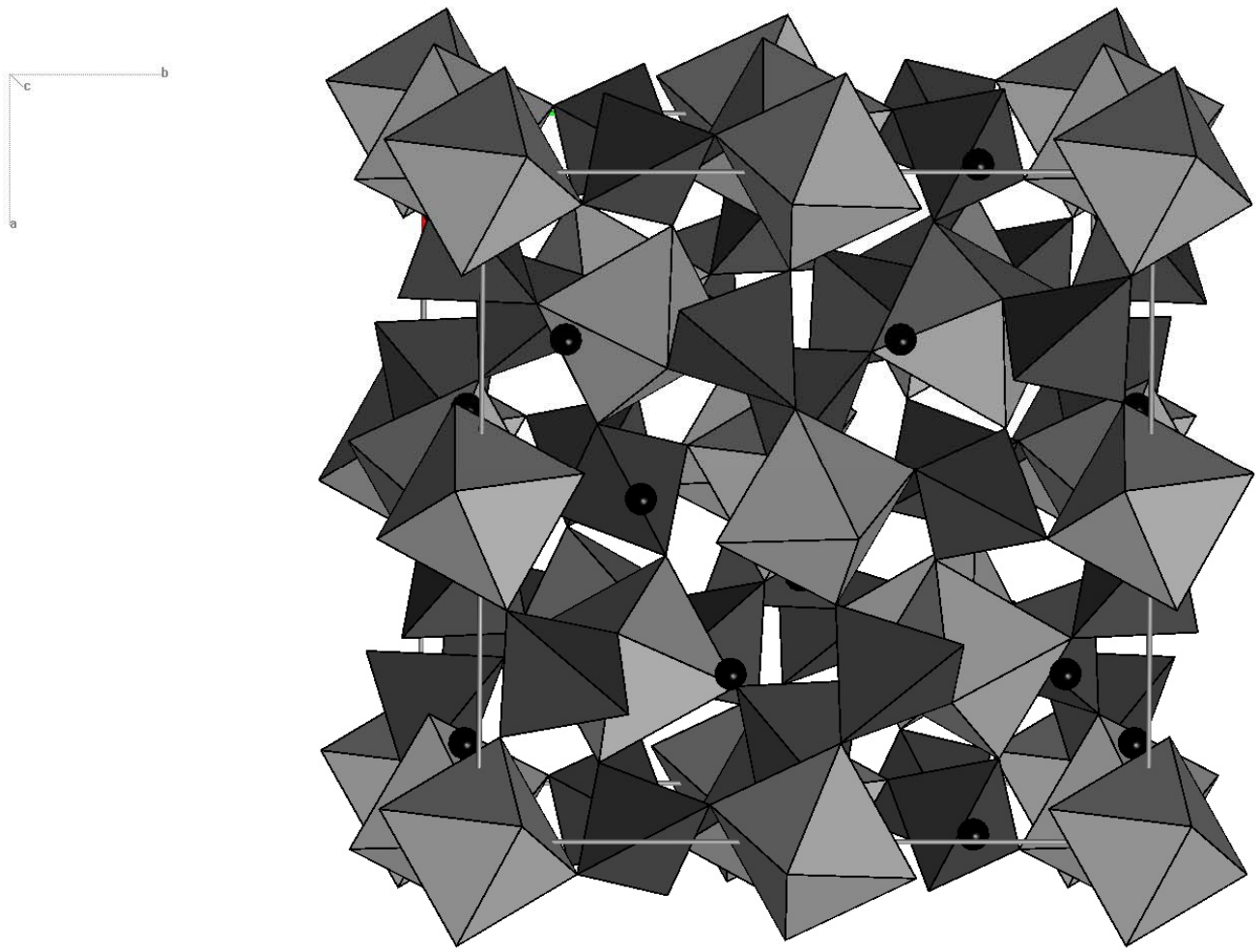

Figure 4.1. Garnet, perspective *a*-axis projection. The divalent cation, Mg, Fe^{2+}, Mn^{2+}, or Ca, is in eight-coordination (sphere) with point symmetry 222. The trivalent cation is in octahedral coordination with point symmetry $\bar{3}$. Si is in tetrahedral coordination with point symmetry $\bar{4}$. Although all Si-O distances are the same, the site is one of the most distorted of all silicates. All oxygen atoms are identical and have point symmetry 1.

Table 4.1.2. Garnet Group Dodecahedral Sites.

End Member	Pyrope	Almandine	Spessartine	Grossular	Andradite	Uvarovite
C.N.	8	8	8	8	8	8
Cation	Mg	Fe	Mn	Ca	Ca	Ca
Point Sym.	222	222	222	222	222	222
Wyckoff Not.	24*c*	24*c*	24*c*	24*c*	24*c*	24*c*
Frac. Coords.						
x	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
y	0	0	0	0	0	0
z	¼	¼	¼	¼	¼	¼
Distances						
1(4)	2.197	2.220	2.245	2.319	2.365	2.360
2(4)	2.343	2.378	2.406	2.490	2.500	2.499
Mean	2.270	2.299	2.236	2.405	2.433	2.429
σ	0.078	0.084	0.086	0.091	0.072	0.075
Poly.Vol.	20.14	20.93	21.65	23.88	24.55	24.48
Elect.Energy	-1126.	-1101.	-1080.	-1022.	-1015.	-1010.

Table 4.1.3. Garnet Group Octahedral Sites.

End Member	Pyrope	Almandine	Spessartine	Grossular	Andradite	Uvarovite
C.N.	6	6	6	6	6	6
Cation	Al	Al	Al	Al	Fe	Cr
Point Sym.	$\bar{3}$	$\bar{3}$	$\bar{3}$	$\bar{3}$	$\bar{3}$	$\bar{3}$
Wyckoff Not.	16*a*	16*a*	16*a*	16*a*	16*a*	16*a*
Frac. Coords.						
x	0	0	0	0	0	0
y	0	0	0	0	0	0
z	0	0	0	0	0	0
Distances						
O(6)	1.887	1.896	1.901	1.924	2.024	1.985
Poly.Vol.	8.937	9.086	9.155	9.491	11.046	10.413
Q.E.	1.0014	1.0004	1.0001	1.0007	1.0004	1.0007
Ang.Var.	4.93	1.38	0.30	2.33	1.36	2.64
Elect. Energy	-2666.	-2655.	-2658.	-2640.	-2455.	-2527.

Table 4.1.4. Garnet Group Tetrahedral Sites.

End Member	Pyrope	Almandine	Spessartine	Grossular	Andradite	Uvarovite
C.N.	4	4	4	4	4	4
Cation	Si	Si	Si	Si	Si	Si
Point Sym.	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$	$\bar{4}$
Wyckoff Not.	24*d*	24*d*	24*d*	24*d*	24*d*	24*d*
Frac. Coords.						
x	$^3/_8$	$^3/_8$	$^3/_8$	$^3/_8$	$^3/_8$	$^3/_8$
y	0	0	0	0	0	0
z	¼	¼	¼	¼	¼	¼
Distances						
O(4)	1.635	1.628	1.636	1.645	1.643	1.643
Poly.Vol.	2.192	2.172	2.206	2.261	2.250	2.257
Q.E.	1.0150	1.0134	1.0117	1.0073	1.0071	1.0058
Ang.Var.	61.6	55.2	48.0	29.8	28.9	23.9
Elect.Energy	-4380.	-4413.	-4400.	-4402.	-4432.	-4426.

Table 4.2.1. Olivine Group Unit Cells.

End Member	Forsterite	Fayalite	Monticellite	Kirschsteinite	Ca-olivine	Tephroite	Co-olivine	Liebenbergite
Formula	Mg_2SiO_4	Fe_2SiO_4	$CaMgSiO_4$	$CaFeSiO_4$	Ca_2SiO_4	Mn_2SiO_4	Co_2SiO_4	Ni_2SiO_4
Form. Wt. (g)	140.708	203.778	156.476	188.011	172.744	201.960	209.959	209.503
Density (g/cm^3)	3.227	4.402	3.040	3.965	2.969	4.127	4.719	4.921
Mol. Vol. (cm^3)	43.603	46.290	51.472	47.415	58.020	48.939	44.493	42.572
Z	4	4	4	4	4	4	4	4
Cryst. Sys.	Orthorh.	Orthorh.	Orthorh.	Orthorh.	Orthorh.	Orthorh.	Orthorh.	Orthorh.
Laue Class	*mmm*	*mmm*	*mmm*	*mmm*	*mmm*	*mmm*	*mmm*	*mmm*
Space Group	*Pbnm*	*Pbnm*	*Pbnm*	*Pbnm*	*Pbnm*	*Pbnm*	*Pbnm*	*Pbnm*
Cell Parameters								
a (Å)	4.7534	4.8195	4.822	4.844	5.078	4.9023	4.7811	4.726
b (Å)	10.1902	10.4788	11.108	10.577	11.225	10.5964	10.2998	10.118
c (Å)	5.9783	6.0873	6.382	6.146	6.760	6.2567	6.0004	5.913
Vol.	289.58	307.42	341.84	314.89	385.32	325.02	295.49	282.75
Ref.	Fujino et al. (1981)	Fujino et al. (1981)	Onken (1971)	Brown (1970)	Czaya (1971)	Fujino et al. (1981)	Brown (1970)	Lager & Meagher(1978)

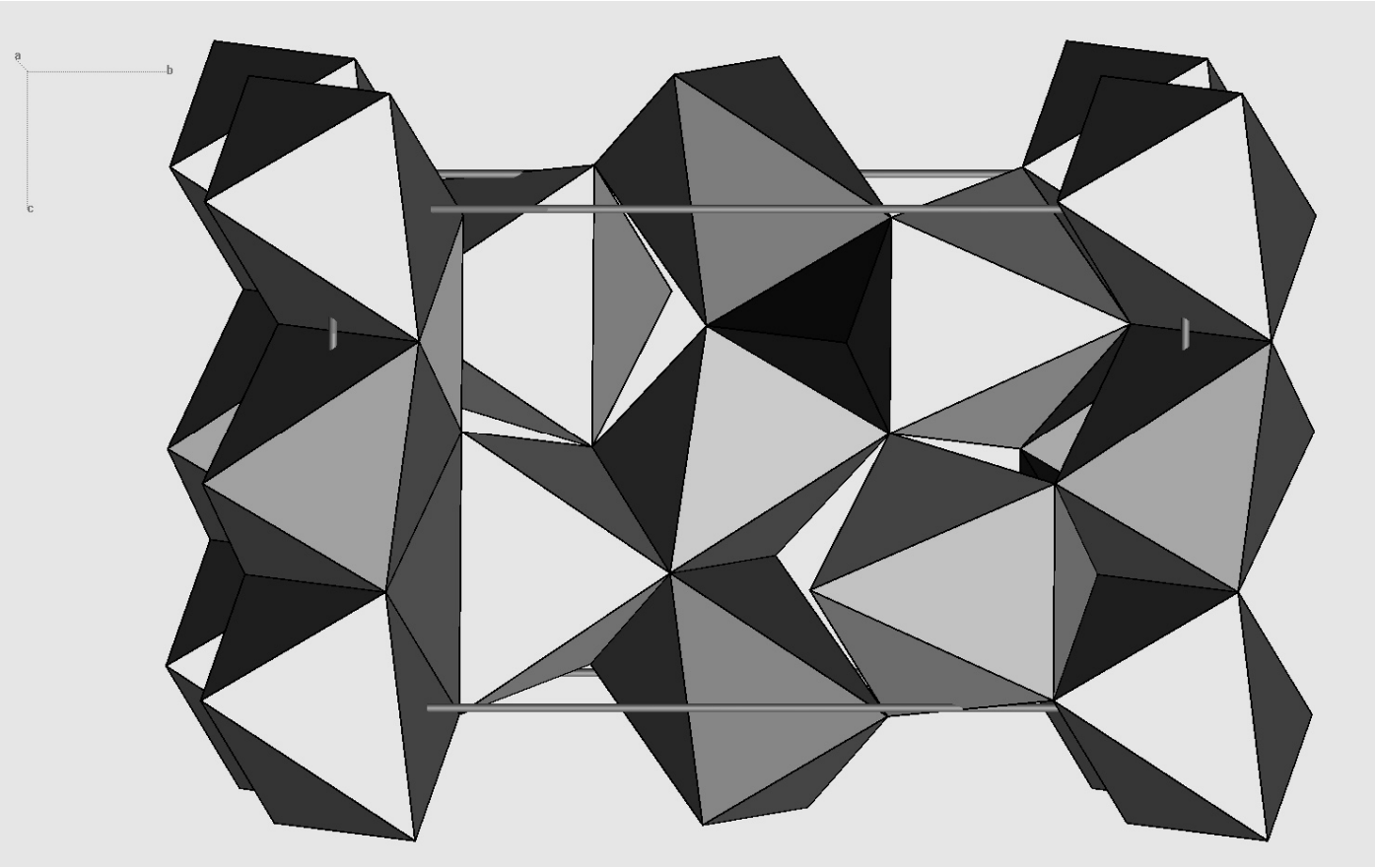

Figure 4.2. Olivine, perspective a-axis projection, c-vertical. There are two distinct octahedral sites, M1 and M2, and a single Si tetrahedron. The space group is *Pbnm* with mirror planes perpendicular to *c* at ¼ and ¾. M2 and Si are on the mirror planes, and M1 at the origin.

Table 4.2.2. Olivine Group M1 Octahedral Sites.

End Member	Forsterite	Fayalite	Monticellite	Kirschsteinite	Ca-olivine	Tephroite	Co-olivine	Liebenbergite
C.N.	6	6	6	6	6	6	6	6
Cation	Mg	Fe^{2+}	Mg	Fe^{2+}	Ca	Mn	Co	Ni
Point Sym.	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$	$\bar{1}$
Wyckoff Not.	4*a*	4*a*	4*a*	4*a*	4*a*	4*a*	4*a*	4*a*
Frac. Coords.								
x	0	0	0	0	0	0	0	0
y	0	0	0	0	0	0	0	0
z	0	0	0	0	0	0	0	0
Distances								
O1(2)	2.0838	2.1207	2.193	2.139	2.356	2.2003	2.098	2.064
O2(2)	2.0678	2.1259	2.090	2.098	2.311	2.1671	2.091	2.060
O3(2)	2.1311	2.2363	2.119	2.154	2.388	2.2498	2.167	2.111
Mean	2.094	2.161	2.134	2.130	2.352	2.206	2.119	2.078
σ	0.029	0.058	0.047	0.026	0.035	0.037	0.037	0.026
Poly.Vol.	11.771	12.737	12.420	12.105	15.896	13.499	12.144	11.531
O.Q.E.	1.0269	1.0379	1.0287	1.0427	1.0601	1.0398	1.0294	1.0254
Ang.Var.	95.3	130.1	100.3	147.9	209.0	138.8	102.9	90.3
Elect.Energy	-1082.	-1041.	-1078.	-1063.	-945.	-1015.	-1064.	-1090.

Table 4.2.3. Olivine Group M2 Octahedral Sites.

