APPENDICES

The division between Appendix A and Appendix B is somewhat arbitrary but conforms to current usage. The majority of structure refinements in Appendix A are based on 2-D data, and those based on 3-D data have been superceded by more recent and more precise refinements. Thus the data listed in Appendix A are limited to "primary data", consisting of chemical compositions, cell contents, atomic positions and site occupancies. For Appendices B, C and D, complete data are listed; all "derivative data", interatomic distances and angles, were recalculated during this study. Where the calculated value(s) differed from those published by the original author(s) by more than two standard deviations, the discrepancy was identified (misprint in atomic position, bond length or bond angle), and the corrected value was used. The site-population Appendices (A3, B3, C3, D3, E3, F3, G2) also contain an outline of the method(s) used to derive the site populations, additional references to the source of the material and chemical data, and an assessment of the results; of course the latter cannot help but be somewhat subjective, good intentions to the contrary. For oxide sums, * indicates that additional oxides are present.

Where relevant, the method of cell-content calculation from the results of the chemical analysis is indicated by a number as follows:

1 24 (O, OH, F)
2 23 oxygen atoms
3 13 cations
4 16 cations
5 Cell contents assumed
6 Not given
7 Normalized on cell volume and density
8 8(Si + Al)
9 8 Si
10 Other (see Appendix B3)

In the numbering system used, [ ] and ( ) respectively designate orthorhombic and monoclinic amphiboles for which crystal-structure data are available; { } denotes an amphibole characterized by Mössbauer spectroscopy; < > denotes an amphibole examined by infrared absorption spectroscopy (but not Mössbauer spectroscopy); - denotes an amphibole examined by vibrational spectroscopy (exclusive of the hydroxyl stretching region); = denotes an amphibole for which magnetic susceptibility data are available.

Appendix A. Early Structural Data

(1)	Tremolite	Warren (1929)
[2]	Anthophyllite	Warren & Modell (1930b)
(3)	Magnesio-riebeckite	Whittaker (1949)
[4]	Anthophyllite	Ito & Morimoto (1950)
(5)	Magnesio-hornblende	Zussman (1955)
(6)	Pargasitic hornblende	Heritsch *et al.* (1957)
(7)	Edenitic hornblende	Heritsch *et al.* (1957)
(8)	Tremolite	Zussman (1959)
(9)	Cummingtonite	Ghose & Hellner (1959)
(10)	Tschermakitic hornblende	Heritsch & Kahler (1960)
(11)	Alumino-pargasitic hornblende	Heritsch & Kahler (1960)
(12)	Potassian titanian magnesio-hastingsite	Heritsch & Riechert (1960)
(13)	Potassian titanian magnesio-hastingsite	Heritsch *et al.* (1960)
(14)	Potassian arfvedsonite	Kawahara (1963)
(15)	$Na_2H_2Co_5Si_8O_{22}(OH)_2$	Prewitt (1963), Gibbs & Prewitt (1968)
(16)	$Na_2H_2Mg_5Si_8O_{22}F_2$	Prewitt (1963), Gibbs & Prewitt (1968)
(17)	Riebeckite	Colville & Gibbs (1964)
(18)	Anthophyllite	Lindeman (1964)
(19)	Pargasitic hornblende	Trojer & Walitzi (1965)

APPENDIX A1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	(1)	[2]	(3)	[4]	(5)	(6)	(7)	(8)	(9)	(10)
SiO_2	–	59.29	56.1	–	50.21	44.60	45.05	57.66	51.0	45.96
TiO_2	–	–	–	–	1.20	1.30	1.40	0.01	–	0.62
Al_2O_3	–	0.59	0.66	–	4.55	14.14	13.78	1.51	0.2	14.84
Fe_2O_3	–	0.29	15.6	–	2.77	1.76	0.99	0.23	–	3.73
FeO	–	0.06	4.06	–	9.03	4.98	9.98	0.33	34.1	4.48
MnO	–	2.77	0.00	–	0.19	–	0.20	0.01	1.6	0.04
MgO	–	30.98	14.5	–	17.85	15.40	12.01	24.34	8.4	14.63
CaO	–	1.26	1.11	–	9.69	11.46	10.28	13.79	0.6	9.51
Na_2O	–	0.37	5.05	–	0.40	3.20	3.84	0.12	0.05	3.25
K_2O	–	0.19	0.71	–	0.23	1.17	0.16	0.02	0.3	0.43
H_2O	–	3.80	(2.21)	–	4.07	2.01	2.48	2.26	–	2.58
F	–	0.20	–	–	0.15	–	–	–	–	–
		99.80	100.00	–	100.44	100.02	100.17	100.28	96.25	100.07
O≡F	–	0.08	–	–	0.06	–	–	–	–	–
Total	–	99.72	100.0		100.38	100.02	100.17	100.28	96.25	100.07
Si	8.00	7.76	7.94	8.00	7.13	6.37	6.54	7.81	8.0	6.47
Al	–	0.09	0.06	–	0.76	1.63	1.46	0.19	tr.	1.53
$\Sigma\ iv$	8.00	7.85	8.00	8.00	7.89	8.00	8.00	8.00	8.00	8.00
Al	–	–	0.05	–	–	0.76	0.90	0.05	–	0.93
Ti	–	–	–	–	0.13	0.17	0.15	–	–	0.07
Fe^{3+}	–	0.03	1.66	–	0.30	0.17	0.10	0.02		0.40
Fe^{2+}	–	0.01	0.48	–	1.07	0.59	1.21	0.04	4.71	0.53
Mn	–	0.31	–	–	0.02	–	0.03	–	0.22	0.01
Mg	5.00	6.04	3.06	7.00	3.78	3.31	2.61	4.92	2.07	3.06
$\Sigma\ vi$	5.00	–	5.25	–	5.30	5.00	5.00	5.03	–	5.00
$\Sigma\ vi_{-5}$	–	–	0.25	–	0.30	–	–	0.03	–	–
Ca	2.00	0.18	0.17	–	1.47	1.75	1.59	2.00	–	1.44
Na	–	0.10	1.38	–	0.11	0.25	0.41	–	–	0.56
$\Sigma^{M(4)}$	2.00	6.67	1.80	7.00	1.88	2.00	2.00	2.03	7.00	2.00
Na	–	–	–	–	–	0.63	0.67	0.03	–	0.33
K	–	0.03	0.13	–	0.04	0.22	0.03	–	–	0.08
Σ^{A}	–	0.03	0.13	–	0.04	0.85	0.70	0.03	–	0.41
Basis	5	1	6	5	7	6	6	1	6	3
a(Å)	9.74	18.5	9.72	18.5	9.87	9.86(6)	9.80(3)	9.840(5)	9.564	9.87(3)
b(Å)	17.8	17.9	17.95	17.9	18.14	17.99(6)	18.04(9)	18.052(9)	18.302	18.01(3)
c(Å)	5.26	5.27	5.31	5.27	5.31	5.300(5)	5.33(1)	5.275(5)	5.348	5.333(9)
β(°)	105.2	90	103.9	90	105.4	105.6(2)	104.6(2)	104.7(1)	101.83	105.7(1)
V(Å^3)	880	1745	899	1745	916.6	905.5	911.9	906.3	916.2	911.9

	(11)	(12)		(13)		(14)	(15)	(16)	(17)	(18)	(19)
SiO_2	43.18	39.24	40.95	39.85	39.66	47.46	–	–	–	–	44.20
TiO_2	0.93	4.28	0.80	4.40	4.60	0.74	–	–	–	–	1.32
Al_2O_3	16.84	14.14	14.31	14.74	14.27	2.43	–	–	–	–	13.93
Fe_2O_3	4.55	10.24	5.81	5.17	5.07	11.85	–	–	–	–	4.27
FeO	7.37	0.26	7.18	5.38	5.10	24.44	–	–	–	–	8.14
MnO	0.04	0.08	–	–	–	0.56	–	–	–	–	0.11
MgO	10.81	13.68	14.06	13.16	14.56	0.46	–	–	–	–	11.53
CaO	9.20	12.55	12.55	11.54	10.78	1.19	–	–	–	–	9.60
Na_2O	3.61	1.88	1.64	2.23	3.52	6.89	–	–	–	–	3.02
K_2O	0.93	1.68	1.54	1.86	2.10	1.59	–	–	–	–	0.80
H_2O	3.44	2.41	0.26	1.86	0.49	2.25	–	–	–	–	3.08
F	–	–	–	–	–	–	–	–	–	–	–
	100.90	100.44	99.10	100.19	100.15	100.02					100.00
O≡F	–	–	–	–	–	–	–	–	–	–	–
Total	100.90	100.44	99.10	100.19	100.15	100.02	–	–	–	–	100.00
Si	6.29	5.83	–	5.85	–	7.50	8.00	8.00	–	–	6.46
Al	1.71	2.17	–	2.15	–	0.45	–	–	–	–	1.54
Σ *iv*	8.00	8.00	–	8.00	–	7.95	8.00	8.00	–	–	8.00
Al	1.16	0.31	–	0.40	–	–	–	–	–	–	0.86
Ti	0.10	0.48	–	0.49	–	0.09	–	–	–	–	0.15
Fe^{3+}	0.50	1.14	–	0.57	–	1.41	–	–	–	–	0.47
Fe^{2+}	0.90	0.03	–	0.66	–	3.23	–	–	–	–	1.00
Mn	0.01	0.01	–	–	–	0.08	5.0Co	–	–	–	0.01
Mg	2.33	3.03	–	2.88	–	0.11	–	5.00	–	–	2.51
Σ *vi*	5.00	5.00	–	5.00	–	4.92	5.00	5.00	–	–	5.00
Σ vi_{-5}	–	–	–	–	–	–	–	–	–	–	–
Ca	1.44	2.00	–	1.82	–	0.20	–	–	–	–	1.50
Na	0.56	0.00	–	0.18	–	1.80	2.00	2.00	–	–	0.50
Σ M(4)	2.00	2.00	–	2.00	–	2.00	2.00	2.00	–	–	2.00
Na	0.46	0.54	–	0.46	–	0.31	2H	2H	–	–	0.36
K	0.17	0.32	–	0.35	–	0.32			–	–	0.15
Σ A	0.63	0.86	–	0.81	–	0.63	–	–	–	–	0.51
Basis	3	3	–	3	–	1	5	5	–	–	3
a (Å)	9.88(3)	9.98(2)		9.98(7)		9.94	9.832(5)	9.650(5)	9.811	18.576(5)	9.86
b (Å)	18.05(7)	17.98(2)		18.22(20)		18.17	18.088(2)	17.920(2)	18.023	18.010(5)	18.07
c (Å)	5.30(1)	5.33(3)		5.365(25)		5.34	5.299(5)	5.270(5)	5.316	5.258(2)	5.333
β (°)	105.5(1)	106.1(2)		105.7(2)		104.4	103.0(2)	102.9(2)	103.77	90	105.48
V (Å^3)	910.7	919.0		939.2		934	918.2	888.3	913.0	1759.1	915.7

APPENDIX A2. ATOMIC POSITIONS

		(1)	[2]		(3)	[4]		(5)	(6)
			A-chain	B-chain		A-chain	B-chain		
O(1)	x	0.14	0.19	0.06	0.117	0.185	0.065	0.117	0.099
	y	0.08	0.18	0.18	0.089	0.178	0.178	0.087	0.092
	z	0.24	0.05	-0.30	(0.207)	0.050	-0.300	(0.217)	(0.219)
O(2)	x	0.14	0.19	0.06	0.120	0.185	0.065	0.120	0.117
	y	0.18	0.07	0.07	0.173	0.072	0.072	0.176	0.176
	z	0.74	-0.44	0.20	(0.740)	-0.450	0.200	(0.720)	(0.727)
O(3)	x	0.14	0.19	0.06	0.110	0.190	0.060	0.112	0.117
	y	0	1/4	1/4	0	1/4	1/4	0	0
	z	0.74	-0.45	0.20	(0.710)	-0.530	0.220	(0.712)	(0.717)
O(4)	x	0.36	0.19	0.06	0.354	0.190	0.060	0.362	0.363
	y	0.25	0.00	0.00	0.246	0.000	0.000	0.249	0.250
	z	0.76	0.05	-0.30	(0.804)	-0.030	-0.280	(0.792)	(0.803)
O(5)	x	0.36	0.20	0.05	0.353	0.200	0.050	0.350	0.349
	y	0.14	-0.13	-0.13	0.140	-0.125	-0.125	0.137	0.138
	z	0.11	0.30	0.05	(0.173)	0.300	0.050	(0.140)	(0.149)
O(6)	x	0.36	0.20	0.05	0.337	0.200	0.050	0.340	0.341
	y	0.11	-0.13	-0.13	0.110	-0.125	-0.125	0.114	0.117
	z	0.61	-0.20	-0.46	(0.677)	-0.200	-0.450	(0.640)	(0.631)
O(7)	x	0.36	0.19	0.06	0.326	0.190	0.060	0.335	0.343
	y	0	-1/4	-1/4	0	-1/4	-1/4	0	0
	z	0.26	0.45	0.20	(0.346)	0.470	0.220	(0.325)	(0.353)
T(1)	x	0.29	0.22	0.03	0.280	0.225	0.025	0.280	0.276
	y	0.08	-0.18	-0.18	0.088	-0.175	-0.175	0.086	0.087
	z	0.30	-0.46	0.29	(0.360)	-0.461	0.289	(0.340)	(0.346)
T(2)	x	0.29	0.22	0.03	0.287	0.225	0.025	0.288	0.293
	y	0.18	-0.08	-0.08	0.170	-0.075	-0.075	0.172	0.170
	z	0.80	0.04	-0.21	(0.877)	0.039	-0.211	(0.838)	(0.863)
M(1)	x	0	0.13		0	0.124		0	0
	y	0.09	0.17		0.090	0.167		0.088	0.089
	z	1/2	0.38		(1/2)	0.385		(1/2)	(1/2)
M(2)	x	0	0.13		0	0.124		0	0
	y	0.17	0.08		0.181	0.083		0.178	0.178
	z	0	-0.13		(0)	-0.115		(0)	(0)
M(3)	x	0	0.13		0	0.124		0	0
	y	0	1/4		0	1/4		0	0
	z	0	-0.13		(0)	-0.115		(0)	(0)
M(4)	x	0	0.13		0	0.124		0	0
	y	0.28	-0.02		0.277	-0.019		0.277	0.279
	z	1/2	0.38		(1/2)	0.385		(1/2)	(1/2)

		(7)	(8)	(9)	(10)	(11)	(12)	(13)	(14)	(19)
	x	0.099	0.1134	0.111	0.098	0.098	0.104	0.099	0.117	0.105
O(1)	y	0.092	0.0873	0.088	0.093	0.093	0.089	0.092	0.089	0.092
	z	(0.219)	–	0.208	(0.208)	(0.208)	(0.224)	(0.219)	–	(0.21)
	x	0.117	0.1195	0.126	0.115	0.115	0.117	0.118	0.122	0.112
O(2)	y	0.176	0.1710	0.174	0.177	0.177	0.173	0.176	0.171	0.175
	z	(0.727)	–	0.715	(0.715)	(0.715)	(0.737)	(0.728)	–	(0.710)
	x	0.117	0.1130	0.114	0.114	0.114	0.110	0.115	0.110	0.109
O(3)	y	0	0	0	0	0	0	0	0	0
	z	(0.717)	–	0.707	(0.714)	(0.714)	(0.710)	(0.715)	–	(0.71)
	x	0.363	0.3651	0.381	0.366	0.366	0.368	0.362	0.354	0.371
O(4)	y	0.250	0.2481	0.245	0.251	0.251	0.250	0.250	0.246	0.250
	z	(0.803)	–	0.771	(0.796)	(0.796)	(0.838)	(0.802)	–	(0.79)
	x	0.349	0.3463	0.349	0.353	0.353	0.349	0.348	0.351	0.352
O(5)	y	0.138	0.1340	0.129	0.139	0.139	0.138	0.138	0.136	0.138
	z	(0.149)	–	0.053	(0.143)	(0.143)	(0.149)	(0.148)	–	(0.14)
	x	0.341	0.3434	0.350	0.337	0.337	0.342	0.342	0.337	0.338
O(6)	y	0.117	0.1179	0.118	0.115	0.115	0.117	0.118	0.114	0.114
	z	(0.631)	–	0.547	(0.647)	(0.647)	(0.637)	(0.632)	–	(0.65)
	x	0.343	0.3376	0.342	0.338	0.338	0.345	0.340	0.326	0.338
O(7)	y	0	0	0	0	0	0	0	0	0
	z	(0.353)	–	0.275	(0.338)	(0.338)	(0.355)	(0.350)	–	(0.33)
	x	0.276	0.2791	0.286	0.279	0.279	0.284	0.275	0.280	0.284
T(1)	y	0.087	0.0838	0.084	0.087	0.087	0.087	0.087	0.083	0.086
	z	(0.346)	–	0.273	(0.339)	(0.339)	(0.334)	(0.345)	–	(0.34)
	x	0.293	0.2880	0.298	0.294	0.294	0.294	0.292	0.289	0.295
T(2)	y	0.170	0.1707	0.168	0.172	0.172	0.172	0.170	0.170	0.173
	z	(0.863)	–	0.781	(0.854)	(0.854)	(0.849)	(0.862)	–	(0.85)
	x	0	0	0	0	0	0	0	0	0
M(1)	y	0.089	0.0877	0.088	0.090	0.090	0.082	0.089	0.091	0.088
	z	(1/2)	–	1/2	(1/2)	(1/2)	(1/2)	(1/2)	–	(1/2)
	x	0	0	0	0	0	0	0	0	0
M(2)	y	0.178	0.1761	0.179	0.177	0.177	0.176	0.178	0.183	0.177
	z	(0)	–	–	(0)	(0)	(0)	(0)	–	(0)
	x	0	0	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0	0	0
	z	(0)	–	0	(0)	(0)	(0)	(0)	–	(0)
	x	0	0	0	0	0	0	0	0	0
M(4)	y	0.279	0.2783	0.259	0.281	0.281	0.280	0.279	0.277	0.280
	z	(1/2)	–	1/2	(1/2)	(1/2)	(1/2)	(1/2)	–	(1/2)

Appendix A3. Site Populations and Annotations

Tremolite(1)

T(1) = T(2) Si
M(1) = M(2) = M(3) Mg
M(4) Ca
O(3) OH

Cation site-populations assigned by analogy with diopside (Warren & Bragg 1928). O(3) assigned as hydroxyl from the second rule of Pauling (1929). No chemical data given. Original structure in *I*2/*m* orientation.

Anthophyllite[2]

T1A = T1B = T2A = T2B Si
M1 = M2 = M3 = M4 Mg
O(3) OH

Cation site-populations assigned by analogy with enstatite (Warren & Modell 1930a). O3A and O3B assigned as hydroxyl from second rule of Pauling (1929).

Magnesio-riebeckite(3)

M(1) = M(3) 0.72Mg + 0.28Fe
M(2) 0.33Mg + 0.02Al + 0.65Fe
M(4) 0.69Na + 0.065K + 0.085Ca + 0.125Mg

Cation site-populations assigned from peak heights on Fourier syntheses, together with the cell contents from the chemical analysis. From the short <M(2)–O> and charge considerations, trivalent cations were considered to be strongly ordered at the M(2) site. Because of the fibrous nature of magnesio-riebeckite, only *hk*0 data could be collected; *z* parameters were derived by assuming that the cation polyhedra would be as regular as the *x* and *y* parameters allowed. Original structure in *I*2/*m*.

Mössbauer spectra of this amphibole are given in Bancroft & Burns (1969) and Ernst & Wai (1970); details are given in Appendix F, #{21}. The X-ray photoelectron spectrum is given by Adams *et al.* (1972), details given earlier in text.

Anthophyllite[4]

No chemical data given, $Mg_7Si_8O_{22}(OH)_2$ assumed. Site populations were presumably assigned after Warren & Modell (1930b).

Magnesio-hornblende(5)

M(1) = M(2) = M(3) 0.72Mg + 0.28Fe
M(4) 0.81Ca + 0.10Mg

Cation site-populations assigned from peak heights on Fourier syntheses, together with the cell contents from the chemical data. The possibility of some Fe at M(4) was not ruled out. Only *hk*0 data were collected; *z* co-ordinates were determined as for magnesio-riebeckite (3). Original structure in *I*2/*m*. The original chemical composition is from Hutton (1940); redetermination of the water by Zussman (1955) gave 3.05 wt. %. The structural formula was calculated from the density and cell volume (Hey 1939), giving $X_{1.62}Y_{5.20}Z_{8.00}O_{22.0}(OH, F)_{1.99}H_{0.92}$, indicating excess hydrogen in the structure. The results of a new analysis were given by Hutton (1956).

Pargasitic hornblende(6)

T(1) = T(2) 0.80Si + 0.20Al
M(1) = M(2) = M(3) 0.66Mg + 0.12Fe^{2+} + 0.03Fe^{3+} + 0.15Al + 0.04Ti
M(4) 0.88Ca + 0.12Na
A 0.63Na + 0.22K
O(3) 0.88 OH + 0.12 O^{2-}

Disordered site-populations were assumed for tetrahedral and octahedral sites. Only *hk*0 data were collected; *z* co-ordinates were determined as for magnesio-riebeckite(3). Chemical data were reported by Koritnig (1940).

Edenitic hornblende(7)

T(1) = T(2) 0.82Si + 0.18Al
M(1) = M(2) = M(3) 0.52Mg+0.24Fe^{2+} + 0.02Fe^{3+} + 0.18Al + 0.04Ti
M(4) 0.80Ca + 0.20Na
A 0.67Na + 0.03K
O(3) 0.94 OH + 0.06 O^{2-}

Disordered site-populations were assumed for tetrahedral and octahedral sites. Only *hk*0 data were collected; *z* co-ordinates were determined as for magnesio-riebeckite(3). Chemical data were reported by Paulitsch (1948).

Tremolite(8)

M(1) = M(2) = M(3) Mg
M(4) Ca

Cation site-populations assumed from analysis. Only *hk*0 data were collected, *x* and *y* values were determined by least-squares refinement; *z* values were not determined or estimated.

Cummingtonite(9)

M(1) = M(2) = M(3) 0.6Fe^{2+} + 0.4Mg
M(4) 1.0Fe^{2+}

Cation site-populations derived by manual adjustment of scattering factors until individual isotropic temperature-factors approximately equal [1.65, 2.23, 1.22 and 1.80 Å^2, respectively, for the M(1), M(2), M(3) and M(4) sites]. Details of the paragenesis are given by Mueller (1960, 1961).

Tschermakitic hornblende(10)

T(1) = T(2) 0.81Si + 0.19Al
M(1) = M(2) = M(3) 0.61Mg + 0.11Fe^{2+} + 0.08Fe^{3+} + 0.19Al + 0.01Ti
M(4) 0.72Ca + 0.28Na
A 0.33Na + 0.08K
O(3) 1.0 OH

Disordered cation site-populations were assumed at tetrahedral and octahedral sites. Only *hk*0 data were collected; *z* co-ordinates determined as for magnesio-riebeckite(3).

Alumino-pargasitic hornblende(11)

T(1) = T(2) 0.79Si + 0.21Al
M(1) = M(2) = M(3) 0.47Mg + 0.18Fe^{2+} + 0.10Fe^{3+} + 0.23Al + 0.02Ti
M(4) 0.72Ca + 0.28Na
A 0.46Na + 0.17K
O(3) 0.89 OH + 0.11 O^{2-}

Disordered cation site-populations were assumed at tetrahedral and octahedral sites. Only *hk*0 data collected; *z* co-ordinates determined as for magnesio-riebeckite(3).

Potassian titanian magnesio-hastingsite(12)

T(1) = T(2) 0.73Si + 0.27Al
M(1) = M(2) = M(3) 0.61Mg + 0.22Fe^{3+} + 0.06Al + 0.10Ti
M(4) 1.0Ca
A 0.54Na + 0.32K
O(3) 0.45 OH + 0.55 O^{2-}

Disordered cation site-populations were assumed at tetrahedral and octahedral sites. Only *hk*0 data were collected; *z* co-ordinates were determined as for magnesio-riebeckite(3). Results of two chemical analyses are given; the structural formula is derived from the more recent data.

Potassian titanian magnesio-hastingsite(13)

T(1) = T(2) 0.73Si + 0.27Al
M(1) = M(2) = M(3) 0.58Mg + 0.13Fe^{2+} + 0.11Fe^{3+} + 0.08Al + 0.10Ti
M(4) 0.91Ca + 0.09Na
A 0.46Na + 0.35K
O(3) 0.79 OH + 0.21 O^{2-}

Disordered cation site-populations were assumed at tetrahedral and octahedral sites. Only *hk*0 data were collected; *z* co-ordinates were determined as for magnesio-riebeckite(3). Results of chemical analyses are given; the structural formula is derived from the more recent data.

Potassian arfvedsonite(14)

M(1) = M(2) = M(3) (Mg, Fe, Mn, Ti)
M(4) (Ca, Na, K)

Site populations not derived. Apparent *c*-glide extinctions in this amphibole ascribed to the Templeton effect (Templeton 1956). Only (*hk*0) data collected, *z* co-ordinates not derived. The structural formula is given only in very general terms, as $(Ca, Na, K)_{2.64}(Si, Al)_8Fe^{3+}{}_{1.42}(Fe, Mn, Mg, Ti)_{3.54}(OH)_{2.15}O_{22}$. For the exact structural formula calculated from the chemical data given, see Appendix A1. Chemical analysis includes 0.16 wt. % P_2O_5.

$Na_2H_2Co_5Si_8O_{22}(OH)_2$(15)

M(1)	1.0Co	0.5Å^2
M(2)	1.0Co	0.5
M(3)	1.0Co	0.5
M(4)	(Na, Co)	1.3

Site populations determined by "population density" refinement (Gibbs & Prewitt 1968); the actual composition apparently departs somewhat from the ideal (Prewitt 1963). No co-ordinates given.

$Na_2H_2Mg_5Si_8O_{22}F_2$(16)

Site populations and co-ordinates not given; Na shows preferential ordering in M(4) site (Prewitt 1963).

Riebeckite(17)

M(1) 1.0Fe^{2+}
M(2) 1.0Fe^{3+}
M(3) 0.25Al + 0.50Fe^{2+} + 0.25Li
M(4) 1.0Na

Cation site-populations quoted by Onuki & Ernst (1969). Positional co-ordinates not given.

Anthophyllite[18]

Abstract only, no information given apart from cell dimensions, physical properties and cell contents.

Pargasitic hornblende(19)

T(1) ~ T(2) 0.81Si + 0.19Al
M(1) 0.63Mg + 0.07Fe^{2+} + 0.03Fe^{3+} + 0.03Ti + 0.24Al
M(2) 0.51Mg + 0.20Fe^{2+} + 0.09Fe^{3+} + 0.03Ti + 0.17Al
M(3) 0.38Mg + 0.32Fe^{2+} + 0.16Fe^{3+} + 0.03Ti + 0.11Al
M(4) 0.75Ca + 0.25Na
A 0.36Na + 0.15K
O(3) ~ OH

Disordered cation site-populations assumed at tetrahedral sites. Octahedral site-populations derived from Fourier maps (presumably in terms of Mg = Mg + Al and Fe = Fe^{2+} + Fe^{3+} + Ti). Only *hk*0 data were collected; *z* coordinates were derived as for edenitic hornblende(7). The chemical data were reported by Machatschki & Walitzi (1963).

Appendix B. Modern Data for Monoclinic Structures ($C2/m$)

(21)	Cummingtonite	Ghose (1961), Fischer (1966), Mitchell *et al.* (1971)
(22)	Grunerite	Finger (1967, 1969a); Finger & Zoltai (1967)
(24)	Potassian titanian magnesio-hastingsite	Papike & Clark (1967), Papike *et al.* (1969) Robinson (1971), Robinson *et al.* (1973)
(26)	Glaucophane	Papike & Clark (1968)
(28)	Tirodite	Papike *et al.* (1969)
(29)	Potassium-magnesio-katophorite	Papike *et al.* (1969), Cameron (1970)
(30)	Tremolite	Papike *et al.* (1969)
(34)	Fluor-richterite	Cameron (1970), Cameron & Gibbs (1971)
(35)	Fluor-richterite	Cameron (1970), Cameron & Gibbs (1971)
(36)	Fluor-tremolite	Cameron (1970), Cameron & Gibbs (1973)
(37)	Manganoan ferro-actinolite	Mitchell (1970), Mitchell *et al.* (1970a, b, 1971)
(38)	Potassian pargasite	Robinson *et al.* (1970, 1973), Robinson (1971)
(39)	Potassian titanian pargasite	Robinson (1971), Robinson *et al.* (1973)
(40)	Potassian oxy-kaersutite	Kitamura & Tokonami (1971), Kitamura *et al.* (1973, 1975)
(41)	Tirodite	Sueno *et al.* (1972a)
(42)	Magnesio-hornblende	Litvin *et al.* (1971a), Litvin (1973)
(43)	Tremolite	Litvin *et al.* (1972a), Litvin (1973)
(44)	Hastingsite	Litvin *et al.* (1972a), Litvin (1973)
(45)	Magnesio-hornblende	Litvin *et al.* (1971b, 1972b), Litvin (1973)
(46)	Magnesio-hornblende	Litvin *et al.* (1972b), Litvin (1973)
(48)	Tschermakite	Litvin (1973)
(49)	Ferro-tschermakitic hornblende	Litvin *et al.* (1973b)
(50)	Tschermakitic hornblende	Litvin *et al.* (1973b)
(51)	Potassian ferri-taramite	Litvin *et al.* (1973c)
(52)	Potassian ferri-tschermakitic hornblende	Kawahara *et al.* (1972)
(53)	Tremolite	Sueno *et al.* (1972b, 1973)
(54)	Ferro-tschermakite	Hawthorne (1973), Hawthorne & Grundy (1973a)
(55)	Potassian oxy-kaersutite	Hawthorne (1973), Hawthorne & Grundy (1973b)
(56)	Tremolite	Hawthorne (1973), Hawthorne & Grundy (1976)
(57)	Zincian tirodite	Hawthorne (1973), Hawthorne & Grundy (1973c, 1977b)
(58)	Subsilicic titanian magnesian hastingsite	Hawthorne (1973), Hawthorne & Grundy (1977a)
(59)	Potassian ferri-taramite	Hawthorne (1973), Hawthorne & Grundy (1978)
(60)	Potassian tschermakite	Litvin *et al.* (1974a)
(61)	Pargasite	Litvin *et al.* (1974b)
(62)	Sodian fluor-clinoholmquistite	Litvin *et al.* (1975a)
(63)	Pargasitic hornblende	Litvin *et al.* (1975b)
(64)	Arfvedsonite	Litvin *et al.* (1976)
(65)	Potassium-arfvedsonite	Litvin *et al.* (1976)
(66)	Potassium-arfvedsonite	Litvin *et al.* (1976)
(67)	Potassium-arfvedsonite	Hawthorne (1976)
(68)	Fluor-riebeckite	Hawthorne (1978b)
(69)	Ferro-glaucophane	Hawthorne (1979)
(70)	Pargasitic hornblende	Bocchio *et al.* (1978)
(71)	Pargasite	Bocchio *et al.* (1978)
(72)	Magnesio-hastingsite	Bocchio *et al.* (1978)
(73)	Ferroan pargasitic hornblende	Hawthorne *et al.* (1980)
(74)	Potassian titanian magnesio-hastingsite	Walitzi & Walter (1981)
(75)	. . .	Ungaretti *et al.* (1978, 1981), Ungaretti (1980)

APPENDIX B1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	(21)	(22)	(24)	(26)	(28)	(29)	(30)
SiO_2	54.0	49.01	40.42	58.04	55.27	52.67	58.90
TiO_2	0.01	0.05	4.43	0.66	0.00	3.53	0.02
Al_2O_3	0.40	0.00	13.90	10.31	0.34	1.72	0.56
Fe_2O_3	-	-	4.84	2.89	-	0.58	-
FeO	20.0	44.99	6.85	6.12	4.52	2.41	0.22
MnO	1.35	0.37	0.10	0.07	16.62	0.06	0.42
MgO	18.5	3.17	12.95	11.71	19.18	21.32	24.74
CaO	2.2	0.31	10.28	1.37	1.19	6.95	13.00
Na_2O	-	0.04	3.04	6.97	0.26	3.64	0.40
K_2O	-	0.00	2.05	0.02	0.00	5.70	0.10
H_2O	2.2	1.59	0.96	1.98	2.46	0.46	1.19
F	-	2.00	0.15	0.02	0.80	1.29	0.30
	98.66	101.21	99.97	100.17	100.73	100.48	99.95*
O ≡ F	-	0.84	0.06	0.01	0.34	0.54	0.13
Total	98.66	100.37	99.91	100.16	100.39	99.94	99.85
Si	7.90	8.00	5.97	7.92	7.95	7.44	7.95
Al	0.10	-	2.03	0.08	0.05	0.29	0.05
$\sum iv$	8.00	8.00	8.00	8.00	8.00	8.00*	8.00
Al	-	-	0.39	1.58	-	-	0.04
Ti^{3+}	-	-	0.49	0.06	-	0.17	-
Fe^{2+}	-	-	0.54	0.30	-	-	-
Fe	2.50	6.14	0.84	0.70	0.54	0.28	0.02
Mn	0.17	0.05	0.01	0.01	2.02	0.01	0.05
Mg	4.05	0.77	2.85	2.38	4.11	4.49	4.97
$\sum vi$	-	-	5.12	5.03	-	4.95	5.08
$\sum vi_{-5}$	-	-	0.12	0.03	-	-	0.08
Ca	0.35	0.06	1.63	0.20	0.18	1.05	1.86
Na	-	-	0.25	1.77	-	1.00	0.04
$\sum$ M(4)	7.07	7.02	2.00	2.00	6.85	2.05	2.00
Na	-	-	0.62	0.07	0.03	-	0.06
K	-	-	0.39	-	-	1.03	0.02
$\sum$ A	-	-	1.01	0.07	0.03	1.02	0.08
Basis	6	1	4	1	1	2	2
a(Å)	9.516(5)	9.5642(7)	9.870(1)	9.541(2)	9.583(2)	10.019(2)	9.818(5)
b(Å)	18.139(10)	18.393(2)	18.058(4)	17.740(3)	18.091(5)	18.036(7)	18.047(8)
c(Å)	5.311	5.3388(3)	5.307(2)	5.295(2)	5.315(4)	5.286(3)	5.275(3)
β(°)	102.1(1)	101.892(3)	105.20(2)	103.67(2)	102.63(2)	104.98(3)	104.66(5)
V(Å^3)	896.4	919.0(2)	912.7(3)	870.9(3)	899.1(6)	922.7(5)	904.2(6)

	(34)	(35)	(36)	(37)		(38)	(39)
SiO_2	–	–	–	50.6	51.0	–	–
TiO_2	–	–	–	0.1	0.04	–	–
Al_2O_3	–	–	–	2.4	2.0	–	–
Fe_2O_3	–	–	–	–	2.8	–	–
FeO	–	–	–	22.4	19.9	–	–
MnO	–	–	–	2.7	2.4	–	–
MgO	–	–	–	8.3	8.6	–	–
CaO	–	–	–	10.8	10.7	–	–
Na_2O	–	–	–	0.5	0.35	–	–
K_2O	–	–	–	0.14	0.16	–	–
H_2O	–	–	–	–	1.71	–	–
F	–	–	–	0.19	0.14	–	–
	–	–	–	98.45	100.08	–	–
O ≡ F	–	–	–	0.08	0.06	–	–
Total	–	–	–	98.37	100.02	–	–
Si	8.00	7.97	8.00	7.66	7.72	6.14	5.84
Al	–	–	–	0.34	0.28	1.86	2.16
$\sum^{iv}$	8.00	7.97	8.00	8.00	8.00	8.00	8.00
Al	–	–	–	0.10	0.08	0.54	0.34
Ti_{3+}	–	–	–	0.01	0.00	0.09	0.44
Fe_{2+}	–	–	–	2.84	0.31	1.08	1.28
Fe	–	1.68	–		2.53		
Mn	–	–	–	0.35	0.31	0.01	0.01
Mg	5.00	3.45	5.00	1.86	1.94	3.26	2.93
$\sum^{vi}$	5.00	5.13	5.00	5.16	5.17	4.98	5.00
$\sum^{vi}{}_{-5}$	–	0.13	–	0.16	0.17	–	–
Ca	1.00	0.90	2.00	1.76	1.74	1.99	1.84
Na	1.00	1.02	–	0.08	0.09	–	0.16
$\sum^{M(4)}$	2.00	2.05	2.00	2.00	2.00	2.00	2.00
Na	1.00	1.00	–	0.01	0.01	0.63	0.39
K	–	–	–	0.03	0.03	0.30	0.40
$\sum^{A}$	1.00	1.00	–	0.04	0.04	0.93	0.79
Basis	5	6	5	7		7	7
a(Å)	9.824(3)	9.846(2)	9.787(3)	9.891(1)		9.910(1)	9.9108(7)
b(Å)	17.968(3)	18.019(3)	18.004(2)	18.200(1)		18.022(1)	18.0487(9)
c(Å)	5.263(1)	5.274(3)	5.263(2)	5.305(1)		5.312(1)	5.3158(9)
β(°)	104.22 (1)	104.25(1)	104.44(2)	104.64(1)		105.78(1)	105.418(6)
V(Å^3)	900.6(4)	906.8(6)	898.1(5)	924.0(1)		912.9(1)	916.7(1)