End Member	Forsterite	Fayalite	Monticellite	Kirschsteinite	Ca-olivine	Tephroite	Co-olivine	Liebenbergite
C.N.	6	6	6	6	6	6	6	6
Cation	Mg	Fe^{2+}	Ca	Ca	Ca	Mn	Co	Ni
Point Sym.	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*
Wyckoff Not.	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*
Frac. Coords.								
x	0.99169	0.98598	0.9770	0.9888	0.9904	0.98792	0.9915	0.9924
y	0.27739	0.28026	0.2767	0.2799	0.2809	0.28041	0.2764	0.2738
z	¼	¼	¼	¼	¼	¼	¼	¼
Distances								
O1(1)	2.1766	2.2331	2.478	2.388	2.441	2.2782	2.187	2.105
O2(1)	2.0454	2.1109	2.308	2.146	2.286	2.1369	2.072	2.043
O3(2)	2.0658	2.0647	2.287	2.212	2.385	2.1547	2.073	2.053
O3(2)	2.2101	2.2946	411	2.325	2.426	2.3194	2.223	2.171
Mean	2.129	2.177	2.364	2.268	2.392	2.227	2.142	2.100
σ	0.078	0.110	0.080	0.092	0.057	0.088	0.077	0.066
Poly.Vol.	12.401	13.072	16.438	14.549	16.930	13.982	12.606	11.966
O.Q.E.	1.0260	1.0370	1.0481	1.0468	1.0516	1.0367	1.0269	1.0215
Ang.Var.	89.5	124.9	165.6	161.1	180.8	127.0	92.7	74.9
Elect.Energy	-1160	-1136.	-1010.	-1061.	-1008.	-1102.	-1153.	-1179.

Table 4.2.4. Olivine Group Tetrahedral Sites.

End Member	Forsterite	Fayalite	Monticellite	Kirschsteinite	Ca-olivine	Tephroite	Co-olivine	Liebenbergite
C.N.	4	4	4	4	4	4	4	4
Cation	Si	Si	Si	Si	Si	Si	Si	Si
Point Sym.	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*
Wyckoff Not.	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*	4*c*
Frac. Coords.								
x	0.42645	0.43122	0.4101	0.4181	0.4293	0.42755	0.4282	0.4276
y	0.09403	0.09765	0.0811	0.0846	0.0959	0.09643	0.0949	0.0944
z	¼	¼	¼	¼	¼	¼	¼	¼
Distances								
O1(1)	1.6139	1.6248	1.614	1.612	1.633	1.6191	1.613	1.620
O2(1)	1.6549	1.6533	1.656	1.568	1.655	1.6578	1.659	1.660
O3(2)	1.6368	1.6333	1.639	1.551	1.647	1.6395	1.656	1.637
Mean	1.636	1.636	1.637	1.570	1.646	1.639	1.636	1.638
σ	0.017	0.012	0.017	0.029	0.009	0.016	0.019	0.016
Poly.Vol.	2.209	2.220	2.220	1.958	2.266	2.232	2.216	2.218
Q.E.	1.0110	1.0085	1.0092	1.0102	1.0062	1.0082	1.0100	1.0118
Ang.Var.	49.4	36.7	40.6	36.8	27.2	36.1	44.3	52.3
Elect.Energy	-4319.	-4348.	-4333.	-4551.	-4377.	-4349.	-4326.	-4305.

Table 4.3.1. Silicate Spinel Unit Cells.

End Member	Ringwoodite	Fe_2SiO_4	Co_2SiO_4	Ni_2SiO_4
Formula	Mg_2SiO_4	Fe_2SiO_4	Co_2SiO_4	Ni_2SiO_4
Form. Wt. (g)	140.708	203.778	209.950	209.503
Density (g/cm^3)	3.563	4.848	5.174	5.346
Mol. Vol. (cm^3)	39.493	42.030	40.577	39.187
Z	8	8	8	8
Cryst. Sys.	Isometric	Isometric	Isometric	Isometric
Laue Class	*m*3*m*	*m*3*m*	*m*3*m*	*m*3*m*
Space Group	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$	$Fd\bar{3}m$
Cell Parameters				
a (Å)	8.0649	8.234	8.138	8.044
Vol.	524.56	558.26	538.96	520.49
Ref.	Sasaki et al. (1982a)	Yagi et al. (1974)	Morimoto et al. (1974)	Yagi et al. (1974)

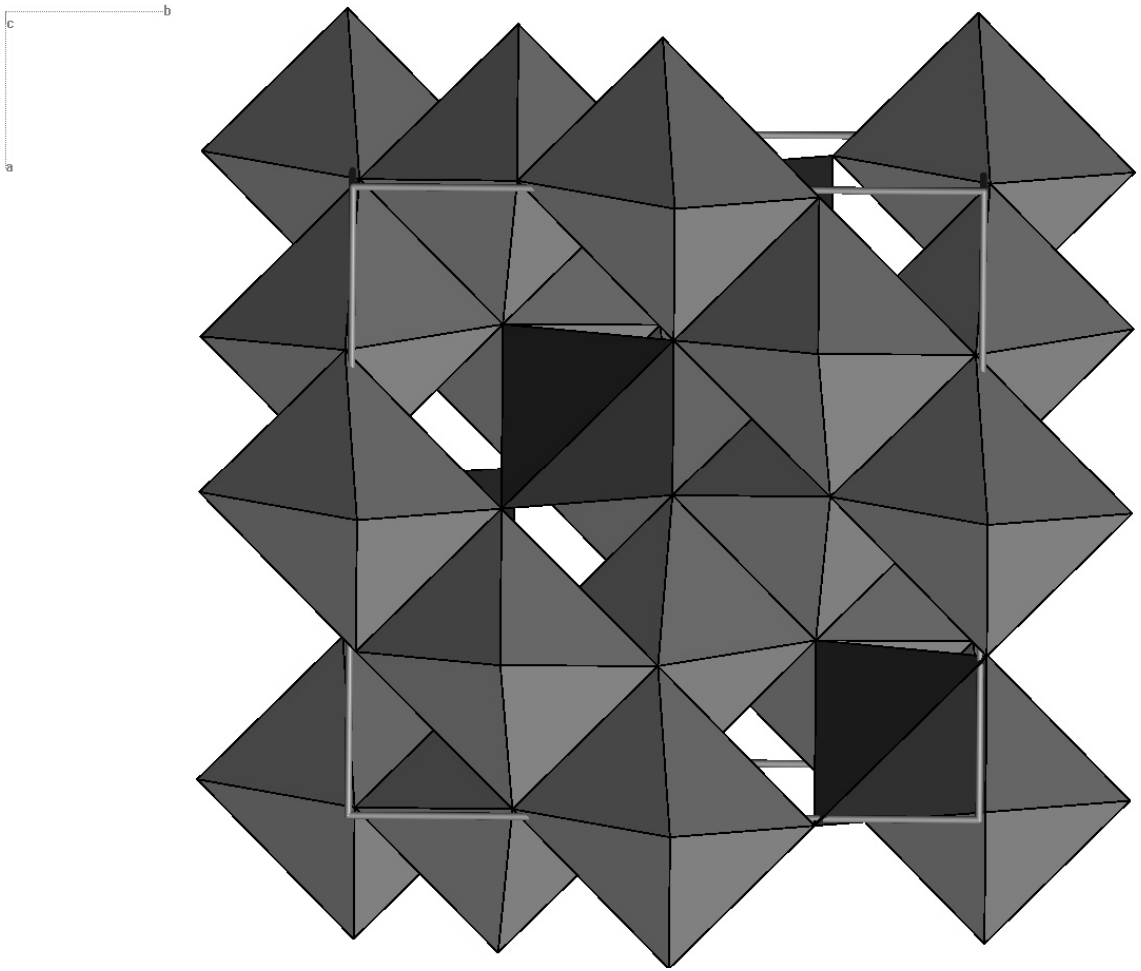

Figure 4.3. Silicate spinel, ringwoodite (Mg_2SiO_4). Divalent cations are in octahedral coordination, Si is in tetrahedral coordination. All oxygens are equivalent and bonded to three Mg and one Si.

Table 4.3.2. Silicate Spinel Octahedral Sites.

End Member	Ringwoodite	Fe_2SiO_4	Co_2SiO_4	Ni_2SiO_4
C.N.	6	6	6	6
Occupant	Mg	Fe2+	Co	Ni
Point SYm.	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$	$\bar{3}m$
Wyckoff Not.	16*d*	16*d*	16*d*	16*d*
Frac.Coord.				
x	½	½	½	½
y	½	½	½	½
z	½	½	½	½
Distances				
O(6)	2.070	2.137	2.103	2.063
Poly.Vol.	11.780	12.912	12.332	11.663
Q.E.	1.0026	1.0051	1.0041	1.0024
Ang.Var.	8.95	17.35	13.95	8.43
Elect. Energy	-1155.	-1101.	-1125.	-1160.

Table 4.3.3. Silicate Spinel Tetrahedral Sites.

End Member	Ringwoodite	Fe_2SiO_4	Co_2SiO_4	Ni_2SiO_4
C.N.	4	4	4	4
Occupant	Si	Si	Si	Si
Point Sym.	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$	$\bar{4}3m$
Wyckoff Not.	8*a*	8*a*	8*a*	8*a*
Frac.Coord.				
x	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
y	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
z	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
Distances				
O(4)	1.655	1.652	1.646	1.654
Poly.Vol.	2.328	2.312	2.290	2.321
Q.E.	1.0000	1.0000	1.0000	1.0000
Ang.Var.	0.0	0.0	0.0	0.0
Elect. Energy	-4417.	-4459.	-4461.	-4419.

Table 4.4 1. Silicate Zircon Unit Cells.

End Member	Zircon	Hafnon	Thorite	Coffinite
Formula	$ZrSiO_4$	$HfSiO_4$	$ThSiO_4$	$USiO_4$
Form. Wt. (g)	183.304	270.574	324.122	330.114
Density (g/cm^3)	4.668	6.976	6.696	7.185
Mol. Vol. (cm^3)	39.270	38.787	48.407	45.945
Z	4	4	4	4
Cryst. Sys.	Tetragonal	Tetragonal	Tetragonal	Tetragonal
Laue Class	4*mm*	4*mm*	4*mm*	4*mm*
Space Group	$I4_1/amd$	$I4_1/amd$	$I4_1/amd$	$I4_1/amd$
Cell Parameters				
a (Å)	6.6042	6.5725	7.1328	6.995
c (Å)	5.9796	5.9632	6.3188	6.236
Vol.	260.80	257.60	321.48	305.13
Ref.	Hazen & Finger (1979)	Speer & Cooper (1982)	Taylor & Ewing (1978)	Keller (1963)

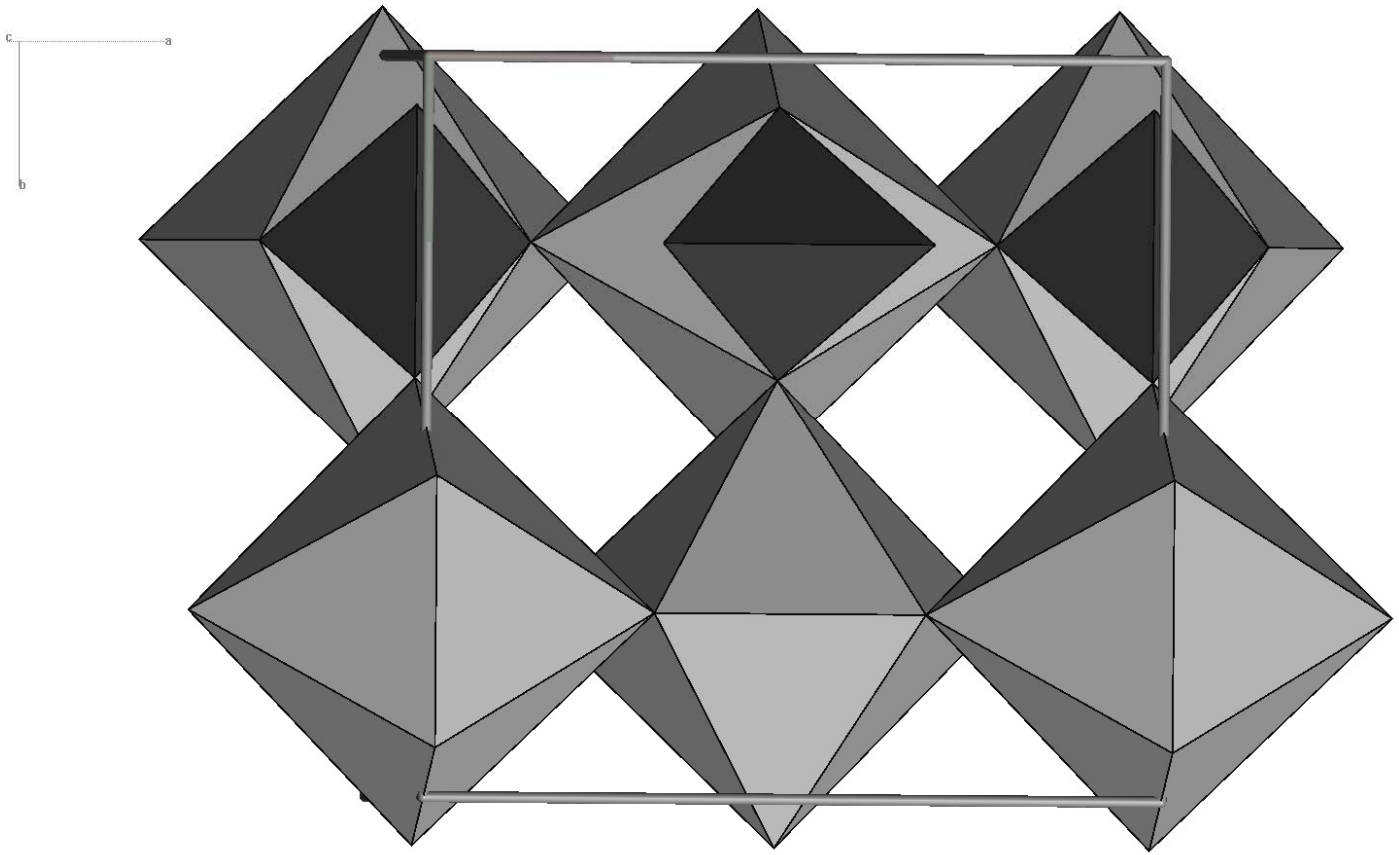

Figure 4.4. Zircon ($ZrSiO_4$). Zr is in 8-coordination, Si in tetrahedral coordination. All oxygens are equivalent and bonded to two Zr and one Si. Both cation sites have point symmetry $\bar{4}2m$.

Table 4.4.2 Zircon M Sites.

End Member	Zircon	Hafnon	Thorite	Coffinite
C.N.	8	8	8	8
Occupant	Zr	Hf	Th	U
Point Sym.	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2m$
Wyckoff Not.	4*a*	4*a*	4*a*	4*a*
Frac. Coord.				
x	0	0	0	0
y	¾	¾	¾	¾
z	$^1/_8$	$^1/_8$	$^1/_8$	$^1/_8$
Distances				
1(4)	2.129	2.115	2.368	2.323
2(4)	2.267	2.260	2.466	2.430
Mean	2.198	2.187	2.417	2.376
σ	0.074	0.077	0.053	0.057
Poly.Vol.	19.00	18.72	25.32	24.02
Elect.Energy	-3884.	-3906.	-3455.	-3518.

Table 4.4.2. Silicate Zircon Tetrahedral Sites.

End Member	Zircon	Hafnon	Thorite	Coffinite
C.N.	4	4	4	4
Occupant	Si	Si	Si	Si
Point Sym.	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2m$
Wyckoff Not.	4*b*	4*b*	4*b*	4*b*
Frac. Coord.				
x	0	0	0	0
y	¼	¼	¼	¼
z	$^3/_8$	$^3/_8$	$^3/_8$	$^3/_8$
Distances0	1.635	1.607		
Poly.Vol.	2.118	2.107	2.205	2.093
Q.E.	1.0237	1.0239	1.0109	1.0118
Elect.Energy	-4513.	-4519.	-4545.	-4626.

Table 4.5.1. Willemite Group Unit Cells

End Member	Willemite	Phenacite
Formula	Zn_2SiO_4	Be_2SiO_4
Form. Wt. (g)	222.824	110.108
Density (g/cm^3)	4.221	2.960
Mol. Vol. (cm^3)	52.795	37.197
Z		
Cryst. Sys.	Trigonal	Trigonal
Laue Class	$\bar{3}$	$\bar{3}$
Space Group	$R\bar{3}$	$R\bar{3}$
ell Parameters		
a (Å)	13.971	12.472
c (Å)	9.334	8.252
Vol.	1577.8	1111.6
Ref.	Simonov (1977)	Zachariasen (1971)

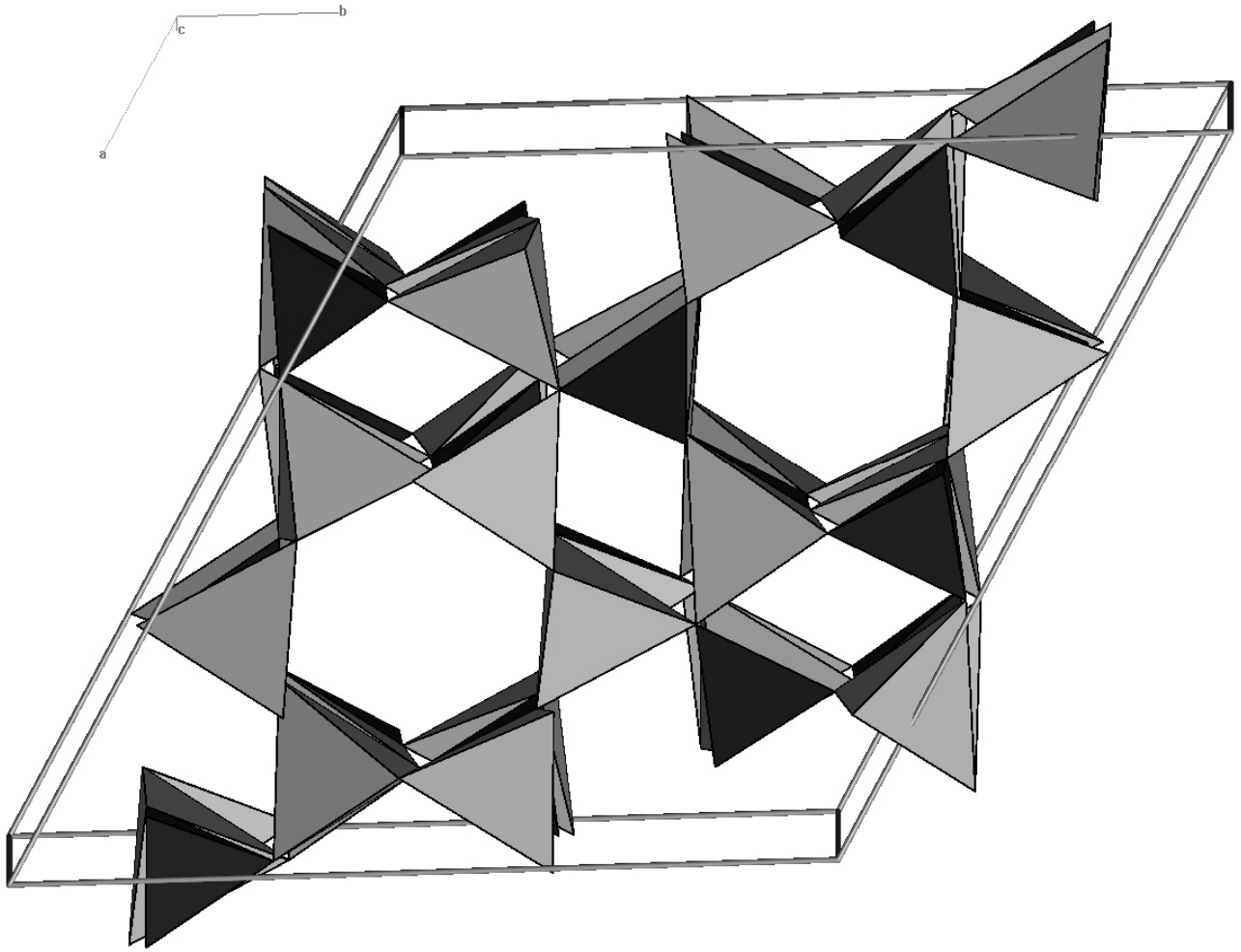

Figure 4.5. Willemite (Zn_2SiO_4). There are two Zn sites, M1 and M2 and a single Si site, all with point symmetry 1. Although all cations are tetrahedral, this is not a framework silicate, because each oxygen atom is bonded to three cations, one Si and two Zn, rather than to two as in the framework silicates.

Table 4.5.2. Willemite Group Divalent Metal Sites.

End Member	Willemite	Phenacite		Willemite	Phenacite
Site	M1	M1		M2	M2
C.N.	4	4		4	4
Occupant	Zn	Be		Zn	Be
Point Sym.	1	1		1	1
Wyckoff Not.	18*f*	18*f*		18*f*	18*f*
Frac. Coord.					
x	0.2087	0.19397		0.2155	0.19386
y	0.0171	0.98412		0.0234	0.98234
z	0.4156	0.41547		0.0815	0.08454
Distances					
O1	1.958	1.640	O1	1.958	1.631
O2	1.952	1.645	O2	1.967	1.643
O4	1.965	1.658	O3	1.972	1.655
O4	1.957	1.637	O3	2.008	1.655
Mean	1.958	1.645		1.976	1.646
σ	0.005	0.009		0.022	0.011
Poly.Vol.	3.821	2.280		3.934	2.283
Q.E.	1.0054	1.0014		1.0048	1.0017
Ang.Var.	21.4	5.4		19.6	7.2
Elect. Energy	-1123.	-1379.		-1109.	-1397.

Table 4.5.3. Willemite Group Si Sites.

End Member	Willemite	Phenacite
C.N.	4	4
Occupant	Si	Si
Point Sym.	1	1
Wyckoff Not.	18*f*	18*f*
Frac. Coord.		
x	0.2118	0.19559
y	0.0155	0.98402
z	0.7490	0.74993
Distances		
O1	1.626	1.630
O2	1.611	1.628
O4	1.637	1.634
O4	1.619	1.631
Mean	1.958	1.645
σ	0.011	0.002
Poly.Vol.	2.191	2.222
Q.E.	1.0009	1.0009
Ang.Var.	3.3	3.8
Elect. Energy	-4445.	-4338.

Table 4.6.1. Aluminosilicate Unit Cells

Polymorph	Andalusite	Sillimanite	Kyanite	Topaz
Formula	Al_2SiO_5	Al_2SiO_5	Al_2SiO_5	$Al_2SiO_4(OH,F)_2$
Form. Wt.	162.046	162.046	162.046	182.052
Density	3.1425	3.2386	3.6640	3.492
Mol. Volume	51.564	50.035	44.227	52.140
Z	4	4	4	4
Cryst.System	Orthorhombic	Orthorhombic	Triclinic	Orthorhombic
Laue Class	*mmm*	*mmm*	$\bar{1}$	*mmm*
Space Group	*Pnnm*	*Pbnm*	$P\bar{1}$	*Pbnm*
Cell Parameters				
a	7.7980	7.4883	7.1262	4.6651
b	7.9031	7.6808	7.8520	8.8381
c	5.5566	5.7774	5.5747	8.3984
α			89.99	
β			101.11	
γ			106.03	
Vol.	342.44	332.29	293.72	346.27
Ref.	Winter & Ghose (1979)	Winter & Ghose (1979)	Winter & Ghose (1979)	Zemann et al. (1979)

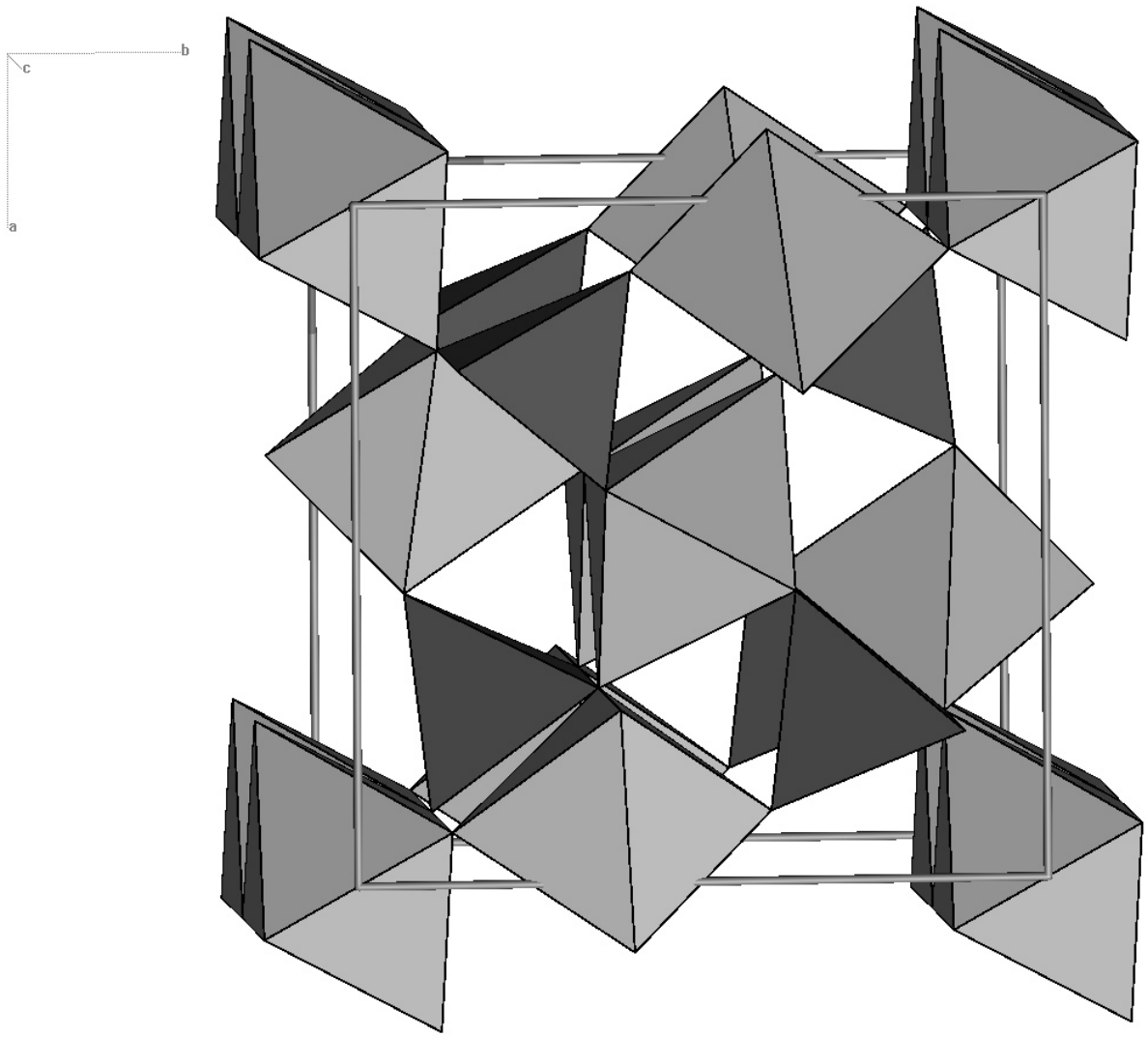

Figure 4.6.1. Andalusite (Al_2SiO_5). There are two Al sites, Al1 is in octahedral coordination on the cell edge in point symmetry 2, whereas the other, Al2, is in 5-coordination with point symmetry *m*. There is a single Si site in tetrahedral coordination with point symmetry m.

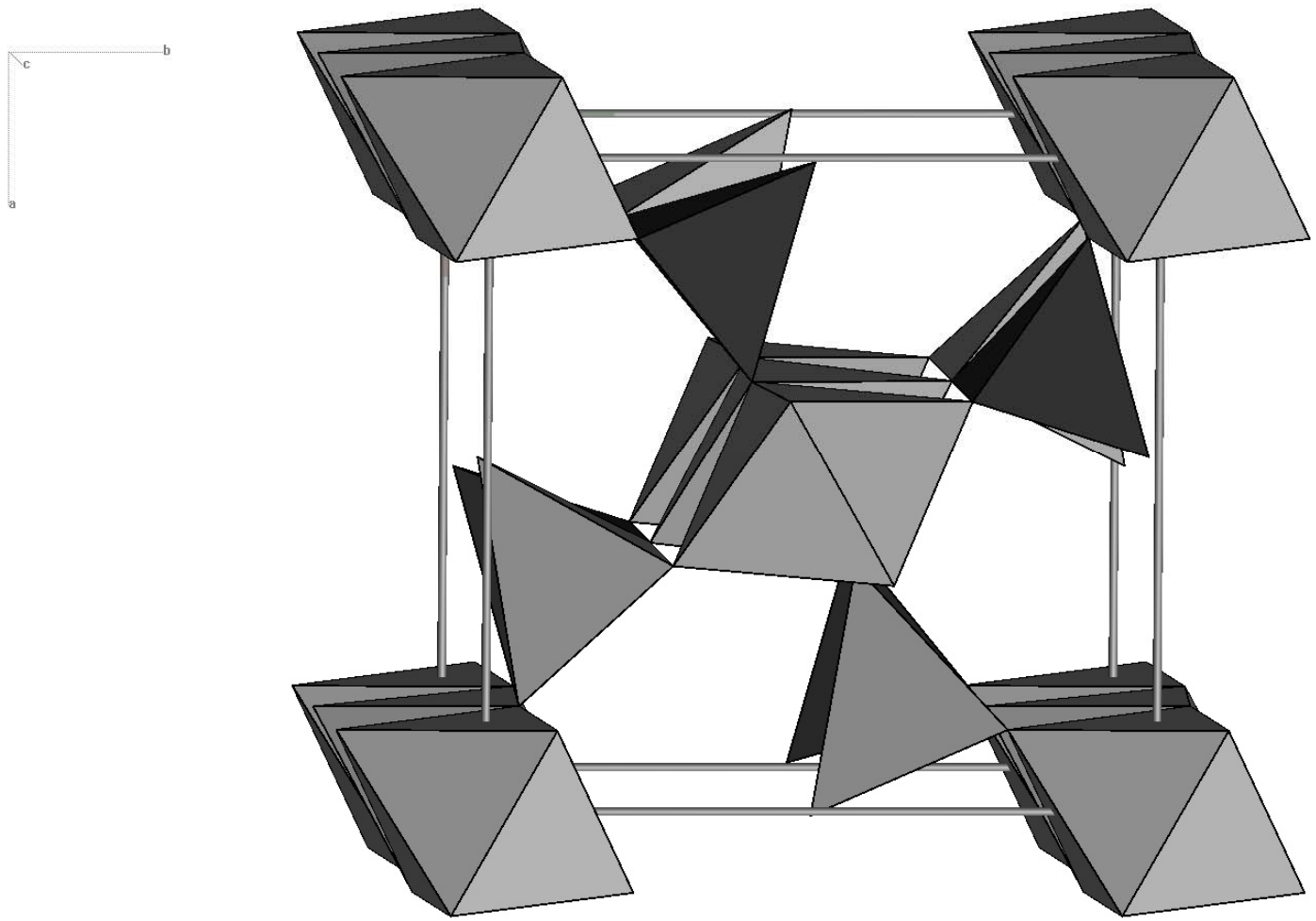

Figure 4.6.2. Sillimanite (Al_2SiO_5). Al1 is in octahedral coordination with point symmetry $\bar{1}$, whereas Al2 is in tetrahedral coordination with point symmetry *m*. There is a single Si site in tetrahedral coordination with point symmetry *m*.