	(40)	(41)	(42)	(43)	(44)		(45)
SiO_2	38.24	58.31	48.40	55.45	37.93	37.10	45.78
TiO_2	5.89	–	0.33	0.04	3.30	3.58	0.78
Al_2O_3	15.48	0.06	11.54	1.24	7.96	9.70	8.23
Fe_2O_3	9.27	–	1.44	1.04	3.96	4.97	2.99
FeO	4.89	0.13	3.59	7.04	28.32	26.85	16.12
MnO	0.16	8.24	0.07	0.59	0.57	0.38	0.44
MgO	10.73	27.17	18.03	21.22	2.56	1.55	10.44
CaO	10.69	2.46	10.70	10.54	9.66	9.87	11.77
Na_2O	2.50	0.22	2.52	0.54	1.71	1.59	0.79
K_2O	1.33	–	0.60	0.09	1.55	1.34	0.64
H_2O	0.53	–	2.63	2.30	2.50	2.41	2.08
F	–	–	–	–	–	–	–
	99.71	96.59	100.23	100.35	100.46	100.32	100.17*
O ≡ F	–	–	–	–	–	–	–
Total	99.71	96.59	100.23	100.35	100.46	100.32	100.17
Si	5.75	8.02	6.73	7.80	6.10	6.03	6.79
Al	2.25	–	1.27	0.20	1.50	1.87	1.21
$\sum iv$	8.00	8.02	8.00	8.00	7.60*	7.90*	8.00
Al	0.48	0.01	0.62	–	–	–	0.23
Ti^{3+}	0.67	–	0.03	–	(0.40)	(0.44)	0.09
Fe^{2+}	1.04	–	0.15	0.10	0.50	0.59	0.34
Fe	0.61	0.01	0.42	0.82	3.80	3.64	2.00
Mn	0.02	0.96	0.01	0.06	0.08	0.05	0.06
Mg	2.42	5.57	3.73	4.44	0.62	0.38	2.28
$\sum vi$	5.24	–	4.96	5.42	5.00	5.00	5.00
$\sum vi - 5$	0.24	–	–	0.42	–	–	–
Ca	1.72	0.36	1.59	1.58	1.68	1.72	1.87
Na	0.04	0.06	0.41	–	0.32	0.28	0.13
$\sum$ M(4)	2.00	6.97	2.00	2.00	2.00	2.00	2.00
Na	0.69	–	0.27	0.15	0.20	0.22	0.10
K	0.25	–	0.10	0.02	0.28	0.28	0.11
$\sum$ A	0.94	–	0.37	0.17	0.48	0.50	0.21
Basis	1	2	3	3	3	3	3
a (Å)	9.807(3)	9.595(1)	9.780(6)	9.830(2)	9.945(6)		9.883(4)
b (Å)	18.017(6)	18.077(2)	17.908(4)	18.084(3)	18.239(2)		18.126(5)
c (Å)	5.307(2)	5.307(1)	5.293(2)	5.281(3)	5.340(3)		5.319(3)
β (°)	105.43(2)	102.61(2)	104.93(7)	104.70(2)	104.95(2)		104.93(8)
V (Å^3)	903.9(7)	898.4(2)	895.8(8)	907.9(6)	935(1)		920.5(6)

	(45)	(46)		(48)	(49)	(50)	(51)	(52)
SiO_2	45.33	44.51	45.45	42.62	44.08	43.33	37.55	43.43
TiO_2	0.96	1.79	1.45	0.45	0.67	0.78	0.89	1.44
Al_2O_3	7.57	8.70	7.85	17.73	13.99	15.98	9.90	10.75
Fe_2O_3	3.95	3.46	3.22	1.00	1.40	1.84	11.89	9.43
FeO	16.22	16.09	16.80	12.96	16.20	13.15	21.40	4.39
MnO	0.49	0.29	0.28	0.04	0.18	0.17	1.25	0.14
MgO	9.17	10.45	10.09	9.90	8.44	9.54	1.31	13.82
CaO	11.99	10.36	11.00	11.84	10.88	10.95	7.28	10.60
Na_2O	0.93	1.47	1.10	0.54	1.35	1.21	4.05	1.72
K_2O	0.92	0.39	0.65	0.40	0.15	0.28	2.11	1.38
H_2O	2.04	2.10	1.96	2.45	2.70	2.70	1.84	2.07
F	–	–	–	–	–	–	–	–
	100.41*	99.84*	100.38*	99.93	100.04	99.99	99.82	99.17
O=F	–	–	–	–	–	–	–	–
Total	100.41	99.84	100.38	99.93	100.04	99.99	99.82	99.17
Si	6.82	6.59	6.80	6.14	6.48	6.30	6.14	6.36
Al	1.18	1.41	1.20	1.86	1.52	1.70	1.86	1.64
Σiv	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Al	0.16	0.10	0.18	1.15	0.91	1.04	0.04	0.22
Ti	0.11	0.18	0.16	0.05	0.07	0.09	0.11	0.16
Fe^{3+}	0.45	0.39	0.36	0.11	0.16	0.20	1.45	1.04
Fe^{2+}	2.04	1.99	2.02	1.56	1.99	1.59	2.92	0.54
Mn	0.06	0.04	0.04	0.01	0.02	0.02	0.18	0.02
Mg	2.18	2.29	2.24	2.13	1.85	2.06	0.30	3.02
Σvi	5.00	4.99	5.00	5.01	5.00	5.00	5.00	5.00
Σvi_{-5}	–	–	–	0.01	–	–	–	–
Ca	1.93	1.62	1.76	1.83	1.71	1.76	1.27	1.66
Na	0.07	0.38	0.24	0.15	0.29	0.24	0.73	0.34
$\Sigma M(4)$	2.00	2.00	2.00	1.99	2.00	2.00	2.00	2.00
Na	0.07	0.01	0.05	–	0.03	0.04	0.55	0.15
K	0.09	0.07	0.12	0.07	0.09	0.04	0.45	0.26
ΣA	0.16	0.08	0.17	0.07	0.12	0.08	1.00	0.41
Basis	3	3	3	3	3	3	3	3
a(Å)		9.842(4)		9.762(6)	9.792(-)	9.753(-)	9.960(8)	9.89
b(Å)		18.114(5)		17.994(12)	18.050(-)	17.989(-)	18.177(8)	18.03
c(Å)		5.318(3)		5.325(6)	5.322(-)	5.321(-)	5.352(2)	5.31
β(°)		104.93(8)		105.10(8)	104.8(-)	104.8(-)	105.07(5)	105.2(1)
V($Å^3$)		915.9(6)		902.2(5)	909.2(-)	902.5(-)	935(1)	913.7

	(53a)	(53b)	(54)	(55)	(56)	(57)	(58)	(59)
SiO_2	58.90		40.12	39.90	56.57	53.60	33.50	39.05
TiO_2	0.02		0.87	4.65	0.01	–	3.26	1.56
Al_2O_3	0.56		18.67	14.35	1.41	0.51	17.89	9.98
Fe_2O_3	–		2.64	9.60	0.01	0.35	6.65	10.98
FeO	0.22		16.75	0.04	0.08	3.50	16.49	18.36
MnO	0.42		0.27	0.08	0.03	12.90	0.26	1.38
MgO	24.74		5.48	14.52	24.41	16.90	5.00	3.76
CaO	13.00		11.65	12.14	12.25	1.66	10.30	6.94
Na_2O	0.40		0.80	1.90	1.44	0.75	3.14	4.56
K_2O	0.10		0.75	2.31	0.68	0.17	1.48	1.88
H_2O	1.19		1.62	0.50	1.46	2.53	1.41	1.81
F	0.30		0.07	0.12	1.52	–	0.25	–
	99.95		99.69	100.11	99.87	99.82*	99.63	100.26
$O \equiv F$	0.13		0.03	0.05	0.64	–	0.10	–
Total	99.85		99.66	100.06	99.23	99.82	99.53	100.26
Si	7.95		6.00	5.878	7.767	7.87	5.27	6.178
Al	0.05		2.00	2.122	0.228	0.09	2.73	1.822
$\sum iv$	8.00		8.00	8.000	7.995	7.94	8.00	8.000
Al	0.04		1.30	0.370	–	–	0.58	0.039
Ti_{3+}	–		0.10	0.515	0.001	–	0.39	0.186
Fe_{2+}	–		0.30	1.064	0.001	0.07	0.79	1.307
Fe	0.02		2.10	–	0.009	0.42	2.17	2.429
Mn	0.05		0.02	0.009	0.003	1.60	0.04	0.185
Mg	4.97		1.22	3.188	4.995	3.70	1.17	0.886
$\sum vi$	5.08		5.04	5.146	5.009		5.14	5.032
						0.75Zn		
$\sum vi_{-5}$	0.08		0.04	0.146	–	–	0.14	0.032
Ca	1.86		1.86	1.916	1.802	0.26	1.74	1.176
Na	0.04		0.10	–	0.198	0.21	0.12	0.792
$\sum M(4)$	2.00		2.00	2.062	2.000	6.97	2.00	2.000
Na	0.06		0.13	0.543	0.184	–	0.83	0.607
K	0.02		0.14	0.434	0.119	0.02	0.30	0.381
$\sum A$	0.08		0.27	0.977	0.303	0.02	1.13	0.988
Basis	2		2	1	1	1	1	1
a (Å)	9.860(1)	9.898(2)	9.8179(7)	9.892(1)	9.863(1)	9.606(1)	9.8659(4)	9.923(1)
b (Å)	18.118(3)	18.190(3)	18.106(2)	18.064(2)	18.048(2)	18.126(1)	18.0139(8)	18.134(2)
c (Å)	5.285(1)	5.296(1)	5.3314(5)	5.3116(7)	5.285(1)	5.317(1)	5.3545(2)	5.352(1)
β (°)	104.57(1)	104.46(1)	105.00(1)	105.388(5)	104.79(1)	102.63(1)	105.08(1)	104.84(1)
V (Å^3)	913.8(2)	923.4(2)	915.4(3)	915.1(4)	909.6(2)	903.4(1)	918.35(9)	930.9(2)

	(60)	(61)	(62)	(63)	(64)	(65)	(66)
SiO_2	41.36	39.49	57.68		47.86	46.45	53.00
TiO_2	1.95	2.02	-		0.64	0.64	0.97
Al_2O_3	12.49	15.56	13.52		1.69	3.44	0.27
Fe_2O_3	4.25	3.07	0.44		17.95	16.70	19.71
FeO	12.36	8.04	5.87		19.91	19.59	4.24
MnO	0.11	2.12	0.45		0.71	0.63	4.27
MgO	11.45	15.56	9.37		0.13	-	2.13
CaO	10.85	12.04	3.00		1.64	1.63	0.52
Na_2O	1.68	2.68	1.74		6.25	5.94	10.97
K_2O	1.50	0.32	0.28		0.61	3.74	2.84
H_2O	1.87	1.66	1.67		1.67	0.95	0.58
F	-	-	1.70		1.16	1.24	1.39
	99.87	100.16	101.07		100.22	100.95	100.89
$O \equiv F$	-	-	0.71		0.49	0.52	0.58
Total	99.87	100.16	100.36		99.73	100.43	100.31
Si	6.10	5.78	8.00	6.42	7.68	7.51	8.00
Al	1.90	2.22	-	1.58	0.32	0.49	-
Σiv	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Al	0.27	0.46	2.21	0.57	-	0.16	0.05
Ti^{3+}	0.22	0.22	Li=0.08	0.01	0.08	0.08	0.11
Fe^{2+}	0.47	0.33	0.05	0.05	2.17	2.02	2.40
Fe	1.52	0.98	0.68	0.27	2.68	2.65	0.53
Mn	0.01	0.01	0.05	0.01	0.10	0.09	0.55
Mg	2.51	3.30	1.93	4.06	0.03	-	0.48
Σvi	5.00	5.30	5.00	5.00	5.06	5.00	4.12
$\Sigma vi-5$	-	0.30	-	-	0.06	-	-
Ca	1.71	1.88	0.21	1.82	0.28	0.28	0.09
Na	0.29	-	Li=1.79	0.18	1.66	1.72	2.79
Σ M(4)	2.00	2.18	2.00	2.00	2.00	2.00	2.88
Na	0.19	0.76	0.45	0.46	0.28	0.14	0.41
K	0.28	0.06	0.04	0.05	0.17	0.77	0.54
Σ A	0.47	0.82	0.54	0.51	0.45	0.91	0.95
Basis	3	4			8	3	9
a (Å)	9.838(5)	9.869(3)	9.334(7)	9.863(3)	9.774(1)	9.935(5)	9.788(4)
b (Å)	18.063(4)	18.040(14)	17.596(10)	18.016(12)	18.032(7)	18.102(2)	17.863(11)
c (Å)	5.313(5)	5.307(3)	5.267(3)	5.291(4)	5.333(4)	5.339(3)	5.285(4)
β (°)	104.8(1)	105.17(3)	102.3(1)	105.2(1)	103.7(1)	103.9(2)	103.80(5)
V ($Å^3$)	912.3(9)	912.0(4)	846.0(5)	907(1)	913(1)	931(1)	897(1)

	(67)		(68)	(69)	(70)	(71)	(72)	(73)	(74)
SiO_2	48.78	49.20	50.45	54.63				43.89	40.26
TiO_2	0.58	0.96	0.14	0.06				0.79	3.16
Al_2O_3	1.61	1.70	1.96	11.02				14.42	11.99
Fe_2O_3	7.53	7.50	17.52	2.76				2.48	7.78
FeO	26.47	26.64	17.90	16.02				12.64	5.52
MnO	0.89	0.98	1.40	0.08				0.29	0.12
MgO	0.49	0.40	0.05	4.75	—	—	—	12.37	13.98
CaO	0.95	0.90	0.08	0.98				9.14	12.01
Na_2O	6.66	7.22	6.80	6.25				2.10	2.54
K_2O	3.95	3.39	1.48	0.01				0.12	1.87
H_2O	-	1.64	0.87	-				-	1.63
F	0.21	-	2.58	-				-	-
	97.21	100.53	101.77	97.56				97.99	100.86
$O \equiv F$	0.11		1.09	-				-	-
Total	99.62		100.68	97.56				97.99	100.86
Si	7.830		7.748	7.94	6.517	6.294	6.253	6.372	5.94
Al	0.170		0.252	0.06	1.483	1.706	1.747	1.628	2.06
$\sum iv$	8.000		8.000	8.00	8.000	8.000	8.000	8.000	8.00
Al	0.143		0.103	1.83	0.665	0.431	0.522	0.840	0.02
Ti	0.093		0.016	0.01	-	-	-	0.086	0.35
Fe^{3+}	0.905		2.025	0.31	0.288	0.429	0.478	0.271	0.86
Fe^{2+}	3.550		2.299	1.94	0.800	0.814	0.687	1.535	0.68
Mn	0.127		0.182	0.01	-	-	-	0.036	0.02
Mg	0.107		0.011	1.03	3.317	3.414	3.373	2.676	3.07
$\sum vi$	4.925		4.970	5.13	5.070	5.088	5.060	5.444	5.00
$\sum vi_{-5}$	-		-	0.13	0.070	0.088	0.060	0.444	—
Ca	0.159		0.013	0.15	1.762	1.872	1.873	1.422	1.90
Na	1.841		1.987	1.72	0.168	0.040	0.067	0.134	0.10
$\sum$ M(4)	2.000		2.000	2.00	2.000	2.000	2.000	2.000	2.00
Na	0.310		0.037	0.03	0.658	0.828	0.714	0.457	0.63
K	0.748		0.290	-	0.041	0.058	0.099	0.022	0.35
$\sum$ A	1.058		0.327	0.03	0.699	0.886	0.813	0.479	0.98
Basis	1		1	2	10	10	10	10	3
a(Å)	10.007(2)		9.811(3)	9.587(4)	9.818(1)	9.851(1)	9.848(1)	9.832(3)	9.880(2)
b(Å)	18.077(2)		18.013(5)	17.832(7)	17.972(2)	17.981(2)	17.974(2)	18.037(5)	18.012(4)
c(Å)	5.332(1)		5.326(2)	5.315(2)	5.300(1)	5.293(1)	5.299(1)	5.302(1)	5.324(2)
β(°)	104.101(7)		103.68(1)	103.47(3)	104.886(3)	105.070(7)	105.057(3)	105.01(2)	105.26(2)
V(Å^3)	935.48(3)		914.5	883.64	903.79	905.44	905.76	908.2	914.1(4)

APPENDIX B2. ATOMIC POSITIONS

		(21)	(22)	(24)	(26)	(28)	(29)	(30)
	x	0.1135(4)	0.1120(5)	0.1064(4)	0.1092(6)	0.1141(3)	0.1102(3)	0.1117(2)
O(1)	y	0.0874(2)	0.0882(2)	0.0885(2)	0.0927(3)	0.0865(2)	0.0855(2)	0.0860(1)
	z	0.2087(9)	0.2044(9)	0.2168(7)	0.2037(11)	0.2110(5)	0.2194(9)	0.2171(3)
	x	0.1232(4)	0.1253(4)	0.1183(4)	0.1177(6)	0.1222(3)	0.1172(3)	0.1185(2)
O(2)	y	0.1721(2)	0.1735(2)	0.1729(2)	0.1714(3)	0.1723(2)	0.1694(2)	0.1712(1)
	z	0.7193(9)	0.7142(8)	0.7308(7)	0.7480(11)	0.7190(5)	0.7269(10)	0.7240(4)
	x	0.1134(7)	0.1147(7)	0.1070(6)	0.1126(9)	0.1128(5)	0.1021(4)	0.1096(2)
O(3)	y	0	0	0	0	0	0	0
	z	0.7067(13)	0.7035(13)	0.7132(11)	0.7088(16)	0.7108(9)	0.7158(12)	0.7152(4)
	x	0.3798(5)	0.3839(5)	0.3664(4)	0.3679(6)	0.3739(4)	0.3612(4)	0.3654(2)
O(4)	y	0.2460(2)	0.2416(2)	0.2502(2)	0.2529(3)	0.2473(2)	0.2482(2)	0.2480(1)
	z	0.7716(9)	0.7689(8)	0.7896(8)	0.8058(11)	0.7772(6)	0.8007(11)	0.7933(3)
	x	0.3514(4)	0.3483(5)	0.3494(4)	0.3548(6)	0.3495(3)	0.3442(5)	0.3465(2)
O(5)	y	0.1310(2)	0.1275(2)	0.1391(2)	0.1318(3)	0.1305(2)	0.1302(2)	0.1343(1)
	z	0.0659(9)	0.0519(8)	0.1090(8)	0.0893(11)	0.0660(6)	0.0993(10)	0.0992(3)
	x	0.3488(5)	0.3478(4)	0.3446(4)	0.3407(6)	0.3491(3)	0.3408(4)	0.3436(2)
O(6)	y	0.1185(2)	0.1182(2)	0.1179(2)	0.1224(3)	0.1214(2)	0.1172(2)	0.1185(1)
	z	0.5597(9)	0.5530(8)	0.6054(8)	0.5814(11)	0.5597(6)	0.5940(10)	0.5884(3)
	x	0.3417(7)	0.3376(6)	0.3389(6)	0.3317(9)	0.3428(5)	0.3333(5)	0.3370(2)
O(7)	y	0	0	0	0	0	0	0
	z	0.2719(13)	0.2700(13)	0.2863(12)	0.3018(16)	0.2806(10)	0.3062(14)	0.2921(5)
	x	0.2874(2)	0.2867(2)	0.2812(1)	0.2831(2)	0.2862(1)	0.2756(1)	0.2804(1)
T(1)	y	0.0842(1)	0.0836(1)	0.0856(1)	0.0871(1)	0.0842(1)	0.0849(1)	0.0840(1)
	z	0.2746(3)	0.2707(3)	0.3035(3)	0.2931(4)	0.2777(2)	0.3021(4)	0.2964(1)
	x	0.2977(2)	0.2993(2)	0.2910(1)	0.2920(2)	0.2952(1)	0.2847(1)	0.2887(1)
T(2)	y	0.1688(1)	0.1667(1)	0.1724(1)	0.1730(1)	0.1700(1)	0.1718(1)	0.1711(1)
	z	0.7817(3)	0.7780(4)	0.8118(3)	0.8087(4)	0.7849(2)	0.8085(4)	0.8042(1)
	x	0	0	0	0	0	0	0
M(1)	y	0.0872(1)	0.08781(8)	0.0857(1)	0.0908(2)	0.0871(1)	0.0886(1)	0.0878(1)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0	0
M(2)	y	0.1773(1)	0.17936(9)	0.1775(1)	0.1807(2)	0.1773(1)	0.1793(1)	0.1766(1)
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(4)	y	0.2597(1)	0.25741(8)	0.2780(1)	0.2772(3)	0.2636(1)	0.2779(1)	0.2776(1)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	-	-	0.0290(7)	-	-	0.0199(7)	-
A(-)	y	-	-	1/2	-	-	1/2	-
	z	-	-	0.0612(24)	-	-	0.0431(11)	-
	x	-	-	-	-	-	-	-
A(-)	y	-	-	-	-	-	-	-
	z	-	-	-	-	-	-	-

		(34)	(35)	(36)	(37)	(38)	(39)	(40)
	x	0.1141(6)	0.1145(7)	0.1126(3)	0.1118(4)	0.1056(3)	0.1059(4)	0.1073(8)
O(1)	y	0.0849(3)	0.0846(3)	0.0847(2)	0.0874(2)	0.0886(1)	0.0884(2)	0.0872(4)
	z	0.2202(13)	0.2179(14)	0.2197(6)	0.2141(8)	0.2163(5)	0.2159(9)	0.2261(16)
	x	0.1179(6)	0.1188(7)	0.1187(3)	0.1209(3)	0.1198(2)	0.1190(3)	0.1170(8)
O(2)	y	0.1688(3)	0.1689(4)	0.1702(2)	0.1730(2)	0.1739(1)	0.1732(2)	0.1706(4)
	z	0.7276(13)	0.7256(14)	0.7239(6)	0.7240(7)	0.7350(5)	0.7313(8)	0.7326(16)
	x	0.1029(6)	0.1022(8)	0.1020(4)	0.1114(5)	0.1078(3)	0.1076(5)	0.1015(12)
O(3)	y	0	0	0	0	0	0	0
	z	0.7097(13)	0.7122(15)	0.7124(8)	0.7129(11)	0.7142(7)	0.7104(12)	0.7177(26)
	x	0.3606(6)	0.3611(7)	0.3644(4)	0.3675(4)	0.3674(2)	0.3670(4)	0.3654(9)
O(4)	y	0.2491(3)	0.2479(4)	0.2484(2)	0.2462(2)	0.2508(1)	0.2503(2)	0.2514(4)
	z	0.7914(12)	0.7928(13)	0.7907(7)	0.7906(8)	0.7923(5)	0.7915(9)	0.7858(19)
	x	0.3500(7)	0.3504(7)	0.3471(3)	0.3457(4)	0.3503(2)	0.3504(4)	0.3493(8)
O(5)	y	0.1302(2)	0.1310(3)	0.1351(2)	0.1335(2)	0.1397(1)	0.1403(2)	0.1396(4)
	z	0.0914(13)	0.0913(15)	0.1001(7)	0.0939(8)	0.1108(5)	0.1109(9)	0.1029(16)
	x	0.3445(6)	0.3448(7)	0.3444(3)	0.3432(4)	0.3440(2)	0.3455(4)	0.3472(8)
O(6)	y	0.1165(2)	0.1175(3)	0.1197(2)	0.1187(2)	0.1182(1)	0.1169(2)	0.1196(4)
	z	0.5908(12)	0.5857(13)	0.5857(6)	0.5841(8)	0.6094(5)	0.6108(8)	0.6056(16)
	x	0.3425(9)	0.3416(10)	0.3408(5)	0.3349(5)	0.3389(4)	0.3383(5)	0.3435(13)
O(7)	y	0	0	0	0	0	0	0
	z	0.2899(18)	0.2896(19)	0.2922(10)	0.2914(12)	0.2861(8)	0.2834(13)	0.2835(28)
	x	0.2803(2)	0.2816(2)	0.2829(1)	0.2807(1)	0.2799(1)	0.2806(1)	0.2842(4)
T(1)	y	0.0843(1)	0.0842(1)	0.0834(1)	0.08399(7)	0.0857(1)	0.0857(1)	0.0855(2)
	z	0.2937(5)	0.2944(5)	0.2960(2)	0.2943(3)	0.3034(2)	0.3042(3)	0.3027(8)
	x	0.2884(2)	0.2892(3)	0.2900(1)	0.2895(1)	0.2908(1)	0.2907(1)	0.2921(4)
T(2)	y	0.1711(1)	0.1704(1)	0.1707(1)	0.17054(7)	0.1734(1)	0.1728(1)	0.1722(2)
	z	0.8037(5)	0.8011(5)	0.8041(2)	0.8022(3)	0.8141(2)	0.8135(3)	0.8107(7)
	x	0	0	0	0	0	0	0
M(1)	y	0.0896(2)	0.0896(2)	0.0885(1)	0.08874(7)	0.0899(1)	0.0868(1)	0.0798(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0	0
M(2)	y	0.1783(2)	0.1797(2)	0.1760(1)	0.17857(7)	0.1766(1)	0.1771(1)	0.1774(3)
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(4)	y	0.2757(2)	0.2749(2)	0.2771(1)	0.27690(8)	0.2802(1)	0.2795(1)	0.2779(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0.0281(14)	0.0277(15)	-	-	0.0267(5)	0.0234(9)	0.0277(18)
A(-)	y	0.4892(12)	0.4871(10)	-	-	1/2	1/2	1/2
	z	0.0760(27)	0.0644(29)	-	-	0.0556(11)	0.0442(22)	0.0690(34)
	x	-	-	-	-	-	-	-
A(-)	y	-	-	-	-	-	-	-
	z	-	-	-	-	-	-	-

		(41)	(42)	(43)	(44)	(45)	(46)	(48)
O(1)	x	0.1131(3)	0.1069(10)	0.1128(9)	0.1043(11)	0.1084(6)	0.1070(11)	0.1042(12)
	y	0.0863(1)	0.0892(6)	0.0862(5)	0.0884(6)	0.0887(3)	0.0902(6)	0.0939(6)
	z	0.2120(6)	0.2063(24)	0.2161(23)	0.2020(31)	0.2137(17)	0.2040(28)	0.2099(28)
O(2)	x	0.1214(3)	0.1209(10)	0.1197(9)	0.1252(11)	0.1194(6)	0.1200(12)	0.1201(11)
	y	0.1719(1)	0.1731(6)	0.1723(5)	0.1757(6)	0.1734(3)	0.1740(6)	0.1761(6)
	z	0.7185(6)	0.7360(25)	0.7249(23)	0.7294(31)	0.7290(16)	0.7350(29)	0.7497(21)
O(3)	x	0.1134(5)	0.1113(15)	0.1103(13)	0.1139(17)	0.1112(8)	0.1080(12)	0.1122(17)
	y	0	0	0	0	0	0	0
	z	0.7096(8)	0.7148(36)	0.7139(32)	0.7167(31)	0.7156(24)	0.7210(41)	0.7113(40)
O(4)	x	0.3742(3)	0.3661(10)	0.3644(9)	0.3640(11)	0.3667(6)	0.3660(12)	0.3713(11)
	y	0.2473(2)	0.2515(6)	0.2473(5)	0.2485(6)	0.2487(3)	0.2500(6)	0.2519(6)
	z	0.7787(6)	0.7972(26)	0.7930(22)	0.7968(30)	0.7951(17)	0.7970(23)	0.7956(27)
O(5)	x	0.3491(3)	0.3499(11)	0.3460(9)	0.3465(11)	0.3482(7)	0.3500(12)	0.3530(12)
	y	0.1303(2)	0.1376(6)	0.1344(5)	0.1364(6)	0.1363(3)	0.1380(6)	0.1409(6)
	z	0.0676(6)	0.1045(27)	0.0965(24)	0.0992(32)	0.1026(18)	0.1040(32)	0.1104(29)
O(6)	x	0.3491(3)	0.3425(11)	0.3415(9)	0.3425(11)	0.3413(6)	0.3420(12)	0.3404(11)
	y	0.1214(2)	0.1182(6)	0.1177(5)	0.1182(6)	0.1179(3)	0.1190(6)	0.1208(6)
	z	0.5597(6)	0.5975(26)	0.5901(24)	0.5946(32)	0.5995(17)	0.5970(32)	0.6059(27)
O(7)	x	0.3427(5)	0.3330(15)	0.3338(13)	0.3342(16)	0.3343(9)	0.3330(16)	0.3285(18)
	y	0	0	0	0	0	0	0
	z	0.2829(9)	0.2827(36)	0.2885(31)	0.2935(43)	0.2962(24)	0.2910(41)	0.2865(43)
T(1)	x	0.2860(1)	0.2792(4)	0.2797(3)	0.2795(4)	0.2801(2)	0.2800(4)	0.2808(4)
	y	0.0843(1)	0.0855(2)	0.0840(2)	0.0841(1)	0.0849(1)	0.0848(2)	0.0866(2)
	z	0.2783(2)	0.2996(9)	0.2961(8)	0.2995(11)	0.2997(7)	0.2980(11)	0.3022(10)
T(2)	x	0.2947(1)	0.2909(4)	0.2894(3)	0.2924(4)	0.2904(2)	0.2920(4)	0.2927(4)
	y	0.1702(1)	0.1723(2)	0.1706(2)	0.1714(2)	0.1719(1)	0.1720(2)	0.1734(2)
	z	0.7851(2)	0.8095(10)	0.8031(8)	0.8071(11)	0.8075(7)	0.8100(12)	0.8171(10)
M(1)	x	0	0	0	0	0	0	0
	y	0.0870(1)	0.0881(3)	0.0876(3)	0.0900(2)	0.0887(1)	0.0866(2)	0.0900(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
M(2)	x	0	0	0	0	0	0	0
	y	0.1767(1)	0.1771(3)	0.1765(2)	0.1787(2)	0.1780(1)	0.1773(2)	0.1776(3)
	z	0	0	0	0	0	0	0
M(3)	x	0	0	0	0	0	0	0
	y	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0
M(4)	x	0	0	0	0	0	0	0
	y	0.2642(1)	0.2793(3)	0.2780(2)	0.2809(7)	0.2794(1)	0.2797(2)	0.2804(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
A(-)	x	-	0	0	0	0	0	0
	y	-	1/2	1/2	1/2	1/2	1/2	1/2
	z	-	0	0	0	0	0	0
A(-)	x	-	-	-	-	-	-	-
	y	-	-	-	-	-	-	-
	z	-	-	-	-	-	-	-

		(49)	(50)	(51)	(52)	(53a)	(53b)	(54)	(55)
	x	0.103(1)	0.103(2)	0.107(2)	0.1077(8)	0.1117(2)	0.1118(3)	0.1046(4)	0.1058(4)
O(1)	y	0.0932(7)	0.0921(8)	0.0915(9)	0.0864(5)	0.0862(1)	0.0863(2)	0.0936(2)	0.0870(2)
	z	0.202(4)	0.204(4)	0.204(3)	0.2198(14)	0.2171(5)	0.2175(6)	0.2099(7)	0.2196(7)
	x	0.120(1)	0.119(2)	0.124(2)	0.1166(9)	0.1190(2)	0.1198(3)	0.1198(4)	0.1184(4)
O(2)	y	0.1761(7)	0.1761(8)	0.1748(7)	0.1701(5)	0.1712(1)	0.1713(2)	0.1766(2)	0.1713(2)
	z	0.737(4)	0.751(4)	0.738(3)	0.7338(15)	0.7235(5)	0.7235(6)	0.7419(7)	0.7291(7)
	x	0.112(2)	0.109(3)	0.108(3)	0.1058(10)	0.1104(3)	0.1106(5)	0.1136(6)	0.1065(5)
O(3)	y	0	0	0	0	0	0	0	0
	z	0.715(6)	0.708(6)	0.718(6)	0.7359(15)	0.7157(7)	0.7179(9)	0.7126(10)	0.7160)10)
	x	0.368(1)	0.370(1)	0.360(2)	0.3655(8)	0.3658(2)	0.3662(3)	0.3713(4)	0.3651(4)
O(4)	y	0.2523(7)	0.2506(7)	0.2500(8)	0.2520(4)	0.2470(1)	0.2461(2)	0.2511(2)	0.2514(2)
	z	0.798(4)	0.810(3)	0.788(3)	0.7747(16)	0.7951(5)	0.7958(7)	0.7951(7)	0.7891(8)
	x	0.349(1)	0.352(1)	0.351(2)	0.3507(9)	0.3451(2)	0.3441(3)	0.3516(4)	0.3504(4)
O(5)	y	0.1385(6)	0.1387(7)	0.1366(7)	0.1407(5)	0.1326(1)	0.1316(2)	0.1401(2)	0.1402(2)
	z	0.105(4)	0.112(4)	0.102(4)	0.1076(16)	0.0950(5)	0.0936(6)	0.1093(7)	0.1107(7)
	x	0.340(1)	0.341(1)	0.340(2)	0.3481(8)	0.3429(2)	0.3420(3)	0.3418(4)	0.3469(4)
O(6)	y	0.1193(7)	0.1179(7)	0.1170(8)	0.1157(4)	0.1192(1)	0.1194(2)	0.1206(2)	0.1181(2)
	z	0.603(4)	0.603(4)	0.612(4)	0.6039(16)	0.5844(5)	0.5820(6)	0.6021(7)	0.6094(8)
	x	0.334(2)	0.333(2)	0.332(2)	0.3465(14)	0.3354(3)	0.3349(5)	0.3323(6)	0.3414(6)
O(7)	y	0	0	0	0	0	0	0	0
	z	0.294(4)	0.286(5)	0.282(5)	0.2740(30)	0.2946(7)	0.2957(10)	0.2861(12)	0.2859(12)
	x	0.2812(5)	0.2774(6)	0.2760(6)	0.2844(4)	0.2798(1)	0.2791(1)	0.2799(1)	0.2823(1)
T(1)	y	0.0864(2)	0.0867(3)	0.0857(3)	0.0849(2)	0.0839(1)	0.0837(1)	0.0864(1)	0.08560(7)
	z	0.298(2)	0.300(1)	0.302(1)	0.3000(10)	0.2955(2)	0.2945(2)	0.3012(3)	0.3045(3)
	x	0.2934(5)	0.2942(5)	0.2936(6)	0.2910(4)	0.2882(1)	0.2880(1)	0.2926(1)	0.2908(1)
T(2)	y	0.1733(3)	0.1731(3)	0.1715(3)	0.1725(2)	0.1707(1)	0.1702(1)	0.1736(1)	0.17304(7)
	z	0.813(1)	0.814(1)	0.811(2)	0.8091(9)	0.8032(2)	0.8027(2)	0.8161(2)	0.8118(3)
	x	0	0	0	0	0	0	0	0
M(1)	y	0.0895(8)	0.0904(4)	0.0897(3)	0.0823(2)	0.0877(1)	0.0878(1)	0.0902(1)	0.0817(1)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0	0	0
M(2)	y	0.1780(7)	0.1777(4)	0.1803(2)	0.1769(3)	0.1770(1)	0.1776(1)	0.1782(1)	0.1767(1)
	z	0	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0	0
M(4)	y	0.2801(7)	0.2802(3)	0.2826(4)	0.2776(3)	0.2776(1)	0.2778(1)	0.2806(1)	0.27890(8)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	–	–	0.020(4)	0	–	–	0.0272(34)	0.0467(11)
A(–)	y	–	–	1/2	1/2	–	–	1/2	1/2
	z	–	–	0.044(6)	0	–	–	0.0621(63)	0.0901(22)
	x	–	–	–	0	–	–	0	0
A(–)	y	–	–	–	1/2	–	–	0.4784(17)	0.4917(8)
	z	–	–	–	0	–	–	0	0