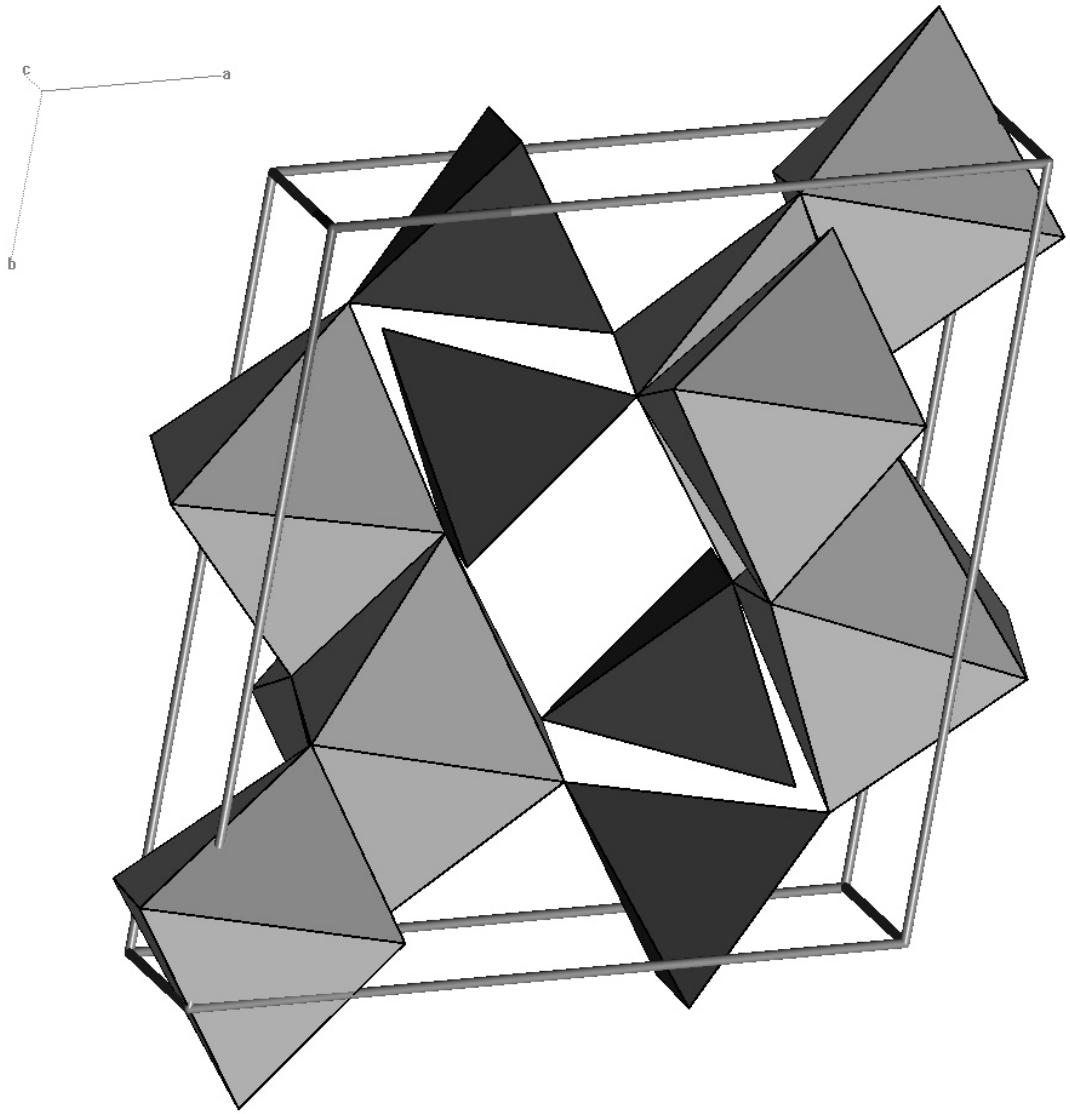

Figure 4.6.3. Kyanite (Al_2SiO_5). There are four Al sites, all in octahedral coordination with point symmetry 1, There are two Si sites in tetrahedral coordination with point symmetry 1.

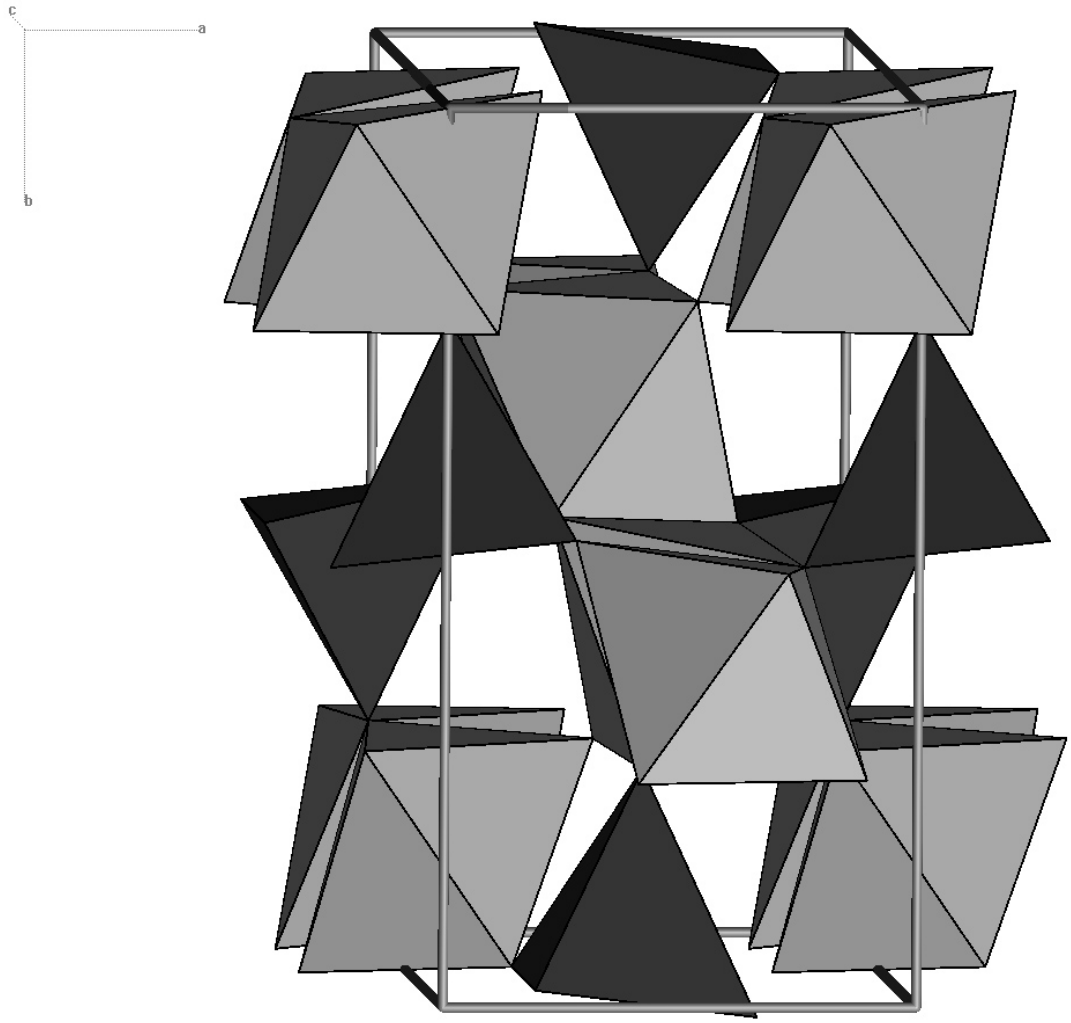

Figure 4.6.4. Topaz ($Al_2SiO_4(F,OH)_2$). There is a single Al site in octahedral coordination with point symmetry 1. There is a single Si site in tetrahedral coordination with point symmetry m. The F site is bonded only to Al.

Table 4.6.2 Aluminosilicate Group Al Sites.

End-Member	Andalusite		Sillimanite		Kyanite				Topaz
Site	Al1	Al2	Al1	Al2	Al1	Al2	Al3	Al4	Al
C.N.	6	5	6	4	6	6	6	6	6
Occupant	Al	Al	Al	Al	Al	Al	Al	Al	Al
Point Sym.	2	*m*	$\bar{1}$	*m*	1	1	1	1	1
Wyckoff Not.	4e	4g	4a	4c	2i	2i	2i	2i	8d
Frac. Coord.									
x	0	0.3705	0	0.1417	0.3254	0.2974	0.0998	0.1120	0.90516
y	0	0.1391	0	0.3449	0.7040	0.6989	0.3862	0.9175	0.13123
z	0.2419	½	0	¼	0.4582	0.9505	0.6403	0.1649	0.08180
Distances									
	(OA) 1.827	(OA) 1.816	(OA) 1.914	(OB) 1.751	(OB) 1.874	(OB) 1.934	(OB) 1.986	(OA) 1.816	(O1) 1.908
	(OB) 1.892	(OC) 1.840	(OB) 1.868	(OC) 1.711	(OF) 1.884	(OC) 1.881	(OC) 1.924	(OA) 1.998	(O2) 1.911
	(OD) 2.086	(OC) 1.899	(OD) 1.954	(OD) 1.796	(OG) 1.971	(OD) 1.889	(OE) 1.862	(OB) 1.846	(O3) 1.894
		(OD) 1.814			(OH) 1.987	(OF) 1.914	(OF) 1.968	(OD) 1.911	(O3) 1.902
					(OK) 1.847	(OK) 1.930	(OF) 1.883	(OE) 1.933	(F) 1.808
					(OM) 1.848	(OM) 1.925	(OG) 1.885	(OH) 1.875	(F) 1.802
Mean	1.935	1.836	1.912	1.764	1.902	1.913	1.918	1.896	1.871
σ	0.121	0.036	0.039	0.041	0.062	0.023	0.050	.0065	0.051
Poly. Vol.	9.531	5.153	9.175	2.791	8.977	9.136	9.164	8.921	8.654
Q.E.	1.0114	--	1.0109	1.0062	1.0155	1.0141	1.0180	1.0139	1.0086
Ang. Var.	18.0	--	36.4	20.5	47.7	50.2	57.0	42.5	20.6
Elect. Energy	-2490.	-2569.	-2573.	-2526.	-2532.	-2563.	-2543.	-2531.	-2506.

Table 4.6.3. Aluminosilicate Group Si Sites.

End-Member	Andalusite	Sillimanite	Kyanite		Topaz
Site	Si	Si	Si1	Si2	Si
C.N.	4	4	4	4	4
Occupant	Si	Si	Si	Si	Si
Point Sym.	*m*	*m*	1	1	*m*
Wyckoff Not.	4g	4c	2i	2i	4c
Frac. Coord.					
x	0.2460	0.1533	0.2692	0.2910	0.39955
y	0.2520	0.3402	0.0649	0.3317	0.94084
z	0	¾	0.7066	0.1892	¼
Distances					
1	(OB) 1.646	(OA) 1.640	(OD) 1.631	(OA) 1.640	(O1) 1.637
2	(OC) 1.618	(OC) 1.573	(OE) 1.643	(OG) 1.627	(O2) 1.651
3	(OD) 1.630 (2)	(OD) 1.645 (2)	(OH) 1.621	(OG) 1.627	(O3) 1.643 (2)
			(OM) 1.647	(OK) 1.649	
Mean	1.631	1.626	1.636	1.636	1.643
σ	0.011	0.0354	0.011	0.010	0.006
Poly. Vol.	2.211	2.203	2.241	2.243	2.277
Q.E.	1.0043	1.0013	1.0012	1.0018	1.0004
Ang. Var.	16.4	3.4	4.8	7.1	1.7
Elect. Energy	-4404.	-4426.	-4443.	-4458.	-4402.

Table 4.7.1. Humite Group Unit Cells.

End-Member	Norbergite	Chondrodite	Humite	Clinohumite
Formula	$Mg_3(SiO_4)F_{1.8}(OH)_{0.2}$	$Mg_{4.95}Fe_{0.05}(SiO_4)_2F_{1.3}(OH)_{0.7}$	$Mg_{6.6}Fe_{0.4}(SiO_4)_3F(OH)$	$Mg_{8.4}Fe_{0.6}(SiO_4)_4F_{1.04}(OH)_{0.96}$
Form. Wt.	203.106	341.73	482.44	640.49
Density	3.186	3.158	3.159	3.259
Mol. Vol.	63.73	1089.20	152.70	196.55
Z	4	2	4	2
Cryst. Sys.	Orthorhombic	Monoclinic	Orthorhombic	Monoclinic
Laue Group	*mmm*	2/*m*	*mmm*	2/*m*
Space Group	*Pbnm*	$P2_1/b$	*Pbnm*	$P2_1/b$
Cell Parameters				
a	4.7104	4.7284	4.7408	4.7441
b	10.2718	10.2539	10.2580	10.2501
c	8.7476	7.8404	20.8526	13.6635
α		109.059		100.786
Vol.	423.25	359.30	1014.09	652.68
Ref.	Gibbs & Ribbe (1969)	Gibbs et al. (1970)	Ribbe & Gibbs (1971)	Robinson et al. (1973a)

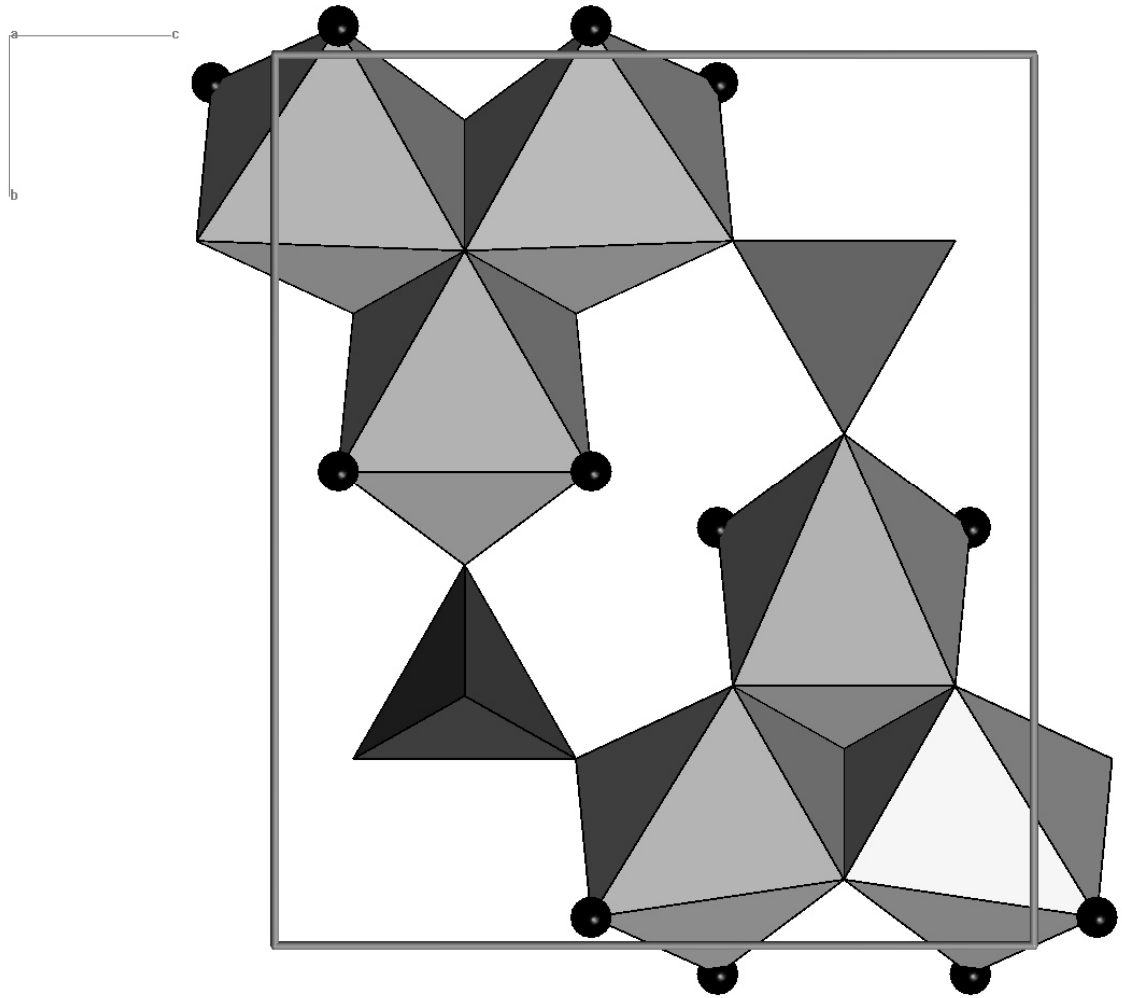

Figure 4.7.1. Norbergite ($Mg_3SiO_4(F,OH)_2$), *a*-axis projection, *b*-vertical. There are two distinct Mg octahedral, M2 (point symmetry m) and M3 (point symmetry 1), and a single Si tetrahedron. The F-OH (sphere) site is bonded only to Mg.

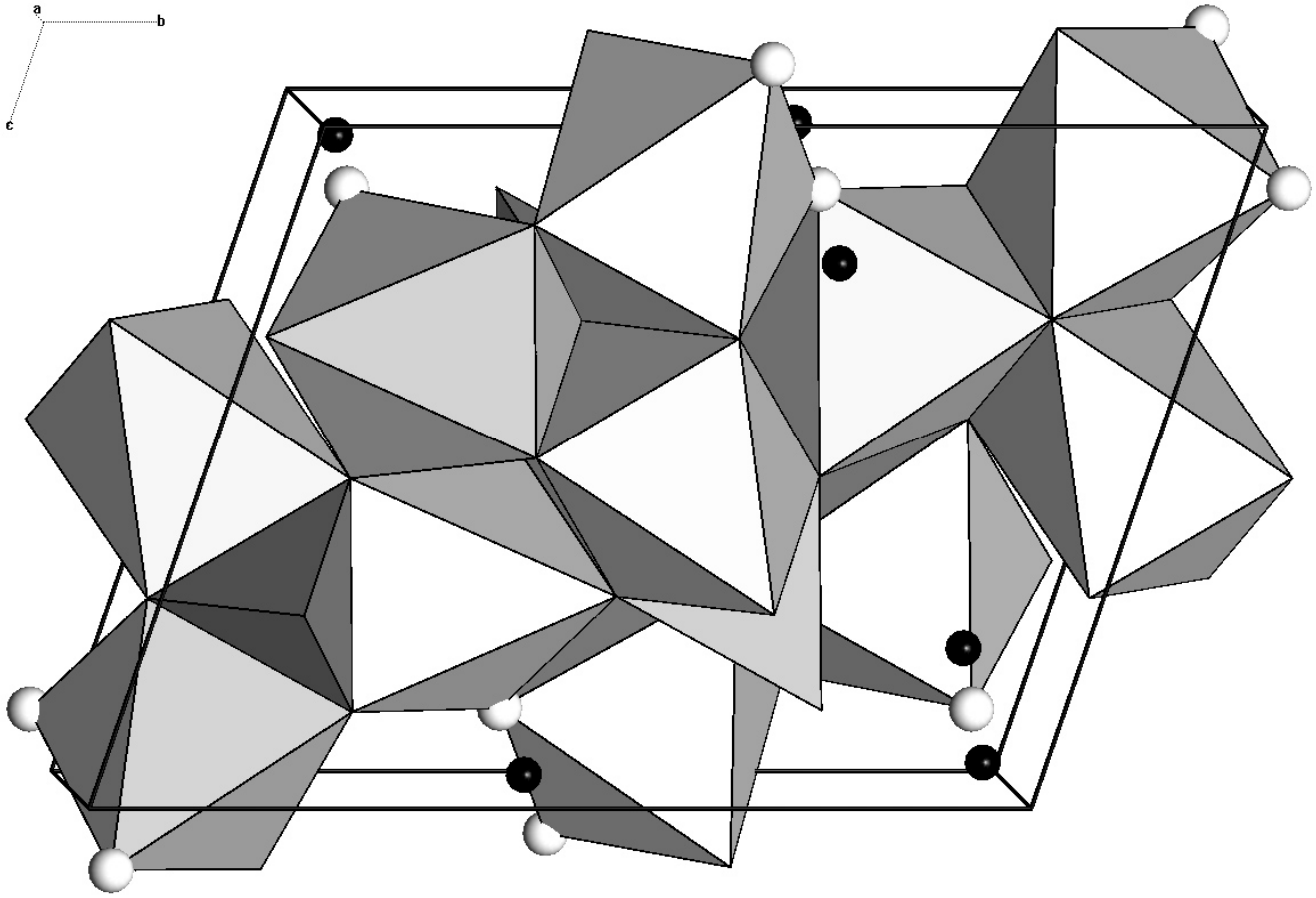

Figure 4.7.2. Chondrodite ($Mg_3SiO_4(F,OH)_2$), *a*-axis projection, *c**-vertical. There are three distinct Mg octahedral, M1 (point symmetry $\bar{1}$), M2, and M3 (both with point symmetry 1), and a single Si tetrahedron. The F-OH (white sphere) site is bonded only to Mg.

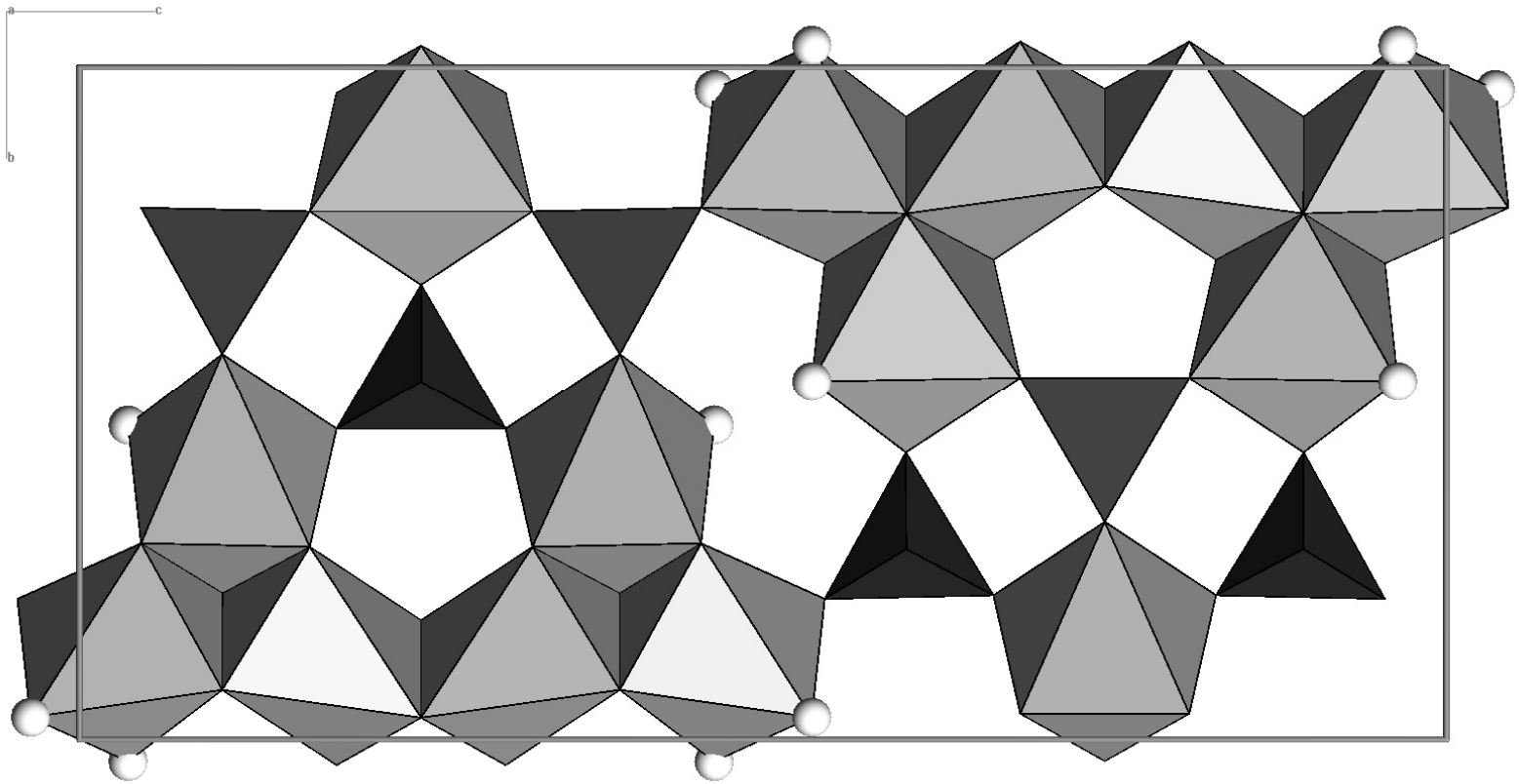

Figure 4.7.3. Humite ($Mg_7(SiO_4)_3(F,OH)_2$), *a*-axis projection, *b*-vertical. There are four distinct Mg octahedral, M1, M3, and M4 (all with point symmetry 1), and M2 with point symmetry m, and two distinct Si tetrahedron, one with point symmetry m and the other in general position. The F-OH (white sphere) site is bonded only to Mg.

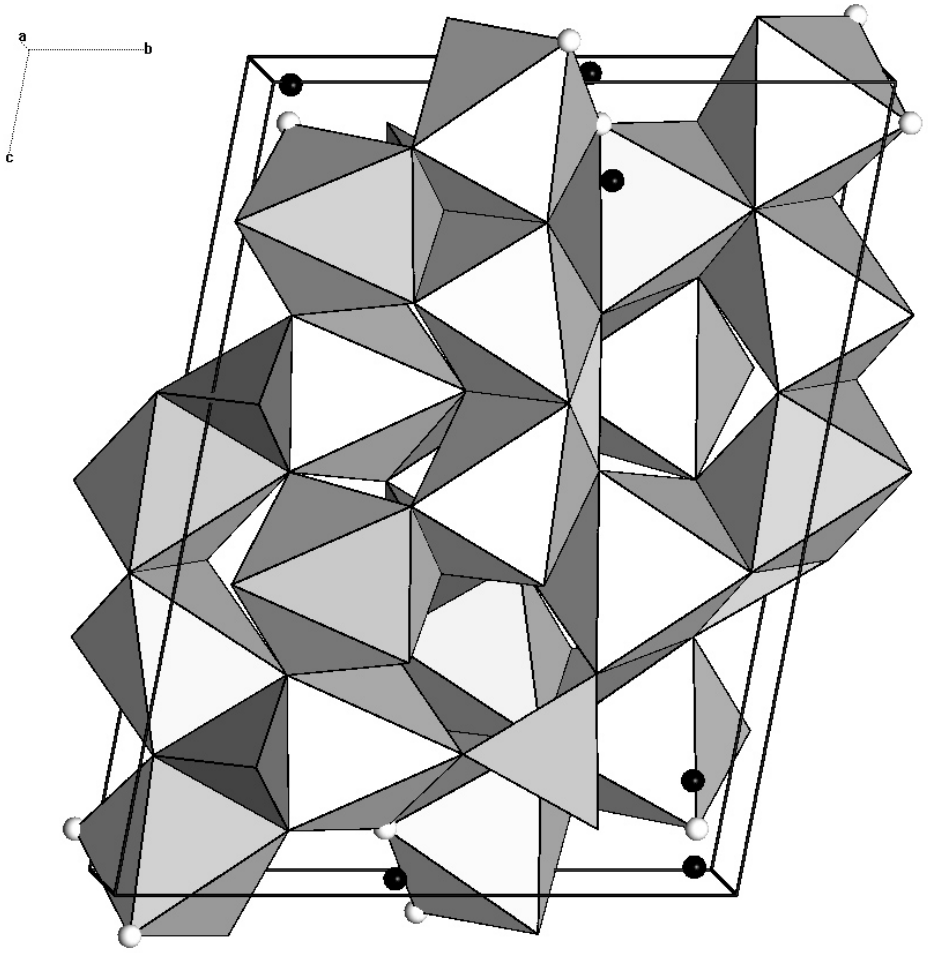

Figure 4.7.4. Clinohumite ($Mg_3SiO_4(F,OH)_2$), *a*-axis projection, *c**-vertical. There are three distinct Mg octahedral, M1 (point symmetry $\bar{1}$), M2, and M3 (both with point symmetry 1), and a single Si tetrahedron. The F-OH (white sphere) site is bonded only to Mg.

Table 4.7.2a. Humite Group (Norbergite and Chondrodite) Octahedral Sites.

End-Member	Norbergite		Chondrodite		
Site	M3	M2	M1	M2	M3
C.N.	6	6	6	6	6
Occupant	Mg	Mg	$Mg_{.95}Fe_{.05}$	Mg	Mg
Point Sym.	1	*m*	$\bar{1}$	1	1
Wyckoff Not.	8d	4c	2d	4e	4e
Frac. Coord.					
x	0.9890	0.9924	½	0.0091	0.4915
y	0.6330	0.9077	0	0.1731	0.8867
z	0.4305	¼	½	0.3055	0.0791
Distances					
Mean	2.068	2.104	2.170	2.116	2.078
σ	0.075	0.100	0.014	0.081	0.072
Poly. Vol.	11.515	12.029	11.965	12.245	11.665
Q.E.	1.0174	1.0236	1.0277	1.0220	1.0179
Ang. Var.	56.5	75.6	100.6	74.0	59.2
Elect. Energy	-1085.	-1086.	-1055.	-1119.	-1095.