		(56a)	(56b)	(57)	(58)	(59)	(60)	(61)
	x	0.1112(2)	0.1114(1)	0.1138(3)	0.1035(3)	0.1063(2)	0.1064(10)	0.1080(12)
O(1)	y	0.0858(1)	0.08570(7)	0.0864(1)	0.0935(1)	0.0912(1)	0.0908(5)	0.0894(6)
	z	0.2184(3)	0.2182(3)	0.2116(5)	0.2109(5)	0.2136(4)	0.2132(23)	0.2071(27)
	x	0.1189(2)	0.1187(1)	0.1224(3)	0.1180(3)	0.1210(2)	0.1200(9)	0.1193(10)
O(2)	y	0.1706(1)	0.17067(6)	0.1723(1)	0.1766(1)	0.1745(1)	0.1730(5)	0.1745(5)
	z	0.7247(3)	0.7251(3)	0.7198(5)	0.7455(6)	0.7356(4)	0.7356(22)	0.7300(24)
	x	0.1072(3)	0.1082(2)	0.1130(4)	0.1111(4)	0.1104(3)	0.1083(14)	0.1111(15)
O(3)	y	0	0	0	0	0	0	0
	z	0.7152(5)	0.7154(4)	0.7104(7)	0.7097(8)	0.7099(6)	0.7157(33)	0.7165(34)
	x	0.3646(2)	0.3642(2)	0.3751(3)	0.3717(3)	0.3662(2)	0.3684(9)	0.3665(11)
O(4)	y	0.2482(1)	0.24818(7)	0.2469(1)	0.2518(1)	0.2499(1)	0.2523(8)	0.2509(6)
	z	0.7931(3)	0.7928(3)	0.7767(5)	0.7946(5)	0.7939(4)	0.8016(21)	0.7907(25)
	x	0.3466(2)	0.3467(1)	0.3501(3)	0.3526(3)	0.3494(2)	0.3479(10)	0.3504(11)
O(5)	y	0.1341(1)	0.13391(7)	0.1307(2)	0.1401(1)	0.1364(1)	0.1370(5)	0.1404(5)
	z	0.1003(3)	0.0998(3)	0.0673(5)	0.1155(6)	0.1004(5)	0.1045(23)	0.1097(25)
	x	0.3437(2)	0.3437(1)	0.3492(3)	0.3418(3)	0.3425(2)	0.3455(9)	0.3422(12)
O(6)	y	0.1183(1)	0.11805(7)	0.1204(2)	0.1181(1)	0.1189(1)	0.1199(4)	0.1156(6)
	z	0.5913(3)	0.5910(3)	0.5616(5)	0.6105(6)	0.6015(5)	0.6013(21)	0.6030(28)
	x	0.3386(3)	0.3380(2)	0.3439(4)	0.3328(4)	0.3353(4)	0.3343(15)	0.3333(15)
O(7)	y	0	0	0	0	0	0	0
	z	0.2913(5)	0.2921(4)	0.2787(8)	0.2807(9)	0.2886(7)	0.2947(33)	0.2650(35)
	x	0.28005(7)	0.2799(2)	0.2864(1)	0.2789(1)	0.27973(9)	0.2807(4)	0.2807(4)
T(1)	y	0.08417(3)	0.08424(4)	0.08426(5)	0.08693(5)	0.08621(5)	0.0851(2)	0.0847(2)
	z	0.2979(1)	0.2974(4)	0.2784(2)	0.3042(2)	0.3005(2)	0.3027(8)	0.3011(9)
	x	0.28803(7)	0.2882(2)	0.2955(1)	0.2920(1)	0.29085(8)	0.2906(3)	0.2924(4)
T(2)	y	0.17132(4)	0.17133(8)	0.16977(5)	0.17394(6)	0.17241(4)	0.1731(2)	0.1723(2)
	z	0.8050(1)	0.8056(4)	0.7853(2)	0.8188(2)	0.8105(1)	0.8102(8)	0.8120(9)
	x	0	0	0	0	0	0	0
M(1)	y	0.08821(7)	0.0883(1)	0.08711(6)	0.09076(6)	0.08945(4)	0.0885(2)	0.0887(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0	0
M(2)	y	0.17678(6)	0.1770(1)	0.17744(7)	0.17904(6)	0.17993(4)	0.1776(2)	0.1769(2)
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(4)	y	0.27797(4)	0.2779(1)	0.26251(5)	0.28193(7)	0.28033(6)	0.2805(2)	0.2792(2)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0.0407(23)	0.0450(40)	–	0.0391(24)	0.0437(8)	0	0.0162(57)
A(–)	y	1/2	1/2	–	1/2	1/2	1/2	1/2
	z	0.0887(42)	0.1030(76)	–	0.0908(52)	0.0906(16)	0	0.0712(93)
	x	0	0	–	0	0	–	–
A(–)	y	0.4901(19)	0.4897(38)	–	0.4848(5)	0.4889(5)	–	–
	z	0	0	–	0	0	–	–

		(62)	(63)	(64)	(65)	(66)	(67)	(68)
	x	0.111(2)	0.1084(13)	0.101(1)	0.114(1)	0.109(2)	0.1096(3)	0.1098(3)
O(1)	y	0.0933(10)	0.0875(7)	0.091(1)	0.093(1)	0.088(1)	0.0914(2)	0.0913(2)
	z	0.185(5)	0.2184(36)	0.183(5)	0.188(4)	0.167(5)	0.2082(7)	0.2047(6)
	x	0.114(2)	0.1183(13)	0.123(2)	0.121(1)	0.118(2)	0.1201(4)	0.1195(3)
O(2)	y	0.1742(9)	0.1727(7)	0.170(1)	0.171(1)	0.171(1)	0.1731(2)	0.1723(2)
	z	0.722(5)	0.7236(36)	0.732(6)	0.728(3)	0.739(4)	0.7332(7)	0.7378(6)
	x	0.107(3)	0.1107(19)	0.124(3)	0.104(2)	0.121(3)	0.1074(5)	0.1118(4)
O(3)	y	0	0	0	0	0	0	0
	z	0.716(7)	0.7125(50)	0.728(8)	0.704(5)	0.705(7)	0.7067(9)	0.7095(8)
	x	0.375(2)	0.3668(12)	0.354(2)	0.360(1)	0.353(2)	0.3643(4)	0.3656(3)
O(4)	y	0.2556(10)	0.2490(7)	0.255(1)	0.249(1)	0.254(1)	0.2473(2)	0.2491(2)
	z	0.787(5)	0.7869(36)	0.821(6)	0.813(5)	0.815(5)	0.7984(7)	0.8013(6)
	x	0.362(2)	0.3476(13)	0.343(2)	0.347(1)	0.351(2)	0.3440(4)	0.3491(3)
O(5)	y	0.1292(9)	0.1393(6)	0.130(1)	0.130(1)	0.130(1)	0.1273(2)	0.1282(2)
	z	0.055(4)	0.1144(35)	0.077(6)	0.075(3)	0.079(5)	0.0827(7)	0.0814(5)
	x	0.345(2)	0.3434(13)	0.337(2)	0.336(1)	0.337(2)	0.3663(4)	0.3399(3)
O(6)	y	0.1246(9)	0.1154(6)	0.120(1)	0.117(1)	0.118(1)	0.1172(2)	0.1206(2)
	z	0.552(4)	0.6054(34)	0.582(6)	0.576(4)	0.582(5)	0.5841(7)	0.5778(5)
	x	0.336(3)	0.3367(18)	0.324(3)	0.327(2)	0.333(3)	0.3262(6)	0.3325(5)
O(7)	y	0	0	0	0	0	0	0
	z	0.275(7)	0.2773(47)	0.297(8)	0.294(4)	0.301(7)	0.2988(10)	0.3004(8)
	x	0.2854(8)	0.2819(5)	0.2753(8)	0.2764(5)	0.2753(7)	0.2738(1)	0.2796(1)
T(1)	y	0.0879(4)	0.0847(3)	0.0844(5)	0.0853(2)	0.0865(4)	0.08618(7)	0.08585(6)
	z	0.282(3)	0.3025(15)	0.289(2)	0.289(1)	0.288(2)	0.2917(3)	0.2905(2)
	x	0.3025(9)	0.2909(5)	0.2964(9)	0.2897(4)	0.2893(7)	0.2864(1)	0.2901(1)
T(2)	y	0.1730(4)	0.1724(2)	0.1707(5)	0.1704(2)	0.1701(4)	0.17104(7)	0.17057(6)
	z	0.792(3)	0.8130(14)	0.800(2)	0.800(1)	0.797(2)	0.8018(2)	0.8015(2)
	x	0	0	0	0	0	0	0
M(1)	y	0.0895(5)	0.0881(5)	0.0917(5)	0.0919(2)	0.0859(4)	0.09205(5)	0.09069(5)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0	0
M(2)	y	0.1777(5)	0.1764(4)	0.1834(5)	0.1837(2)	0.1804(3)	0.18443(5)	0.18262(5)
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0	0
	z	0	0	0	0	0	0	0
	x	0	0	0	0	0	0	0
M(4)	y	0.2911(26)	0.2782(3)	0.2850(9)	0.2802(3)	0.2864(8)	0.2779(2)	0.2782(1)
	z	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	x	0.034(10)	0	0	0.031(-)	0	0.0172(5)	0.0387(11)
A(-)	y	1/2	1/2	1/2	1/2	1/2	1/2	1/2
	z	0.063(27)	0	0	0.075(-)	0	0.0402(9)	0.0833(19)
	x	-	-	-	-	-	-	-
A(-)	y	-	-	-	-	-	-	-
	z	-	-	-	-	-	-	-

		(69)	(70)	(71)	(72)	(73)	(74)
	x	0.1089(3)	0.1069(1)	0.1062(1)	0.1069(1)	0.1061(4)	0.1044(5)
O(1)	y	0.0947(1)	0.08979(6)	0.08926(6)	0.08831(7)	0.0895(2)	0.0883(3)
	z	0.2016(5)	0.2142(2)	0.2146(2)	0.2152(2)	0.2134(7)	0.218(1)
	x	0.1178(3)	0.1196(1)	0.1197(1)	0.1202(1)	0.1203(4)	0.1188(5)
O(2)	y	0.1730(1)	0.17378(6)	0.17400(6)	0.17360(7)	0.1743(2)	0.1728(3)
	z	0.7478(4)	0.7356(2)	0.7352(2)	0.7338(2)	0.7351(7)	0.733(1)
	x	0.1129(4)	0.1089(2)	0.1087(2)	0.1085(2)	0.1094(6)	0.1061(8)
O(3)	y	0		0	0	0	0
	z	0.7077(7)	0.7127(3)	0.7136(3)	0.7144(4)	0.7132(11)	0.713(2)
	x	0.3695(3)	0.3691(1)	0.3683(1)	0.3678(1)	0.3696(4)	0.3661(5)
O(4)	y	0.2520(1)	0.25024(6)	0.25026(6)	0.24970(7)	0.2498(2)	0.2505(3)
	z	0.8064(5)	0.7904(2)	0.7895(2)	0.7871(3)	0.7879(8)	0.788(1)
	x	0.3550(3)	0.3506(1)	0.3504(1)	0.3501(1)	0.3506(4)	0.3498(6)
O(5)	y	0.1307(1)	0.13927(6)	0.13981(6)	0.13963(7)	0.1403(2)	0.1409(3)
	z	0.0884(5)	0.1086(2)	0.1103(2)	0.1097(3)	0.1107(7)	0.114(1)
	x	0.3398(3)	0.3426(1)	0.3430(1)	0.3435(1)	0.3436(4)	0.3454(6)
O(6)	y	0.1224(1)	0.11701(6)	0.11653(6)	0.11570(7)	0.1168(2)	0.1169(3)
	z	0.5793(5)	0.6049(2)	0.6087(2)	0.6089(3)	0.6066(8)	0.611(1)
	x	0.3288(4)	0.3371(2)	0.3381(2)	0.3395(2)	0.3394(6)	0.3369(8)
O(7)	y	0	0	0	0	0	0
	z	0.3022(7)	0.2780(3)	0.2770(3)	0.2732(4)	0.2750(12)	0.280(2)
	x	0.2824(1)	0.28061(4)	0.28025(4)	0.28063(5)	0.2812(1)	0.2802(3)
T(1)	y	0.08732(5)	0.08576(2)	0.08569(2)	0.08545(2)	0.08559(7)	0.0856(2)
	z	0.2922(2)	0.30064(8)	0.30178(8)	0.3013(1)	0.3008(3)	0.3037(6)
	x	0.2926(1)	0.29146(4)	0.29105(4)	0.29112(5)	0.2921(1)	0.2912(2)
T(2)	y	0.17268(5)	0.17283(2)	0.17310(2)	0.17282(2)	0.17282(7)	0.1728(1)
	z	0.8079(2)	0.81182(8)	0.81279(8)	0.8116(1)	0.8125(3)	0.8137(4)
	x	0	0	0	0	0	0
M(1)	y	0.09176(7)	0.08952(3)	0.08945(3)	0.08931(4)	0.0892(1)	0.0864(3)
	z	1/2	1/2	1/2	1/2	1/2	1/2
	x	0	0	0	0	0	0
M(2)	y	0.18168(7)	0.17755(3)	0.17734(3)	0.17741(3)	0.1773(1)	0.1772(3)
	z	0	0	0	0	0	0
	x	0	0	0	0	0	0
M(3)	y	0	0	0	0	0	0
	z	0	0	0	0	0	0
	x	0	0	0	0	0	0
M(4)	y	0.2772(1)	0.27872(3)	0.27921(3)	0.27857(3)	0.2783(1)	0.2792(1)
	z	1/2	1/2	1/2	1/2	1/2	1/2
	x	-	0.0283(13)	0.0332(11)	0.0346(11)	0.037(5)	0.044(4)
A(-)	y	-	1/2	1/2	1/2	1/2	1/2
	z	-	0.0845(24)	0.0864(20)	0.0866(21)	0.088(9)	0.092(9)
	x	-	0	0	0	0	0
A(-)	y	-	0.4748(3)	0.4710(2)	0.4717(2)	0.4762(13)	0.489(2)
	z	-	0	0	0	0	0

APPENDIX B3. SITE POPULATIONS AND ANNOTATIONS

Cummingtonite(21)

M(1) $0.84Mg + 0.16Fe^{2+}$
M(2) $0.95Mg + 0.05Fe^{2+}$
M(3) $0.84Mg + 0.16Fe^{2+}$
M(4) $0.13Mg + 0.87Fe^{2+}$
O(3) 1.0(OH)

(0.67Mg + 0.33Fe²⁺) (0.85Mg + 0.15Fe²⁺) (0.67Mg + 0.33Fe²⁺) (0.25Mg + 0.75Fe²⁺)

Values in parentheses were given by Ghose (1961), and were derived by manually adjusting the site populations until the individual isotropic temperature-factors were approximately equal [1.00(5), 0.95(6), 0.99(6), 0.84(5) Å², respectively]. The first values given were derived by least-squares refinement of the site populations (Fischer 1966), with the isotropic temperature-factors refining to 0.23, 0.27, 0.22 and 0.88 Å², respectively.

Mössbauer examination of this amphibole (Hafner & Ghose 1971) indicates an $Fe^{2+}{}_{M(4)}/Fe^{2+}{}_{M(1,2,3)}$ ratio of 0.73/0.20; the above refinements give 0.75/0.26 (Ghose 1961) and 0.87/0.12 (Fischer 1966). These three studies give the following values for total Fe^{2+} in the crystal:

Ghose (1961)	$2.79Fe^{2+}$ p.f.u.
Fischer (1966)	$2.32Fe^{2+}$ p.f.u.
Hafner & Ghose (1971)	$2.46Fe^{2+}$ p.f.u.

The chemical analysis shows 0.35 Ca p.f.u. that has been attributed to admixed actinolite. Assuming a Ca content of 0.1 atoms p.f.u. and normalizing to seven cations gives an M-site bulk composition of $(Mg_{4.16}Fe^{2+}{}_{2.57}Mn_{0.17}Ca_{0.10})$. None of the values given above for total Fe^{2+} agree with this site content. Using the $Fe^{2+}{}_{M(4)}/Fe^{2+}{}_{M(1,2,3)}$ value of Hafner & Ghose (1971) together with $Fe^{2+}{}_{M(1)}/Fe^{2+}{}_{M(2)}/Fe^{2+}{}_{M(3)}$ proportions of Fischer (1966) and the total site-contents indicated above gives the following site-populations:

M(1) $0.29Fe^{2+} + 0.71Mg$
M(2) $0.09Fe^{2+} + 0.91Mg$
M(3) $0.29Fe^{2+} + 0.71Mg$
M(4) $0.76Fe^{2+} + 0.09Mn + 0.05Ca + 0.10Mg$

Mn was assumed to be ordered in the M(4) site as has been shown by combined Mössbauer and infrared absorption studies (Bancroft *et al.* 1967a) and combined Mössbauer and crystal-structure-refinement studies (Hawthorne & Grundy 1977b). O(3) was assumed to be completely occupied by OH. The mean observed octahedral bond-lengths are in good agreement with those calculated from the curves of Hawthorne (1978a) using the site-populations given above [<M(1)–O> obs. 2.094, calc. 2.093; <M(2)–O> obs. 2.083, calc. 2.088; <M(3)–O> obs. 2.090, calc. 2.085 Å]. Cell dimensions are from Viswanathan & Ghose (1965).

Grunerite(22)

M(1)	0.848(8)Fe + 0.152Mg	0.51(3) Å²
M(2)	0.773(7)Fe + 0.227Mg	0.51(4)
M(3)	0.888(12)Fe + 0.112Mg	0.56(5)
M(4)	0.985(8)Fe + 0.015Mg	0.92(4)
O(3)	0.70(OH) + 0.26F	

A Mössbauer study (Hafner & Ghose 1971) of this amphibole gave statistically equal site-populations for M(4) and the weighted average of the M(1), M(2) and M(3) sites; this study also indicated ~0.06 Fe^{3+} p.f.u., but there is no information as to where this occurs. The small amount of Ca indicated by the chemical analysis (Klein 1964, sample no. 1) presumably occurs in the M(4) site; thus, M(4) could be completely occupied by Fe^{2+} and Ca with even less Mg than indicated above. Chemical analysis total includes 0.1 wt. % P_2O_5.

Potassian titanian magnesio-hastingsite(24)

T(1)	0.58Si + 0.42Al	0.49(2) Å²
T(2)	0.92Si + 0.08Al	0.46(2)
M(1)	0.65Mg + 0.35Fe	0.91(3)
M(2)	0.24Ti+0.20Al +0.45Mg+0.11Fe	0.56(3)
M(3)	0.65Mg+0.35Fe	0.48(3)
M(4)	0.82Ca+0.11Na+ 0.06Fe+0.01Mn	0.87(2)
A	0.63Na+0.30K	3.34(13)

Cation site-populations from Robinson *et al.* (1973), all other data from Robinson (1971); no standard deviations given for site populations. The site populations of Si and Mg were refined over the T and M(1, 2, 3) sites, respectively, with octahedral Al and Ti assigned to the M(2) site and bulk-chemical constraints operative. The isotropic temperature-factors at the M(1), M(2) and M(3) sites differ significantly, and suggest that there is too much scattering power at the M(1) site. Both the analyses by Mason (1968) and White *et al.* (1972) show ~1.0 wt. % H_2O; as F = 0.15 wt. %, this suggests that the O(3) position is occupied by 0.47 OH + 0.04 F + 0.49 O^{2-}. Robinson *et al.* (1973) suggested that the Fe at the M(2) site is in the trivalent state on the basis of the short <M(2)–O> value. This leaves $0.32Fe^{3+}$ p.f.u. to be distributed over the M(1) and M(3) sites.

Using the equations of Hawthorne (1978a)

and assuming that the Fe at the M(1) and M(3) sites is in the divalent state, the following mean octahedral bond-lengths are obtained:

<M(1)–O> obs. 2.077, calc. 2.102 Å
<M(2)–O> obs. 2.047, calc. 2.041 Å
<M(3)–O> obs. 2.079, calc. 2.093 Å

The agreement is not good, particularly for the M(1) site. The occupancy of the O(3) position indicated by the analysis (Mason 1968) suggests that this amphibole is partially oxidized, a fact that is not surprising in view of its paragenesis. Kitamura *et al.* (1975) showed that Ti is strongly ordered in the M(1) site in potassian oxy-kaersutite(40). The oxidized nature of potassian titanian magnesio-hastingsite (24), the high Ti content and short <M(1)–O> suggest a similar ordering in this amphibole. From the observed bond-lengths, mean cation-radii at the three M sites may be calculated from the equations of Hawthorne (1978a); the following values were obtained for M(1), M(2) and M(3): 0.715, 0.670 and 0.725 Å, respectively. Using these values together with the total site-scattering powers indicated by the site populations of Robinson *et al.* (1973), cation site-populations may be obtained. Assuming M(1) is occupied by Mg, Ti^{4+} and Fe^{2+}, and M(3) is occupied by Mg, Fe^{3+} and Fe^{2+}, site populations may be calculated that result in mean cation-radii of 0.715 and 0.725 Å, respectively. The M(2) site-populations are obtained by difference, assuming that Mn and $0.12Fe^{2+}$ occupy the M(4) site; the resulting mean cation-radius for the M(2) site is 0.665 Å, in good agreement with the ideal value of 0.670 Å. The calculated site-populations are:

M(1) $0.65Mg+0.15Ti^{4+}+0.20Fe^{2+}$
M(2) $0.45Mg+0.20Al+0.09Ti^{3+}+0.21Fe^{3+}+0.05Fe^{2+}$
M(3) $0.65Mg+0.12Fe^{3+}+0.23Fe^{2+}$

These values are, of course, highly speculative, but the overall pattern is in agreement with current knowledge of oxy-amphiboles. One supporting factor is that the total number of higher-valence-state cations (Fe^{3+} and Ti^{4+}) co-ordinated to O(3) is approximately equal to the O^{2-} site-populations at the O(3) site: ($Ti^{4+}+Fe^{3+}$) at M(1) and M(3) = 0.42 atoms p.f.u.; O^{2-} site-occupancy of O(3) = 0.49 atoms p.f.u.

Glaucophane(26)

M(1)	$0.84(2)Mg+0.16Fe^{2+}$	0.38(5) Å²
M(2)	$0.91(2)Al+0.09Fe^{3+}$	0.26(4)
M(3)	$0.71(2)Mg+0.29Fe^{2+}$	0.24(3)
M(4)	$0.98(4)Na+0.02Ca$	0.80(7)

Cation site-populations from Papike & Clark (1968), derived by unconstrained refinement of site occupancies; Fe was assumed to be in the trivalent state at the M(2) site on the basis of the short <M(2)–O> and by analogy with crocidolite (Whittaker 1949). The total M-site contents obtained by unconstrained refinement differ significantly from those indicated by the chemical analysis:

refinement:

$(Na_{1.96}Ca_{0.04})(Mg_{2.39}Al_{1.82}Fe^{2+}_{0.61}Fe^{3+}_{0.18})$

analysis:

$(Na_{1.84}Ca_{0.20})\,(Mg_{2.38}Al_{1.58}Fe^{2+}_{0.70}Fe^{3+}_{0.30}Ti_{0.06}Mn_{0.01})$

No supporting evidence was given for the validity of the refined composition. Finger (1969a) and Burnham *et al.* (1971) have shown that unconstrained site-population refinement can lead to significant differences between refined and analyzed cell-contents; this may be the case for glaucophane. However, there is some evidence to support the results of the refinement. Comparison of <M(2)–O> in glaucophane and ferroglaucophane (Hawthorne 1979) together with the M(2) site-populations indicates that the mean constituent-cation radius in glaucophane is essentially correct. Bancroft & Burns (1969) obtained site populations for this glaucophane by Mössbauer spectroscopy; their results for the M(1) and M(3) sites are statistically identical to those indicated by the X-ray site-populations. This additional evidence supports the site populations assigned for glaucophane. The chemical analysis includes 0.01 Cl.

Tirodite(28)

M(1)	$0.208(9)(Fe+Mn)+0.792Mg =$ $0.79Mg+0.03Fe+0.18Mn$	0.45 Å²
M(2)	$0.158(8)\ (Fe+Mn)+0.842Mg =$ $0.84Mg+0.12Fe+0.04Mn$	0.39
M(3)	$0.125(14)\ (Fe+Mn)+0.875Mg =$ $0.88Mg+0.07Fe+0.05Mn$	0.27
M(4)	$0.88\ (Fe+Mn)+0.03Mg+0.09Ca =$ $0.78Mn+0.09Fe+0.03Mg+0.09Ca+0.01Na$	0.81
O(3)	$0.92(OH)+0.08F$	

Cation site-populations were refined in terms of the scattering species (Fe+Mn) and Mg, with bulk-chemical constraints operative; the spread in the equivalent isotropic temperature-factors at the M(1), M(2) and M(3) site suggests that the scattering power at the M(3) site is less than it should be. Cation site-occupancies were assigned by comparison of the <M–O> with

similar distances in ordered end-member pyroxenes and amphiboles containing these cations. Using these site occupancies together with the curves of Hawthorne (1978a) gives the following <M–O> distances:

<M(1)–O> obs. 2.096, calc. 2.096 Å
<M(2)–O> obs. 2.088, calc. 2.093 Å
<M(3)–O> obs. 2.080, calc. 2.077 Å

This supports the assigned site-populations, although it should be noted that the following site-populations

M(1) $0.792Mg+0.025Fe^{2+}+0.183Mn$
M(2) $0.842Mg+0.158Fe^{2+}$
M(3) $0.875Mg+0.125Mn$

provide an even better agreement. The O(3) site-population was taken from the analysis by Klein (1964) and normalized to a total of 1.0. The analysis total includes 0.09 P_2O_5.

Potassium-magnesio-katophorite(29)

T(1)	0.06(4)Al+0.96Si	0.54(2) Å²
T(2)	0.01Al+0.99Si	0.54(2)
M(1)	0.91Mg+0.05(2)Ti +0.04(Fe+Mn)	0.77(3)
M(2)	0.89Mg+0.11(Fe+Mn)	0.60(3)
M(3)	0.94Mg+0.06Ti	0.69(5)
M(4)	0.50Ca+0.50Na	0.80(3)
A(m)	0.5K	1.58(6)

Cation site-populations from Cameron (1970); the relative ordering of Ti and (Fe+Mn) was derived by the partitioned matrix method (see previous section on site occupancies from X-ray data) and is unlikely to be statistically significant. The cell contents indicate that all Fe^{3+} and 0.07 Ti must be assigned to the T sites to fill them up; whether this is the case or a result of error in the analysis is difficult to assess, as the presence of cations other than Si, Al and Be in the T sites has not been incontrovertibly proven in the amphiboles. <T(2)–O> is quite large: 1.646 Å. However, the isotropic temperature-factor at this site (see above) does not suggest any substitution of transition metals at this site. The large <T(2)–O> value is compatible with complete Si occupancy when the bond-length distortion Δ is considered, as potassian magnesio-katophorite(29) agrees with the general trend (Δ *vs.* <T–O>) of Figure 37 for non-^{iv}Al *C*2/*m* amphiboles. Comparison of <M(2)–O> for this amphibole (2.092 Å) and fluor-richterite(34) (2.085 Å) supports the premise that the mean radius of the constituent M(2) cation in this amphibole is larger than 0.720 Å, the value for Mg. Mn is negligible, and assuming $M(2) = 0.89Mg + 0.11Fe^{2+}$, the following values for <M(2)–O> are obtained: <M(2)–O> obs. 2.095, calc. 2.089 Å. This suggests that no trivalent cations occur in the M(2) site of potassium-magnesio-katophorite (29).

The chemical analysis (Prider 1939) indicates an O(3) site-occupancy $O(3)=0.22(OH)+0.29F + 0.42\ O^{2-}$ [<r> = 1.338 Å]; H_2O^- was not determined in the analysis. If this site population is correct, it indicates that this amphibole is considerably oxidized, suggesting that higher valence cations may occupy the M(1) and M(3) sites. The analysis total includes 0.15 SrO.

Tremolite(30)

M(1)	Mg	0.33 Å²
M(2)	Mg (0.98Mg+0.02Al)	0.31
M(3)	Mg	0.33
M(4)	0.95Ca+0.05Na	0.57
O(3)	0.94(OH)+0.06F	0.46

Site populations assigned; equality of octahedral-site isotropic temperature-factors is in agreement with this. The cell content from the chemical analysis (Ross *et al.* 1969) indicates a small amount of octahedral Al that may be assigned to the M(2) site on the basis of the observed site-preference of octahedral Al in other *C*2/*m* amphiboles and on mean bond-length considerations. The analysis total includes 0.10 CO_2 (Ross *et al.* 1968b).

Fluor-richterite(34)

M(1)	Mg	0.50(7) Å²
M(2)	Mg	0.50(7)
M(3)	Mg	0.24(8)
M(4)	0.5Ca+0.5Na	0.61(4)
A(1)	0.25Na	3.0(4)
O(3)	1.00F	0.49(11)

The stoichiometry of this synthetic amphibole (Cameron 1970) forces this assignment, assuming that all Ca occurs at the M(4) site. The isotropic temperature-factor at the M(3) site is less than that at the M(1) and M(2) sites, but the difference is only $\sim 2\sigma$, and hence not significant.

Fluor-richterite(35)

M(1)	0.80(2)Mg+0.20Fe	0.77(6) Å²
M(2)	0.48(2)Mg+0.52Fe	0.76(5)
M(3)	0.85Mg+0.15Fe	0.79(8)
M(4)	0.51Na+0.45Ca+0.04Fe	0.93(6)
A(1)	0.25Na	2.3(3)
O(3)	1.00F	0.74(12)

Cation site-populations (Cameron 1970)

derived by constrained site-occupancy refinement. The octahedral-site isotropic temperature-factors are statistically equal, supporting these results. The cell contents calculated from the chemical composition indicates a slight deficiency from the ideal Ca content and a slight excess of octahedral cations; excess Fe was thus assigned to the M(4) site. Charge-balance considerations (Cameron 1970) indicate that little if any of the Fe is in the trivalent state.

One rather puzzling factor is seen when the <M(3)–O> and constituent M(3) cation radii for the two fluor-richterites(34) and (35) are compared:

fluor-richterite(34):

$$<M(3)\text{–}O> = 2.057,\ r_{M(3)} = 0.720\ \text{Å}$$

fluor-richterite(35):

$$<M(3)\text{–}O> = 2.051,\ r_{M(3)} = 0.729\ \text{Å}.$$

The reason for the smaller <M(3)–O> associated with the larger constituent-cation radius is unclear.

Fluor-tremolite(36)

M(1)	Mg	0.40(4) Å²
M(2)	Mg	0.51(4)
M(3)	Mg	0.37(5)
M(4)	Ca	0.73(2)
O(3)	F	0.60(6)

Cation site-populations for this synthetic amphibole were assumed; the octahedral-site isotropic temperature-factors are statistically equal and support this assignment.

Manganoan ferro-actinolite(37)

T(1)	0.92Si+0.08Al	0.56(3) Å²
T(2)	1.00Si	0.58(3)
M(1)	$0.39Mg+0.61Fe^{2+}$	0.59(3)
M(2)	$0.34Mg+0.46Fe^{2+}+0.16Fe^{3+}+0.04Al$	0.55(3)
M(3)	$0.42Mg+0.58Fe^{2+}$	0.68(3)
M(4)	0.88Ca+O.08Mn+0.04Na	0.97(3)
O(3)	0.03F+0.97(OH)	

Cation site-populations (Mitchell *et al.* 1971) were derived by constrained site-occupancy refinement; no standard deviations were given. Tetrahedral Al occupancy of T(1) supported by comparison of <T–O> distances with those in tremolite(30). Octahedral-site temperature-factors are statistically equal and support the assigned populations. The "C-type" cation sum is 5.16 atoms p.f.u.; 0.16 Mn was assigned to the M(4) site.

Fe site-occupancies have also been obtained for this actinolite by Mössbauer methods (Burns & Greaves 1971):

M(1)	$0.765Fe^{2+}+(Fe^{3+}>0.00)$
M(2)	$0.20Fe^{2+}+(Fe^{3+}<0.16)$
M(3)	$0.58Fe^{2+}+(Fe^{3+}>0.00)$

The agreement between the X-ray and Mössbauer results is poor. The problems associated with deriving Fe site-populations by Mössbauer spectroscopy have been examined earlier, and for these reasons the X-ray results are considered more reliable.

Potassian pargasite(38)

T(1)	0.62Si+0.38Al	0.49(2) Å²
T(2)	0.91Si+0.09Al	0.48(2)
M(1)	0.77Mg+0.23Fe	0.40(2)
M(2)	0.48Mg+0.20Fe+0.27Al+0.05Ti	0.37(2)
M(3)	0.76Mg+0.24Fe	0.29(3)
M(4)	1.00Ca	0.68(2)
A(m)	0.315Na+0.15K	3.45(11)
O(3)	$0.42F+(0.58-x)O^{2-}+x(OH)$	0.91(5)

Cation site-populations (Robinson *et al.* 1973) were derived by constrained site-occupancy refinement; no standard deviations were given. There is a slight difference in the isotropic temperature-factors at the M(1) and M(3) sites, but this is of marginal (3σ) significance. Robinson *et al.* (1973) assumed that most of the Fe at the M(2) site is trivalent, with Fe at M(1) and M(3) divalent. This is a potassian pargasite, assuming Fe^{3+} < Al (*cf.* analyses 492 and 1011, Leake 1968).

Potassian titanian pargasite(39)

T(1)	0.54Si+0.46Al	0.55(3) Å²
T(2)	0.92Si+0.08Al	0.55(3)
M(1)	0.68Mg+0.32Fe	1.10(4)
M(2)	0.44Mg+0.22Ti+0.17Al+0.17Fe	0.62(3)
M(3)	0.68Mg+0.32Fe	0.69(4)
M(4)	0.92Ca+0.08Na	0.71(3)
A	0.39Na+0.40K	—

Cation site-populations from Robinson *et al.* (1973); no standard deviations given for site populations. The site populations of Si and Mg were refined over the T and M(1, 2,3) sites, respectively, with octahedral Al and Ti assigned to the M(2) site and bulk-chemical constraints operative. The isotropic temperature-factors at the M(1), M(2) and M(3) sites differ significantly, and suggest that there is too much scattering power at the M(1) site. The O(3) occupancy is not given. However, this "titanian pargasite" is from Boulder Dam, Arizona and was originally called kaersutite. A kaersutite from Boulder

Dam, Arizona (Leake 1968, #512) has a similar chemical composition and a site occupancy $O(3) = 0.11(OH)+0.19F+0.70\ O^{2-}$.

Although the mean bond-lengths suggest that this O(3) occupancy is not directly applicable to the titanian pargasite, it does suggest that the O(3) position is deficient in (OH) and partly occupied by O^{2-}. This suggests that the amphibole is at least partially oxidized; unfortunately the Fe^{3+}/Fe^{2+} ratio is not known, and so confirmatory evidence for this is lacking. However, oxidation can be accompanied by Ti disordering; this questions the assumption that Ti is ordered in the M(2) site. Robinson *et al.* (1973) proposed that the Fe in the M(2) site is predominantly Fe^{3+}; the <M(2)–O> distance is compatible with this assumption.

Potassium oxy-kaersutite(40)

T(1)	0.55Si+0.45Al	0.49(6) Å²
T(2)	0.89Si+0.11Al	0.31(6)
M(1)	0.40MG+0.33Fe+0.27Ti	0.35(7)
M(2)	0.75MG+0.23Fe+0.02Ti	0.22(8)
M(3)	0.50MG+0.46Fe+0.04Ti	0.38(9)
M(4)	0.12MC+0.86Ca	0.60(7)
A	0.73Na+0.25K	3.6(4)
O(3)	$0.25(OH)+0.75\ O^{2-}$	1.1(3)

where

MG = 0.83Mg+0.17Al

MC = $0.20Fe^{3+}+0.12Fe^{2+}+0.13Ti$ +0.46Mg+0.09Al

Tetrahedral site-populations were derived from considerations of mean bond-lengths; the agreement with the curves of Hawthorne & Grundy (1977a) is not good.

$Al_{T(1)}$ assigned 0.45, forecast 0.45

$Al_{T(2)}$ assigned 0.11, forecast 0.01

$^{iv}Al_{total}$ analysis 2.25, forecast 1.82 atoms p.f.u.

The reasons for this are not clear. Site occupancies of octahedral sites were determined from Fourier maps, and thus no standard deviations are available. Site occupancies from the X-ray study (Kitamura & Tokonami 1971) were determined in terms of the joint scattering species MG (Mg+Al) and Fe ($Fe^{2+}+Fe^{3+}+Ti$). The authors discussed the distribution of these joint species, but the discussion has no meaning as the ordering patterns of the different chemical species within a given scattering species are not necessarily correlated. A subsequent 2–D neutron structure-refinement (Kitamura *et al.* 1975) showed Ti to be strongly ordered in the M(1) site. However, the relative ordering of Mg–Al and Fe^{2+}–Fe^{3+} is not known.

Tirodite(41)

M(1)	Mg	0.89 Å²
M(2)	Mg	1.00
M(3)	Mg	0.96
M(4)	0.49Mn+0.19Ca+0.01Fe +0.28Mg+0.03Na	1.36

X-ray-diffraction data collected at 270°C, well above the $P2_1/m \rightarrow C2/m$ transition at 100°C. Material identical with (27), site populations were assigned by analogy with the room-temperature structure and confirmed by site-occupancy refinement. The similarity of the octahedral-cation temperature-factors supports the assigned occupancies.

Magnesio-hornblende(42)

T(1)	0.68Si+0.32Al	0.33(8) Å²
T(2)	1.00Si	0.22(8)
M(1)	$0.29Fe^{2+}+0.71Mg$	0.61(11)
M(2)	0.33Al+0.67Mg	0.59(11)
M(3)	1.00Mg	0.38(14)
M(4)	0.80Ca+0.20Na	0.40(8)
A	0.27Na+0.10K	—
O(3)	1.00(OH)	0.33(23)

Tetrahedral site-occupancies assigned on the basis of mean bond-lengths. The *R* index is not sensitive to the site occupancies (Litvin *et al.* 1971b) in this crystal, and the refinement was completed with the cation species statistically distributed over the octahedral sites. Octahedral site-occupancies assigned on the basis of observed mean bond-lengths. The unit formula was supposedly calculated on the basis of 13 cations but the sum of the tetrahedral- and octahedral-type cations equals 12.96, and the formula agrees with that calculated on the basis of 24(O, OH).

These results show poor agreement with the curves of Hawthorne & Grundy (1977a) and Hawthorne (1978a). The total observed ^{iv}Al is 1.27 atoms p.f.u.; the value forecast from the grand mean tetrahedral bond-length is 0.60 atoms p.f.u. Similarly, the agreement for the octahedral sites is not good.

Tremolite(43)

T(1)	0.95Si+0.05Al	0.30(5) Å²
T(2)	1.00Si	0.27(5)
M(1)	$0.89Mg+0.09Fe^{2+}+0.02Fe^{3+}$	0.66(8)
M(2)	$0.89Mg+0.09Fe^{2+}+0.02Fe^{3+}$	0.52(8)
M(3)	$0.89Mg+0.09Fe^{2+}+0.02Fe^{3+}$	0.38(10)
M(4)	$0.79Ca+0.03Mn+0.18Fe^{2+}$	0.33(50)
A	0.15Na+0.02K	—

Tetrahedral site-occupancies assigned on the basis of mean bond-lengths. Octahedral site-populations statistically distributed during structure refinement (Litvin 1973). The values are in good agreement with the curves of Hawthorne (1978a):

<M(1)–O>	obs.	2.089 Å,	calc.	2.081 Å
<M(2)–O>	obs.	2.086 Å,	calc.	2.088 Å
<M(3)–O>	obs.	2.076 Å,	calc.	2.073 Å

Even better agreement can be obtained by assigning all Fe^{3+} to M(2). Chemical analysis includes 0.14 P_2O_5.

Hastingsite(44)

T(1)	0.51Si+0.11Ti+0.38Al	0.82 Å²
T(2)	1.00Si	0.71
M(1)	1.00Fe^{2+}	0.92
M(2)	0.59Fe^{2+}+0.17Mg+0.18Fe^{3+} +0.06Al	0.79
M(3)	0.59Fe^{2+}+0.17Mg+0.18Fe^{3+} +0.06Al	0.74
M(4)	0.85Ca+0.15Na	0.74
A	0.21Na+0.30K	—

Tetrahedral site-populations assigned on the basis of mean bond-lengths; there is no direct evidence for tetrahedral occupancy of Ti. There is no information on the cation distribution assumed during refinement.

Site occupancies of octahedral cations derived from mean bond-lengths, by assuming ideal mean bond-lengths for complete occupancy by a single cation and then proportionally assigning the cations. Agreement with the curves of Hawthorne (1978a) is as follows, *assuming* complete occupancy of O(3) by hydroxyl:

<M(1)–O>	obs.	2.145 Å,	calc.	2.133 Å
<M(2)–O>	obs.	2.077 Å,	calc.	2.092 Å
<M(3)–O>	obs.	2.080 Å,	calc.	2.079 Å

Chemical analyses include 0.33 and 0.45 wt. % SO_3, and 0.11 and 0.52 wt. % P_2O_5 respectively. Kukovskii & Litvin (1970) give the infrared spectrum of this amphibole, #9 in Appendix G.

Magnesio-hornblende(45)

T(1)	0.70Si+0.30Al	0.65(3) Å²
T(2)	1.00Si	0.70(3)
M(1)	0.41Mg+0.46Fe^{2+}+0.08Fe^{3+} +0.05Al	0.72(3)
M(2)	0.51Mg+0.35Fe^{2+}+0.07Fe^{3+} +0.07Al	0.71(8)
M(3)	0.38Mg+0.48Fe^{2+}+0.09Fe^{3+} +0.05Al	0.51(4)
M(4)	0.95Ca+0.05Na	0.90(3)
A	0.08Na+0.10K	4.0(8)
O(3)	1.00(OH)	0.76(12)

Tetrahedral site-occupancies assigned on the basis of mean bond-lengths. Site populations of Mg* (Mg+^{vi}Al) and Fe* (Fe^{2+}+Fe^{3+}+Mn+Ti) derived by manual adjustment during refinement procedure; chemical species within these two groups were assumed to be disordered over all three sites. Using the site populations given above together with the curves of Hawthorne (1978a):

<M(1)–O>	obs.	2.102 Å,	calc.	2.088 Å
<M(2)–O>	obs.	2.058 Å,	calc.	2.086 Å
<M(3)–O>	obs.	2.095 Å,	calc.	2.081 Å

Much better agreement is obtained if the same Mg*/Fe* populations are retained but the trivalent cations are assumed to be ordered in the M(2) site.

M(1)	0.41Mg+0.59Fe^{2+}	calc.	2.110 Å
M(2)	0.51Mg+0.20Fe^{3+}+0.05Ti +0.10Al+0.14Fe^{3+}	calc.	2.063 Å
M(3)	0.38Mg+0.62Fe^{2+}	calc.	2.103 Å

Chemical analyses include — and 0.18 wt. % SO_3 and 0.14 and 0.11 wt. % P_2O_5, respectively.

Magnesio-hornblende(46)

T(1)	0.68Si+0.32Al	0.34(8) Å²
T(2)	1.00Si	0.33(8)
M(1)	0.51Mg+0.49Fe^{2+}	0.69(9)
M(2)	0.43Mg+0.42Fe^{2+}+0.15Al	0.66(9)
M(3)	0.35Mg+0.27Fe^{2+}+0.38Fe^{3+}	0.43(8)
M(4)	0.85Ca+0.15Na	0.37(?)
A	0.03Na+0.10K	—
O(3)	1.00(OH)	0.70(27)

Site populations assigned as for (44). Agreement with the curves of Hawthorne (1978a) is not good:

<M(1)–O>	obs.	2.119 Å,	calc.	2.104 Å
<M(2)–O>	obs.	2.027 Å,	calc.	2.082 Å
<M(3)–O>	obs.	2.071 Å,	calc.	2.059 Å

In particular, the agreement for the M(2) site is very poor; the curves indicate a mean constituent-cation radius of ~0.64 as compared with the value of 0.717 calculated from the site-population given. The cell contents would not appear to allow the constituent M(2) cation radius to be that small no matter what the cation distribution, and the duplicate chemical analyses support the Fe^{3+}/Fe^{2+} used; thus the source of this discrepancy is not clear. The chemical analyses indicate 0.12 and 0.30 wt. % SO_3 and 0.11 and 0.23 wt. % P_2O_5, respectively. This amphibole has been examined by Mössbauer and P.M.R. spectroscopy (Kalinichenko *et al.*

1977), and a comparison of the site-occupancy results is given below:

	PMR	Mössbauer	X-ray
M(1)	0.59Fe	$0.53Fe^{2+}$	$0.49Fe^{2+}$
M(2)	0.38Fe	$0.34Fe^{2+}$	$0.42Fe^{2+}$
M(3)	0.61Fe	$0.51Fe^{2+}$	$0.30Fe^{2+}+0.35Fe^{3+}$

The infrared vibrational spectrum is given by Kukovskii & Litvin (1970), *#8* in Appendix G.

Tschermakite(48)

T(1)	0.54Si+0.45Al+0.01Ti	0.87 Å²
T(2)	1.00Si	0.77
M(1)	$0.48Mg+0.52Fe^{2+}$	0.98
M(2)	$0.35Mg+0.05Fe^{3+}+0.60Al$	1.41
M(3)	$0.48Mg+0.52Fe^{2+}$	0.26
M(4)	0.92Ca+0.08Na	0.96
A	0.07K	—

Site populations as for (44). The isotropic temperature-factors at the three octahedral sites are very disparate, and suggest too much scattering power at M(2) and insufficient scattering power at M(3). However, this appears inconsistent with the fact that the Fe content of M(2) is very low; it is difficult to see how the scattering power at the M(2) site could be significantly reduced without resorting to vacancies, a possibility that is very unlikely on crystallochemical grounds. The agreement with the curves of Hawthorne (1978a) is as follows:

<M(1)–O>	obs.	2.116, calc.	2.106 Å
<M(2)–O>	obs.	2.013, calc.	1.997 Å
<M(3)–O>	obs.	2.116, calc.	2.097 Å

Ferro-tschermakitic hornblende(49)

T(1)	0.38Al+0.62Si	0.30 Å²
T(2)	1.00Si	0.13
M(1)	$0.3Mg+0.7Fe^{2+}$	0.52
M(2)	$0.4Mg+0.1Fe^{3+}+0.5Al$	1.26
M(3)	0.4Mg+0.6Fe	0.17
M(4)	0.86Ca+.14Na	0.06
A	0.02Na+0.05K	—

Site populations assigned as for (44). If the site populations quoted above were used in the last stages of refinement, the disparity in the octahedral cation temperature-factors does not support this distribution. However, the large isotropic temperature-factor for the M(2) cation(s) suggests a smaller scattering power at this site, and it is difficult to see how this could occur. The very small isotropic temperature-factor for the M(3) cation(s) suggests a larger scattering power at this site. The very small temperature-factor of the M(4) cation(s) could be a misprint. Agreement with the curves of Hawthorne (1978a) is as follows:

<M(1)–O>	obs.	2.122, calc.	2.116 Å
<M(2)–O>	obs.	1.988, calc.	2.009 Å
<M(3)–O>	obs.	2.103, calc.	2.102 Å

Agreement is good for the M(1) and M(3) sites, the disparity between the M(2) values is difficult to evaluate because of similar disparities in other structures.

Tschermakitic hornblende(50)

T(1)	——	0.94 Å²
T(2)	——	0.30
M(1)	$0.4Mg+0.6Fe^{2+}$	0.29
M(2)	$0.3Mg+0.1Fe^{3+}+0.6Al$	1.60
M(3)	$0.6Mg+0.4Fe^{2+}$	0.99
M(4)	0.88Ca+0.12Na	0.96
A	0.04Na+0.05K	—

Site populations assigned as for (44). The isotropic temperature-factors do not support this distribution, but any redistribution of cations would probably not lead to equal isotropic temperature-factors at the octahedral sites. Agreement with the curves of Hawthorne (1978a) is as follows:

<M(1)–O>	obs.	2.114, calc.	2.111 Å
<M(2)–O>	obs.	1.958, calc.	1.995 Å
<M(3)–O>	obs.	2.093, calc.	2.091 Å

As with (49), the agreement for the M(1) and M(3) sites is extremely close, with a large disparity between the M(2)-site values.

Potassian ferri-taramite(51)

T(1)	0.43Al+0.03Ti+0.54Si	0.79(9) Å²
T(2)	1.00Si	0.84(9)
M(1)	$0.85Fe^{2+}+0.09Mn+0.06Mg$	0.53(9)
M(2)	$0.18Fe^{2+}+0.69Fe^{3+}$ $+0.09Mg+0.04Al$	0.52(8)
M(3)	$0.85Fe^{2+}+0.07Fe^{3+}+0.08Al$	1.05(13)
M(4)	0.64Ca+0.36Na	1.16(13)
A	0.55Na+0.45K	3.79(48)
O(3)	$0.92(OH)+0.08(O^{2-})$	1.98(51)

Site populations assigned from refinement together with a consideration of mean bond-lengths and a cosmetically appealing Mössbauer spectrum. The isotropic temperature-factor for the M(3) cation(s) is a trifle large for comfort. Agreement with the curves of Hawthorne (1978a) is as follows:

<M(1)–O>	obs.	2.14, calc.	2.136 Å
<M(2)–O>	obs.	2.06, calc.	2.048 Å
<M(3)–O>	obs.	2.10, calc.	2.099 Å

As can be seen, the agreement is close. Kukovskii & Litvin (1970) gave the infrared vibrational

spectrum for this amphibole, *#10* in Appendix G.

Potassian ferri-tschermakitic hornblende(52)

No precise cation site-occupancies were given by Kawahara *et al.* (1972); "T(1) contains more Al than T(2)" but <T–O> is not consistent with ^{iv}Al from the cell contents. The mean atomic numbers of the cations at the M sites are: M(1) 17.6, M(2) 13.8, M(3) 16.3, M(4) 19.8; Fe was considered to be ordered at the M(1) and M(3) sites, with Mg ordered at M(2).

Tremolite(53)

M(1)	Mg	1.02(3) Å^2	1.38(4) Å^2
M(2)	Mg	0.95(3)	1.38(4)
M(3)	Mg	0.97(4)	1.34(5)
M(4)	Ca	1.53(2)	2.27(4)
O(3)	1.0(OH)	1.26(6)	1.79(8)

Amphibole identical with (29), site populations assigned by analogy and confirmed by equality of isotropic temperatures at the octahedrally co-ordinated sites. Structure refinements done at 400 and 700°C.

Ferro-tschermakite(54)

T(1)	0.45Al+0.55Si	0.59(2) Å^2
T(2)	0.05Al+0.95Si	0.59(2)
M(1)	0.610(5)Fe^{2+}+0.390Mg	0.65(2)
M(2)	0.15Fe^{3+}+0.05Ti+0.65Al	
	0.050(5)Fe^{2+}+0.100Mg	0.55(2)
M(3)	0.780(7)Fe^{2+}+0.220 Mg	0.60(2)
M(4)	0.93Ca+0.05Na+0.01Mn	
	+0.10(6)Mg	0.85(2)
A	0.23Na+0.14K	—
O(3)	1.0(OH)	0.99(5)

Tetrahedral site-occupancies assigned by method 2 of Papike *et al.* (1969). Trivalent cations assigned to M(2) site on the basis of mean bond-lengths, Mg–Fe^{2+} site-populations derived by constrained least-squares refinement. Comparison of the observed <M(1)–O> and <M(3)–O> with the values forecast from the equations of Hawthorne (1978a):

<M(1)–O> obs. 2.123 Å, calc. 2.112 Å
<M(3)–O> obs. 2.132 Å, calc. 2.112 Å

suggest that there may be an error in the chemical analysis, although the structure looks satisfactory in all other respects.

Potassian oxy-kaersutite(55)

T(1)	0.47(4)Al+0.53Si	0.47(2) Å^2
T(2)	0.06Al+0.94Si	0.48(2)
M(1)	0.343(9)Fe^{3+}+0.657Mg	0.66(4)
M(2)	0.056(9)Fe^{3+}+0.502Mg	
	+0.185Al+0.257Ti	0.63(4)
M(3)	0.235(14)Fe^{3+} +0.765Mg	0.64(6)
M(4)	0.958Ca+0.009Mn	
	+0.010(15)Fe^{3+}+0.025Mg	0.84(3)
A	0.543Na+0.434K	—
O(3)	0.25(OH)+0.03F+0.72 O^{2-}	0.94(7)

Tetrahedral site-populations derived by constrained least-squares refinement of occupancies; the standard deviation is unreasonably low and probably results from site refinement with temperature factors held constant. Octahedral site-populations were derived as follows: it was assumed that this amphibole crystallized as a normal hydroxy-amphibole and oxidized upon eruption; thus prior to oxidation, octahedral trivalent cations would be confined to the M(2) site, with Fe^{2+} and Mg occurring at M(1) and M(3). Furthermore, it was assumed that oxidation occurred sufficiently rapidly to prevent a reordering of the octahedral cations. Thus the present arrangement of cations would reflect the preoxidation distribution with the exception that Fe^{2+} was oxidized to Fe^{3+} during the dehydroxylation. Thus Ti was assigned to the M(2) site and Fe^{3+} was refined over the octahedral sites with bulk-chemical constraints operative. The statistical equality of the equivalent isotropic temperature-factors of the cations at the M(1), M(2) and M(3) sites indicates that the scattering power at each site is correct. In a previous refinement of a kaersutitic amphibole, Kitamura & Tokonami (1971) assumed that cation disordering would occur upon oxidation, and suggested preferential ordering of Ti in the M(1) and M(3) sites. X rays cannot distinguish between these two possibilities, but a neutron structure-refinement (Kitamura *et al.* 1975) showed that the latter is correct. Thus the site-populations given above are not correct. An attempt was made to derive better site-populations (this study), but the agreement between the observed and calculated mean bond-lengths is not good.

Tremolite(56)

T(1)	0.94(4)Si+0.06Al	0.43(1)	0.32(2) Å^2
T(2)	1.00Si+0.00Al	0.42(1)	0.37(3)
M(1)	1.00Mg	0.54(2)	0.37(3)
M(2)	1.00Mg	0.51(2)	0.39(3)
M(3)	1.00Mg	0.53(2)	0.35(4)
M(4)	0.910Ca+0.01Fe^{2+}		
	+0.089Na	0.72(2)	0.72(3)
A	0.185Na+0.119K	—	—
O(3)	0.665(OH)+0.329F		
	+0.006Cl	0.76(3)	0.62(3)

Tetrahedral site-populations were derived by constrained site-occupancy refinement using neutron data. Octahedral site-populations assigned, equality of octahedral cation isotropic temperature-factors for both X-ray (larger values) and neutron (smaller values above) is in agreement with this assignment. The hydrogen position derived from the neutron crystal-structure refinement is: 0.2088(6) 0 0.7628(14), giving an O(3)–H distance of 0.960(6) Å.

Zincian tirodite(57)

T(1)	0.978Si+0.022Al	0.58(1) Å²
T(2)	0.99Si+0.01Fe^{3+}	0.60(1)
M(1)	0.252(42)Zn+0.708(80)Mg +0.039(65)Mn	0.70(2)
M(2)	0.165Fe^{2+}+0.020Fe^{3+} +0.034(53)Zn+0.781(53)Mg	0.72(3)
M(3)	0.177(83)Zn+0.722(98)Mg +0.101(91)Mn	0.73(4)
M(4)	0.710Mn+0.045Fe^{2+} +0.140Ca+0.105Na	0.92(1)
O(3)	1.00(OH)	0.72(5)

Unconstrained site-population refinement indicated no Mg at M(4). Fe^{2+} was divided between M(4) and M(1, 2, 3) by Mössbauer spectroscopy; thus M(4) site-occupancy was known. The Mössbauer spectra also suggest the presence of $^{iv}Fe^{3+}$, which was assigned to T(2) on the basis of bonding arguments and by analogy with ferridiopside (Hafner & Huckenholz 1971). On the basis of mean bond-lengths, Fe^{2+} was assigned to M(2), and the distribution of Zn, Mg and Mn was refined over the octahedral M(1, 2, 3) sites with bulk-chemical constraints operative. The equality of octahedral-cation equivalent isotropic temperature-factors supports these site populations. Note the very large standard deviations associated with the full-matrix refinement of three scattering species over the octahedral sites. The chemical analysis includes 6.95% ZnO.

Subsilicic titanian magnesian hastingsite(58)

T(1)	0.51(11)Si+0.49Al	0.46(4) Å²
T(2)	0.81Si+0.19Al	0.43(4)
M(1)	0.691(8)Fe*+0.309Mg	0.66(3)
M(2)	0.301(8)Fe*+0.214Mg +0.195Ti+0.290Al	0.62(3)
M(3)	0.839(12)Fe*+0.161Mg	0.64(3)
M(4)	0.870Ca+0.060Na +0.070(15)Fe*	0.81(2)
A	0.70Na+0.30K	—
O(3)	1.0(OH)	0.91(6)

Ti and Al assigned to M(2) site, Al–Si and Fe*–Mg (Fe*=Fe^{2+}+Fe^{3+}+Mn) distributions determined by constrained least-squares refinement; the equality of the equivalent isotropic temperature-factors supports this distribution. There are several peculiar aspects to the site chemistry of this amphibole, and because of this, no attempt was made to determine the relative ordering of Fe^{2+} and Fe^{3+} over the octahedral sites. The refined tetrahedral site-populations are compatible with the mean bond-length arguments of Hawthorne & Grundy (1977a), and the grand mean tetrahedral bond-length is compatible with the unusual tetrahedral site-chemistry. The total Fe^{3+} p.f.u. (0.79) is greater than the refined Fe* (M2) site-population, indicating that some Fe^{3+} must occur at the M(1) or M(3) sites (or both). Supposing that all the Fe at the M(1) and M(3) sites was Fe^{2+}, the curves of Hawthorne (1978a) predict the following values:

<M(1)–O> obs. 2.116 Å, calc. 2.116 Å
<M(3)–O> obs. 2.131 Å, calc. 2.114 Å

These results suggest that any Fe^{3+} at the M(1) and M(3) sites in this amphibole should be concentrated in the M(1) site. This conclusion is in agreement with results from other structures; however, the agreement between the observed and calculated <M–O> distances is not good for the M(1) and M(3) octahedra. There is also a significant difference between the observed and calculated <M(2)–O> distance [obs. 1.980(2), calc.(Ti^{3+}) 2.023, calc.(Ti^{4+}) 2.013 Å]; this experimental result was confirmed by a second complete crystal-structure refinement on a different crystal from the same separate.

Potassian ferri-taramite(59)

T(1)	0.57Si+0.43Al	0.56(1) Å²
T(2)	0.98Si+0.02Al	0.53(1)
M(1)	0.730(5)Fe^{2+}+0.270Mg	0.84(2)
M(2)	0.131(5)Fe^{2+}+0.654Fe^{3+}+ 0.102Mg+0.093Ti+0.020Al	0.66(2)
M(3)	0.706(8)Fe^{2+}+0.153Mn^{2+} +0.141Mg	0.74(2)
M(4)	0.589Ca+0.395Na +0.016Mn	0.89(2)
A	0.607Na+0.381K	—
O(3)	0.96(OH)+0.04(F,O^{2-})	0.94(5)

Tetrahedral site-populations were assigned using the curves of Hawthorne & Grundy (1977a). The site populations of Fe* (Fe^{2+}+Fe^{3+}+Mn+Ti) were determined by constrained least-squares refinement. There is some difference in the equivalent isotropic temperature-factors at the M(1, 2,3) sites; this suggests slightly too much scattering power at M(1) and

slightly too little scattering power at M(2). On the basis of mean bond-lengths, all trivalent cations were assigned to M(2), and Mn^{2+} was *tentatively* assigned to M(3). Consideration of results from a series of amphibole structures led to the proposal that K occupies the A(m) site, and Na occupies the A(2) site. The optical absorption spectra of this amphibole are given by Faye & Nickel (1970).

Potassian tschermakite(60)

T(1)	0.64Si+0.36Al	0.91 Å²
T(2)	0.89Si+0.11Al	0.91
M(1)	$0.36Fe^{2+}+0.64Mg$	1.26
M(2)	$0.18Fe^{2+}+0.41Mg+0.16Fe^{3+}$ $+0.14Al+0.11Ti$	1.12
M(3)	$0.45Fe^{2+}+0.15Fe^{3+}+0.40Al$	0.90
M(4)	0.85Ca+0.15Na	1.09
A	0.19Na+0.28K	2.55

Site populations were assigned on the basis of mean bond-lengths and equality of isotropic temperature-factors. The agreement with the curves of Hawthorne & Grundy (1977a) and Hawthorne (1978a) is as follows:

^{iv}Al	obs.	1.90, calc.	1.62 atoms p.f.u.
<M(1)–O>	obs.	2.093, calc.	2.092 Å
<M(2)–O>	obs.	2.012, calc.	2.060 Å
<M(3)–O>	obs.	2.091, calc.	2.019 Å

The agreement is reasonable for the M(1) site only; the assignment of considerable amounts of Al to the M(3) site is not in accord with the observed bond-lengths. Assigning all [6]-co-ordinate trivalent cations to the M(2) site, the deviant values are much improved: <M(2)–O> obs. 2.012, calc. 2.047 Å; <M(3)–O> obs. 2.091, calc. 2.102 Å.

Pargasite(61)

T(1)	0.60Si+0.40Al	−0.08(7) Å²
T(2)	0.84Si+0.16Al	0.12(7)
M(1)	$0.30Fe^{2+}+0.70Mg$	0.47(10)
M(2)	$0.07Fe^{2+}+0.08Fe^{3+}+0.11Ti$ $+0.23Al+0.51Mg$	−0.22(10)
M(3)	$0.24Fe^{2+}+0.18Fe^{3+}$ $+0.58Mg$	0.45(11)
M(4)	0.85Ca+0.15Mg	0.39(7)
A	0.76Na+0.06K+0.18Ca	5.8(1.1)

Site occupancies were assigned on the basis of mean bond-lengths and similarity of isotropic temperature-factors; however, the observed isotropic temperature-factors do not appear to bear out the latter contention. Agreement with mean bond-length – ionic radius curves is as follows:

^{iv}Al	obs.	2.22, calc.	1.79 atoms p.f.u.
<M(1)–O>	obs.	2.112, calc.	2.094 Å
<M(2)–O>	obs.	2.037, calc.	2.046 Å
<M(3)–O>	obs.	2.081, calc.	2.070 Å

There is some discrepancy, particularly with regard to the tetrahedral Al.

Sodium-fluor-clinoholmquisite(62)

T(1) = T(2)	Si	1.75, 1.71 Å²
M(1)	$0.25Fe^{2+}+0.75Mg$	1.92
M(2)	1.00Al	1.92
M(3)	$0.30Fe^{2+}+0.20Al$ $+0.50Mg$	3.25
M(4)	0.90Li+0.10Ca	14.75
A	0.45Na+0.04K+0.05Ca	0.65

Site populations were assigned on the basis of mean bond-lengths and equality of isotropic temperature-factors at similar sites. The isotropic temperature-factors listed above do not appear satisfactory, but the authors comment on the extremely poor quality of the crystals. The chemical composition is taken from Ginsburg (1965) and includes 3.37 wt. % Li_2O and 1.98 wt. % CO_2. The latter value, together with the high CaO value (3.00 wt. %), suggests that there was some admixture of calcite in the material analyzed. Note that the cell dimensions and space group given in the latter reference are incorrect.

Pargasitic hornblende(63)

T(1)	0.75Si+0.25Al	1.07 Å²
T(2)	0.85Si+0.15Al	1.07

Tetrahedral site-occupancies derived from mean bond-lengths; agreement with the curve of Hawthorne & Grundy (1977a) is as follows: ^{iv}Al obs. 1.58, calc. 1.27 atoms p.f.u. During the refinement, octahedral site-populations were assumed to be disordered. From an examination of the mean bond-lengths, small C-type cations were considered to be ordered at M(2); however, the authors suggested that some Al may occur at M(1) or M(3) (or both). The chemical data are taken from Udovkina (1971).

Arfvedsonite(64)

T(1)	0.92Si+0.08Al	0.55 Å²
T(2)	1.00Si	0.33
M(1)	$1.00Fe^{2+}$	0.07
M(2)	$1.00Fe^{3+}$	0.07
M(3)	$0.67Fe^{2+}+0.17Fe^{3+}+0.03Mg$ $+0.05Li+0.08Ti$	0.77

M(4)	0.71Na+0.14Ca+0.05Mn +0.10Li	4.05
A	0.53Na+0.17K	—

The authors commented that the high standard deviations make assignment of cation site-populations on the basis of mean bond-lengths rather difficult. The site occupancies above were derived from *both* X-ray and Mössbauer data; a comparison of X-ray and Mössbauer results is given below:

M(1) X-ray: Fe^{2+} 0.92, Mössbauer: Fe^{2+} 2.00
M(3) X-ray: Fe^{2+} 0.97, Mössbauer: Fe^{2+} 0.67
Fe^{3+} analysis: Fe^{3+} 2.04, Mössbauer: Fe^{3+} 2.17

The authors noted also that the mean bond-lengths are not in close agreement with those expected for these occupancies; similar results are obtained using the mean bond-length – ionic radius curves of Hawthorne (1978a). Note that the isotropic temperature-factors at the M(1, 2, 3) sites are not satisfactory. However, any rearrangement of the C-type cations does not lead to any improvement in the situation.

Potassium-arfvedsonite(65)

T(1)	0.88Si+0.12Al	0.35 Å²
T(2)	1.00Si	0.24
M(1)	0.93Fe^{2+}+0.07Fe^{3+}	0.01
M(2)	0.34Fe^{2+}+0.54Fe^{3+} +0.08Al+0.04Ti	0.36
M(3)	0.88Fe^{2+}+0.12Fe^{3+}	2.93
M(4)	0.86Na+0.14Ca	1.54
A	0.77K+0.14Na	—

As with arfvedsonite(63), high standard deviations make assignment of cation site-occupancies on the basis of mean bond-lengths rather difficult. Mössbauer studies showed that Fe^{2+} occurred in the M(1), M(2) and M(3) sites and that the Fe^{3+}/Fe^{2+} ratio obtained from the chemical analysis was incorrect. The Fe^{3+} content by Mössbauer spectroscopy (chemical analysis) is 1.35 (2.02) atoms p.f.u. Comparison of the X-ray and Mössbauer site-occupancies is as follows:

M(1) X-ray: Fe^{2+} 0.93, Mössbauer: Fe^{2+} 0.97
M(2) X-ray: Fe^{2+} 0.34, Mössbauer: Fe^{2+} 0.19
M(3) X-ray: Fe^{2+} 0.88, Mössbauer: Fe^{2+} 1.00

The mean bond-lengths show good agreement with calculated values according to the method of Litvin (1973) and reasonable agreement with the curves of Hawthorne (1978a). The isotropic temperature-factors at the M(1), M(2) and M(3) sites are in poor agreement; however, this cannot be improved by any redistribution of the C-type cations over these three sites.

Potassium-arfvedsonite(66)

T(1) = T(2)	Si	0.41, 0.46, Å²
M(1)	0.75Fe^{2+}+0.25Mn	0.17
M(2)	1.00Fe^{3+}	0.09
M(3)	1.00Na	7.57
M(4)	1.00Na	3.12
A	1.00(Na+K)	—

This is a very peculiar amphibole, and the assigned name does not really reflect the unusual chemical composition. The isotropic temperature-factors suggest that Na is ordered at the M(3) site, as indicated by the authors. Fourier sections through the M(3) site show very anisotropic density elongate along *Z*. *R* indices for non-split- and split-site models are 16.9% and 15.5%, respectively, with corresponding isotropic temperature-factors of 7.57 Å² and 4.12 Å². However, the authors' confidence in the split-atom model is low because of the high *R*-index, and only the single-site refinement results are given. The authors suggest that the mean bond-lengths are not compatible with the cell contents calculated from the results of a chemical analysis, and suggest the site occupancies given above on the basis of mean bond-lengths.

The <M(3)–O> value of 2.05 Å observed here cannot be compatible with complete occupancy of Na, which would involve a mean bond-length of ~2.4 Å. In fact the mean bond-lengths at the M(1), M(2) and M(3) sites are not compatible with significant occupancy of these sites by Na. Additional confirmatory chemical data for this amphibole are required.

Potassimu-arfvedsonite(67)

T(1)	0.96Si+0.04Al	0.46(2) Å²
T(2)	1.00Si	0.48(2)
M(1)	1.00Fe^{2+}	0.66(2)
M(2)	0.460Fe^{3+}+0.420Fe^{2+} +0.073Al+0.047Ti	0.60(2)
M(3)	0.760Fe^{2+}+0.130Mn +0.110Mg	0.65(3)
M(4)	0.921Na+0.079Ca	1.23(5)
A	0.293Na+0.707K	—
O(3)	0.88(OH)+0.05F+0.07(O^{2-})	0.74(7)

Tetrahedral site-occupancies assigned. Octahedral site-populations in terms of Fe* (Fe^{2+}+Fe^{3+}+Mn) were determined by constrained least-squares refinement. Slight negative occupancies of Mg occurred at the M(1) and M(2) sites; however, these were found to be within one standard deviation (0.006) of zero and hence not significant. Thus the Mg occupancies of M(1) and M(2) were set equal to zero

for the final cycle of refinement. The equality of the equivalent isotropic temperature-factors supports this distribution. On the basis of the observed mean bond-lengths and the curves of Hawthorne (1978a), all octahedral trivalent cations were assigned to M(2), and Mn^{+2} was *tentatively* assigned to M(3).

Hawthorne & Grundy (1978) proposed a slightly different composition for this arfvedsonite, using the microprobe value for Na_2O instead of the average value (Hawthorne 1976) because of the possibility of contamination of the separate by aenigmatite. This gives a unit formula $(K_{0.694}Na_{0.200})$ $(Na_{1.871}Ca_{0.129})$ $(Ca_{0.031}Mg_{0.108}Mn_{0.128}Fe^{2+}_{3.562}Fe^{3+}_{0.908}Ti_{0.093}Al_{0.170})$ $(Al_{0.144}Si_{7.856})$ $O_{22}(OH)_{1.754}F_{0.107}O_{0.139}$ with refined A(m) and A(2) occupancies of 0.62 and 0.05 Na, respectively. The other results are not materially affected.

Fluor-riebeckite(68)

T(1)	0.95Si+0.05Al	0.51(2) Å²
T(2)	0.99Si+O.01Al	0.50(2)
M(1)	$0.066Fe^{3+}+0.934Fe^{2+}$	0.63(2)
M(2)	$0.057Al+0.943Fe^{3+}$	0.42(1)
M(3)	$0.336Li+0.182Mn+0.482Fe^{2+}$	0.70(4)
M(4)	0.007Ca+0.993Na	1.32(4)
A	0.037Na+0.290K	—
O(3)	0.892(OH)+1.253F	0.96(6)

Tetrahedral site-occupancies assigned on the basis of bulk chemistry and the curves of Hawthorne & Grundy (1977a). Octahedral site-populations in terms of Li and Fe* ($Fe^{2+}+Fe^{3+}+Mn$) were determined by constrained least-squares refinement. The Li occupancy of M(1) was found to be equal to zero within one standard deviation (0.004) and thus was set to zero. Remaining occupancies (Fe^{2+}–Fe^{3+}–Mn) were assigned according to mean bond-length criteria and are thus tentative. Chemical analysis includes 0.54 wt. % Li_2O, and the formula unit includes 0.334 Li, which is included in the Σ^{vi} value.

Ferro-glaucophane(69)

T(1)	0.99Si+0.01Al	0.45(1) Å²
T(2)	1.00Si	0.45(1)
M(1)	$0.585(6)Fe^{2+}+0.348Mg+0.067Al$	0.60(2)
M(2)	$0.156(6)Fe^{3+}+0.844Al$	0.58(3)
M(3)	$0.795(9)Fe^{2+}+0.205Mg$	0.61(3)
M(4)	$0.860Na+0.075Ca+0.065Mg$	1.27(5)

The occupancies of the M sites in terms of Fe* ($Fe^{2+}+Fe^{3+}+Mn$) and Mg, with Al assigned to M(2) and Na+Ca assigned to M(4); the Mg occupancy of M(2) became negative with the Fe content of the M(2) site exactly equal to the Fe^{3+} content of the unit formula. The refinement was completed with M(2) occupied by Fe* and Al only, the final results indicating a small amount of Al resident at M(1) or M(3) (or both). On the basis of mean bond-lengths, the M(2) site appears completely occupied by trivalent cations; by the same criterion, any ^{vi}Al not occurring at M(2) will be strongly ordered at M(1), although the author suggests that this result is rather tentative. In fact, using the equations of Table 27, it seems unlikely that any Al occurs at the M(1) or M(3) sites. Thus the cell contents of this amphibole may be slightly in error.