Table 4.7.2b. Humite Group (Humite and Clinohumite) Octahedral Sites.

End-Member	Humite				Clinohumite				
Site	M1	M2	M3	M4	$M1_c$	$M1_n$	$M2_5$	$M2_6$	M3
C.N.	6	6	6	6	6	6	6	6	6
Occupant	$Mg_{.9}Fe_{.1}$	$Mg_{.9}Fe_{.1}$	$Mg_{.96}Fe_{.04}$	$Mg_{.99}Fe_{.01}$	$Mg_{.94}Fe_{.06}$	$Mg_{.94}Fe_{.06}$	$Mg_{.91}Fe_{.09}$	$Mg_{.94}Fe_{.06}$	$Mg_{.97}Fe_{.03}$
Point Sym.	1	*m*	1	1	$\bar{1}$	1	1	1	1
Wyckoff Not.	8d	4c	8d	8d	2d	4e	4e	4e	4e
Frac. Coord.									
x	0.0017	0.5108	0.0087	0.4925	½	0.4977	0.0101	0.5101	0.4939
y	0.3773	0.1540	0.0976	0.8665	0	0.9463	0.1398	0.2503	0.8780
z	0.1767	¼	0.1092	0.0278	½	0.2738	0.1703	0.3888	0.0428
Distances									
Mean	2.108	2.137	2.122	2.086	2.107	2.109	2.119	2.136	2.080
σ	0.023	0.086	0.082	0.074	0.027	0.024	0.083	0.083	0.072
Poly. Vol.	11.970	12.483	12.345	11.780	11.295	11.978	12.280	12.483	11.703
Q.E.	1.0293	1.0291	1.0223	1.0189	1.0301	1.0297	1.0230	1.0283	1.0181
Ang. Var.	105.0	99.4	74.9	62.5	107.4	106.5	77.1	97.1	59.5
Elect. Energy	-1057.	-1135.	-1122.	-1099.	-1046.	-1058.	-1135.	-1131.	-1119.

Table 4.7.3. Humite Group Tetrahedral Sites.

End-Member	Norbergite	Chondrodite	Humite		Clinohumite	
Site	Si	Si	Si1	Si2	Si1	Si2
C.N.	4	4	4	4	4	4
Occupant	Si	Si	Si	Si	Si	Si
Point Sym.	*m*	1	*m*	1	1	1
Wyckoff Not.	4c	4e	4c	8d	4c	4c
Frac. Coord.						
x	0.4195	0.0768	0.0752	0.5765	0.0741	0.0759
y	0.7196	0.1441	0.9691	0.2819	0.0663	0.1771
z	¼	0.7038	¼	0.1059	0.3891	0.8354
Distances						
Mean	1.630	1.633	1.629	1.627	1.626	1.638
σ	0.012	0.012	0.009	0.011	0.004	0.014
Poly. Vol.	2.193	2.202	2.188	2.180	2.175	2.219
Q.E.	1.0093	1.0102	1.0090	1.0096	1.0094	1.0109
Ang. Var.	41.3	45.2	38.2	42.5	39.7	48.6
Elect. Energy	-4321.	-4305.	-4293.	-4346.	-4299.	-4333.

Table 4.8.1. Titanite Group Unit Cells.

End-Member	Titanite	Malayaite
Formula	$CaTiSiO_5$	$CaSnSiO_5$
Form. Wt.	196.063	266.853
Density	3.517	4.546
Mol. Vol.	55.748	58.704
Z	4	4
Cryst. Sys.	Monoclinic	Monoclinic
Laue Class	2/*m*	2/m
Space Group	$P2_1/a$	$A2/a$
Cell Parameters		
a	7.069	7.149
b	8.722	8.906
c	6.586	6.667
β	113.86	113.3
Vol.	370.23	389.86
Ref.	Speer & Gibbs (1976)	Higgins & Ribbe (1977)

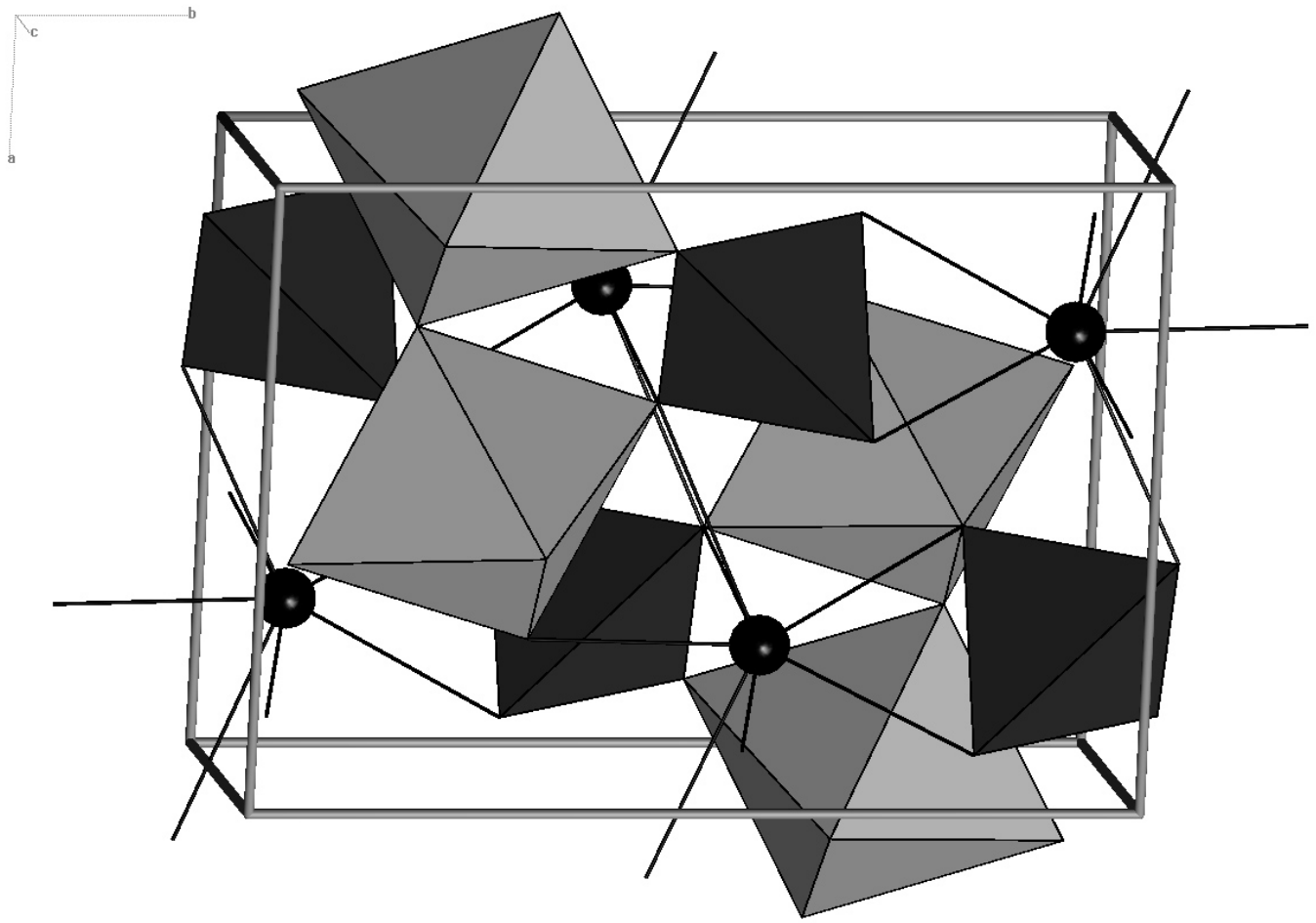

Figure 4.8.1. Titanite ($CaTiSiO_5$), *c*-axis projection, *a*-vertical. Ca (black sphere) is in irregular 7-coordination, Ti is octahedral, and Si tetrahedral.

Table 4.8.2. Titanite Group Cation Sites.

End-Member	Titanite			Malayaite		
C.N.	7	6	4	7	6	4
Occupant	Ca	Ti	Si	Ca	Sn	Si
Point Sym.	1	1	1	2	$\bar{1}$	2
Wyckoff Not.	4e	4e	4e	8e	4c	4e
Frac. Coord.						
x	0.2424	0.5134	0.7486	¼	½	¾
y	0.9184	0.2495	0.7490	¾	¼	¾
z	0.7512	0.2495	0.7490	¾	¼	¾
Distances						
Mean	2.485	1.959	1.645	2.490	2.042	1.641
σ	0.130	0.096	0.003	0.188	0.074	0.009
Poly. Vol.	19.713	9.978	2.273	20.688	11.300	2.253
Q.E.	--	1.0052	1.0032	--	1.0046	1.0044
Ang. Var.	--	7.6	12.1	--	8.5	17.4
Elect. Energy	-999.	-4160.	-4420.	-1007.	-3934.	-4448.

Table 4.9.1. Staurolite Unit Cell.

End-Member	Staurolite
Formula	$Fe_4Al_{18}Si_8O_{46}(OH)_2$
Form. Wt.	1703.73
Density	3.823
Mol. Volume	445.67
Z	1
Cryst. Sys.	Monoclinic
Laue Class	2/*m*
Space Group	*C*2/*m*
Cell Parameters	
a	7.8713
b	16.6204
c	5.6560
α	90.0
Vol.	739.94
Ref.	Smith (1968)

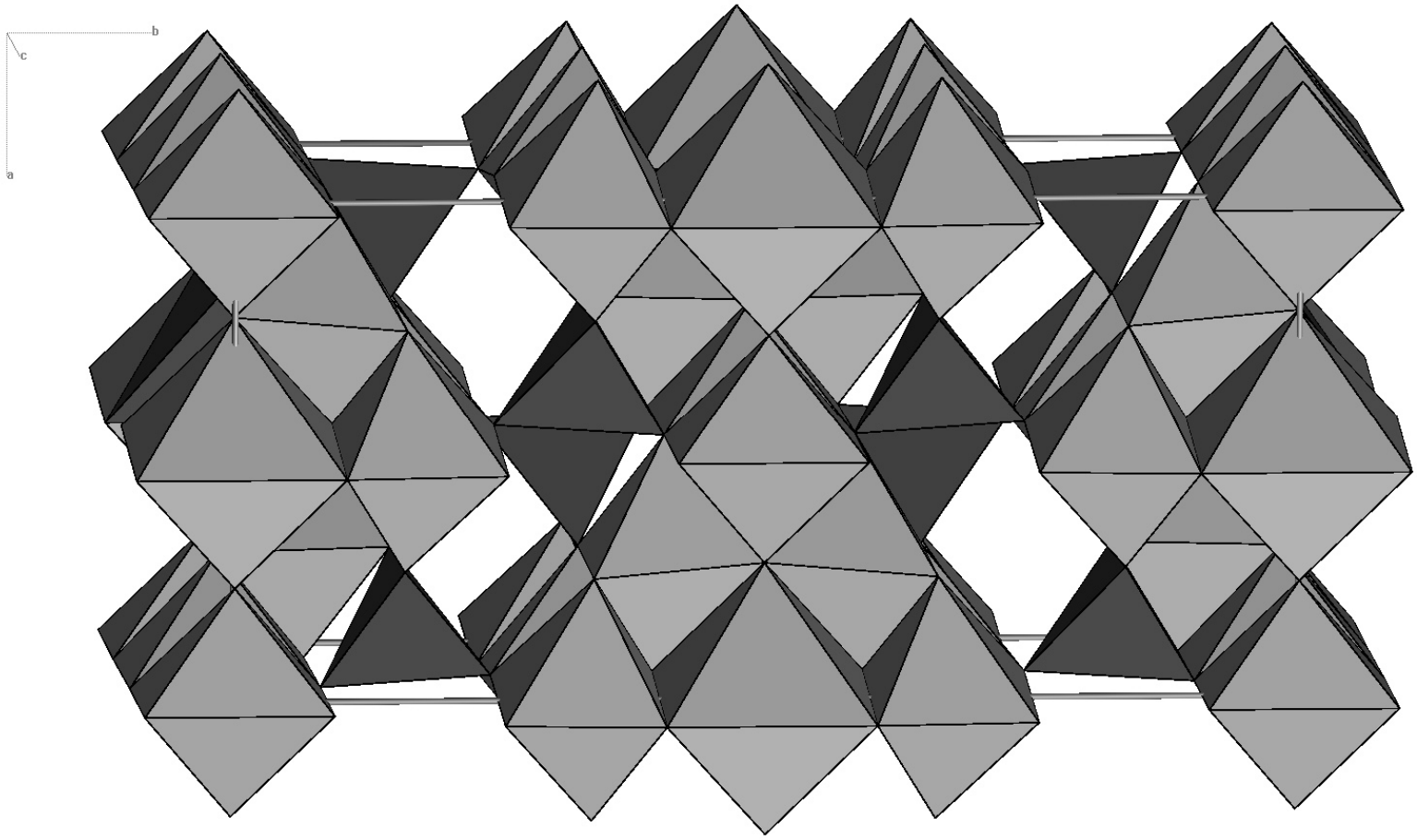

Figure 4.9.1. Staurolite ($Fe_4Al_{18}Si_8O_{46}(OH)_2$), *c*-axis projection, *a*-vertical. Al and Fe are octahedral and Si is tetrahedral.

Table 4.9.1. Staurolite Fully Occupied Cation Sites.

Site	Al1A	Al1B	Al2	Si
C.N.	6	6	6	4
Occupant	Al	Al	Al	Si
Point Sym.	2	2	2	2
Wyckoff Not.	4g	4h	8j	8j
Frac. Coord.				
x	½	½	0.26536	0.13414
y	0.17511	0.17477	0.41042	0.16612
z	0	½	0.25122	0.24902
Distances				
Mean	1.911	1.914	1.905	1.641
σ	0.021	0.022	0.029	0.008
Poly. Vol.	9.127	9.169	9.031	2.266
Q.E.	1.0133	1.0132	1.0139	1.0004
Ang. Var.	45.5	45.3	46.3	1.7
Elect. Energy	-2365.	-2365.	-2619.	-4361.
Model Charge	3.0	3.0	3.0	4.0

Table 4.9.1. Staurolite Partially Occupied Cation Sites.

Site	Fe	U1	U2	Al3A	Al3B
C.N.	4	6	6	6	6
Occupant	$Fe_{.64}Al_{.36}$	$Fe_{.68}Mn_{.32}$	$Fe_{.68}Mn_{.32}$	$Al_{.67}Fe_{.33}$	$Al_{.67}Fe_{.33}$
Occupancy	0.916	0.080	0.038	0.415	0.282
Point Sym.	*m*	2/*m*	2/*m*	2/*m*	2/*m*
Wyckoff Not.	4i	2b	2d	2a	2c
Frac. Coord.					
x	0.39281	½	½	0	0
y	0	0	0	0	0
z	0.24815	0	½	0	½
Distances					
Mean	2.008	2.165	2.163	1.972	1.992
σ	0.042	0.040	0.049	0.100	0.106
Poly. Vol.	4.141	12.960	12.957	10.125	10.441
Q.E.	1.0026	1.0299	1.0286	1.0092	1.0083
Ang. Var.	11.5	90.4	85.8	16.6	12.2
Elect. Energy	-1395.	+12.	+6.	-622.	-369.
Model Charge	2.36	0.16	0.08	1.11	0.75

Table 5.1.1. Epidote Group Unit Cells.