Pargasitic hornblende(70)

T(1)	0.61Si+0.39Al
T(2)	1.00Si
M(1)	$0.17Fe^{2+}+0.83Mg$
M(2)	$0.15Fe^{3+}+0.53Mg+0.32Al$
M(3)	$0.22Fe^{2+}+0.05Fe^{3+}+0.73Mg$
M(4)	$0.91Ca+0.06Na+0.03Fe^{2+}$
A	0.56Na+0.10K

The chemical analysis of this amphibole was derived from the site occupancies calculated according to the method of Ungaretti *et al.* (1981) that is outlined on page 263. It can be argued that the small amount of Fe^{3+} at M(3) is due to a postcrystallization post-cation-equilibration process (see text on Fe^{3+} distributions). Atomic co-ordinates and bond lengths are from Ungaretti (pers. comm.).

Pargasite(71)

T(1)	0.54Si+0.46Al
T(2)	1.00Si
M(1)	$0.19Fe^{2+}+0.81Mg$
M(2)	$0.11Fe^{3+}+0.25Al+0.58Mg+0.06Ti^{4+}$
M(3)	$0.16Fe^{2+}+0.12Fe^{3+}+0.72Mg$
M(4)	$0.95Ca+0.03Na+0.02Fe^{2+}$
A	0.74Na+0.07K

The chemical analysis of this amphibole was derived from the site occupancies calculated according to the method of Ungaretti *et al.* (1981) outlined on page 263. It can be argued that the small amount of Fe^{3+} at M(3) is due to a post-cation-equilibration process (see section on Fe^{3+} distribution).

Magnesio-hastingsite(72)

T(1)	0.56Si+0.44Al

T(2)	1.00Si
M(1)	$0.17Fe^{2+}+0.79Mg+0.04Fe^{3+}$
M(2)	$0.16Fe^{3+}+0.18Al+0.66Mg$
M(3)	$0.08F^{2+}+0.21Fe^{3+}+0.71$ Mg
M(4)	$0.92Ca+0.04Na+0.04Fe^{2+}$
A	$0.82Na+0.05K$

The chemical analysis of this amphibole was derived from the site occupancies calculated according to the method of Ungaretti *et al.* (1981) that is outlined on page 263. It can be argued that the Fe^{3+} at M(1) and M(3) is the result of post-cation-equilibration oxidation (see section on Fe^{3+} distribution).

Ferroan pargasitic hornblende(73)

T(1)	$0.60Si+0.40Al$	0.53(2) Å²
T(2)	$0.98Si+0.02Al$	0.54(2)
M(1)	$0.32Fe^{2+}+0.68Mg$	0.67(4)
M(2)	$0.07Fe^{2+}+0.14Fe^{3+}+0.04Ti$ $+0.42Al+0.33Mg$	0.54(4)
M(3)	$0.45Fe^{2+}+0.55Mg$	0.56(5)
M(4)	$0.71Ca+0.07Na+0.17Fe^{2+}$ $+0.05Mg$	1.15(3)
A	$0.46Na+0.02K$	—

Tetrahedral site-occupancies assigned on the basis of bulk chemistry and the curves of Hawthorne & Grundy (1977a). Octahedral site-populations were determined by constrained least-squares refinement in terms of Mg and Fe* ($Fe^{2+}+Fe^{3+}+Mn$) with Al and Ti assigned to M(2). The ratio $Fe^{3+}/(Fe^{2+}+Fe^{3+})$ was not known from chemical analysis; the refinement was done for a series of cell contents with different $Fe^{3+}/(Fe^{2+}+Fe^{3+})$ ratios, the final solution giving a ratio of 0.15 and best overall agreement with the data and a variety of crystal-chemical criteria.

Potassian titanian magnesio-hastingsite(74)

T(1)	$0.60Si+0.40Al$	0.44 Å²
T(2)	$0.89Si+0.11Al$	0.44
M(1)	$0.290Fe^{2+}+0.710Mg$	0.97
M(2)	$0.059Fe^{2+}+0.572Mg$ $+0.264Fe^{3+}+0.105Ti$	0.99
M(3)	$0.059Fe^{2+}+0.572Mg$ $+0.264Fe^{3+}+0.105Ti$	0.93
M(4)	$0.950Ca+0.050Na$	0.82
A(2)	$0.170Na+0.075K$	1.89
A(m)	$0.145Na+0.100K$	1.84

Site occupancies are from Walitzi (pers. comm.). Tetrahedral site-occupancies assigned on the basis of bulk chemistry and the curves of Hawthorne & Grundy (1977a). There is some discrepancy between the sum of the site occupancies and the cell content from the chemical analysis. The agreement with the bond-length – ionic radius curves of Table 27 is as follows, assuming O(3) = (OH):

<M(1)–O>	obs.	2.071, calc	2.108 Å
<M(2)–O>	obs.	2.047, calc	2.060
<M(3)–O>	obs.	2.073, calc	2.058

The isotropic temperature-factors suggest that the relative scattering-powers at the M(1, 2, 3) sites are correct; the bond-length comparisons suggest more trivalent and quadrivalent cations at M(1) and M(2), which would suggest that the amphibole has undergone partial oxidation and dehydroxylation.

APPENDIX B4. CATION-ANION AND CATION-CATION DISTANCES (Å)

		(21)	(22)	(24)	(26)	(28)	(29)	(30)
T(1)-O(1)		1.619(7)	1.637(4)	1.666(4)	1.618(6)	1.610(3)	1.602(4)	1.602(2)
T(1)-O(5)		1.614(7)	1.627(5)	1.679(4)	1.616(7)	1.622(4)	1.633(5)	1.632(2)
T(1)-O(6)		1.628(7)	1.630(4)	1.665(5)	1.621(6)	1.633(3)	1.620(5)	1.629(2)
T(1)-O(7)		1.613(7)	1.613(2)	1.658(2)	1.611(3)	1.616(2)	1.635(2)	1.616(1)
⟨T(1)-O⟩		1.619	1.627	1.667	1.616	1.620	1.622	1.620
T(2)-O(2)		1.625(7)	1.633(4)	1.646(4)	1.618(6)	1.618(3)	1.622(4)	1.616(2)
T(2)-O(4)		1.609(7)	1.604(4)	1.607(4)	1.594(3)	1.594(3)	1.583(4)	1.586(2)
T(2)-O(5)		1.639(7)	1.611(5)	1.645(4)	1.637(7)	1.634(3)	1.676(5)	1.653(2)
T(2)-O(6)		1.643(7)	1.638(5)	1.659(4)	1.654(7)	1.655(4)	1.704(5)	1.672(2)
⟨T(2)-O⟩		1.629	1.622	1.639	1.626	1.625	1.646	1.632
M(1)-O(1)	x2	2.064(7)	2.082(5)	2.047(4)	2.078(6)	2.071(3)	2.066(4)	2.064(2)
M(1)-O(2)	x2	2.128(7)	2.160(4)	2.142(4)	2.082(6)	2.124(3)	2.051(4)	2.078(2)
M(1)-O(3)	x2	2.091(7)	2.122(4)	2.041(4)	2.100(5)	2.092(3)	2.073(4)	2.083(2)
⟨M(1)-O⟩		2.094	2.121	2.077	2.087	2.096	2.063	2.075
M(2)-O(1)	x2	2.134(7)	2.161(5)	2.092(4)	2.038(6)	2.148(3)	2.183(4)	2.133(2)
M(2)-O(2)	x2	2.083(7)	2.128(4)	2.070(4)	1.943(6)	2.092(3)	2.095(4)	2.083(2)
M(2)-O(4)	x2	2.033(7)	2.075(4)	1.980(4)	1.849(6)	2.024(3)	1.998(4)	2.014(2)
⟨M(2)-O⟩		2.083	2.121	2.047	1.943	2.088	2.092	2.077
M(3)-O(1)	x4	2.099(7)	2.118(5)	2.084(4)	2.103(5)	2.089(3)	2.069(4)	2.070(2)
M(3)-O(3)	x2	2.073(7)	2.103(6)	2.068(5)	2.077(5)	2.063(5)	2.024(6)	2.057(3)
⟨M(3)-O⟩		2.083	2.113	2.079	2.094	2.080	2.054	2.066
M(4)-O(2)	x2	2.164(7)	2.135(5)	2.394(4)	2.411(6)	2.204(3)	2.431(4)	2.397(2)
M(4)-O(4)	x2	2.023(7)	1.988(4)	2.328(5)	2.337(6)	2.109(4)	2.414(5)	2.321(2)
M(4)-O(5)	x2	3.143(7)	3.298(5)	2.665(4)	2.798(6)	3.101(3)	2.822(4)	2.767(2)
M(4)-O(6)	x2	2.691(7)	2.757(5)	2.582(5)	2.446(6)	2.592(4)	2.604(4)	2.539(2)
⟨M(4)-O⟩ [8]		2.505	2.545	2.492	2.498	2.502	2.568	2.506
⟨M(4)-O⟩ [6]		2.293	2.293	2.435	2.398	2.302	2.483	2.419
A-O(5)	x4	2.824(4)	2.801	3.049(5)	2.814(6)	2.828(3)	2.945(7)	2.970(2)
A-O(6)	x4	3.278(5)	3.333	3.086(4)	3.216(5)	3.303(3)	3.152(8)	3.156(2)
A-O(7)	x2	2.295(8)	2.327	2.459(8)	2.519(10)	2.340(6)	2.605(12)	2.486(3)
A-O(7)	x2	3.845(9)	3.887	3.714(7)	3.666(8)	3.791(6)	3.605(13)	3.672(3)
⟨A-O⟩ [12]		3.057	3.080	3.074	3.041	3.066	3.067	3.068
⟨A-O⟩ [10]		2.900	2.919	2.946	2.916	2.920	2.960	2.948
M(1)-M(1)		3.163(3)	3.230	3.103(3)	3.221(4)	3.151(3)	3.196(4)	3.169(2)
M(1)-M(2)		3.118(4)	3.156	3.129(2)	3.091(2)	3.118(2)	3.109(2)	3.086(2)
M(1)-M(3)		3.091(4)	3.120	3.074(1)	3.099(2)	3.089(2)	3.088(1)	3.077(1)
M(1)-M(4)		3.129(3)	3.119	3.468(3)	3.307(6)	3.191(2)	3.414(3)	3.423(2)
M(2)-M(3)		3.216(3)	3.299	3.210(2)	3.206(3)	3.207(2)	3.234(2)	3.187(2)
M(2)-M(4)		3.047(4)	3.031	3.211(2)	3.153(3)	3.080(2)	3.185(2)	3.204(1)
T(1)-T(2)[1]		3.083(4)	3.091	3.099(2)	3.110(3)	3.094(3)	3.083(2)	3.086(2)
T(1)-T(2)[2]		3.054(4)	3.066	3.068(2)	3.003(3)	3.060(2)	3.065(2)	3.051(2)
T(1)-T(1)		3.055(3)	3.075	3.092(2)	3.090(3)	3.046(2)	3.063(2)	3.030(2)

[1] through O(6): [2] through O(5).

	(34)	(35)	(36)	(37)	(38)	(39)	(40)
T(1)-O(1)	1.582(6)	1.594(6)	1.614(3)	1.618(4)	1.663(3)	1.670(4)	1.677(9)
T(1)-O(5)	1.625(6)	1.636(7)	1.628(3)	1.643(4)	1.693(3)	1.698(4)	1.683(9)
T(1)-O(6)	1.641(7)	1.624(7)	1.630(4)	1.632(4)	1.682(3)	1.682(4)	1.684(9)
T(1)-O(7)	1.636(3)	1.631(4)	1.606(2)	1.621(2)	1.663(2)	1.663(2)	1.659(6)
⟨T(1)-O⟩	1.621	1.621	1.620	1.628	1.675	1.678	1.676
T(2)-O(2)	1.625(6)	1.626(7)	1.623(3)	1.614(3)	1.631(2)	1.640(4)	1.661(9)
T(2)-O(4)	1.578(5)	1.572(7)	1.587(3)	1.587(4)	1.608(2)	1.608(4)	1.618(9)
T(2)-O(5)	1.658(7)	1.660(8)	1.648(4)	1.651(4)	1.642(3)	1.643(5)	1.618(9)
T(2)-O(6)	1.681(6)	1.674(7)	1.659(3)	1.679(4)	1.662(3)	1.669(4)	1.636(9)
⟨T(2)-O⟩	1.636	1.633	1.629	1.633	1.636	1.640	1.633
M(1)-O(1) x2	2.060(6)	2.078(7)	2.051(3)	2.090(4)	2.056(3)	2.055(4)	2.005(9)
M(1)-O(2) x2	2.031(6)	2.036(7)	2.054(4)	2.115(3)	2.111(2)	2.136(4)	2.188(8)
M(1)-O(3) x2	2.069(5)	2.077(6)	2.057(3)	2.114(4)	2.097(2)	2.052(4)	1.950(8)
⟨M(1)-O⟩	2.053	2.064	2.054	2.106	2.088	2.081	2.048
M(2)-O(1) x2	2.186(6)	2.212(6)	2.146(4)	2.151(3)	2.069(3)	2.085(4)	2.131(8)
M(2)-O(2) x2	2.059(6)	2.082(7)	2.077(3)	2.114(4)	2.074(3)	2.082(4)	2.045(9)
M(2)-O(4) x2	2.011(6)	2.008(7)	2.024(4)	2.022(4)	1.966(3)	1.976(4)	1.977(8)
⟨M(2)-O⟩	2.085	2.101	2.082	2.096	2.036	2.048	2.051
M(3)-O(1) x4	2.071(5)	2.068(6)	2.055(3)	2.100(3)	2.076(3)	2.079(4)	2.089(7)
M(3)-O(3) x2	2.028(6)	2.017(8)	2.011(4)	2.093(5)	2.080(3)	2.093(6)	2.001(15)
⟨M(3)-O⟩	2.057	2.051	2.040	2.098	2.077	2.084	2.060
M(4)-O(2) x2	2.405(6)	2.397(7)	2.400(4)	2.388(3)	2.414(2)	2.410(4)	2.420(8)
M(4)-O(4) x2	2.336(6)	2.338(6)	2.308(3)	2.301(4)	2.358(3)	2.348(4)	2.313(10)
M(4)-O(5) x2	2.846(6)	2.851(7)	2.756(3)	2.823(5)	2.625(2)	2.635(4)	2.689(8)
M(4)-O(6) x2	2.582(5)	2.577(6)	2.514(3)	2.561(4)	2.563(2)	2.582(4)	2.529(9)
⟨M(4)-O⟩ [8]	2.542	2.541	2.459	2.518	2.490	2.494	2.488
⟨M(4)-O⟩ [6]	2.441	2.437	2.407	2.417	2.445	2.447	2.421
A-O(5) x4	2.866(5)	2.886(6)	2.971	2.977	3.060(4)	3.070(8)	3.037(8)
A-O(6) x4	3.114(6)	3.153(7)	3.172	3.195	3.080(4)	3.065(8)	3.108(7)
A-O(7) x2	2.413(9)	2.432(10)	2.447	2.516	2.486(8)	2.582(14)	2.409(15)
A-O(7) x2	3.684(10)	3.690(11)	3.662	3.701	3.693(7)	3.719(12)	3.724(11)
⟨A-O⟩ [12]	3.010	3.033	3.066	3.094	3.076	3.095	3.071
⟨A-O⟩ [10]	2.875	2.902	2.947	2.972	2.953	2.970	2.940
M(1)-M(1)	3.218(8)	3.227(8)	3.187(4)	3.230(2)	3.240	3.133	2.875(5)
M(1)-M(2)	3.077(3)	3.097(3)	3.067(2)	3.116(1)	3.082	3.118	3.183(3)
M(1)-M(3)	3.084(2)	3.091(2)	3.076(1)	3.105(1)	3.111	3.085	3.018(2)
M(1)-M(4)	3.345(5)	3.339(5)	3.395(3)	3.424(2)	3.430	3.478	3.570(5)
M(2)-M(3)	3.204(4)	3.238(3)	3.168(2)	3.250(1)	3.183	3.196	3.196(4)
M(2)-M(4)	3.161(3)	3.145(3)	3.200(2)	3.200(1)	3.247	3.237	3.213(3)
T(1)-T(2)	3.088(4)	3.076(4)	3.088(2)	3.103(2)	3.116(1)	3.109(2)	3.099(6)
T(1)-T(2)	3.031(4)	3.046(4)	3.045(2)	3.069(2)	3.068(1)	3.070(2)	3.061(6)
T(1)-T(1)	3.029(5)	3.034(3)	3.002(2)	3.057(2)	3.089(1)	3.094(2)	3.080(5)

	(41)	(42)	(43)	(44)	(45)	(46)	(48)
T(1)-O(1)	1.613(4)	1.630	1.586	1.687	1.640	1.649	1.670
T(1)-O(5)	1.613(5)	1.669	1.648	1.694	1.668	1.683	1.693
T(1)-O(6)	1.627(5)	1.646	1.634	1.658	1.663	1.669	1.686
T(1)-O(7)	1.617(2)	1.629	1.613	1.630	1.632	1.626	1.635
⟨T(1)-O⟩	1.617	1.644	1.621	1.667	1.651	1.657	1.672
T(2)-O(2)	1.625(4)	1.608	1.614	1.609	1.633	1.636	1.629
T(2)-O(4)	1.588(5)	1.606	1.577	1.586	1.592	1.599	1.626
T(2)-O(5)	1.646(5)	1.641	1.644	1.641	1.655	1.640	1.627
T(2)-O(6)	1.658(5)	1.657	1.654	1.664	1.649	1.653	1.628
⟨T(2)-O⟩	1.629	1.628	1.622	1.625	1.632	1.632	1.628
M(1)-O(1) x2	2.063(4)	2.085	2.079	2.112	2.075	2.107	2.060
M(1)-O(2) x2	2.112(5)	2.125	2.106	2.169	2.117	2.169	2.176
M(1)-O(3) x2	2.087(4)	2.081	2.083	2.154	2.113	2.080	2.112
⟨M(1)-O⟩	2.087	2.097	2.089	2.145	2.102	2.119	2.116
M(2)-O(1) x2	2.141(5)	2.044	2.134	2.091	2.102	2.046	1.990
M(2)-O(2) x2	2.082(4)	2.051	2.090	2.138	2.086	2.059	1.991
M(2)-O(4) x2	2.031(5)	1.944	2.033	2.002	1.987	1.976	1.912
⟨M(2)-O⟩	2.084	2.013	2.086	2.077	2.058	2.027	1.964
M(3)-O(1) x4	2.084(4)	2.062	2.078	2.064	2.099	2.089	2.132
M(3)-O(3) x2	2.072(6)	2.076	2.071	2.112	2.086	2.035	2.107
⟨M(3)-O⟩	2.080	2.067	2.076	2.080	2.095	2.071	2.124
M(4)-O(2)	2.215(4)	2.412	2.396	2.439	2.413	2.421	2.419
M(4)-O(4)	2.109(5)	2.357	2.330	2.396	2.349	2.365	2.329
M(4)-O(5)	3.090(5)	2.677	2.775	2.737	2.722	2.689	2.611
M(4)-O(6)	2.584(5)	2.533	2.567	2.551	2.575	2.542	2.522
⟨M(4)-O⟩ [8]	2.500	2.495	2.517	2.530	2.515	2.504	2.470
⟨M(4)-O⟩ [6]	2.303	2.434	2.431	2.462	2.446	2.443	2.423
A-O(5) x4	2.828	2.992	2.976	3.037	3.013	3.025	3.045
A-O(6) x4	3.301	3.114	3.147	3.167	3.136	3.153	3.138
A-O(7) x2	2.350	2.483	2.505	2.552	2.547	2.531	2.542
A-O(7) x2	3.775	3.727	3.691	3.704	3.679	3.703	3.733
⟨A-O⟩ [12]	3.064	3.070	3.074	3.111	3.085	3.098	3.107
⟨A-O⟩ [8]	2.922	2.939	2.950	2.992	2.969	2.977	2.982
M(1)-M(1)	3.147(6)	3.155	3.168	3.284	3.216	3.137	3.238
M(1)-M(2)	3.109(2)	3.089	3.091	3.120	3.110	3.126	3.094
M(1)-M(3)	3.085(1)	3.081	3.079	3.133	3.108	3.087	3.116
M(1)-M(4)	3.202(4)	3.424	3.443	3.480	3.453	3.498	3.427
M(2)-M(3)	3.195(3)	3.171	3.191	3.259	3.226	3.212	3.196
M(2)-M(4)	3.089(2)	3.218	3.216	3.256	3.231	3.241	3.242
T(1)-T(2)	3.087(2)	3.091	3.083	3.117	3.104	3.124	3.131
T(1)-T(2)	3.065(2)	3.052	3.061	3.104	3.079	3.066	3.046
T(1)-T(1)	3.050(3)	3.062	3.038	3.068	3.078	3.072	3.116

	(49)	(50)	(51)	(52)	(53a)	(53b)	(54)	(55)
T(1)-O(1)	1.689	1.647	1.63	1.69	1.604(2)	1.605(3)	1.668(4)	1.684(4)
T(1)-O(5)	1.657	1.665	1.73	1.69	1.630(2)	1.626(3)	1.692(4)	1.689(4)
T(1)-O(6)	1.686	1.672	1.71	1.67	1.628(3)	1.628(3)	1.679(4)	1.682(5)
T(1)-O(7)	1.644	1.657	1.67	1.67	1.616(1)	1.620(2)	1.656(2)	1.665(2)
⟨T(1)-O⟩	1.669	1.660	1.68	1.68	1.620	1.620	1.674	1.680
T(2)-O(2)	1.639	1.658	1.64	1.67	1.615(2)	1.612(3)	1.640(4)	1.644(4)
T(2)-O(4)	1.611	1.580	1.59	1.65	1.586(2)	1.587(3)	1.620(4)	1.615(4)
T(2)-O(5)	1.634	1.659	1.64	1.65	1.653(3)	1.658(3)	1.636(4)	1.651(5)
T(2)-O(6)	1.632	1.650	1.60	1.69	1.676(2)	1.679(3)	1.656(4)	1.663(4)
⟨T(2)-O⟩	1.629	1.637	1.62	1.67	1.633	1.634	1.638	1.643
M(1)-O(1) x2	2.088	2.074	2.13	2.05	2.068(2)	2.071(3)	2.067(5)	2.037(5)
M(1)-O(2) x2	2.160	2.172	2.17	2.16	2.089(2)	2.100(3)	2.170(5)	2.173(5)
M(1)-O(3) x2	2.118	2.095	2.13	2.05	2.094(2)	2.110(4)	2.131(4)	1.988(5)
⟨M(1)-O⟩	2.122	2.114	2.14	2.09	2.084	2.094	2.123	2.066
M(2)-O(1) x2	1.993	1.999	2.08	2.13	2.145(2)	2.161(3)	2.014(4)	2.106(5)
M(2)-O(2) x2	2.046	1.967	2.09	2.05	2.094(2)	2.105(3)	2.029(5)	2.085(5)
M(2)-O(4) x2	1.924	1.909	2.01	2.01	2.024(2)	2.033(4)	1.928(5)	1.981(5)
⟨M(2)-O⟩	1.988	1.958	2.06	2.06	2.088	2.100	1.990	2.057
M(3)-O(1) x4	2.110	2.093	2.12	2.07	2.082(2)	2.093(3)	2.141(4)	2.070(4)
M(3)-O(3) x2	2.089	2.094	2.07	1.96	2.065(3)	2.061(4)	2.115(6)	2.060(6)
⟨M(3)-O⟩	2.103	2.093	2.10	2.03	2.076	2.082	2.132	2.067
M(4)-O(2) x2	2.398	2.419	2.48	2.42	2.406(2)	2.421(3)	2.410(4)	2.424(5)
M(4)-O(4) x2	2.364	2.387	2.41	2.28	2.328(2)	2.331(3)	2.330(5)	2.351(5)
M(4)-O(5) x2	2.679	2.637	2.69	2.67	2.814(2)	2.841(4)	2.636(6)	2.642(6)
M(4)-O(6) x2	2.548	2.550	2.59	2.59	2.538(2)	2.544(3)	2.519(4)	2.560(4)
⟨M(4)-O⟩ [8]	2.465	2.498	2.54	2.49	2.521	2.534	2.474	2.494
⟨M(4)-O⟩ [6]	2.437	2.452	2.49	2.43	2.424	2.432	2.420	2.445
A-O(5) x4	3.028	3.017	3.01	3.07	2.957(2)	2.956(3)	3.056(4)	3.068(4)
A-O(6) x4	3.141	3.113	3.11	3.07	3.190(2)	3.215(4)	3.159(3)	3.079(3)
A-O(7) x2	2.528	2.497	2.52	2.37	2.516(3)	2.530(4)	2.518(4)	2.456(4)
A-O(7) x2	3.693	3.732	3.77	3.76	3.673(3)	3.680(5)	3.735(4)	3.700(4)
⟨A-O⟩ [12]	3.093	3.082	3.09	3.07	3.081	3.091	3.114	3.075
⟨A-O⟩ [10]	2.973	2.951	2.95	2.93	2.962	2.974	2.990	2.950
M(1)-M(1)	3.232	3.252	3.26	2.97	3.178(3)	3.196(4)	3.266(2)	2.950(4)
M(1)-M(2)	3.103	3.089	3.14	3.16	3.099(1)	3.111(2)	3.106(1)	3.163(1)
M(1)-M(3)	3.113	3.118	3.14	3.05	3.084(1)	3.093(1)	3.126(1)	3.038(1)
M(1)-M(4)	3.439	3.414	3.50	3.53	3.440(2)	3.455(3)	3.448(2)	3.563(3)
M(2)-M(3)	3.214	3.196	3.28	3.19	3.208(1)	3.230(2)	3.226(2)	3.192(2)
M(2)-M(4)	3.236	3.237	3.26	3.22	3.210(1)	3.215(1)	3.247(1)	3.234(1)
T(1)-T(2)	3.132	3.114	3.10	3.13	3.093	3.100	3.140(2)	3.106(2)
T(1)-T(2)	3.051	3.056	3.10	3.13	3.059	3.063	3.060(2)	3.077(2)
T(1)-T(1)	3.117	3.117	3.11	3.06	3.039	3.047	3.130(3)	3.091(3)

	(56a)	(56b)	(57)	(58)	(59)	(60)	(61)
T(1)-O(1)	1.611(2)	1.607(2)	1.618(3)	1.675(3)	1.666(2)	1.662	1.648
T(1)-O(5)	1.637(2)	1.637(2)	1.626(3)	1.688(3)	1.683(2)	1.667	1.697
T(1)-O(6)	1.639(2)	1.637(2)	1.632(4)	1.692(4)	1.680(2)	1.673	1.654
T(1)-O(7)	1.629(1)	1.628(2)	1.624(2)	1.669(2)	1.664(1)	1.629	1.642
⟨T(1)-O⟩	1.629	1.627	1.625	1.681	1.673	1.658	1.660
T(2)-O(2)	1.613(2)	1.617(2)	1.623(3)	1.660(3)	1.630(2)	1.623	1.650
T(2)-O(4)	1.589(2)	1.586(2)	1.600(3)	1.630(3)	1.604(2)	1.629	1.613
T(2)-O(5)	1.662(2)	1.658(2)	1.637(3)	1.661(4)	1.646(2)	1.654	1.637
T(2)-O(6)	1.675(2)	1.681(2)	1.658(3)	1.668(3)	1.658(2)	1.660	1.674
⟨T(2)-O⟩	1.635	1.635	1.630	1.655	1.635	1.642	1.644
M(1)-O(1) x2	2.061(2)	2.063(1)	2.069(4)	2.065(4)	2.072(2)	2.058	2.102
M(1)-O(2) x2	2.071(2)	2.072(2)	2.129(4)	2.163(4)	2.153(2)	2.130	2.127
M(1)-O(3) x2	2.082(2)	2.087(2)	2.096(4)	2.120(3)	2.113(2)	2.092	2.103
⟨M(1)-O⟩	2.071	2.074	2.097	2.116	2.113	2.093	2.111
M(2)-O(1) x2	2.143(2)	2.146(2)	2.155(4)	2.023(4)	2.096(2)	2.058	2.056
M(2)-O(2) x2	2.091(2)	2.087(1)	2.092(4)	2.010(4)	2.080(2)	2.055	2.079
M(2)-O(4) x2	2.018(2)	2.018(2)	2.026(4)	1.907(4)	1.962(2)	1.922	1.975
⟨M(2)-O⟩	2.084	2.084	2.091	1.980	2.046	2.012	2.037
M(3)-O(1) x4	2.071(2)	2.070(1)	2.092(3)	2.135(2)	2.130(2)	2.112	2.081
M(3)-O(3) x2	2.047(2)	2.054(2)	2.069(5)	2.122(5)	2.117(3)	2.059	2.081
⟨M(3)-O⟩	2.063	2.065	2.084	2.131	2.126	2.094	2.081
M(4)-O(2) x2	2.415(2)	2.413(2)	2.195(4)	2.425(4)	2.437(2)	2.445	2.386
M(4)-O(4) x2	2.336(2)	2.337(2)	2.099(4)	2.345(4)	2.368(2)	2.378	2.340
M(4)-O(5) x2	2.766(2)	2.770(2)	3.109(5)	2.602(6)	2.729(3)	2.696	2.640
M(4)-O(6) x2	2.548(1)	2.552(2)	2.630(3)	2.551(3)	2.552(3)	2.502	2.602
⟨M(4)-O⟩ [8]	2.516	2.518	2.508	2.481	2.522	2.505	2.492
⟨M(4)-O⟩ [6]	2.433	2.434	2.308	2.440	2.454	2.441	2.443
A-O(5) x4	2.973(2)	2.968(1)	2.835(4)	3.055(4)	3.008(2)	3.015	3.063
A-O(6) x4	3.148(2)	3.146(1)	3.289(4)	3.101(4)	3.152(2)	3.136	3.082
A-O(7) x2	2.480(3)	2.488(2)	2.327(5)	2.504(5)	2.520(4)	2.532	2.428
A-O(7) x2	3.680(4)	3.676(3)	3.800(5)	3.775(6)	3.739(4)	3.684	3.816
⟨A-O⟩ [12]	3.067	3.065	3.062	3.099	3.097	3.086	3.089
⟨A-O⟩ [10]	2.944	2.943	2.915	2.963	2.968	2.967	2.944
M(1)-M(1)	3.184(2)	3.186(4)	3.158(2)	3.270(2)	3.244(2)	3.197	3.200
M(1)-M(2)	3.088(1)	3.090(2)	3.122(1)	3.114(1)	3.139(1)	3.106	3.094
M(1)-M(3)	3.085(1)	3.086(1)	3.092(1)	3.137(1)	3.129(1)	3.100	3.099
M(1)-M(4)	3.425(1)	3.422(3)	3.179(1)	3.444(1)	3.461(1)	3.468	3.437
M(2)-M(3)	3.191(1)	3.195(2)	3.216(1)	3.225(1)	3.263(1)	3.208	3.191
M(2)-M(4)	3.212(1)	3.209(2)	3.073(1)	3.256(1)	3.237(1)	3.242	3.232
T(1)-T(2)	3.091(1)	3.095(3)	3.094(1)	3.143(1)	3.123(1)	3.110	3.114
T(1)-T(2)	3.061(1)	3.057(3)	3.063(1)	3.066(1)	3.079(1)	3.084	3.067
T(1)-T(1)	3.038(1)	3.041(3)	3.055(2)	3.132(2)	3.127(2)	3.074	3.056

		(62)	(63)	(64)	(65)	(66)	(67)	(68)	(69)
T(1)-O(1)		1.60	1.652	1.67	1.58	1.61	1.598(4)	1.623(3)	1.625(3)
T(1)-O(5)		1.69	1.649	1.65	1.69	1.66	1.634(4)	1.627(3)	1.615(3)
T(1)-O(6)		1.55	1.654	1.67	1.61	1.63	1.632(4)	1.630(3)	1.623(3)
T(1)-O(7)		1.61	1.635	1.59	1.62	1.64	1.641(2)	1.628(2)	1.617(1)
<T(1)-O>		1.61	1.648	1.65	1.63	1.64	1.626	1.627	1.620
T(2)-O(2)		1.72	1.643	1.65	1.63	1.63	1.615(4)	1.627(3)	1.631(3)
T(2)-O(4)		1.60	1.592	1.62	1.59	1.62	1.585(4)	1.598(3)	1.596(3)
T(2)-O(5)		1.58	1.657	1.62	1.61	1.64	1.667(4)	1.652(3)	1.651(3)
T(2)-O(6)		1.64	1.682	1.61	1.69	1.63	1.680(4)	1.656(3)	1.655(3)
<T(2)-O>		1.64	1.644	1.63	1.63	1.63	1.637	1.633	1.633
M(1)-O(1)	x2	2.14	2.049	2.15	2.23	2.27	2.110(3)	2.106(3)	2.093(2)
M(1)-O(2)	x2	2.05	2.089	2.06	2.06	2.14	2.100(4)	2.106(3)	2.101(2)
M(1)-O(3)	x2	2.07	2.082	2.23	2.12	2.08	2.136(3)	2.130(3)	2.124(2)
<M(1)-O>		2.09	2.073	2.15	2.14	2.16	2.115	2.114	2.106
M(2)-O(1)	x2	1.95	2.096	2.06	2.11	2.06	2.161(4)	2.121(3)	2.030(3)
M(2)-O(2)	x2	1.99	2.098	2.09	2.11	2.00	2.084(4)	2.034(3)	1.950(2)
M(2)-O(4)	x2	1.85	2.007	1.88	1.94	1.93	1.953(4)	1.926(3)	1.850(3)
<M(2)-O>		1.93	2.067	2.01	2.05	2.00	2.066	2.027	1.943
M(3)-O(1)	x4	2.07	2.078	2.03	2.13	1.98	2.138(4)	2.121(3)	2.138(2)
M(3)-O(3)	x2	1.97	2.092	2.10	2.09	2.17	2.103(5)	2.098(4)	2.090(4)
<M(3)-O>		2.04	2.083	2.05	2.12	2.04	2.126	2.113	2.122
M(4)-O(2)	x2	2.49	2.377	2.57	2.48	2.54	2.419(4)	2.432(4)	2.403(3)
M(4)-O(4)	x2	2.25	2.306	2.58	2.47	2.55	2.374(4)	2.357(3)	2.332(3)
M(4)-O(5)	x2	2.80	2.650	2.85	2.90	2.79	2.937(4)	2.906(3)	2.828(3)
M(4)-O(6)	x2	2.13	2.611	2.45	2.57	2.44	2.614(4)	2.504(4)	2.457(3)
<M(4)-O>[8]		2.42	2.486	2.61	2.61	2.58	2.586	2.550	2.505
<M(4)-O> [6]		2.29	2.431	2.53	2.51	2.51	2.469	2.431	2.397
A-O(5)	x4	2.66	3.066	2.89	2.89	2.83	2.755(3)	2.832(3)	2.809(3)
A-O(6)	x4	3.32	3.063	3.23	3.23	3.20	3.212(3)	3.252(3)	3.244(3)
A-O(7)	x2	2.32	2.446	2.60	2.59	2.53	2.629(2)	2.550(3)	2.549(4)
A-O(7)	x2	3.80	3.742	3.74	3.75	3.67	3.720(2)	3.700(4)	3.690(4)
<A-O> [12]		3.01	3.074	3.10	3.10	3.04	3.047	3.070	3.058
<A-O> [10]		2.86	2.940	2.97	2.97	2.92	2.913	2.944	2.931
M(1)-M(1)		3.15	3.174	3.31	3.33	3.07	3.328(2)	3.267(2)	3.272(2)
M(1)-M(2)		3.06	3.088	3.14	3.14	3.14	3.146(1)	3.136(1)	3.104(1)
M(1)-M(3)		3.07	3.086	3.14	3.15	3.06	3.143(1)	3.124(1)	3.121(1)
M(1)-M(4)		3.55	3.425	3.49	3.41	3.58	3.360(3)	3.377(3)	3.307(2)
M(2)-M(3)		3.13	3.178	3.31	3.33	3.22	3.334(1)	3.290(1)	3.240(1)
M(2)-M(4)		3.30	3.220	3.24	3.19	3.25	3.157(2)	3.171(2)	3.157(1)
T(1)-T(2)		3.05	3.112	3.10	3.11	3.06	3.098(2)	3.100(2)	3.117(1)
T(1)-T(2)		3.02	3.057	3.08	3.06	3.03	3.059(2)	3.041(2)	3.012(1)
T(1)-T(1)		3.09	3.050	3.04	3.09	3.09	3.116(2)	3.093(2)	3.114(2)

		(70)	(71)	(72)	(73)	(74)
T(1)-O(1)		1.650(1)	1.657(1)	1.654(1)	1.664(4)	1.676(6)
T(1)-O(5)		1.671(1)	1.679(1)	1.675(1)	1.677(4)	1.688(7)
T(1)-O(6)		1.668(1)	1.677(1)	1.676(1)	1.675(4)	1.691(7)
T(1)-O(7)		1.653(1)	1.659(1)	1.663(1)	1.664(3)	1.656(4)
<T(1)-O>		1.661	1.668	1.667	1.670	1.678
T(2)-O(2)		1.631(1)	1.630(1)	1.626(1)	1.632(4)	1.644(5)
T(2)-O(4)		1.604(1)	1.602(1)	1.597(1)	1.605(4)	1.605(6)
T(2)-O(5)		1.645(1)	1.645(1)	1.646(1)	1.644(4)	1.654(6)
T(2)-O(6)		1.656(1)	1.659(1)	1.661(1)	1.660(4)	1.663(7)
<T(2)-O>		1.634	1.634	1.632	1.635	1.642
M(1)-O(10	x2	2.053(1)	2.050(1)	2.051(1)	2.054(4)	2.032(6)
M(1)-O(2)	x2	2.116(1)	2.119(1)	2.114(1)	2.132(4)	2.137(6)
M(1)-O(3)	x2	2.094(1)	2.094(1)	2.093(1)	2.096(4)	2.044(6)
<M(1)-O>		2.088	2.088	2.086	2.094	2.071
M(2)-O(1)	x2	2.065(1)	2.068(1)	2.086(1)	2.065(4)	2.085(7)
M(2)-O(2)	x2	2.048(1)	2.055(1)	2.064(1)	2.057(4)	2.071(6)
M(2)-O(4)	x2	1.959(1)	1.967(1)	1.980(1)	1.973(4)	1.985(6)
<M(2)-O>		2.024	2.030	2.043	2.032	2.047
M(3)-O(1)	x4	2.093(1)	2.084(1)	2.075(1)	2.088(4)	2.076(5)
M(3)-O(3)	x2	2.073(2)	2.072(2)	2.065(2)	2.077(6)	2.068(9)
<M(3)-O>		2.086	2.080	2.072	2.084	2.073
M(4)-O(2)	x2	2.396(1)	2.399(1)	2.395(1)	2.388(4)	2.412(5)
M(4)-O(4)	x2	2.304(1)	2.313(1)	2.300(1)	2.290(4)	2.334(6)
M(4)-O(5)	x2	2.658(1)	2.641(1)	2.651(1)	2.646(4)	2.624(5)
M(4)-O(6)	x2	2.579(1)	2.588(1)	2.605(1)	2.592(4)	2.580(6)
<M(4)-O> [8]		2.484	2.485	2.488	2.479	2.487
<M(4)-O> [6]		2.426	2.433	2.433	2.423	2.442
A-O(5)	x4	3.030(1)	3.045(1)	3.044(1)	3.058(3)	3.081(8)
A-O(6)	x4	3.087(1)	3.068(1)	3.055(1)	3.081(4)	3.064(7)
A-O(7)	x2	2.438(1)	2.432(2)	2.404(2)	2.411(3)	2.467(8)
A-O(7)	x2	3.749	3.748	3.761	3.758(3)	3.746(8)
<A-O> [12]		3.070	3.068	3.061	3.075	3.084
<A-O> [10]		2.934	2.931	2.920	2.938	2.951
M(1)-M(1)		3.218	3.216	3.212	3.217(3)	3.113(8)
M(1)-M(2)		3.086	3.085	3.084	3.091(1)	3.124(4)
M(1)-M(3)		3.100	3.099	3.096	3.101(1)	3.084(3)
M(1)-M(4)		3.400	3.411	3.403	3.411(3)	3.473(6)
M(2)-M(3)		3.191	3.188	3.190	3.198(2)	3.191(6)
M(2)-M(4)		3.214	3.221	3.211	3.217(1)	3.235(4)
T(1)-T(2)		3.107	3.108	3.103	3.114(2)	3.114(4)
T(1)-T(2)		3.052	3.056	3.056	3.055(2)	3.072(4)
T(1)-T(1)		3.083	3.080	3.073	3.088(3)	3.084(4)

APPENDIX B4 (ADDENDUM). CATION-ANION DISTANCES (Å) FOR SPLIT A-SITE MODELS

		(24)	(29)	(38)	(39)	(40)	(51)	(54)	(55)
A(m)-O(5)	x2	3.022(11)	2.911(5)	3.032	3.034	3.030(12)	2.98	3.042(4)	3.026(6)
A(m)-O(5)	x2	3.121(11)	2.996(5)	3.124	3.131	3.095(11)	3.06	3.114(4)	3.210(7)
A(m)-O(6)	x2	2.829(9)	2.940(6)	2.847	2.870	2.836(12)	2.93	2.905(5)	2.705(8)
A(m)-O(6)	x2	3.364(10)	3.351(8)	3.332	3.272	3.405(14)	3.30	3.433(6)	3.507(11)
A(m)-O(7)		2.464(19)	2.598(8)	2.490	2.486	2.369(22)	2.53	2.504(7)	2.515(11)
A(m)-O(7)		2.510(18)	2.649(9)	2.527	2.494	2.511(24)	2.54	2.584(7)	2.527(11)
A(m)-O(7)		3.376(14)	3.356(9)	3.387	3.471	3.367(16)	3.55	3.391(8)	3.204(12)
A(m)-O(7)		4.059(14)	3.883(13)	4.004	3.972	4.155(15)	4.02	4.084(10)	4.104(12)
⟨A-O⟩ XII		3.090	3.074	3.090	3.086	3.094	3.10	3.129	3.104
⟨A-O⟩ VIII		2.865	2.868	2.878	2.881	2.850	2.88	2.901	2.864
A(2)-O(5)	x2	–	–	–	–	–	–	2.739(27)	2.945(11)
A(2)-O(5)	x2	–	–	–	–	–	–	3.388(30)	3.192(12)
A(2)-O(6)	x2	–	–	–	–	–	–	2.901(22)	2.978(11)
A(2)-O(6)	x2	–	–	–	–	–	–	3.441(27)	3.185(12)
A(2)-O(7)	x2	–	–	–	–	–	–	2.548(9)	2.460(7)
A(2)-O(7)	x2	–	–	–	–	–	–	3.756(9)	3.703(9)
⟨A-O⟩ XII		–	–	–	–	–	–	3.129	3.077
⟨A-O⟩ X		–	–	–	–	–	–	3.003	2.952

		(56a)	(56b)	(58)	(59)	(61)	(62)	(65)	(67)
A(m)-O(5)	x2	2.94(1)	2.95(2)	3.057(9)	2.974(5)	3.059	2.599	2.849	2.846(5)
A(m)-O(5)	x2	3.10(1)	3.11(2)	3.146(11)	3.145(5)	3.118	2.778	2.980	2.923(5)
A(m)-O(6)	x2	2.78(1)	2.73(3)	2.737(19)	2.773(6)	2.833	3.036	2.919	3.037(5)
A(m)-O(6)	x2	3.56(1)	3.62(3)	3.510(14)	3.580(7)	3.354	3.625	3.586	3.397(5)
A(m)-O(7)		2.49(2)	2.49(4)	2.501(15)	2.554(8)	2.299	2.355	2.572	2.616(8)
A(m)-O(7)		2.58(2)	2.63(4)	2.620(17)	2.609(8)	2.603	2.359	2.685	2.666(8)
A(m)-O(7)		3.19(2)	3.11(4)	3.273(19)	3.231(9)	3.445	3.438	3.325	3.491(7)
A(m)-O(7)		4.10(2)	4.11(4)	4.285(19)	4.261(9)	4.185	4.168	4.175	3.950(8)
⟨A-O⟩ XII		3.09	3.10	3.132	3.133	3.105	3.033	3.119	3.094
⟨A-O⟩ VIII		2.84	2.84	2.875	2.868	2.865	2.692	2.844	2.862
A(2)-O(5)	x2	2.83(3)	2.82(5)	2.834(8)	2.845(8)	–	–	–	–
A(2)-O(5)	x2	3.12(3)	3.12(5)	3.285(8)	3.177(8)	–	–	–	–
A(2)-O(6)	x2	3.03(2)	3.02(4)	2.921(8)	3.017(7)	–	–	–	–
A(2)-O(6)	x2	3.27(2)	3.27(5)	3.295(8)	3.294(7)	–	–	–	–
A(2)-O(7)	x2	2.486(4)	2.495(6)	2.519(6)	2.528(4)	–	–	–	–
A(2)-O(7)	x2	3.684(3)	3.681(4)	3.785(8)	3.744(4)	–	–	–	–
⟨A-O⟩ XII		3.070	3.068	3.107	3.101	–	–	–	–
⟨A-O⟩ X		2.947	2.945	2.971	2.972	–	–	–	–

		(68)	(70)	(71)	(72)	(73)	(74)
A(m)-O(5)	x2	2.788(7)	3.058(1)	3.055(1)	3.047(1)	3.05(2)	3.06(3)
A(m)-O(5)	x2	2.964(7)	3.073(1)	3.113(1)	3.121(1)	3.15(2)	3.21(3)
A(m)-O(6)	x2	2.894(7)	2.769(1)	2.731(1)	2.713(1)	2.72(3)	2.69(3)
A(m)-O(6)	x2	3.646(9)	3.439	3.441	3.435	3.48(4)	3.49(3)
A(m)-O(7)		2.556(12)	2.360(2)	2.392(2)	2.378(2)	2.40(4)	2.51(5)
A(m)-O(7)		2.645(11)	2.597(2)	2.565(2)	2.528(2)	2.53(4)	2.56(5)
A(m)-O(7)		3.225(11)	3.296(2)	3.281(2)	3.293(2)	3.27(5)	3.24(5)
A(m)-O(7)		4.183(12)	4.266	4.289	4.308	4.25(5)	4.27(4)
$\langle A\text{-}O \rangle_{VIII}^{XII}$		3.099	3.100	3.100	3.095	3.10	3.09
$\langle A\text{-}O \rangle$		2.812	2.845	2.854	2.834	2.85	2.87
A(2)-O(5)	x2	-	2.668(1)	2.631(1)	2.640(1)	2.715(16)	2.92(2)
A(2)-O(5)	x2	-	3.414	3.488	3.476	3.421(18)	3.25(3)
A(2)-O(6)	x2	-	2.799(1)	2.738(1)	2.734(1)	2.806(13)	2.93(2)
A(2)-O(6)	x2	-	3.412	3.445	3.422	3.388(15)	3.20(2)
A(2)-O(7)	x2	-	2.479(2)	2.487(2)	2.457(2)	2.448(7)	2.48(1)
A(2)-O(7)	x2	-	3.776	3.784	3.795	3.783(8)	3.75(1)
$\langle A\text{-}O \rangle^{XII}_{X}$		-	3.091	3.096	3.087	3.094	3.09
$\langle A\text{-}O \rangle$		-	2.954	2.959	2.946	2.956	2.96

APPENDIX B5. ANION-ANION DISTANCES (Å)

		(21)	(22)	(24)	(26)	(28)	(29)	(30)
O(1)-O(5)		2.654(6)	2.656(6)	2.764(6)	2.648(8)	2.660(5)	2.705(5)	2.681(3)
O(1)-O(6)		2.656(6)	2.669(6)	2.747(5)	2.659(7)	2.661(4)	2.687(6)	2.666(3)
O(1)-O(7)		2.652(7)	2.664(6)	2.742(7)	2.638(8)	2.652(5)	2.657(5)	2.649(2)
O(5)-O(6)		2.638(8)	2.682(6)	2.682(7)	2.646(9)	2.629(5)	2.634(6)	2.602(3)
O(5)-O(7)		2.626(5)	2.629(5)	2.690(5)	2.627(7)	2.628(4)	2.604(5)	2.638(2)
O(6)-O(7)		2.630(6)	2.638(6)	2.718(6)	2.617(8)	2.642(5)	2.594(6)	2.639(2)
⟨O-O⟩ T(1)		2.643	2.656	2.726	2.639	2.645	2.647	2.646
O(2)-O(4)		2.748(6)	2.733(6)	2.767(6)	2.745(8)	2.725(5)	2.767(5)	2.736(2)
O(2)-O(5)		2.642(6)	2.633(6)	2.687(5)	2.635(8)	2.638(4)	2.692(6)	2.670(3)
O(2)-O(6)		2.653(7)	2.657(6)	2.683(6)	2.636(9)	2.664(5)	2.684(5)	2.665(3)
O(4)-O(5)		2.654(6)	2.649(6)	2.662(6)	2.640(8)	2.652(5)	2.682(6)	2.645(2)
O(4)-O(6)		2.562(6)	2.536(6)	2.576(6)	2.588(8)	2.542(5)	2.590(6)	2.560(2)
O(5)-O(6)		2.693(6)	2.668(6)	2.682(7)	2.666(8)	2.695(5)	2.673(7)	2.702(3)
⟨O-O⟩ T(2)		2.659	2.646	2.676	2.652	2.653	2.681	2.663
$O(1^u)$-$O(2^d)$	x2	2.818(7)	2.865	2.764(4)	2.639	2.836	2.811(5)	2.815(2)
$O(1^u)$-$O(2^u)$	x2	3.101(8)	3.121	3.100(6)	3.186	3.101	3.061(6)	3.070(3)
$O(1^u)$-$O(3^d)$	x2	2.790(7)	2.831	2.745(5)	2.804	2.783	2.719(5)	2.765(3)
$O(1^u)$-$O(3^u)$	x2	3.084(7)	3.115	3.079(7)	3.133	3.085	3.063(7)	3.056(3)
O(2)-O(2)		2.938(8)	2.952	2.908(8)	3.026	2.919	2.885(9)	2.867(3)
O(2)-O(3)	x2	3.123(8)	3.193	3.124(4)	3.047	3.118	3.059(3)	3.090(2)
O(3)-O(3)		2.737(13)	2.751	2.660(11)	2.695	2.753	2.642(11)	2.704(3)
⟨O-O⟩ M(1)		2.959	2.995	2.933	2.945	2.960	2.913	2.908
$O(1^u)$-$O(1^d)$		2.752(9)	2.725	2.678(8)	2.621	2.769	2.758(8)	2.741(3)
$O(1^u)$-$O(2^d)$	x2	2.819(7)	2.865	2.764(4)	2.639	2.836	2.811(5)	2.815(2)
$O(1^u)$-$O(2^u)$	x2	3.037(8)	3.076	3.025(6)	2.805	3.057	3.032(6)	3.037(3)
$O(1^u)$-O(4)	x2	3.024(7)	3.134	2.928(5)	2.749	3.009	3.016(5)	3.006(2)
$O(2^u)$-$O(4^d)$	x2	2.814(7)	2.852	2.935(5)	2.815	2.863	3.076(5)	2.982(3)
$O(2^u)$-$O(4^u)$	x2	3.090(7)	3.188	2.869(6)	2.693	3.040	2.869(7)	2.904(3)
O(4)-O(4)		2.964(12)	2.960	2.975(8)	2.852	2.991	3.024(9)	2.970(3)
⟨O-O⟩ M(2)		2.940	2.993	2.891	2.740	2.948	2.949	2.922
$O(1^u)$-$O(1^d)$	x2	2.751(9)	2.725	2.678(8)	2.621	2.769	2.758(8)	2.741(3)
$O(1^u)$-$O(1^u)$	x2	3.171(9)	3.245	3.195(7)	3.289	3.130	3.085(6)	3.104(2)
$O(1^u)$-$O(3^d)$	x4	2.789(14)	2.831	2.745(5)	2.804	2.783	2.719(5)	2.765(3)
$O(1^u)$-$O(3^u)$	x4	3.102(15)	3.132	3.115	3.100	3.083	3.063(7)	3.064(3)
⟨O-O⟩ M(3)		2.951	2.983	2.932	2.953	2.939	2.901	2.892
O(2)-O(2)		2.938	2.952	2.908(8)	3.026	2.919	2.885(9)	2.867(3)
$O(2^u)$-$O(4^d)$	x2	2.814	2.852	2.935(5)	2.815	2.863	3.076(5)	2.982(3)
$O(2^u)$-$O(4^u)$	x2	2.996	3.001	3.131(6)	3.258	3.020	3.212(7)	3.133(3)
$O(2^u)$-$O(5^u)$	x2	3.741	3.859	3.494(5)	3.590	3.738	3.726(5)	3.626
$O(4^u)$-$O(5^d)$	x2	3.273	3.297	3.375(5)	3.351	3.350	3.567(5)	3.424
$O(4^u)$-$O(6^u)$	x2	2.562	2.537	2.569(6)	2.587	2.542	2.590(6)	2.560(2)
$O(5^u)$-$O(6^d)$	x2	3.125	3.225	3.027(5)	3.019	3.133	3.162(5)	3.085
$O(5^u)$-$O(6^u)$	x2	2.638	2.682	2.682(7)	2.646	2.629	2.634(6)	2.602
O(6)-O(6)		3.074	3.078	3.530(8)	3.350	3.094	3.578(8)	3.426(3)
⟨O-O⟩ M(4)		3.019	3.059	3.053	3.057	3.035	3.150	3.070

		(34)	(35)	(36)	(37)	(38)	(39)	(40)
O(1)-O(5)		2.695(8)	2.702(9)	2.680(4)	2.685(5)	2.789(4)	2.789(5)	2.785(12)
O(1)-O(6)		2.661(9)	2.662(9)	2.664(5)	2.673(5)	2.747(4)	2.768(6)	2.722(10)
O(1)-O(7)		2.663(8)	2.655(9)	2.651(5)	2.667(5)	2.750(4)	2.746(5)	2.750(13)
O(5)-O(6)		2.654(10)	2.633(11)	2.578(5)	2.621(6)	2.694(4)	2.703(6)	2.697(13)
O(5)-O(7)		2.570(6)	2.592(7)	2.641(4)	2.658(4)	2.697(3)	2.706(4)	2.697(9)
O(6)-O(7)		2.622(8)	2.627(8)	2.647(4)	2.650(5)	2.729(4)	2.724(6)	2.745(12)
<O-O> T(1)		2.644	2.645	2.644	2.661	2.734	2.738	2.733
O(2)-O(4)		2.735(8)	2.725(8)	2.732(4)	2.723(5)	2.762(3)	2.768(5)	2.790(12)
O(2)-O(5)		2.684(9)	2.687(10)	2.666(5)	2.666(5)	2.665(3)	2.688(5)	2.642(10)
O(2)-O(6)		2.673(8)	2.676(9)	2.652(4)	2.681(5)	2.683(3)	2.692(5)	2.679(12)
O(4)-O(5)		2.674(7)	2.647(9)	2.642(4)	2.650(5)	2.657(4)	2.646(6)	2.656(12)
O(4)-O(6)		2.594(7)	2.579(9)	2.543(4)	2.551(5)	2.567(4)	2.579(5)	2.549(11)
O(5)-O(6)		2.633(11)	2.664(12)	2.715(5)	2.711(6)	2.675(4)	2.680(6)	2.658(13)
<O-O> T(2)		2.666	2.663	2.658	2.663	2.668	2.676	2.662
$O(1^u)$-$O(2^d)$	x2	2.803(6)	2.831(7)	2.818(4)	2.865(5)	2.782(4)	2.779(5)	2.721
$O(1^u)$-$O(2^u)$	x2	3.059(10)	3.069(12)	3.064(5)	3.102(5)	3.125(3)	3.111(6)	3.059
$O(1^u)$-$O(3^d)$	x2	2.720(6)	2.721(8)	2.694(4)	2.826(6)	2.753(4)	2.759(6)	2.660
$O(1^u)$-$O(3^u)$	x2	3.020(10)	3.048(11)	3.040(5)	3.088(6(	3.085(4)	3.071(7)	3.059
O(2)-O(2)		2.896(12)	2.898(14)	2.867(6)	2.915(7)	2.940(5)	2.920(7)	2.889
O(2)-O(3)	x2	3.038(5)	3.048(6)	3.069(3)	3.149(3)	3.138(2)	3.129(3)	3.077
O(3)-O(3)		2.602(13)	2.615(15)	2.600(7)	2.728(10)	2.664(6)	2.649(11)	2.618
<O-O> M(1)		2.898	2.912	2.903	2.973	2.948	2.939	2.888
O(1)-$O(1)_d$		2.801(12)	2.796(13)	2.757(6)	2.741(7)	2.654(5)	2.667(8)	2.739
$O(1^u)$-$O(2^d)$	x2	2.803(6)	2.831(7)	2.818(4)	2.865(5)	2.782(4)	2.779(5)	2.721
$O(1^u)$-$O(2^u)$	x2	3.007(10)	3.017(12)	3.036(5)	3.051(5)	3.020(3)	3.030(6)	3.043
O(1)-)$(4)_d$	x2	2.995(7)	3.029(8)	3.015(4)	3.034(5)	2.908(3)	2.926(5)	2.922
$O(2^u)$-$O(4^d)$	x2	3.016(8)	3.043(9)	2.984(5)	3.003(5)	2.932(3)	2.945(5)	2.918
$O(2^u)$-$O(4^u)$	x2	2.892(9)	2.914(10)	2.914(5)	2.943(5)	2.826(4)	2.859(6)	2.881
O(4)-O(4)		3.061(12)	3.052(13)	2.997(7)	2.977(8)	2.936(5)	2.959(7)	2.991
<O-O> M(2)		2.941	2.960	2.941	2.959	2.877	2.892	2.892
$O(1^u)$-$O(1^d)$	x2	2.801(12)	2.796(13)	2.757(6)	2.741(7)	2.654(5)	2.667(8)	2.739
$O(1^u)$-$O(1^u)$	x2	3.051(9)	3.049(12)	3.049(6)	3.183(7)	3.193(5)	3.190(7)	3.142
$O(1^u)$-$O(3^d)$	x4	2.720(6)	2.720(8)	2.694(4)	2.825(6)	2.753(4)	2.759(6)	2.660
$O(1^u)$-$O(3^u)$	x4	3.068(10)	3.048(11)	3.054(5)	3.098(6)	3.114(4)	3.129(7)	3.110
<O-O> M(3)		2.905	2.897	2.884	2.962	2.930	2.939	2.904
O(2)-$O(2)_d$		2.895(12)	2.898(14)	2.867(6)	2.915(7)	2.940(5)	2.920(5)	2.889
$O(2^u)$-$O(4^d)$	x2	3.016(8)	3.043(9)	2.984(5)	3.003(5)	2.932(3)	2.945(5)	2.918
$O(2^u)$-$O(4^u)$	x2	3.157(9)	3.167(10)	3.119(5)	3.128(6)	3.145(4)	3.139(6)	3.135
$O(2^u)$-$O(5^d)$	x2	3.728(7)	3.725(8)	3.619(5)	3.646	3.451(3)	3.463(5)	3.535
$O(4^u)$-$O(5^u)$	x2	3.488(7)	3.467(9)	3.414(5)	3.428	3.364(3)	3.359(5)	3.370
$O(4^u)$-$O(6^u)$	x2	2.594(7)	2.597(9)	2.543(4)	2.551(5)	2.567(4)	2.579(5)	2.548
$O(5^u)$-$O(6^d)$	x2	3.066(6)	3.074(8)	3.072(3)	3.131	3.014(3)	3.013(5)	2.989
$O(5^u)$-$O(6^u)$	x2	2.654(11)	2.633(11)	2.578(5)	2.621	2.694(4)	2.703(6)	2.698
O(6)-O(6)		3.418(11)	3.394(12)	3.386(6)	3.437(8)	3.586(5)	3.561(8)	3.468
<O-O> M(4)		3.107	3.107	3.057	3.086	3.054	3.055	3.046

		(41)	(42)	(43)	(44)	(45)	(46)	(48)	(49)	(50)	(51)
O(1)-O(5)		2.657(6)	2.711	2.674	2.750	2.725	2.721	2.751	2.715	2.729	2.751
O(1)-O(6)		2.663(6)	2.722	2.650	2.780	2.710	2.738	2.732	2.763	2.756	2.781
O(1)-O(7)		2.654(6)	2.672	2.622	2.738	2.695	2.702	2.711	2.761	2.733	2.734
O(5)-O(6)		2.618(6)	2.652	2.636	2.676	2.678	2.665	2.698	2.697	2.668	2.783
O(5)-O(7)		2.620(5)	2.659	2.649	2.711	2.694	2.711	2.735	2.713	2.684	2.688
O(6)-O(7)		2.638(6)	2.680	2.647	2.677	2.667	2.688	2.744	2.701	2.699	2.752
<O-O> T(1)		2.641	2.683	2.646	2.722	2.695	2.704	2.729	2.725	2.712	2.748
O(2)-O(4)		2.741(6)	2.752	2.705	2.665	2.741	2.730	2.761	2.737	2.738	2.672
O(2)-O(5)		2.645(6)	2.641	2.656	2.647	2.681	2.666	2.643	2.661	2.660	2.664
O(2)-O(6)		2.672(6)	2.650	2.651	2.664	2.660	2.670	2.657	2.643	2.697	2.634
O(4)-O(5)		2.656(8)	2.638	2.629	2.640	2.647	2.634	2.643	2.661	2.609	2.676
O(4)-O(6)		2.538(7)	2.597	2.564	2.598	2.574	2.586	2.553	2.602	2.614	2.583
O(5)-O(6)		2.699(6)	2.688	2.680	2.703	2.680	2.699	2.682	2.673	2.709	2.620
<O-O> T(2)		2.658	2.661	2.648	2.653	2.664	2.664	2.657	2.663	2.671	2.642
$O(1^u)$-$O(2^d)$	x2	2.821	2.769	2.847	2.884	2.804	2.788	2.697	2.734	2.701	2.838
$O(1^u)$-$O(2^u)$	x2	3.087	3.153	3.091	3.193	3.116	3.179	3.200	3.183	3.248	3.200
$O(1^u)$-$O(3^d)$	x2	2.779	2.782	2.790	2.827	2.805	2.782	2.821	2.816	2.781	2.827
$O(1^u)$-$O(3^u)$	x2	3.067	3.121	3.062	3.165	3.110	3.196	3.143	3.189	3.140	3.212
O(2)-O(2)		2.906	2.965	2.888	3.008	2.920	2.963	3.053	2.976	3.059	3.053
O(2)-O(3)	x2	3.108	3.102	3.118	3.206	3.145	3.154	3.175	3.181	3.176	3.182
O(3)-O(3)		2.752	2.713	2.706	2.789	2.735	2.738	2.701	2.736	2.649	2.732
<O-O> M(1)		2.949	2.961	2.951	3.029	2.968	2.992	2.986	2.993	2.983	3.025
$O(1)_u$-$O(1)_d$		2.764	2.605	2.749	2.578	2.691	2.605	2.601	2.545	2.554	2.625
$O(1^u)$-$O(2^d)$	x2	2.821	2.769	2.847	2.884	2.804	2.788	2.697	2.734	2.701	2.838
$O(1^u)$-$O(2^u)$	x2	3.058	2.941	3.041	3.035	3.024	2.950	2.901	2.933	2.883	2.960
$O(1)_u$-$O(4)_d$	x2	3.010	2.865	3.021	2.989	2.957	2.907	2.786	2.803	2.845	2.899
$O(2^u)$-$O(4^d)$	x2	2.862	2.925	2.999	3.046	2.968	2.945	2.819	2.876	2.850	3.036
$O(2^u)$-$O(4^u)$	x2	3.034	2.790	2.901	2.858	2.869	2.816	2.728	2.768	2.661	2.849
O(4)-O(4)		2.978	2.928	2.988	2.998	2.954	2.946	2.864	2.910	2.811	3.104
<O-O> M(2)		2.943	2.843	2.946	2.933	2.907	2.864	2.777	2.807	2.770	2.908
$O(1^u)$-$O(1^d)$	x2	2.764	2.605	2.749	2.578	2.691	2.605	2.601	2.545	2.554	2.625
$O(1^u)$-$O(1^u)$	x2	3.120	3.195	3.117	3.225	3.216	3.268	3.379	3.365	3.314	3.326
$O(1^u)$-$O(3^d)$	x4	2.779	2.782	2.790	2.827	2.805	2.782	2.821	2.816	2.781	2.827
$O(1^u)$-$O(3^u)$	x4	3.090	3.063	3.071	3.073	3.105	3.046	3.165	3.110	3.129	3.090
<O-O> M(3)		2.937	2.915	2.931	2.934	2.955	2.922	2.992	2.960	2.948	2.964
$O(2)_u$-$O(2)_d$		2.906	2.965	2.889	3.009	2.923	2.964	3.053	2.967	3.059	3.053
$O(2^u)$-$O(4^d)$	x2	2.862	2.925	3.000	3.045	2.968	2.946	2.819	2.876	2.850	3.036
$O(2^u)$-$O(4^u)$	x2	3.024	3.161	3.136	3.158	3.159	3.181	3.201	3.156	3.290	3.171
$O(2^u)$-$O(5^d)$	x2	3.743	3.487	3.615	3.540	3.555	3.503	3.372	3.445	3.407	3.523
$O(4^u)$-$O(5^d)$	x2	3.353	3.377	3.431	3.457	3.405	3.383	3.284	3.381	3.317	3.464
$O(4^u)$-$O(6^u)$	x2	2.543	2.597	2.563	2.596	2.575	2.586	2.553	2.602	2.614	2.583
$O(5^u)$-$O(6^d)$	x2	3.134	3.035	3.112	3.121	3.088	3.058	3.003	3.065	3.014	3.081
$O(5^u)$-$O(6^u)$	x2	2.617	2.652	2.636	2.676	2.678	2.665	2.698	2.697	2.668	2.783
O(6)-O(6)		3.096	3.492	3.481	3.531	3.558	3.519	3.579	3.574	3.544	3.682
<O-O> M(4)		3.035	3.058	3.085	3.108	3.084	3.071	3.031	3.062	3.058	3.126

	(52)	(53a)	(53b)	(54)	(55)
O(1)-O(5)	2.800	2.676(3)	2.674(4)	2.748(5)	2.803(5)
O(1)-O(6)	2.748	2.664(3)	2.661(4)	2.741(9)	2.770(9)
O(1)-O(7)	2.780	2.649(3)	2.657(5)	2.750(6)	2.755(6)
O(5)-O(6)	2.680	2.603(3)	2.601(4)	2.677(5)	2.688(6)
O(5)-O(7)	2.690	2.635(3)	2.633(4)	2.730(4)	2.707(4)
O(6)-O(7)	2.721	2.638(3)	2.640(4)	2.745(5)	2.731(5)
⟨O-O⟩ T(1)	2.737	2.644	2.644	2.732	2.742
O(2)-O(4)	2.830	2.736(3)	2.735(4)	2.763(5)	2.782(5)
O(2)-O(5)	2.678	2.667(3)	2.668(4)	2.673(8)	2.688(9)
O(2)-O(6)	2.740	2.668(3)	2.666(4)	2.679(5)	2.683(5)
O(4)-O(5)	2.703	2.648(3)	2.655(5)	2.655(5)	2.667(5)
O(4)-O(6)	2.610	2.554(3)	2.553(5)	2.563(5)	2.579(5)
O(5)-O(6)	2.706	2.704(3)	2.713(4)	2.704(5)	2.684(6)
⟨O-O⟩ T(2)	2.711	2.663	2.668	2.673	2.680
$O(1^u)$-$O(2^d)$ x2	2.747	2.829(3)	2.846(4)	2.733(5)	2.764(5)
$O(1^u)$-$O(2^u)$ x2	3.100	3.073(3)	3.077(4)	3.178(5)	3.079(6)
$O(1^u)$-$O(3^d)$ x2	2.683	2.785(3)	2.794(5)	2.844(5)	2.718(5)
$O(1^u)$-$O(3^u)$ x2	3.157	3.066(4)	3.083(5)	3.153(6)	3.064(6)
O(2)-O(2)	2.912	2.881(4)	2.903(6)	3.007(11)	2.896(10)
O(2)-O(3) x2	3.069	3.103(2)	3.117(3)	3.201(3)	3.097(4)
O(3)-O(3)	2.812	2.727(6)	2.756(10)	2.738(11)	2.666(13)
⟨O-O⟩ M(1)	2.936	2.923	2.940	2.998	2.917
$O(1)_u$-O(1)	2.717	2.752(4)	2.767(6)	2.617(10)	2.689(10)
$O(1^u)$-$O(2^d)$ x2	2.747	2.829(3)	2.846(4)	2.733(5)	2.764(5)
$O(1^u)$-$O(2^u)$ x2	3.011	3.045(3)	3.057(4)	2.949(5)	3.049(6)
$O(1)_u$-O(4) x2	2.925	3.032(3)	3.057(4)	2.822(5)	2.935(5)
$O(2^u)$-$O(4^d)$ x2	2.910	3.008(3)	3.031(4)	2.847(5)	2.958(5)
$O(2^u)$-$O(4^u)$ x2	2.928	2.915(3)	2.930(4)	2.776(5)	2.881(5)
O(4)-O(4)	3.076	2.968(4)	2.972(7)	2.822(11)	2.994(11)
⟨O-O⟩ M(2)	2.903	2.935	2.951	2.813	2.905
$O(1^u)$-$O(1^d)$ x2	2.717	2.752(4)	2.767(6)	2.617(10)	2.689(10)
$O(1^u)$-$O(1^u)$ x2	3.116	3.125(4)	3.141(6)	3.390(7)	3.142(7)
$O(1^u)$-$O(3^d)$ x4	2.683	2.785(3)	2.794(5)	2.844(5)	2.718(5)
$O(1^u)$-$O(3^u)$ x4	3.001	3.073(4)	3.075(5)	3.167(6)	3.107(6)
⟨O-O⟩ M(3)	2.867	2.906	2.916	3.004	2.914
O(2)-O(2)	2.912	2.881(4)	2.903(6)	3.007(11)	2.896(10)
$O(2^u)$-$O(4^d)$ x2	2.910	3.008(3)	3.031(4)	2.847(5)	2.958(5)
$O(2^u)$-$O(4^u)$ x2	3.090	3.153(3)	3.167(4)	3.170(5)	3.128(5)
$O(2^u)$-$O(5^u)$ x2	3.508	3.677	3.707	3.407(5)	3.504(5)
$O(4^u)$-$O(5^d)$ x2	3.373	3.453	3.473	3.314(5)	3.383(6)
$O(4^u)$-$O(6^u)$ x2	2.610	2.554(3)	2.553(5)	2.563(5)	2.579(5)
$O(5^u)$-$O(6^d)$ x2	3.005	3.126	3.160	3.026(8)	2.994(8)
$O(5^u)$-$O(6^u)$ x2	2.680	2.603	2.601	2.677(5)	2.688(6)
O(6)-O(6)	3.462	3.433(4)	3.449(6)	3.547(8)	3.519(8)
⟨O-O⟩ M(4)	3.045	3.090	3.109	3.035	3.055