End Member	Zoisite	Clinozoisite	Epidote	Epidote	Allanite
Formula	$Ca_2Al_3Si_3O_{12}(OH)$	$Ca_2Al_3Si_3O_{12}(OH)$	$Ca_2Al_{2.16}Fe_{0.84}Si_3O_{12}(OH)$	$Ca_2Al_{2.6}Fe_{0.4}Si_3O_{12}(OH)$	$Ca_{1.26}RE_{0.76}Al_{1.83}Fe_{1.17}Si_3O_{12}(OH)$
Form. Wt. (g)	454.363	454.363	478.610	465.909	565.2
Density (g/cm^3)	3.336	3.321	3.465	3.392	3.960
Mol. Vol. (cm^3)\	136.19	136.83	138.146	137.370	142.737
Z	4	2	2	2	2
Cryst. Sys.	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Laue Class	*mmm*	2/*m*	2/*m*	2/*m*	2/*m*
Space Group	*Pnna*	$P2_1/m$	$P2_1/m$	$P2_1/m$	$P2_1/m$
Cell Parameters					
a (Å)	16.212	8.879	8.8877	8.8802	8.927
b (Å)	5.559	5.583	5.6275	5.6043	5.761
c (Å)	10.036 `	10.155	10.1517	10.1541	10.150
β		115.50	115.383	115.455	10.150
Vol.	904.47	454.36	458.73	456.15	114.77
Ref.	Dollase (1968)	Dollase (1968)	Gabe et al. (1973)	Gabe et al. (1973)	Dollase (1971)

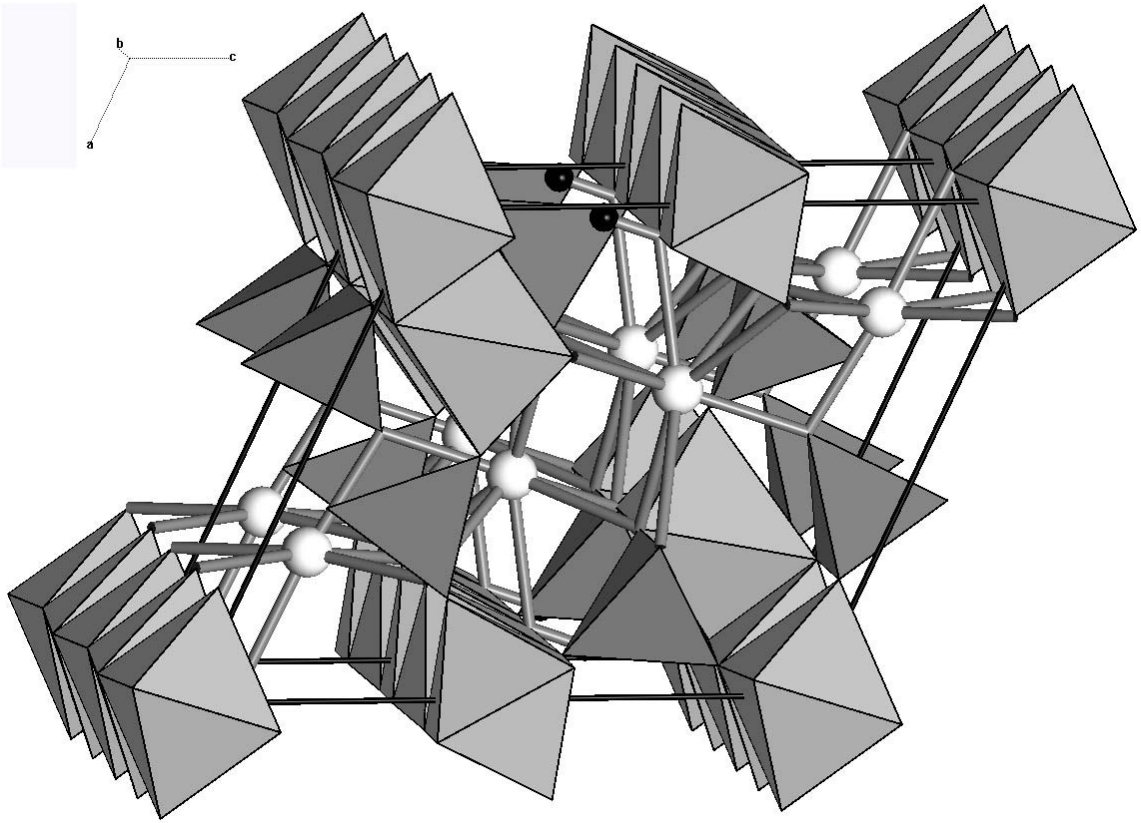

Figure 5.1. Edidote, $Ca_2(Al,Fe)_3Si_3O_{12}(OH)$, perspective *b*-axis projection, *a* vertical. There are two distinct Ca sites, A1 and A2, both with eight-coordination and point symmetry *m*. Rare earth elements occupy the A2 site in allanite. The unusually deep electrostatic potential of this site for its size may explain why this site strongly fractionates lanthanides in natural systems. The three octahedral sites M1, M2, and M3, are occupied by Al and smaller amounts of ferric iron. M1 and M2 lie on inversion centers, and M3 lies on the mirror. There are three distinct tetrahedral sites, T1, T2, and T3, all of which lie on the mirror.

Table 5.1.2. Epidote Group Ca Sites.

End Member	Zoisite		Clinozoisite		Epidote		Epidote		Allanite	
Site	A1	A2	A1	A2	A1	A2	A1	A2	A1	A2
C.N.	9	7	9	8	9	8	9	8	9	11
Cation	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	Ca	$RE_{.74}Ca_{.26}$
Point Sym.	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*
Wyckoff Not.	4*c*	4*c*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*
Frac. Coords.										
x	0.3667	0.4518	0.7617	0.6063	0.7572	0.6049	0.7597	0.6066	0.6585	0.5936
y	¼	¼	¾	¾	¾	¾	¾	¾	¾	¾
z	0.4376	0.1150	0.1555	0.4234	0.1516	0.4240	0.1537	0.4236	0.1517	0.4286
Distances										
O1(2)	2.504		2.491		2.459		2.478		2.373	
O2(2)		2.789		2.818		2.784		2.810		2.642
O2(2)		2.521		2.543		2.527		2.536		2.516
O3(2)	2.416	2.468	2.368	2.532	2.323	2.653	2.345	2.575	2.337	2.801
O5(1)	2.588		2.522		2.556		2.534		2.592	
O6(1)	2.552		2.745		2.861		2.789		2.911	
O7(1)	2.252	2.305	2.283	2.267	2.295	2.248	2.284	2.262	2.369	2.329
O8(2)										3.017
O8(2)										3.127
O9(2)	2.916		2.952		3.000		2.973		3.112	
O10(1)				2.575		2.531		2.551		2.611
Mean	2.562	2.551	2.575	2.579	2.586	2.588	2.578	2.582	2.613	2.729
σ	0.223	0.178	0.250	0.177	0.291	0.174	0.268	0.174	0.338	0.248
Poly.Vol.	28.095	31.011	27.608	32.980	27.249	33.079	27.405	32.977	27.521	54.860
Elect.Energy	-957.	-1040	-958.	-1053.	-961.	-1071.	-972.	-1044.	-966.	-1105.

Table 5.1.3. Epidote Group Octahedral Sites.

End Member	Zoisite		Clinozoisite			Epidote			Epidote			Allanite		
Site	M1,2	M3	M1	M2	M3	M1	M2	M3	M1	M2	M3	M1	M2	M3
C.N.	6	6	6	6	6	6	6	6	6	6	6	6	6	6
Cation	Al	Al	Al	Al	Al,Fe	Al	Al	Al,Fe	Al	Al	Al,Fe	Al	Al	Al,Fe
Point Sym.	$\bar{1}$	*m*	$\bar{1}$	$\bar{1}$	*m*	$\bar{1}$	$\bar{1}$	*m*	$\bar{1}$	$\bar{1}$	*m*	$\bar{1}$	$\bar{1}$	*m*
Wyckoff Not.	8*d*	4*c*	2*a*	2*c*	2*e*	2*a*	2*c*	2*e*	2*a*	2*c*	2*e*	2*a*	2*c*	2*e*
Frac. Coords.														
x	0.2496	0.1054	0	0	0.2873	0	0	0.29386	0	0	0.29085	0	0	0.3030
y	0.9971	¾	0	0	¼	0	0	¼	0	0	¼	0	0	¼
z	0.1899	0.3006	0	½	0.2238	0	½	0.2242	0	½	0.2242	0	½	0.2148
Distances														
O1(2)	1.964	2.133	1.930		2.184	1.939		2.224	1.931		2.200	1.992		2.304
O2(2)		1.965			1.926			1.985			1.956			2.195
O3(2)	1.850			1.859			1.854			1.858			1.876	
O4(2)	1.843	1.822	1.850		1.861	1.843		1.935	1.847		1.903	1.878		2.002
O5(1)	1.900		1.936			1.956			1.943			2.026		
O6(1)	1.926			1.923			1.927			1.926			1.920	
O8(1)		1.784			1.781			1.860			1.810			1.941
O10(1)	1.849			1.852			1.870			1.864			1.914	
Mean	1.888	1.967	1.906	1.878	1.977	1.913	1.883	2.036	1.907	1.883	2.004	1.965	1.904	2.157
σ	0.050	0.148	0.043	0.035	0.169	0.054	0.034	0.153	0.047	0.034	0.161	0.069	0.021	0.153
Poly.Vol.	8.899	9.866	9.146	8.773	10.009	9.252	8.853	10.864	9.167	8.847	10.395	10.053	9.110	12.637
O.Q.E.	1.0066	1.0237	1.0065	1.0045	1.0259	1.0065	1.0045	1.0283	1.0064	1.0042	1.0271	1.0055	1.0064	1.0433
Ang.Var.	20.1	54.9	19.7	14.0	58.1	17.9	14.0	74.8	18.9	13.1	66.3	11.9	22.1	125.5
Elect.Energy	-2573.	-2541.	-2435.	-2633.	-2545.	-2410.	-2614.	-2413.	-2427.	-2684.	-2452.	-2298.	-2640.	-2203.

Table 5.1.2. Epidote Group Tetrahedral Sites.

End Member	Zoisite			Clinozoisite			Epidote			Epidote			Allanite		
Site	T1	T2	T3	T1	T2	T3	T1	T2	T3	T1	T2	T3	T1	T2	T3
C.N.	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4
Cation	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si	Si
Point Sym.	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*	*m*
Wyckoff Not.	4*c*	4*c*	4*c*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*	2*e*
Frac. Coords.															
x	0.0816	0.4104	0.1601	0.3328	0.6776	0.1822	0.3396	0.6843	0.1839	0.3388	0.6805	0.1830	0.3389	0.6866	0.1880
y	¼	¾	¼	¾	¼	¾	¾	¼	¾	¾	¼	¾	¾	¼	¾
z	0.1064	0.2821	0.4356	0.0478	0.2753	0.3158	0.0477	0.2745	0.3184	0.0480	0.2751	0.3169	0.0369	0.2799	0.3240
Distances															
O1(2)	1.656			1.652			1.650			1.652			1.645		
O2(2)			1.619			1.629			1.627			1.625			1.604
O3(2)		1.621			1.620			1.618			1.619			1.631	
O5(1)			1.651			1.662			1.668			1.667			1.657
O6(1)			1.672			1.657			1.638			1.648			1.661
O7(1)	1.586			1.566			1.564			1.562			1.581		
O8(1)		1.580			1.593		1.588			1.592			1.603		
O9(1)	1.640	1.624		1.627	1.627		1.634	1.631		1.633	1.627		1.651	1.627	
Mean	1.635	1.612	1.640	1.625	1.615	1.644	1.624	1.614	1.640	1.625	1.614	1.641	1.630	1.623	1.632
σ	0.033	0.021	0.026	0.041	0.015	0.018	0.041	0.019	0.019	0.043	0.016	0.020	0.033	0.014	0.032
Poly.Vol.	2.226	2.143	2.227	2.190	2.157	2.261	2.190	2.155	2.249	2.191	2.155	2.251	2.217	2.192	2.201
T.Q.E.	1.0049	1.0018	1.0114	1.0034	1.0014	1.0060	1.0033	1.0009	1.0046	1.0035	1.0012	1.0055	1.0027	1.0011	1.0086
Ang.Var.	17.5	7.4	44.3	10.5	6.0	23.9	9.9	3.7	18.4	10.5	5.0	22.2	8.9	4.1	33.5
Elect.Energy	-4368.	-4529.	-4400.	-4380.	-4540.	-4395.	-4348.	-4542.	-4427.	-4373.	-4564.	-4390.	-4286.	-4504.	-4518.

Table 5.2.1. Melilite Group Unit Cells.

End Member	Na-Melilite	Gehlenite	Akermanite
Formula	$CaNaAlSi_2O_7$	$Ca_2Al(Al,Si)_2O_7$	$Ca_2MgSi_2O_7$
Form. Wt. (g)	258.219	274.205	272.640
Density (g/cm^3)	2.912	3.006	2.944
Mol. Vol. (cm^3)	88.662	91.220	92.619
Z	2	2	2
Cryst. Sys.	Tetragonal	Tetragonal	Tetragonal
Laue Class	$\bar{4}2m$	$\bar{4}2m$	$\bar{4}2m$
Space Group	$P\bar{4}2_1m$	$P\bar{4}2_1m$	$P\bar{4}2_1m$
Cell Parameters			
a (Å)	7.6344	7.7173	7.835
c (Å)	5.0513	5.0860	5.010
Vol.	294.41	302.91	307.55
Ref.	Louisnathan (1970b)	Louisnathan (1970a)	Kimata & Ii (1981)

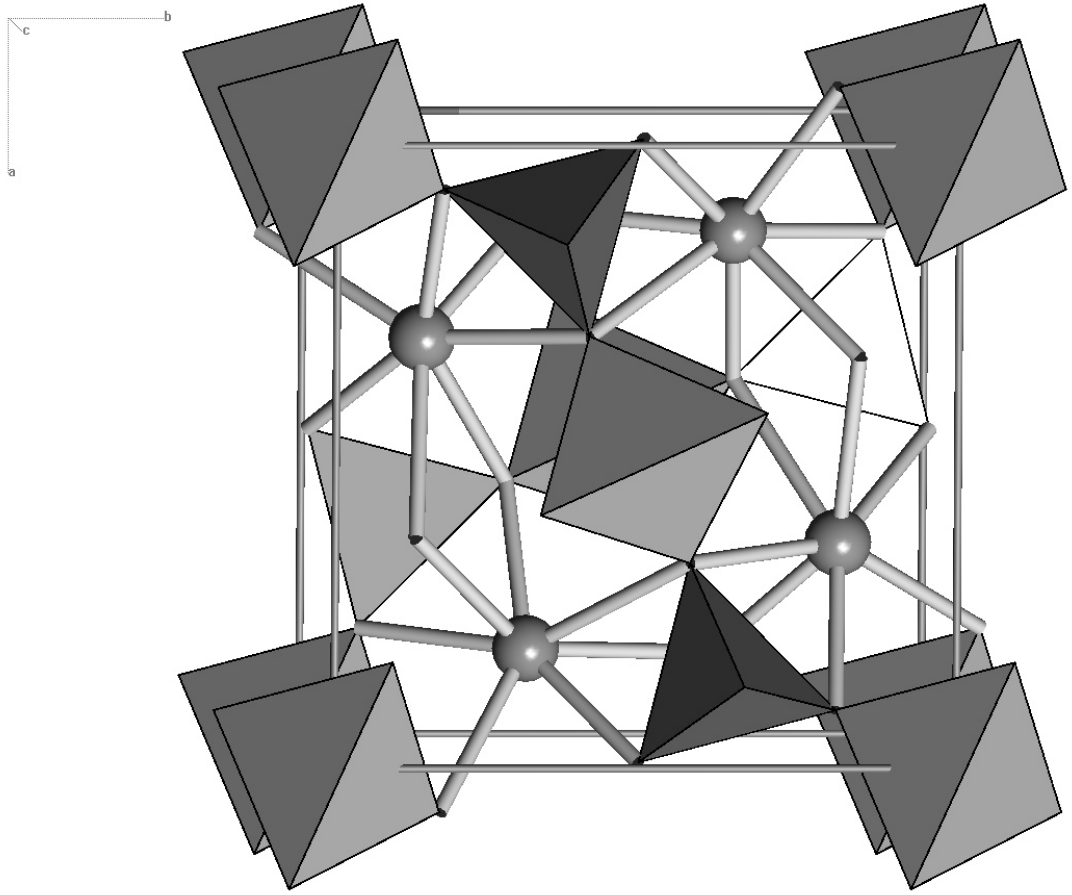

Figure 5.2. Melilite, $Ca_2MgSi_2O_7$, perspective *c*-axis projection, *a* vertical. The structure resembles a layered structure with layers of Mg and Si tetrahedral held together with bonds to the Na/Ca atoms (spheres).

Table 5.2.2. Melilite Group Ca-Na Sites.

End Member	Na-Melilite	Gehlenite	Akermanite
C.N.	8	8	8
Cation	Ca.5Na.5	Ca	Ca
Point Sym.	*m*	*m*	*m*
Wyckoff Not.	4*e*	4*e*	4*e*
Frac. Coords.			
x	0.3399	0.3375	0.3318
y	0.1601	0.1625	0.1682
z	0.5134	0.5110	0.5067
Distances			
O1(1)	2.453	2.416	2.484
O2(1)	2.470	2.430	2.465
O2(2)	2.572	2.576	2.712
O3(2)	2.463	2.438	2.425
O3(2)	2.793	2.816	2.695
Mean	2.572	2.563	2.577
σ	0.144	0.168	0.137
Poly.Vol.	32.893	32.475	32.909
Elect.Energy	-604.	-991.	-952.
Model Charge	1.5	2.0	2.0

Table 5.2.3. Melilite Group Al-Mg Tetrahedral Sites.

End Member	Na-Melilite	Gehlenite	Akermanite
C.N.	4	4	4
Cation	Al	Al	Mg
Point Sym.	$\bar{4}$	$\bar{4}$	$\bar{4}$
Wyckoff Not.	2*a*	2*a*	2*a*
Frac. Coords.			
x	0	0	0
y	0	0	0
z	0	0	0
Distances			
O3(4)	1.762	1.785	1.915
Poly.Vol.	2.788	2.916	3.599
T.Q.E.	1.0040	1.0010	1.0010
Ang.Var.	16.8	3.6	5.8
Elect.Energy	-2442.	-2431.	-1184.
Model Charge	3.0	3.0	2.0

Table 5.2.4. Melilite Group Al-Si Tetrahedral Sites.

End Member	Na-Melilite	Gehlenite	Akermanite
C.N.	4	4	4
Cation	Si	Al.5Si.5	Si
Point Sym.	*m*	*m*	*m*
Wyckoff Not.	4*e*	4*e*	4*e*
Frac. Coords.			
x	0.1416	0.1431	0.1397
y	0.3584	0.3569	0.3603
z	0.9531	0.9528	0.9352
Distances			
O1(1)	1.648	1.719	1.650
O2(1)	1.577	1.680	1.595
O3(2)	1.631	1.683	1.616
Mean	1.622	1.691	1.619
σ	0.031	0.019	0.023
Poly.Vol.	2.788	2.916	3.599
T.Q.E.	1.0081	1.0143	1.0110
Elect.Energy	-4341.	-3338.	-4378.
Model Charge	4.0	3.5	4.0

Table 5.3.1. Wadsleyite Group Unit Cells.

End Member	Wadsleyite	Co_2SiO_4
Formula	Mg_2SiO_4	Co_2SiO_4
Form. Wt. (g)	140.708	209.950
Density (g/cm^3)	3.4729	5.044
Mol. Vol. (cm^3)	40.515	41.628
Z	8	8
Cryst. Sys.	Orthorhombic	Orthorhombic
Laue Class	*mmm*	*mmm*
Space Group	*Imma*	*Imma*
Cell Parameters		
a (Å)	5.6983	5.753
b (Å)	11.4380	11.524
c (Å)	8.2566	8.340
Vol.	538.14	552.92
Ref.	Horiuchi & Sawamoto(1981)	Morimoto et al. (1974)

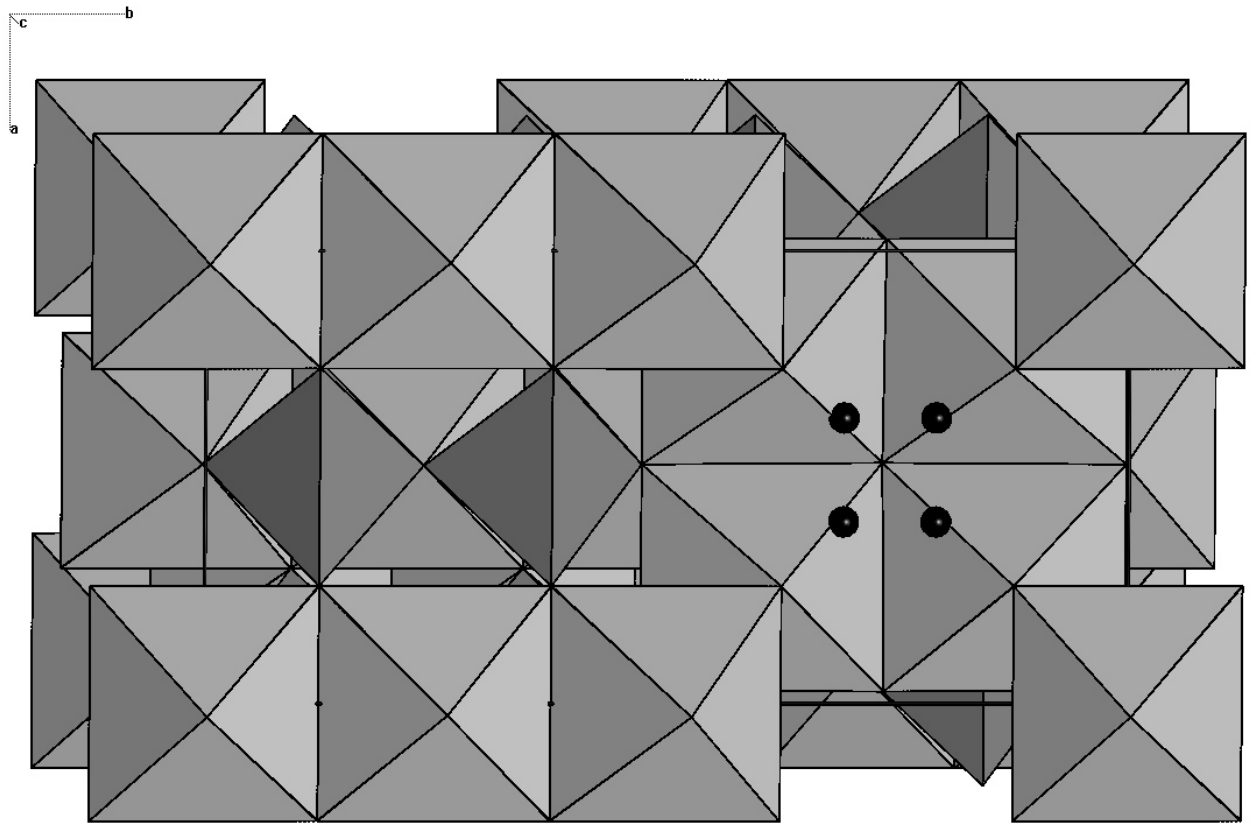

Figure 5.3. Wadsleyite (Mg_2SiO_4) is a polymorph of olivine but is a sorosilicate with Si_2O_7 groups and a non-silicate oxygen. The structure can incorporate significant amounts of OH at the non-silicate oxygen position with protons (sphere) shown on the O1-O3 octahedral edge. The structure can incorporate up to 3.3% H_2O by weight with charge compensation by Mg vacancy at M3.

Table 5.3.2. Wadsleyite Group Octahedral Sites.

End Member	Wadsleyite			Co_2SiO_4		
Site	M1	M2	M3	M1	M2	M3
C.N.	6	6	6	6	6	6
Cation	Mg	Mg	Mg	Co	Co	Co
Point Sym.	2/*m*	*mm*	2	2/*m*	*mm*	2
Wyckoff Not.	4*c*	4*e*	8*f*	4*c*	4*e*	8*f*
Frac. Coords.						
x	0	0	¼	0	0	¼
y	0	¼	0.1276	0	¼	0.1241
z	0	0.9701	¼	0	-.0286	¼
Distances						
O1(1)		2.035			2.052	
O1(2)			2.016			2.061
O2(1)		2.095			2.135	
O3(2)	2.115		2.123	2.147		2.147
O4(4)	2.046	2.093		2.086	2.128	
O4(2)			2.128			2.156
Mean	2.069	2.084	2.089	2.106	2.117	2.121
σ	0.036	0.024	0.056	0.032	0.031	0.047
Poly.Vol.	11.731	11.966	12.039	12.321	12.549	12.614
O.Q.E.	1.0050	1.0055	1.0072	1.0077	1.0051	1.0064
Ang.Var.	15.2	19.3	q23.4	24.5	17.4	21.0
Elect.Energy	-1172.	-1165.	-1193.	-1132.	-1141.	-1164.

Table 5.3.3. Wadsleyite Group Tetrahedral Sites.

End Member	Wadsleyite	Co_2SiO_4
C.N.	4	4
Cation	Si	Si
Point Sym.	*m*	*m*
Wyckoff Not.	8*i*	8*i*
Frac. Coords.		
x	0	0.1331
y	0.1198	0.1211
z	0.6168	¼
Distances		
O2(1)	1.701	1.697
O3(1)	1.638	1.622
O4(2)	1.632	1.621
Mean	1.651	1.641
σ	0.034	0.038
Poly.Vol.	2.297	2.257
O.Q.E.	1.0037	1.0029
Ang.Var.	14.7	11.6
Elect.Energy	-4322.	-4366.

Table 5.3.1. Lawsonite Unit Cell.

End Member	Lawsonite
Formula	$CaAl_2Si_2O_7(OH)_2H_2O$
Form.Wt.	314.241
Density (g/cm^3)	3.088
Mol. Vol. (cm^3)	101.76
Z	4
Cryst. Sys.	Orthorhombic
Laue Class	*mmm*
Space Group	*Ccmm*
Cell Parameters	
a (Å)	8.795
b (Å)	5.847
c (Å)	13.142
Vol.	675.82
Ref.	Baur (1978)

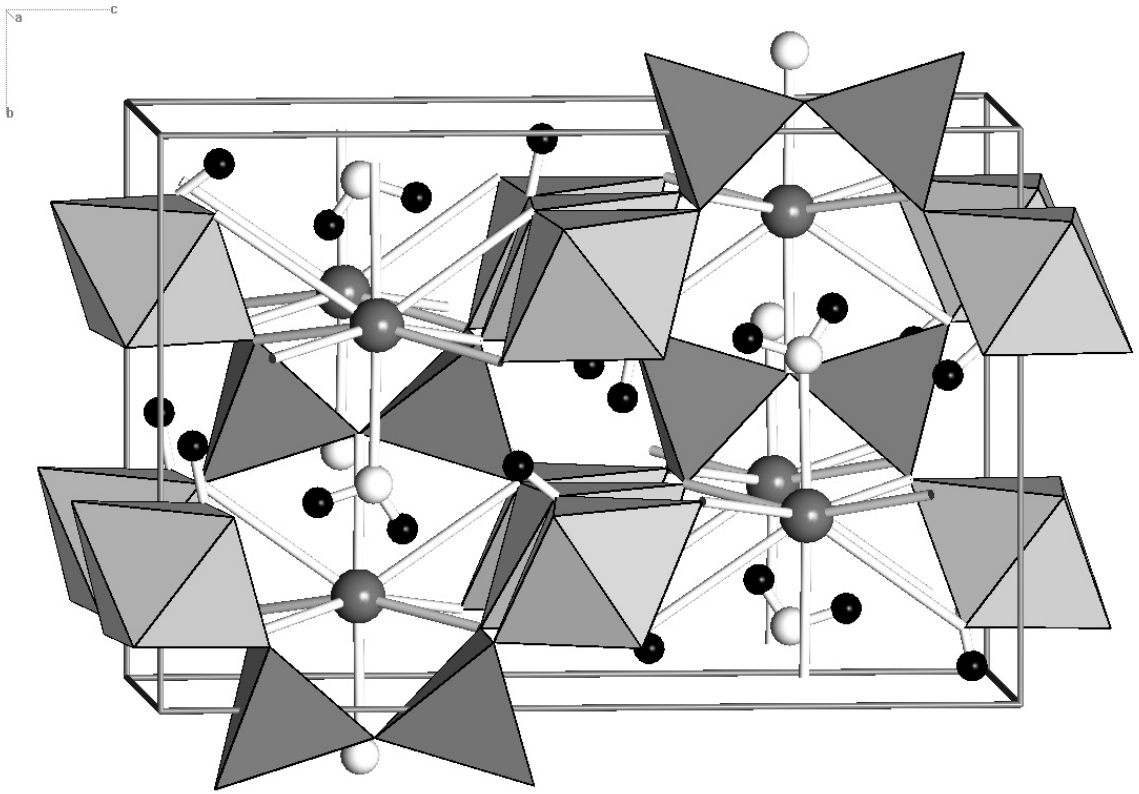

Figure 5.3. Lawsonite, $CaAl_2Si_2O_7(OH)_2H_2O$,. Ca (gray sphere) is in irregular 6-coordination with point symmetry mm. Al is in octahedral coordination with point symmetry -1, and Si has point symmetry m in tetrahedral coordination as part of an Si_2O_7 group. Despite the presence of molecular water, the structure is relatively dense at 3.09 g/cm^3.

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Table 5.4.2. Lawsonite Cation Sites.

End Member	Lawsonite		
Site	Ca	Al	Si
C.N.	6	6	4
Cation	Ca	Al	Si
Point Sym.	*mm*	$\bar{1}$	*m*
Wyckoff Not.	4*c*	8*d*	8*f*
Frac. Coords.			
x	0.33305	¼	0.9804
y	0	¼	0
z	¼	0	0.13298
Distances			
Mean	2.421	1.913	1.633
σ	0.038	0.042	0.020
Poly.Vol.	18.315	9.190	2.219
Q.E.	1.0255	1.0112	1.0049
Ang.Var.	78.4	36.7	19.61
Elect.Energy	-1170.	-2679.	-4779.
Model Charge	2.0	3.0	4.0