		(56a)	(56b)	(57)	(58)	(59)	(60)	(61)
O(1)-O(5)		2.697(2)	2.696(2)	2.673(4)	2.766(4)	2.758(3)	2.716	2.736
O(1)-O(6)		2.682(2)	2.680(2)	2.667(8)	2.772(8)	2.750(3)	2.753	2.727
O(1)-O(7)		2.671(3)	2.664(2)	2.668(4)	2.767(4)	2.755(4)	2.722	2.698
O(5)-O(6)		2.618(3)	2.620(2)	2.637(4)	2.710(4)	2.719(3)	2.664	2.678
O(5)-O(7)		2.632(3)	2.632(1)	2.629(3)	2.698(3)	2.688(3)	2.689	2.682
O(6)-O(7)		2.652(2)	2.644(2)	2.645(4)	2.752(4)	2.720(3)	2.695	2.737
⟨O-O⟩ T(1)		2.659	2.656	2.653	2.744	2.732	2.707	2.710
O(2)-O(4)		2.742(2)	2.740(2)	2.737(4)	2.798(4)	2.738(3)	2.776	2.747
O(2)-O(5)		2.675(2)	2.675(2)	2.646(7)	2.707(8)	2.676(3)	2.654	2.690
O(2)-O(6)		2.663(2)	2.670(2)	2.672(5)	2.709(4)	2.677(3)	2.676	2.683
O(4)-O(5)		2.656(3)	2.656(2)	2.655(4)	2.685(4)	2.663(3)	2.671	2.647
O(4)-O(6)		2.562(2)	2.566(2)	2.551(4)	2.590(4)	2.575(3)	2.604	2.623
O(5)-O(6)		2.698(3)	2.697(2)	2.693(4)	2.707(4)	2.672(3)	2.685	2.706
⟨O-O⟩ T(2)		2.666	2.667	2.659	2.699	2.667	2.678	2.683
$O(1^u)$-$O(2^d)$	x2	2.817(2)	2.817(2)	2.840(4)	2.709(4)	2.786(3)	2.748	2.809
$O(1^u)$-$O(2^u)$	x2	3.067(2)	3.072(2)	3.104(4)	3.200(4)	3.147(3)	3.120	3.148
$O(1^u)$-$O(3^d)$	x2	2.747(3)	2.756(2)	2.788(4)	2.823(4)	2.824(3)	2.775	2.811
$O(1^u)$-$O(3^u)$	x2	3.057(3)	3.056(2)	3.081(4)	3.143(4)	3.120(4)	3.129	3.141
O(2)-O(2)		2.884(3)	2.884(3)	2.930(9)	3.024(10)	3.005(4)	2.970	2.915
O(2)-O(3)	x2	3.081(2)	3.082(1)	3.125(3)	3.188(3)	3.168(2)	3.128	3.149
O(3)-O(3)		2.685(5)	2.697(4)	2.756(9)	2.699(11)	2.707(6)	2.701	2.730
⟨O-O⟩ M(1)		2.926	2.928	2.964	2.969	2.984	2.956	2.980
O(1)-$O(1)_d$		2.752(3)	2.753(2)	2.774(9)	2.622(9)	2.685(4)	2.663	2.631
$O(1^u)$-$O(2^d)$	x2	2.817(2)	2.817(2)	2.840(4)	2.709(4)	2.786(3)	2.748	2.809
$O(1^u)$-$O(2^u)$	x2	3.043(2)	3.040(2)	3.060(4)	2.942(4)	3.007(3)	2.972	2.988
O(1)-$O(4)_d$	x2	3.007(2)	3.010(2)	3.022(4)	2.797(4)	2.897(3)	2.848	2.892
$O(2^u)$-$O(4^d)$	x2	3.005(2)	3.005(2)	2.862(4)	2.822(4)	2.963(3)	2.918	2.926
$O(2^u)$-$O(4^u)$	x2	2.909(2)	2.906(2)	3.046(4)	2.757(4)	2.842(3)	2.781	2.849
O(4)-O(4)		2.992(4)	2.999(3)	2.984(9)	2.890(9)	2.986(5)	2.891	2.969
⟨O-O⟩ M(2)		2.942	2.942	2.952	2.797	2.888	2.819	2.853
$O(1^u)$-$O(1^d)$	x2	2.752(3)	2.753(2)	2.774(9)	2.622(9)	2.685(4)	2.663	2.631
$O(1^u)$-$O(1^u)$	x2	3.097(3)	3.093(2)	3.133(5)	3.370(5)	3.306(4)	3.280	3.226
$O(1^u)$-$O(3^d)$	x4	2.747(3)	2.756(2)	2.788(4)	2.823(4)	2.824(3)	2.775	2.811
$O(1^u)$-$O(3^u)$	x4	3.069(3)	3.068(2)	3.090(4)	3.186(4)	3.172(4)	3.115	3.070
⟨O-O⟩ M(3)		2.914	2.916	2.944	3.002	2.997	2.954	2.937
O(2)-$O(2)_d$		2.884(3)	2.884(3)	2.930(9)	3.024(10)	3.005(4)	2.970	2.915
$O(2^u)$-$O(4^d)$	x2	3.005(2)	3.005(2)	2.862(4)	2.822(4)	2.963(3)	2.918	2.926
$O(2^u)$-$O(4^u)$	x2	3.144(2)	3.147(2)	3.023(4)	3.191(4)	3.180(3)	3.185	3.110
$O(2^u)$-$O(5^u)$	x2	3.638(3)	3.640(2)	3.737(4)	3.380(4)	3.533(3)	3.530	3.440
$O(4^u)$-$O(5^d)$	x2	3.444(3)	3.448(2)	3.337(5)	3.317(4)	3.420(3)	3.415	3.359
$O(4^u)$-$O(6^u)$	x2	2.562(2)	2.566(2)	2.551(4)	2.590(4)	2.575(3)	2.604	2.623
$O(5^u)$-$O(6^d)$	x2	3.082(3)	3.090(3)	3.128(9)	3.017(7)	3.081(3)	3.037	3.051
$O(5^u)$-$O(6^u)$	x2	2.618(3)	2.620(3)	2.637(4)	2.710(4)	2.719(3)	2.664	2.678
O(6)-O(6)		3.457(3)	3.455(3)	3.107(6)	3.615(7)	3.563(5)	3.475	3.559
⟨O-O⟩ M(4)		3.084	3.086	3.037	3.043	3.094	3.072	3.053

		(62)	(63)	(64)	(65)	(66)	(67)	(68)	(69)
O(1)-O(5)		2.654	2.724	2.654	2.616	2.630	2.672(5)	2.667(4)	2.646(3)
O(1)-O(6)		2.647	2.708	2.790	2.674	2.783	2.677(5)	2.684(4)	2.665(3)
O(1)-O(7)		2.628	2.699	2.680	2.657	2.653	2.675(5)	2.686(5)	2.657(4)
O(5)-O(6)		2.657	2.644	2.714	2.713	2.703	2.700(5)	2.670(4)	2.651(4)
O(5)-O(7)		2.587	2.665	2.648	2.656	2.627	2.600(4)	2.610(4)	2.631(3)
O(6)-O(7)		2.625	2.698	2.630	2.588	2.573	2.596(5)	2.619(4)	2.622(3)
⟨O-O⟩ T(1)		2.633	2.690	2.701	2.651	2.662	2.653	2.656	2.646
O(2)-O(4)		2.783	2.753	2.676	2.706	2.685	2.734(5)	2.734(4)	2.748(3)
O(2)-O(5)		2.707	2.702	2.578	2.651	2.648	2.673(5)	2.665(4)	2.664(3)
O(2)-O(6)		2.653	2.667	2.574	2.648	2.651	2.678(5)	2.672(4)	2.652(3)
O(4)-O(5)		2.651	2.667	2.651	2.589	2.620	2.681(5)	2.666(4)	2.653(3)
O(4)-O(6)		2.603	2.579	2.734	2.687	2.711	2.598(5)	2.588(4)	2.591(4)
O(5)-O(6)		2.621	2.717	2.633	2.651	2.606	2.647(5)	2.666(4)	2.680(4)
⟨O-O⟩ T(2)		2.670	2.680	2.641	2.655	2.654	2.669	2.665	2.665
$O(1^u)$-$O(2^d)$	x2	2.668	2.794	2.739	2.855	2.812	2.813(5)	2.759(4)	2.649(3)
$O(1^u)$-$O(2^u)$	x2	3.161	3.062	3.217	3.196	3.349	3.114(5)	3.173(5)	3.204(3)
$O(1^u)$-$O(3^d)$	x2	2.750	2.775	2.872	2.908	2.954	2.852(5)	2.849(4)	2.844(4)
$O(1^u)$-$O(3^u)$	x2	3.250	3.048	3.298	3.250	3.226	3.134(6)	3.148(5)	3.169(4)
O(2)-O(2)		2.806	2.855	3.012	2.983	2.989	3.009(7)	3.018(6)	3.045(5)
O(2)-O(3)	x2	3.066	3.112	3.066	3.101	3.060	3.134(4)	3.107(3)	3.091(2)
O(3)-O(3)		2.688	2.693	2.997	2.618	2.803	2.678(9)	2.735(8)	2.709(7)
⟨O-O⟩ M(1)		2.940	2.928	3.033	2.988	3.050	2.982	2.985	2.973
O(1)-$O(1)_d$		2.523	2.707	2.424	2.641	2.423	2.714(7)	2.678(6)	2.621(5)
$O(1^u)$-$O(2^d)$	x2	2.668	2.794	2.739	2.855	2.812	2.813(5)	2.759(4)	2.649(3)
$O(1^u)$-$O(2^u)$	x2	2.829	3.058	2.847	2.848	2.724	2.956(5)	2.904(4)	2.805(3)
O(1)-$O(4)_d$	x2	2.665	2.957	2.812	2.872	2.845	2.929(5)	2.884(4)	2.742(4)
$O(2^u)$-$O(4^d)$	x2	2.635	2.948	3.092	3.097	3.030	3.030(5)	2.953(4)	2.811(3)
$O(2^u)$-$O(4)^u$	x2	2.848	2.919	2.703	2.814	2.667	2.854(5)	2.807(4)	2.699(3)
O(4)-O(4)		2.871	2.981	3.033	3.009	3.069	3.025(7)	2.965(6)	2.846(5)
⟨O-O⟩ M(2)		2.724	2.920	2.820	2.885	2.804	2.909	2.855	2.740
$O(1^u)$-$O(1^d)$	x2	2.523	2.707	2.424	2.641	2.423	2.714(7)	2.678(6)	2.621(5)
$O(1^u)$-$O(1^u)$	x2	3.283	3.153	3.282	3.367	3.144	3.305(7)	3.290(6)	3.378(5)
$O(1^u)$-$O(3^d)$	x4	2.750	2.775	2.872	2.908	2.954	2.852(2)	2.849(4)	2.844(4)
$O(1^u)$-$O(3^u)$	x4	2.960	3.112	2.982	3.066	2.930	3.139(6)	3.112(5)	3.129(4)
⟨O-O⟩ M(3)		2.871	2.939	2.902	2.993	2.889	3.000	2.983	2.991
O(2)-$O(2)_d$		2.806	2.855	3.012	2.983	2.989	3.009(7)	3.018(6)	3.045(5)
$O(2^u)$-$O(4^d)$	x2	2.635	2.948	3.092	3.097	3.030	3.030(5)	2.953(4)	2.811(3)
$O(2^u)$-$O(4^u)$	x2	2.973	3.085	3.300	3.277	3.293	3.217(5)	3.235(4)	3.263(3)
$O(2^u)$-$O(5^u)$	x2	3.645	3.488	3.740	3.745	3.676	3.733(5)	3.714(4)	3.602(4)
$O(4^u)$-$O(5^d)$	x2	3.285	3.368	3.658	3.556	3.582	3.567(5)	3.484(4)	3.359(4)
$O(4^u)$-$O(6^u)$	x2	2.603	2.579	2.734	2.687	2.711	2.598(5)	2.588(4)	2.591(4)
$O(5^u)$-$O(6^d)$	x2	3.058	3.050	3.227	3.260	3.158	3.264(5)	3.163(4)	3.049(3)
$O(5^u)$-$O(6^u)$	x2	2.657	2.644	2.714	2.713	2.703	2.700(5)	2.670(4)	2.651(4)
O(6)-O(6)		3.058	3.548	3.499	3.542	3.500	3.602(7)	3.433(6)	3.369(5)
⟨O-O⟩ M(4)		2.974	3.045	3.215	3.223	3.187	3.177	3.129	3.067

		(70)	(71)	(72)	(73)	(74)
O(1)-O(5)		2.742	2.758	2.756	2.756(5)	2.791(8)
O(1)-O(6)		2.724	2.741	2.738	2.742(5)	2.773(7)
O(1)-O(7)		2.726	2.740	2.739	2.754(6)	2.741(8)
O(5)-O(6)		2.682	2.694	2.694	2.682(6)	2.693(9)
O(5)-O(7)		2.674	2.677	2.666	2.688(4)	2.702(6)
O(6)-O(7)		2.716	2.727	2.730	2.737(5)	2.734(8)
<O-O> T(1)		2.711	2.723	2.721	2.727	2.739
O(2)-O(4)		2.758	2.755	2.746	2.754(5)	2.763(7)
O(2)-O(5)		2.671	2.673	2.669	2.671(5)	2.688(7)
O(2)-O(6)		2.663	2.668	2.667	2.672(5)	2.685(9)
O(4)-O(5)		2.648	2.649	2.649	2.651(5)	2.662(8)
O(4)-O(6)		2.576	2.576	2.576	2.573(5)	2.570(7)
O(5)-O(6)		2.680	2.673	2.670	2.689(6)	2.701(9)
<O-O> T(2)		2.666	2.666	2.663	2.668	2.678
$O(1^u)$-$O(2^d)$	x2	2.757	2.766	2.783	2.772(5)	2.749(8)
$O(1^u)$-$O(2^u)$	x2	3.123	3.124	3.117	3.133(6)	3.104(8)
$O(1^u)$-$O(3^d)$	x2	2.769	2.760	2.752	2.769(5)	2.718(9)
$O(1^u)$-$O(3^u)$	x2	3.092	3.088	3.079	3.096(6)	3.072(9)
O(2)-O(2)		2.956	2.953	2.948	2.959(7)	2.930(7)
O(2)-O(3)	x2	3.126	3.130	3.124	3.147(3)	3.116(5)
O(3)-O(3)		2.680	2.682	2.684	2.687(11)	2.651(9)
<O-O> M(1)		2.948	2.948	2.945	2.957	2.925
O(1)-O(1)		2.666	2.660	2.671	2.651(7)	2.671(7)
$O(1^u)$-$O(2^d)$	x2	2.757	2.766	2.783	2.772(5)	2.749(8)
$O(1^u)$-$O(2^u)$	x2	2.982	2.994	3.006	2.996(6)	3.037(8)
O(1)-O(4)	x2	2.885	2.896	2.924	2.909(5)	2.920(7)
$O(2^u)$-$O4^d)$	x2	2.893	2.904	2.921	2.895(5)	2.935(8)
$O(2^u)$-$O(4^u)$	x2	2.837	2.838	2.862	2.855(5)	2.874(8)
O(4)-O(4)		2.935	2.949	2.969	2.941(8)	2.995(8)
<O-O> M(2)		2.859	2.867	2.886	2.871	2.891
$O(1^u)$-$O(1^d)$	x2	2.666	2.660	2.671	2.651(7)	2.671(7)
$O(1^u)$-$O(1^u)$	x2	3.227	3.209	3.176	3.227(8)	3.180(7)
$O(1^u)$-$O(3^d)$	x4	2.769	2.760	2.752	2.769(5)	2.718(9)
$O(1^u)$-$O(3^u)$	x4	3.114	3.107	3.093	3.112(6)	3.129(9)
<O-O> M(3)		2.943	2.934	2.923	2.940	2.924
O(2)-O(2)		2.956	2.953	2.948	3.147(3)	2.930(7)
$O(2^u)$-$O(4^d)$	x2	2.893	2.904	2.921	2.895(5)	2.935(8)
$O(2^u)$-$O(4^u)$	x2	3.131	3.125	3.112	3.117(5)	3.133(9)
$O(2^u)$-$O(5^u)$	x2	3.454	3.440	3.453	3.436(5)	3.447(7)
$O(4^u)$-$O(5^d)$	x2	3.329	3.336	3.339	3.315(5)	3.358(7)
$O(4^u)$-$O(6^u)$	x2	2.576	2.576	2.576	2.573(5)	2.570(7)
$O(5^u)$-$O(6^d)$	x2	3.031	3.028	3.030	3.022(5)	3.013(7)
$O(5^u)$-$O(6^u)$	x2	2.687	2.694	2.694	2.682(6)	2.693(9)
O(6)-O(6)		3.543	3.569	3.561	3.542(6)	3.554(9)
<O-O> M(4)		3.044	3.046	3.047	3.048	3.049

APPENDIX B6. INTERATOMIC ANGLES (°)

		(21)	(22)	(24)	(26)	(28)	(29)	(30)
O(1)-T(1)-O(5)		110.4(2)	108.9(2)	111.4(2)	110.0(3)	110.8(2)	113.5(2)	111.9(1)
O(1)-T(1)-O(6)		109.7(3)	109.6(2)	110.7(2)	110.4(3)	110.3(2)	113.0(2)	111.1(1)
O(1)-T(1)-O(7)		110.3(3)	110.1(3)	110.9(3)	109.6(4)	110.6(2)	110.3(2)	110.7(1)
O(5)-T(1)-O(6)		108.9(3)	110.9(2)	106.4(2)	109.7(3)	107.8(2)	108.1(2)	105.8(1)
O(5)-T(1)-O(7)		108.9(3)	108.5(3)	107.4(3)	109.0(4)	108.5(2)	105.6(3)	108.5(1)
O(6)-T(1)-O(7)		108.7(3)	108.9(3)	109.3(3)	108.2(4)	108.9(2)	105.7(3)	108.7(1)
<O-T(1)-O>		109.5	109.5	109.4	109.5	109.5	109.4	109.4
O(2)-T(2)-O(4)		116.3(2)	115.2(2)	116.3(2)	117.5(3)	116.0(2)	119.4(2)	117.3(1)
O(2)-T(2)-O(5)		108.1(2)	108.5(2)	109.3(2)	108.1(3)	108.4(2)	109.4(2)	109.4(1)
O(2)-T(2)-O(6)		108.5(2)	108.7(2)	108.6(2)	107.4(3)	109.0(2)	107.6(2)	108.2(1)
O(4)-T(2)-O(5)		109.6(2)	110.9(2)	109.6(2)	109.6(3)	110.4(2)	110.8(2)	109.4(1)
O(4)-T(2)-O(6)		103.9(3)	103.0(2)	104.0(3)	105.6(3)	102.9(2)	103.9(2)	103.5(1)
O(5)-T(2)-O(6)		110.3(2)	110.4(2)	108.9(2)	108.2(3)	110.0(2)	104.5(2)	108.6(1)
<O-T(2)-O>		109.5	109.5	109.4	109.4	109.4	109.3	109.4
T(1)-O(5)-T(2)		139.7(3)	142.4(3)	134.4(3)	134.7(4)	140.0(2)	135.7(2)	136.5(1)
T(1)-O(6)-T(2)		141.0(3)	142.1(3)	137.6(3)	143.5(4)	140.4(2)	136.1(2)	138.4(1)
T(1)-O(7)-T(1)		142.4(5)	144.8(4)	137.3(4)	147.2(6)	141.0(3)	139.0(3)	139.3(2)
O(5)-O(6)-O(5)		170.2(2)	172.7(3)	163.5(2)	170.8(3)	172.9(2)	169.8(2)	167.6(1)
$O(1^u)$-M(1)-$O(2^d)$	x2	84.5	85.0	82.8(2)	78.7(2)	85.1(1)	86.1(2)	85.6(1)
$O(1^u)$-M(1)-$O(2^u)$	x2	95.4	94.8	95.5(2)	100.0(2)	95.3(1)	96.1(2)	95.7(1)
$O(1^u)$-M(1)-$O(3^d)$	x2	84.3	84.7	84.5(2)	84.3(3)	83.9(2)	82.1(2)	83.7(1)
$O(1^u)$-M(1)-$O(3^u)$	x2	95.8	95.6	97.8(2)	97.2(3)	95.7(2)	95.5(2)	95.0(1)
O(2)-M(1)-O(2)		87.3	86.3	85.4(2)	93.2(2)	86.8(1)	89.4(2)	87.2(1)
O(2)-M(1)-O(3)	x2	95.5	96.7	96.6(2)	93.6(2)	95.4(1)	95.8(2)	95.9(1)
O(3)-M(1)-O(3)		81.7	80.9	81.2(2)	79.8(2)	82.3(1)	79.2(2)	81.0(1)
<O-M(1)-O>		90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-$O(1)_d$		80.3	78.2	79.4(2)	80.0(2)	80.3(1)	78.3(2)	80.0(1)
$O(1^u)$-M(2)-$O(2^d)$	x2	83.9	83.8	83.0(2)	83.0(2)	84.0(1)	82.1(1)	83.7(1)
$O(1^u)$-M(2)-$O(2^u)$	x2	92.2	91.7	93.2(2)	89.6(2)	92.3(1)	90.2(2)	92.1(1)
O(1)-M(2)-O(4)	x2	93.0	95.4	91.8(2)	89.9(2)	92.2(1)	92.2(2)	92.8(1)
$O(2^u)$-M(2)-$O(4^d)$	x2	86.3	85.4	92.9(2)	95.8(3)	88.1(1)	97.4(2)	93.4(1)
$O(2^u)$-M(2)-$O(4^u)$	x2	97.3	98.7	90.3(2)	90.4(3)	95.2(1)	89.0(2)	90.3(1)
O(4)-M(2)-O(4)		93.6	91.0	97.5(2)	100.9(3)	95.3(1)	98.4(4)	95.0(1)
<O-M(2)-O>		89.9	90.0	90.0	89.9	89.9	89.9	90.0
$O(1^u)$-M(3)-$O(1^d)$	x2	81.9	80.0	80.2(2)	77.1(2)	83.0(1)	83.6(2)	82.9(1)
$O(1^u)$-M(3)-$O(1^u)$	x2	98.1	100.0	99.8(2)	102.9(2)	97.0(1)	96.4(2)	97.1(1)
$O(1^u)$-M(3)-$O(3^d)$	x2	83.9	84.2	82.6(2)	84.2(2)	84.2(1)	83.3(1)	84.1(1)
$O(1^u)$-M(3)-$O(3^u)$	x4	96.1	95.8	97.4(2)	95.8(2)	95.8(1)	96.7(1)	95.9(1)
<O-M(3)-O>		90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-O(2)		85.5	87.5	74.9	77.7	82.9	72.8(2)	73.5
$O(2^u)$-M(4)-$O(4^d)$	x2	84.4	87.4	76.9	72.7	83.1	78.8(1)	78.4
$O(2^u)$-M(4)-$O(4^u)$	x2	91.3	93.3	83.1	86.6	88.1	83.2	83.2
$O(2^u)$-M(4)-$O(5^u)$	x2	87.6	87.8	87.1	86.8	87.9	90.0(1)	88.9
$O(4^u)$-M(4)-$O(5^d)$	x2	75.2	72.4	84.6	80.9	77.4	85.5(1)	84.1
$O(4^u)$-M(4)-$O(6^u)$	x2	64.0	62.2	62.9	65.5	64.5	62.0(1)	63.4
$O(5^u)$-M(4)-$O(6^d)$	x2	64.2	63.6	70.4	69.9	66.1	71.2(1)	70.9
$O(5^u)$-M(4)-$O(6^u)$	x2	53.1	51.6	61.2	60.2	54.1	57.9(1)	58.6
O(6)-M(4)-O(6)		69.7	67.9	86.4	86.5	73.3	86.8(2)	84.9
<O-M(4)-O>		74.7	74.5	75.9	75.6	74.9	76.0	75.8
O(7)-O(7)-O(7)		58.7	59.2	64.5(2)	66.8(2)	60.3(1)	69.9(1)	65.9(1)
△		0.348	0.342	0.283	0.258	0.330	0.223	0.268

		(34)	(35)	(36)	(37)	(38)	(39)	(40)
O(1)-T(1)-O(5)		114.3(3)	113.6(4)	111.6(2)	110.8(2)	112.4(1)	111.9(2)	111.9(4)
O(1)-T(1)-O(6)		111.3(3)	111.6(4)	110.4(2)	110.7(2)	110.4(1)	111.3(2)	109.2(5)
O(1)-T(1)-O(7)		111.6(3)	110.8(4)	110.8(2)	110.8(2)	111.5(1)	110.9(2)	111.1(5)
O(5)-T(1)-O(6)		108.7(3)	107.7(4)	104.6(2)	106.3(2)	105.9(1)	106.2(2)	106.5(4)
O(5)-T(1)-O(7)		104.0(3)	105.0(4)	109.5(2)	109.0(2)	106.9(2)	107.3(2)	107.6(6)
O(6)-T(1)-O(7)		106.3(4)	107.6(4)	109.7(2)	109.1(2)	109.3(2)	109.0(3)	110.4(6)
⟨O-T(1)-O⟩		109.4	109.4	109.4	109.5	109.4	109.4	109.5
O(2)-T(2)-O(4)		117.3(3)	116.9(4)	116.7(2)	116.5(2)	117.0(1)	116.9(2)	116.6(4)
O(2)-T(2)-O(5)		109.7(3)	109.7(4)	109.2(2)	109.5(2)	109.1(1)	109.9(2)	108.4(5)
O(2)-T(2)-O(6)		107.9(3)	108.3(4)	107.8(2)	109.0(2)	109.1(1)	108.9(2)	108.7(4)
O(4)-T(2)-O(5)		111.4(3)	110.0(4)	109.5(2)	109.8(2)	109.7(1)	109.0(2)	110.3(5)
O(4)-T(2)-O(6)		105.5(3)	105.2(3)	103.1(2)	102.7(2)	103.4(1)	103.8(2)	103.1(5)
O(5)-T(2)-O(6)		104.1(3)	106.1(3)	110.3(2)	109.0(2)	108.1(1)	108.0(2)	109.5(4)
⟨O-T(2)-O⟩		109.3	109.4	109.4	109.4	109.4	109.4	109.4
T(1)-O(5)-T(2)		134.9(4)	135.2(5)	136.7(2)	137.4(2)	133.9(2)	133.6(3)	136.0(5)
T(1)-O(6)-T(2)		136.8(4)	137.6(4)	139.7(2)	139.1(2)	137.5(2)	136.2(2)	138.0(5)
T(1)-O(7)-T(1)		135.7(5)	137.0(6)	138.3(3)	141.1(4)	136.5(2)	136.9(3)	136.4(9)
O(5)-O(6)-O(5)		169.1(3)	169.2(3)	167.9(2)	168.4(2)	163.2(1)	161.8(2)	164.5(4)
$O(1^u)$-M(1)-$O(2^d)$	x2	86.5(2)	87.0(3)	86.5(1)	85.9(1)	83.7(1)	83.0(2)	80.7(3)
$O(1^u)$-M(1)-$O(2^u)$	x2	96.8(2)	96.5(3)	96.3(1)	95.1(1)	97.2(1)	95.8(2)	93.6(3)
$O(1^u)$-M(1)-$O(3^d)$	x2	82.4(2)	81.8(3)	81.8(1)	84.5(2)	83.1(1)	84.4(2)	84.4(5)
$O(1^u)$-M(1)-$O(3^u)$	x2	94.0(3)	94.4(3)	95.2(1)	94.5(2)	95.9(1)	96.8(2)	101.3(5)
O(2)-M(1)-O(2)		90.9(4)	90.8(4)	88.5(2)	87.1(2)	88.3(1)	86.2(2)	83.0
O(2)-M(1)-O(3)	x2	95.6(2)	95.6(3)	96.6(1)	96.3(1)	96.4(1)	96.7(2)	96.3
O(3)-M(1)-O(3)		77.9(3)	78.0(3)	78.4(2)	80.4(2)	78.9(1)	80.4(2)	84.6
⟨O-M(1)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-O(1)		79.7(3)	78.4(3)	80.0(2)	79.1(2)	79.8(1)	79.5(2)	80.6(3)
$O(1^u)$-M(2)-$O(2^d)$	x2	82.6(2)	82.4(2)	83.7(1)	84.4(1)	84.4(1)	83.7(2)	81.2(3)
$O(1^u)$-M(2)-$O(2^u)$	x2	90.2(2)	89.2(3)	91.9(1)	91.3(1)	93.6(1)	93.5(2)	93.5(3)
O(1)-M(2)-O(4)	x2	91.0(2)	91.6(2)	92.6(1)	93.2(1)	92.2(1)	92.2(1)	90.6(8)
$O(2^u)$-M(2)-$O(4^d)$	x2	95.6(2)	96.1(3)	93.3(1)	93.1(2)	93.0(1)	93.0(2)	92.9(4)
$O(2^u)$-M(2)-$O(4^u)$	x2	90.5(2)	90.9(2)	90.5(1)	90.7(2)	88.7(1)	89.6(2)	91.5(4)
O(4)-M(2)-O(4)		99.1(3)	98.9(4)	95.5(2)	94.8(1)	96.6(1)	97.0(2)	99.2(4)
⟨O-M(2)-O⟩		89.9	89.8	90.0	90.0	90.0	90.0	89.9
$O(1^u)$-M(3)-$O(1^d)$	x2	85.1(3)	85.0(4)	84.2(2)	81.5(2)	79.5(1)	79.8(2)	82.5(3)
$O(1^u)$-M(3)-$O(1^u)$	x2	94.9(3)	95.0(4)	95.8(2)	98.5(2)	100.5(1)	100.2(2)	97.5(3)
$O(1^u)$-M(3)-$O(3^d)$	x4	83.1(2)	83.5(2)	83.0(1)	84.7(1)	83.0(1)	82.8(2)	81.0(3)
$O(1^u)$-M(3)-$O(3^u)$	x4	96.9(2)	96.5(2)	97.0(1)	95.3(1)	97.0(1)	97.2(2)	99.0(3)
⟨O-M(3)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-O(2)		74.0(3)	74.4(3)	73.4(2)	75.2(2)	75.0(1)	74.6(2)	73.5
$O(2^u)$-M(4)-$O(4^d)$	x2	79.0(2)	80.0(2)	78.6(1)	79.6(1)	75.8(1)	76.5(1)	76.1
$O(2^u)$-M(4)-$O(4^u)$	x2	83.5(2)	84.0(2)	83.0(1)	83.7(1)	82.5(1)	82.5(1)	82.9
$O(2^u)$-M(4)-$O(5^u)$	x2	90.1(2)	90.0(2)	88.9(1)	88.4	86.3(1)	86.6(1)	87.4
$O(4^u)$-M(4)-$O(5^d)$	x2	84.0(2)	83.2(2)	84.3(1)	83.3	84.8(1)	84.6(1)	84.4
$O(4^u)$-M(4)-$O(6^u)$	x2	63.4(2)	63.1(2)	63.5(1)	63.0(1)	62.7(1)	62.9(1)	63.2
$O(5^u)$-M(4)-$O(6^d)$	x2	68.6(2)	68.8(2)	71.2(1)	70.9	71.0(1)	70.5(1)	69.9
$O(5^u)$-M(4)-$O(6^u)$	x2	58.3(2)	57.8(2)	58.4(1)	58.0	62.6(1)	62.4(1)	62.3
O(6)-M(4)-O(6)		82.9(2)	82.4(3)	84.7(1)	84.3(2)	88.8(1)	87.2(1)	86.4
⟨O-M(4)-O⟩		75.7	75.7	75.9	75.8	76.0	75.9	75.8
O(7)-O(7)-O(7)		63.8	64.2	64.9	66.3	69.5	67.3	63.0(4)
Δ		0.291	0.287	0.279	0.263	0.228	0.252	0.300

		(41)	(42)	(43)	(44)	(45)	(46)	(48)	(49)	(50)	(51)
O(1)-T(1)-O(5)		110.8(2)	110.5	111.5	108.8	110.9	109.5	109.7	108.6	110.8	110.1
O(1)-T(1)-O(6)		110.5(2)	112.3	110.7	112.5	110.3	111.2	109.0	109.7	112.3	112.5
O(1)-T(1)-O(7)		110.4(3)	110.2	110.0	111.2	110.8	111.2	110.2	111.6	111.4	112.0
O(5)-T(1)-O(6)		107.7(2)	106.3	106.8	106.0	107.2	105.3	105.9	107.8	106.2	108.1
O(5)-T(1)-O(7)		108.5(3)	107.5	108.6	109.3	109.4	110.0	110.5	110.7	107.6	104.8
O(6)-T(1)-O(7)		108.8(3)	109.9	109.2	109.0	108.1	109.4	111.4	108.4	108.3	109.0
⟨O-T(1)-O⟩		109.5	109.5	109.5	109.5	109.5	109.4	109.5	109.5	109.4	109.4
O(2)-T(2)-O(4)		117.0(2)	116.0	115.9	113.1	116.4	115.1	116.0	114.4	115.5	111.9
O(2)-T(2)-O(5)		107.8(2)	108.8	109.2	109.1	109.3	109.0	108.5	108.6	106.6	109.0
O(2)-T(2)-O(6)		108.9(2)	108.5	108.4	108.9	108.2	108.5	109.3	107.6	109.4	108.8
O(4)-T(2)-O(5)		110.4(2)	108.7	109.4	109.8	109.2	108.8	108.7	110.0	107.2	111.8
O(4)-T(2)-O(6)		102.8(2)	105.4	104.9	106.1	105.2	105.3	103.4	106.5	108.1	107.7
O(5)-T(2)-O(6)		109.5(2)	109.2	108.8	109.8	108.3	110.1	110.9	109.7	109.9	107.5
⟨O-T(2)-O⟩		109.4	109.4	109.4	109.5	109.4	109.5	109.5	109.5	109.5	109.5
T(1)-O(5)-T(2)		140.2(3)	134.5	136.8	137.2	135.8	134.6	133.0	136.1	133.5	134.1
T(1)-O(6)-T(2)		140.0(3)	138.8	139.2	139.5	139.2	140.2	141.8	141.5	139.6	138.4
T(1)-O(7)-T(1)		141.0(4)	140.1	140.6	140.3	141.3	141.8	144.8	142.9	140.1	138.2
O(5)-O(6)-O(5)		173.0(3)	164.8	166.8	165.7	165.4	164.9	163.7	164.7	163.4	164.2
$O(1^u)$-M(1)-$O(2^d)$	x2	85.1	82.2	85.8	84.6	84.0	81.4	79.1	80.2	79.0	82.6
$O(1^u)$-M(1)-$O(2^u)$	x2	95.5	97.0	95.3	96.5	96.1	96.0	98.1	97.1	99.8	96.2
$O(1^u)$-M(1)-$O(3^d)$	x2	84.1	83.8	84.2	82.9	84.1	83.2	85.1	84.1	83.6	83.3
$O(1^u)$-M(1)-$O(3^u)$	x2	95.3	97.0	94.7	95.8	96.0	99.5	97.9	98.7	97.7	98.1
O(2)-M(1)-O(2)		86.9	88.5	86.6	87.8	87.2	86.2	89.2	87.2	89.5	89.2
O(2)-M(1)-O(3)	x2	95.4	95.1	96.2	95.7	96.0	95.8	95.7	96.2	96.1	95.4
O(3)-M(1)-O(3)		82.4	81.4	81.0	80.7	80.8	82.1	79.7	80.5	78.3	79.9
⟨O-M(1)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-O(1)		80.5	79.2	80.2	76.1	79.5	79.1	81.6	79.5	79.3	78.2
$O(1^u)$-M(2)-$O(2^d)$	x2	83.7	85.1	84.7	85.9	84.0	85.6	85.3	85.3	85.7	85.6
$O(1^u)$-M(2)-$O(2^u)$	x2	92.7	91.8	92.1	91.8	92.4	91.9	93.5	93.2	93.1	90.2
O(1)-M(2)-$O(4)_d$	x2	92.5	91.9	92.9	93.8	92.6	92.5	91.1	91.5	93.4	90.4
$O(2^u)$-M(2)-$O(4^d)$	x2	88.2	94.1	93.4	94.6	93.5	93.7	92.4	92.9	94.6	95.5
$O(2^u)$-M(2)-$O(4^u)$	x2	95.1	88.5	89.5	87.3	89.6	88.5	88.6	88.4	86.6	88.0
O(4)-M(2)-O(4)		94.6	97.7	94.6	97.0	96.1	96.4	96.9	98.3	94.9	101.6
⟨O-M(2)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.1	89.9
$O(1^u)$-M(3)-$O(1^d)$	x2	83.1	78.4	82.8	77.3	79.9	77.1	75.2	74.2	75.2	76.6
$O(1^u)$-M(3)-$O(1^u)$	x2	96.9	101.6	97.2	102.7	100.1	102.9	104.8	105.8	104.8	103.4
$O(1^u)$-M(3)-$O(3^d)$	x4	84.0	84.5	84.5	85.2	84.1	84.8	83.4	84.3	83.3	84.9
$O(1^u)$-M(3)-$O(3^u)$	x4	96.0	95.5	95.5	94.8	95.9	95.2	96.6	95.7	96.7	95.1
⟨O-M(3)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-O(2)		82.1	75.9	74.2	76.2	74.5	75.5	78.3	76.8	78.5	75.8
$O(2^u)$-M(4)-$O(4^d)$	x2	82.8	75.7	78.8	78.1	77.0	76.0	72.8	74.4	72.8	76.8
$O(2^u)$-M(4)-$O(4^u)$	x2	88.7	83.0	83.2	81.6	83.1	83.3	84.7	83.1	86.4	80.8
$O(2^u)$-M(4)-$O(5^u)$	x2	88.2	86.4	88.4	86.1	87.4	86.4	84.1	85.3	84.6	85.8
$O(4^u)$-M(4)-$O(5^d)$	x2	77.7	84.0	84.0	84.4	84.0	83.8	83.1	84.0	82.5	85.4
$O(4^u)$-M(4)-$O(6^u)$	x2	64.7	64.0	62.9	63.3	62.9	63.5	63.4	63.9	63.8	62.1
$O(5^u)$-M(4)-$O(6^d)$	x2	66.4	71.2	71.1	72.2	71.2	71.5	71.6	71.7	71.1	71.3
$O(5^u)$-M(4)-$O(6^u)$	x2	54.0	61.1	59.0	60.7	60.7	61.2	63.4	62.1	61.9	63.5
O(6)-M(4)-O(6)		73.6	87.1	85.4	87.6	87.4	87.6	90.4	89.1	88.1	90.6
⟨O-M(4)-O⟩		75.0	75.9	75.9	76.0	75.9	75.9	75.9	75.9	75.8	76.1
O(7)-O(7)-O(7)		60.8	65.2	66.2	67.0	67.3	66.6	66.6	66.6	65.4	65.4
△		0.324	0.276	0.264	0.256	0.252	0.260	0.260	0.260	0.273	0.273

		(52)	(53a)	(53b)	(54)	(55)	(56a)	(56b)	(57)
O(1)-T(1)-O(5)		112.3	111.7(1)	111.7(2)	109.8(2)	112.4(2)	112.3(1)	112.4(1)	111.0(2)
O(1)-T(1)-O(6)		110.0	111.0(1)	110.8(2)	109.9(3)	110.8(3)	111.2(1)	111.4(2)	110.3(2)
O(1)-T(1)-O(7)		111.9	110.7(1)	111.0(2)	111.2(3)	110.7(2)	111.1(1)	110.9(1)	110.8(2)
O(5)-T(1)-O(6)		106.3	106.1(1)	106.1(2)	105.2(2)	105.8(2)	106.1(1)	106.3(1)	108.1(2)
O(5)-T(1)-O(7)		106.7	108.5(2)	108.4(2)	109.6(3)	107.6(3)	107.4(1)	107.5(1)	108.0(2)
O(6)-T(1)-O(7)		109.4	108.8(2)	108.7(2)	111.0(3)	109.4(3)	108.6(1)	108.2(2)	108.7(2)
<O-T(1)-O>		109.4	109.5	109.5	109.4	109.5	109.5	109.5	109.5
O(2)-T(2)-O(4)		117.5	117.5(1)	117.5(2)	115.9(2)	117.2(2)	117.8(1)	117.6(1)	116.3(2)
O(2)-T(2)-O(5)		108.1	109.4(1)	109.4(2)	109.6(2)	109.3(3)	109.5(1)	109.5(1)	108.5(2)
O(2)-T(2)-O(6)		109.2	108.3(1)	108.2(2)	108.6(2)	108.5(2)	108.2(1)	108.1(1)	109.0(2)
O(4)-T(2)-O(5)		110.7	109.7(1)	109.8(2)	109.1(2)	109.5(2)	109.6(1)	109.9(2)	110.2(2)
O(4)-T(2)-O(6)		102.8	103.0(1)	102.8(2)	103.0(2)	103.8(2)	103.4(1)	103.5(1)	103.0(2)
O(5)-T(2)-O(6)		108.2	108.6(1)	108.8(2)	110.5(2)	108.2(2)	107.9(1)	107.7(1)	109.6(2)
<O-T(2)-O>		109.4	109.4	109.4	109.5	109.4	109.4	109.4	109.4
T(1)-O(5)-T(2)		134.0	137.3(1)	137.6(2)	133.7(2)	134.3(3)	136.2(1)	136.1(1)	139.7(2)
T(1)-O(6)-T(2)		135.9	138.8(1)	139.1(2)	140.7(2)	136.4(2)	137.8(1)	137.7(1)	140.2(2)
T(1)-O(7)-T(1)		133.1	140.2(2)	140.2(2)	141.9(2)	136.4(3)	137.8(2)	138.2(2)	140.3(3)
O(5)-O(6)-O(5)		160.7	169.5(1)	170.4(2)	164.4(2)	162.9(2)	167.6(1)	167.6(1)	172.0(2)
$O(1^u)$-M(1)-$O(2^d)$	x2	81.7	85.8(1)	86.0(1)	80.3(1)	82.0(1)	85.9(1)	85.9(1)	85.2(1)
$O(1^u)$-M(1)-$O(2^u)$	x2	95.2	95.3(1)	95.1(1)	97.2(1)	94.0(1)	95.8(1)	96.0(1)	95.4(1)
$O(1^u)$-M(1)-$O(3^d)$	x2	82.0	84.0(1)	83.9(2)	85.3(2)	84.9(2)	83.1(1)	83.2(1)	84.0(1)
$O(1^u)$-M(1)-$O(3^u)$	x2	101.0	94.9(1)	95.0(2)	97.4(2)	99.1(2)	95.1(1)	94.8(1)	95.4(1)
O(2)-M(1)-O(2)		85.2	87.2(1)	87.4(2)	87.7(2)	83.6(2)	88.2(1)	88.2(1)	87.0(2)
O(2)-M(1)-O(3)	x2	94.0	95.8(1)	95.5(1)	96.2(2)	96.1(2)	95.8(1)	95.7(1)	95.4(2)
O(3)-M(1)-O(3)		86.9	81.3(1)	81.6(2)	79.9(3)	84.2(3)	80.3(1)	80.5(1)	82.2(2)
<O-M(1)-O>		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-$O(1)_d$		79.6	79.8(1)	79.7(2)	81.0(3)	79.4(3)	79.9(1)	79.8(1)	80.1(2)
$O(1^u)$-M(2)-$O(2^d)$	x2	82.3	83.7(1)	83.7(1)	85.1(1)	82.5(1)	83.4(1)	83.4(1)	83.9(1)
$O(1^u)$-M(2)-$O(2^u)$	x2	92.4	91.8(1)	91.5(1)	93.7(1)	93.4(1)	91.9(1)	91.8(1)	92.2(1)
O(1)-M(2)-$O(4)_d$	x2	90.3	93.3(1)	93.6(1)	91.4(2)	91.7(2)	92.5(1)	92.5(1)	92.5(2)
$O(2^d)$-M(2)-$O(4^d)$	x2	91.8	93.8(1)	94.2(1)	92.0(1)	93.3(2)	94.0(1)	94.1(1)	88.0(1)
$O(2^u)$-M(2)-$O(4^u)$	x2	92.6	90.1(1)	90.1(1)	89.1(1)	90.2(1)	90.1(1)	90.1(1)	95.4(1)
O(4)-M(2)-O(4)		100.4	94.3(1)	93.9(2)	96.8(3)	98.2(3)	95.5(2)	95.9(2)	94.9(2)
<O-M(2)-O>		89.9	90.0	90.0	90.0	90.0	90.0	90.0	89.9
$O(1^u)$-M(3)-$O(1^d)$	x2	82.2	82.7(1)	82.8(2)	75.3(2)	81.1(3)	83.2(2)	83.3(2)	83.0(2)
$O(1^u)$-M(3)-$O(1^u)$	x2	97.8	97.3(1)	97.2(2)	104.7(2)	98.9(3)	96.8(2)	96.7(2)	97.0(2)
$O(1^u)$-M(3)-$O(3^d)$	x4	83.6	84.4(1)	84.5(1)	83.9(1)	82.3(1)	83.8(1)	83.9(1)	84.1(1)
$O(1^u)$-M(3)-$O(3^u)$	x4	96.4	95.6(1)	95.5(1)	96.2(1)	97.7(1)	96.2(1)	96.1(1)	95.9(1)
<O-M(3)-O>		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-O(2)		73.8	73.6(1)	73.7(2)	77.2(2)	73.4(2)	73.3(2)	73.3(2)	83.8(2)
$O(2^u)$-M(4)-$O(4^d)$	x2	76.4	78.9(1)	79.3(1)	73.8(1)	76.6(1)	78.6(1)	78.5(1)	83.6(1)
$O(2^u)$-M(4)-$O(4^u)$	x2	82.0	83.5(1)	83.6(1)	83.9(1)	81.9(1)	82.9(1)	83.0(1)	89.5(1)
$O(2^u)$-M(4)-$O(5^u)$	x2	87.1	89.2	89.2	84.8(2)	87.4(2)	89.0(2)	89.0(2)	87.8(2)
$O(4^u)$-M(4)-$O(5^d)$	x2	85.7	83.8	83.8	83.5(1)	85.1(1)	84.5(1)	84.5(1)	77.0(1)
$O(4^u)$-M(4)-$O(6^u)$	x2	64.5	63.1(1)	63.0(1)	63.7(1)	63.2(1)	63.0(1)	63.1(1)	64.1(1)
$O(5^u)$-M(4)-$O(6^d)$	x2	69.9	71.3	71.6	71.8(2)	70.3(2)	71.0(1)	70.9(1)	65.4(1)
$O(5^u)$-M(4)-$O(6^u)$	x2	61.4	57.9	57.5	62.5(1)	62.2(1)	58.8(1)	58.8(1)	53.9(1)
O(6)-M(4)-O(6)		84.0	85.1(1)	85.4(2)	89.5(2)	86.8(2)	85.5(1)	85.2(1)	72.4(1)
<O-M(4)-O>		75.7	75.9	75.9	75.9	75.9	75.9	75.9	74.9
O(7)-O(7)-O(7)		59.3	66.7	66.9	65.8(1)	64.5(1)	65.8(1)	65.9(1)	59.9(1)
△		0.341	0.259	0.257	0.269	0.283	0.269	0.268	0.334

		(58)	(59)	(60)	(61)	(62)	(63)	(64)	(65)	(66)
O(1)-T(1)-O(5)		110.7(2)	110.9(1)	109.4	109.7	107.7	111.3	106.0	106.5	107.4
O(1)-T(1)-O(6)		110.8(3)	110.6(1)	111.3	111.4	114.1	110.0	113.8	113.9	119.1
O(1)-T(1)-O(7)		111.7(2)	111.6(1)	111.6	110.3	109.3	110.3	110.6	112.1	109.9
O(5)-T(1)-O(6)		106.6(2)	107.9(1)	105.7	106.1	110.3	106.5	109.6	110.9	110.5
O(5)-T(1)-O(7)		107.0(2)	106.8(1)	109.3	106.9	103.1	108.5	109.1	106.9	105.3
O(6)-T(1)-O(7)		109.9(2)	108.9(2)	109.4	112.3	111.6	110.2	107.7	106.4	103.9
⟨O-T(1)-O⟩		109.5	109.5	109.5	109.5	109.4	109.5	109.5	109.5	109.4
O(2)-T(2)-O(4)		116.5(1)	115.7(1)	117.3	114.7	113.6	116.6	110.2	115.1	111.5
O(2)-T(2)-O(5)		109.2(2)	109.5(1)	108.2	109.8	110.3	110.0	104.4	109.6	108.4
O(2)-T(2)-O(6)		109.0(2)	109.0(1)	109.2	107.7	104.2	106.7	104.8	106.1	109.2
O(4)-T(2)-O(5)		109.3(2)	110.0(1)	108.9	109.0	112.7	110.3	110.3	108.2	107.4
O(4)-T(2)-O(6)		103.5(2)	104.2(1)	104.7	105.9	106.6	103.9	116.4	110.8	113.7
O(5)-T(2)-O(6)		108.9(1)	108.0(1)	108.3	109.6	109.0	109.0	109.9	106.8	106.4
⟨O-T(2)-O⟩		109.4	109.4	109.4	109.5	109.4	109.4	109.3	109.4	109.4
T(1)-O(5)-T(2)		132.6(2)	135.3(1)	136.4	133.7	135.3	135.2	141.1	136.1	133.2
T(1)-O(6)-T(2)		138.7(2)	138.7(2)	137.8	138.6	145.4	137.7	143.6	141.2	139.9
T(1)-O(7)-T(1)		139.5(3)	139.9(2)	141.3	137.2	145.4	137.8	145.8	144.3	140.7
O(5)-O(6)-O(5)		162.6(2)	166.2(1)	166.7	160.6	172.4	161.4	171.9	169.0	169.1
$O(1^u)$-M(1)-$O(2^d)$	x2	79.6(1)	82.5(1)	82.0	83.3	79.2	85.0	81.0	83.2	79.5
$O(1^u)$-M(1)-$O(2^u)$	x2	98.4(1)	96.3(1)	96.3	96.2	98.1	95.5	99.5	96.1	99.2
$O(1^u)$-M(1)-$O(3^d)$	x2	84.8(1)	84.9(1)	83.9	83.9	81.6	84.4	81.9	84.0	85.6
$O(1^u)$-M(1)-$O(3^u)$	x2	97.3(1)	96.4(1)	97.9	96.7	101.2	95.1	97.6	96.8	95.8
O(2)-M(1)-O(2)		88.7(2)	88.5(1)	88.4	86.6	86.5	86.3	93.7	92.3	89.0
O(2)-M(1)-O(3)	x2	96.2(2)	95.9(1)	95.6	96.3	96.3	96.6	91.0	95.7	93.0
O(3)-M(1)-O(3)		79.1(3)	79.7(1)	80.4	80.9	81.0	80.6	84.4	76.4	84.8
⟨O-M(1)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-O(1)		80.8(2)	79.7(1)	80.7	79.6	80.7	80.4	72.1	77.6	72.6
$O(1^u)$-M(2)-$O(2^d)$	x2	84.4(1)	83.7(1)	83.9	85.6	85.4	83.6	82.6	85.2	87.8
$O(1^u)$-M(2)-$O(2^u)$	x2	93.7(1)	92.1(1)	92.6	92.6	91.9	93.6	86.7	85.0	84.4
O(1)-M(2)-O(4)	x2	90.7(2)	91.0(1)	91.4	91.7	88.9	92.2	91.0	90.4	91.3
$O(2^u)$-M(2)-$O(4^d)$	x2	92.1(1)	94.2(1)	94.4	92.3	86.6	91.8	102.2	99.9	100.6
$O(2^u)$-M(2)-$O(4^u)$	x2	89.5(1)	89.3(1)	88.7	89.2	95.7	90.6	85.7	88.1	85.3
O(4)-M(2)-O(4)		98.5(2)	99.1(1)	97.6	97.5	101.5	95.9	107.6	102.0	105.3
⟨O-M(2)-O⟩		90.0	90.0	90.0	90.0	89.9	90.0	89.7	89.7	89.7
$O(1^u)$-M(3)-$O(1^d)$	x2	75.8(2)	78.2(1)	78.1	78.4	75.1	81.3	72.9	76.2	75.3
$O(1^u)$-M(3)-$O(1^u)$	x2	104.2(2)	101.8(1)	101.9	101.6	104.9	98.7	107.1	103.8	104.7
$O(1^u)$-M(3)-$O(3^d)$	x4	83.1(1)	83.4(1)	83.4	85.0	85.8	83.5	87.9	87.0	90.5
$O(1^u)$-M(3)-$O(3^u)$	x4	96.9(1)	96.6(1)	96.6	95.0	94.2	96.5	92.1	93.0	89.5
⟨O-M(3)-O⟩		90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-O(2)		77.1(2)	76.1(1)	74.8	75.3	68.6	73.8	72.0	74.1	71.9
$O(2^u)$-M(4)-$O(4^d)$	x2	72.5(1)	76.1(1)	74.5	76.5	67.3	78.0	73.9	77.5	73.0
$O(2^u)$-M(4)-$O(4^u)$	x2	84.0(1)	82.9(1)	82.7	82.3	77.5	82.4	79.9	82.9	80.5
$O(2^u)$-M(4)-$O(5^u)$	x2	84.4(2)	86.1(1)	86.6	86.2	86.9	87.7	87.2	87.8	87.1
$O(4^u)$-M(4)-$O(5^d)$	x2	84.1(1)	84.0(1)	84.4	84.6	80.4	85.3	84.5	82.3	84.2
$O(4^u)$-M(4)-$O(6^u)$	x2	63.7(1)	63.0(1)	64.5	63.9	72.8	62.9	65.8	64.4	65.7
$O(5^u)$-M(4)-$O(6^d)$	x2	71.7(1)	71.3(1)	71.4	71.2	75.4	70.9	74.5	72.8	74.0
$O(5^u)$-M(4)-$O(6^u)$	x2	63.4(1)	61.9(1)	61.5	61.4	63.6	60.3	61.0	59.0	61.8
O(6)-M(4)-O(6)		90.2(1)	88.6(1)	88.0	86.3	91.7	85.6	91.2	87.2	91.4
⟨O-M(4)-O⟩		75.9	75.9	75.9	75.9	75.5	75.9	76.0	75.9	76.0
O(7)-O(7)-O(7)		64.9(1)	69.0(1)	66.9	62.8	60.2	64.0	68.1	67.6	67.4
△		0.279	0.233	0.257	0.302	0.331	0.289	0.243	0.249	0.251

	(67)	(68)	(69)	(70)	(71)	(72)	(73)	(74)
O(1)-T(1)-O(5)	111.5(2)	110.3(2)	109.5(1)	111.3	111.6	111.8	111.2(2)	112.1(3)
O(1)-T(1)-O(6)	112.0(2)	111.2(2)	110.3(1)	110.4	110.6	110.7	110.4(2)	110.9(3)
O(1)-T(1)-O(7)	111.3(2)	111.4(2)	110.0(2)	111.3	111.5	111.4	111.7(2)	110.6(3)
O(5)-T(1)-O(6)	111.5(2)	110.1(2)	109.8(1)	106.9	106.8	107.1	106.3(2)	105.7(3)
O(5)-T(1)-O(7)	105.1(2)	106.6(2)	109.0(2)	107.1	106.6	106.1	107.1(2)	107.8(4)
O(6)-T(1)-O(7)	105.0(2)	107.0(2)	108.1(2)	109.8	109.6	109.7	110.1(2)	109.5(4)
<O-T(1)-O>	109.4	109.4	109.5	109.5	109.5	109.5	109.5	109.4
O(2)-T(2)-O(4)	117.4(2)	115.9(2)	116.8(1)	117.0	117.0	116.9	116.6(2)	116.5(3)
O(2)-T(2)-O(5)	109.0(2)	108.7(2)	108.5(1)	109.2	109.4	109.3	109.2(2)	109.2(3)
O(2)-T(2)-O(6)	108.7(2)	108.9(2)	107.6(1)	108.2	108.4	108.4	108.5(2)	108.6(3)
O(4)-T(2)-O(5)	111.0(2)	110.2(2)	109.6(1)	109.2	109.3	109.6	109.3(2)	109.5(3)
O(4)-T(2)-O(6)	105.4(2)	105.4(2)	105.7(1)	104.4	104.3	104.5	104.0(2)	103.7(3)
O(5)-T(2)-O(6)	104.5(2)	107.4(2)	108.3(1)	108.6	108.0	107.7	109.0(2)	109.1(2)
<O-T(2)-O>	109.3	109.4	109.4	109.4	109.4	109.4	109.4	109.4
T(1)-O(5)-T(2)	135.8(2)	136.1(2)	134.5(2)	134.0	133.7	133.9	133.8(2)	133.6(3)
T(1)-O(6)-T(2)	138.6(2)	141.4(2)	143.9(2)	138.3	137.4	136.9	138.0(2)	136.4(4)
T(1)-O(7)-T(1)	143.4(3)	143.6(3)	148.7(3)	137.7	136.3	135.1	136.1(2)	137.1(6)
O(5)-O(6)-O(5)	171.5(2)	173.0(2)	171.2(1)	162.5	161.8	161.3	161.6(2)	161.5(3)
$O(1^u)$-M(1)-$O(2^d)$ x2	83.8(1)	81.8(1)	78.4(1)	82.8	83.1	83.8	82.9(2)	82.4(2)
$O(1^u)$-M(1)-$O(2^u)$ x2	96.6(1)	97.7(1)	99.6(1)	97.0	97.0	96.9	97.0(2)	96.2(2)
$O(1^u)$-M(1)-$O(3^d)$ x2	84.4(2)	84.5(1)	84.8(1)	83.8	83.5	83.2	83.7(2)	83.6(3)
$O(1^u)$-M(1)-$O(3^u)$ x2	95.1(2)	96.0(1)	97.4(1)	96.4	96.3	96.0	96.5(2)	97.8(3)
O(2)-M(1)-O(2)	91.5(2)	91.5(2)	92.9(1)	88.6	88.3	88.4	87.9(2)	86.5(3)
O(2)-M(1)-O(3) x2	95.4(1)	94.3(1)	94.1(1)	95.9	96.0	95.9	96.2(2)	96.3(2)
O(3)-M(1)-O(3)	77.7(2)	79.9(2)	79.2(1)	79.6	79.7	79.8	79.7(2)	80.8(3)
<O-M(1)-O>	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(1)-M(2)-$O(1)_d$	77.8(2)	78.3(2)	80.4(1)	80.4	80.1	79.6	79.8(2)	79.7(3)
$O(1^u)$-M(2)-$O(2_d)$ x2	83.0(1)	83.2(1)	83.4(1)	84.2	84.3	84.2	84.5(2)	82.8(2)
$O(1^u)$-M(2)-$O(2^u)$ x2	88.3(1)	88.7(1)	89.6(1)	92.9	93.2	92.8	93.2(2)	93.9(3)
O(1)-M(2)-$O(4)_d$ x2	90.7(2)	90.8(1)	89.8(1)	91.6	91.7	91.9	92.2(2)	91.7
$O(2^u)$-M(2)-$O(4_d)$ x2	97.2(2)	96.4(1)	95.4(1)	92.4	92.5	92.4	91.8(2)	92.6(3)
$O(2^u)$-M(2)-$O(4^u)$ x2	89.9(2)	90.3(1)	90.5(1)	90.1	89.8	90.1	90.2(2)	90.2(3)
O(4)-M(2)-O(4)	101.5(2)	100.7(1)	100.6(1)	97.0	97.1	97.1	96.4(2)	97.5(2)
<O-M(2)-O>	89.8	89.8	89.9	90.0	90.0	90.0	90.0	90.0
$O(1^u)$-M(3)-$O(1^d)$ x2	78.8(2)	78.3(2)	75.6(1)	79.1	79.3	80.1	78.8(2)	80.1(2)
$O(1^u)$-M(3)-$O(1_u)$ x2	101.2(2)	101.7(2)	104.4(1)	100.9	100.7	99.9	101.2(2)	99.9(2)
$O(1^u)$-M(3)-$O(3^d)$ x2	84.5(1)	84.9(1)	84.5(1)	83.3	83.2	83.3	83.3(2)	81.9(2)
$O(1^u)$-M(3)-$O(3^u)$ x4	95.5(1)	95.1(1)	95.5(1)	96.7	96.8	96.7	96.7(2)	98.1(2)
<O-M(3)-O>	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
O(2)-M(4)-$O(2)_d$	76.9(2)	76.7(2)	78.6(1)	76.2	76.0	76.0	76.6(2)	74.8(2)
$O(2^u)$-M(4)-$O(4^d)$ x2	78.4(1)	76.1(1)	72.8(1)	75.9	76.1	76.9	76.4(2)	76.4(2)
$O(2^u)$-M(4)-$O(4^u)$ x2	84.3(1)	85.0(1)	87.1(1)	83.5	83.1	83.0	83.5(2)	82.6(2)
$O(2^u)$-M(4)-$O(5^u)$ x2	87.8(1)	87.7(1)	86.6(1)	86.1	85.9	86.2	85.9(2)	86.3(2)
$O(4^u)$-M(4)-$O(5^d)$ x2	83.6(1)	82.2(1)	80.6(1)	84.0	84.4	84.5	84.0(2)	85.0(2)
$O(4^u)$-M(4)-$O(6^u)$ x2	62.6(1)	64.3(1)	65.5(1)	63.4	63.1	63.0	63.2(2)	62.8(2)
$O(5^u)$-M(4)-$O(6^d)$ x2	71.8(1)	71.1(1)	70.0(1)	70.7	70.8	70.4	70.5(2)	70.7(2)
$O(5^u)$-M(4)-$O(6^u)$ x2	57.8(1)	58.6(1)	59.7(1)	61.6	62.0	61.7	61.6(2)	62.3(2)
O(6)-M(4)-O(6)	87.1(2)	86.6(2)	86.5(1)	86.8	87.2	86.3	86.2(2)	87.1(2)
<O-M(4)-O>	76.0	75.8	75.6	75.8	75.9	75.9	75.8	75.9
O(7)-O(7)-O(7)	65.7(1)	67.1(1)	67.2(2)	63.7	63.5	62.6	62.8(3)	64.3(4)
Δ	0.270	0.254	0.253	0.292	0.294	0.304	0.302	0.285

APPENDIX B7. REFINEMENT DETAILS FOR C2/m AMPHIBOLES

	#E_o	#$E_o > 0$	R_{obs}	R_w^{obs}	R_{all}	R_w^{all}	B	Abs	Wts
(21)	1161	1087	7.7	–	10.2	–		No	1
(22)	1505	1216	3.9	3.4	5.8	4.0	A	Yes	1
(24)	–	1122	4.7	3.2	–	–	A	Yes	w
(26)	1389	963	8.0	–	–	–	I	Yes	1
(28)	–	1611	4.8	–	–	–	A	Yes	1
(29)	1511/985		6.9	–	–	–	I	Yes	1
(30)	–	1701	3.5	–	–	–	A	Yes	1
(34)	~1200	959	8.5	–	–	–	I	No	w
(35)	~1200	971	9.2	–	–	–	I	No	w
(36)	~1200	865	4.2	–	–	–	A	No	w
(37)	719	633	4.0	–	–	–	I	No	w
(38)	> 885	825	3.0	3.6	–	–	A	Yes	w
(39)	> 736	736	6.2	6.4	–	–	I	Yes	w
(40)	1072	971	–	–	–	7.9	A	No	w
(41)	828	753	5.6	4.4	–	–	I	No	w
(42)		860	12.1	–	–	–	I	No	–
(43)		838	11.1	–	–	–	I	No	–
(44)		920	12.8	–	–	–	I	No	–
(45)		927	10.0	–	–	–	I	No	–
(46)		840	11.8	–	–	–	I	No	–
(48)		1021	11.5	–	–	–	I	No	–
(49)		480	10.4	–	–	–	I	No	–
(50)		510	9.7	–	–	–	I	No	–
(51)		450	9.3	–	–	–	I	No	–
(52)		–	14.8	–	–	–	A	Yes	–
(53a)	869	818	3.1	3.5	–	–	A	No	1
(53b)	795	732	4.4	4.8	–	–	A	No	1
(54)	1767	1217	4.5	4.9	–	–	A	Yes	1
(55)	1681	1041	4.0	4.7	–	–	A	Yes	1
(56a)	1640	1376	3.2	3.5	4.4	4.6	A	Yes	1
(56b)	731	709	2.1	2.7	2.3	3.2	A	No	1
(57)	1761	1383	3.7	4.5	4.4	–	A	Yes	1
(58)	1826	1263	4.1	4.4	–	–	A	Yes	1
(59)	1626	1421	3.6	4.1	–	–	A	Yes	1
(60)	854	818	10.2	–	12.0	–	I	No	–
(61)		734	10.2	–	–	–	I	No	–
(62)	427	369	14.0	–	18.0	–	I	No	–
(63)		650	12.0	–	–	–	I	No	–
(64)	–	554	14.9	–	–	–	I	No	1
(65)	–	924	11.9	–	–	–	I	No	1
(66)	–	701	16.9	–	–	–	I	No	1
(67)	1565	1193	4.7	4.8	7.0	6.9	A	Yes	1
(68)	1628	1158	3.6	3.7	5.6	5.4	A	Yes	1
(69)	1257	1015	3.2	3.4	4.5	4.4	A	Yes	1
(70)	1373	1068	2.4	–	3.8	–	A	Yes	1
(71)	1373	1068	2.4	–	3.8	–	A	Yes	1
(72)	1369	1035	2.5	–	4.0	–	A	Yes	1
(73)	1557	1098	4.8	5.1	–	–	A	Yes	1
(74)	1714	1191	4.7	–	–	–	A	Yes	–

B: temperature-factor type, I: isotropic, A: anisotropic, 1: unit weights, w: statistical weights.

APPENDIX C. MODERN DATA FOR ORTHORHOMBIC STRUCTURES *(Pnma)*

[23]	Anthophyllite	Finger (1967, 1970a, b)
[31]	Holmquistite	Whittaker (1969), Irusteta & Whittaker (1975)
[32]	Gedrite	Papike & Ross (1970)
[33]	Gedrite	Papike & Ross (1970)
[47]	Holmquistite	Litvin *et al.* (1973a)

APPENDIX C1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	[23]		[31]		[32]		[33]	[47]
SiO_2	57.14	-	59.06		44.22	45.52	40.75	-
TiO_2	-	-	0.20		-	0.62	0.25	-
Al_2O_3	1.94	-	12.38		23.79	18.33	19.81	-
Fe_2O_3	-	-	2.36		0.20	9.93	1.22	-
FeO	11.12	-	10.84		9.21		19.29	-
MnO	0.11	-	0.25		0.16	0.13	0.25	-
MgO	26.82	-	8.82		20.69	22.09	13.81	-
CaO	0.64	-	0.21		0.62	0.22	0.27	-
Na_2O	0.27	-	0.11		-	1.78	1.92	-
K_2O	0.06	-	0.05		-	-	0.04	-
H_2O	2.06	-	2.16		1.42	-	2.68	-
F	-	-	0.18		-	-	0.01	-
	100.16	-	99.95		100.31	98.62	100.38	-
O = F	-	-	0.08		-	-	-	-
Total	100.16	-	99.87		100.31	98.62	100.38*	-
Si	8.00	7.87	7.89	7.91	6.00	6.25	5.953	8.00
Al	-	0.13	0.11	0.09	2.00	1.75	2.047	-
$\sum iv$	8.00	8.00	8.00	8.00	8.00	8.00	8.000*	8.00
Al	-	0.05	1.84	1.85	1.78	1.21	1.365	2.09
Ti^{3+}	-	-	0.02	-	-	0.06	0.026	-
Fe^{3+}	-	-	0.24	0.24	0.02	1.14	0.140	0.23
Fe^{2+}	1.47	1.17	1.21	1.20	1.04		2.351	1.00
Mn	-	-	0.03	0.03	0.02	0.02	0.031	0.02
Mg	5.53	5.79	1.76	1.75	4.16	4.52	3.009	1.91
Ca	-	0.09	0.03	-	0.09	0.03	0.042	0.11
Na	-	0.05	0.03	0.02	-	-	-	-
Li	-	-	1.79	1.82	-	-	0.018	1.75
$\sum vi$	7.00	7.10	6.95	6.91	7.11	6.98	6.966*	7.11
Na	-	0.05	-	-	-	0.47	0.544	0.04
K	-	-	0.01	0.01	-	-	0.007	0.02
$\sum$ A	-	0.05	0.01	0.01	-	0.47	0.551	0.06
Basis			1					
a (Å)	18.560(3)		18.29		18.531(4)		18.601(4)	18.27
b (Å)	18.013(2)		17.67		17.741(4)		17.839(3)	17.67
c (Å)	5.2818(9)		5.28		5.249(5)		5.284(2)	5.30
V ($Å^3$)	1765.8(7)		1706.4		1725.8(14)		1753.2(6)	1711.0

APPENDIX C2. ATOMIC POSITIONS

		[23]		[31]		[32]	
		A-chain	B-chain	A-chain	B-chain	A-chain	B-chain
O1	x	0.1825(2)	0.0685(2)	0.1803(5)	0.0698(5)	0.1796(4)	0.0695(5)
	y	0.1635(2)	0.1635(2)	0.1562(5)	0.1563(5)	0.1603(4)	0.1584(5)
	z	0.0573(6)	-0.2746(6)	0.0492(16)	-0.2611(15)	0.0312(15)	-0.2860(17)
O2	x	0.1855(2)	0.0630(2)	0.1848(5)	0.0653(5)	0.1840(5)	0.0622(4)
	y	0.0777(2)	0.0773(2)	0.0747(5)	0.0744(5)	0.0737(5)	0.0742(4)
	z	-0.4377(6)	0.2187(6)	-0.4087(17)	0.1971(18)	-0.4436(18)	0.1875(14)
O3	x	0.1822(3)	0.0694(3)	0.1822(8)	0.0683(7)	0.1797(7)	0.0700(6)
	y	1/4	1/4	1/4	1/4	1/4	1/4
	z	-0.4437(8)	0.2267(9)	-0.4468(24)	0.2322(24)	-0.4571(27)	0.2087(23)
O4	x	0.1869(2)	0.0668(2)	0.1873(5)	0.0653(5)	0.1868(4)	0.0679(4)
	y	-0.0011(2)	-0.0065(2)	0.0042(4)	0.0013(5)	0.0022(4)	-0.0046(4)
	z	0.0721(6)	-0.2920(6)	0.0612(15)	-0.2692(16)	0.0425(16)	-0.2985(16)
O5	x	0.1978(2)	0.0508(2)	0.1943(4)	0.0548(4)	0.1968(5)	0.0549(4)
	y	-0.1168(2)	-0.1112(2)	-0.1146(5)	-0.1134(5)	-0.1090(5)	-0.1026(4)
	z	0.3293(6)	0.0570(6)	0.3373(14)	0.0505(15)	0.3206(17)	0.0943(15)
O6	x	0.2009(2)	0.0484(2)	0.2034(4)	0.0462(4)	0.2022(4)	0.0472(5)
	y	-0.1303(2)	-0.1402(2)	-0.1297(5)	-0.1335(5)	-0.1313(4)	-0.1450(5)
	z	-0.1739(6)	-0.4493(6)	-0.1686(16)	-0.4494(15)	-0.1752(15)	-0.4097(18)
O7	x	0.2027(3)	0.0450(3)	0.2054(7)	0.0424(7)	0.2030(6)	0.0454(7)
	y	-1/4	-1/4	-1/4	-1/4	-1/4	-1/4
	z	0.5397(8)	0.2221(9)	0.5451(21)	0.2424(23)	0.5138(21)	0.2153(26)
T1	x	0.23039(7)	0.01863(8)	0.2305(2)	0.0190(2)	0.2315(2)	0.0202(2)
	y	-0.16540(7)	-0.16626(7)	-0.1621(2)	-0.1622(2)	-0.1631(2)	-0.1645(2)
	z	-0.4344(2)	0.2760(2)	-0.4327(6)	0.2770(2)	-0.4487(6)	0.2971(6)
T2	x	0.22731(8)	0.02469(8)	0.2262(2)	0.0244(2)	0.2278(2)	0.0266(2)
	y	-0.07956(7)	-0.08177(7)	-0.0761(2)	-0.0769(2)	-0.0760(2)	-0.0802(2)
	z	0.0622(2)	-0.2227(2)	0.0735(6)	-0.2146(6)	0.0502(6)	-0.1985(6)
M1	x	0.12489(9)		0.1248(2)		0.1244(2)	
	y	0.16329(7)		0.1590(1)		0.1611(2)	
	z	0.3911(3)		0.3944(6)		0.3737(8)	
M2	x	0.12488(9)		0.1255(2)		0.1248(2)	
	y	0.07317(7)		0.0687(2)		0.0731(2)	
	z	-0.1099(3)		-0.1045(7)		-0.1281(7)	
M3	x	0.12579(14)		0.1255(2)		0.1249(3)	
	y	1/4		1/4		1/4	
	z	-0.1089(5)		-0.1061(8)		-0.1248(10)	
M4	x	0.12371(4)		0.1221(10)		0.1189(1)	
	y	-0.00982(4)		-0.0086(8)		-0.0145(1)	
	z	0.3877(2)		0.3988(37)		0.3636(5)	
A	x	-		-		0.1151(3)	
	y	-		-		-1/4	
	z	-		-		0.8533(47)	

		[33]		[47]	
		A-chain	B-chain	A-chain	B-chain
O1	x	0.1790(4)	0.0701(4)	0.179(1)	0.069(1)
	y	0.1581(4)	0.1568(4)	0.157(1)	0.153(1)
	z	0.0315(15)	-0.2900(15)	0.030(6)	-0.278(5)
O2	x	0.1850(4)	0.0635(4)	0.185(1)	0.064(1)
	y	0.0731(4)	0.0739(4)	0.075(1)	0.075(1)
	z	-0.4409(15)	0.1808(15)	-0.420(5)	0.189(5)
O3	x	0.1811(6)	0.0701(6)	0.184(2)	0.072(1)
	y	1/4	1/4	1/4	1/4
	z	-0.4662(22)	0.2111(22)	-0.458(8)	0.224(7)
O4	x	0.1863(4)	0.0685(4)	0.1883(5)	0.0649(5)
	y	0.0028(4)	-0.0049(4)	0.0106(4)	0.0018(4)
	z	0.0445(16)	-0.2986(15)	0.069(2)	-0.263(2)
O5	x	0.1973(4)	0.0545(4)	0.190(1)	0.054(1)
	y	-0.1100(4)	-0.1014(4)	-0.115(1)	-0.117(1)
	z	0.3215(14)	0.0989(14)	0.345(6)	0.051(5)
O6	x	0.2030(4)	0.0473 (4)	0.201(1)	0.049(1)
	y	-0.1320(4)	-0.1461(4)	-0.130(1)	-0.125(1)
	z	-0.1763(16)	-0.4036(15)	-0.175(5)	-0.439(5)
O7	x	0.2050(6)	0.0453(6)	0.208(2)	0.042(1)
	y	-1/4	-1/4	-1/4	-1/4
	z	0.5141(22)	0.2154(21)	0.544(8)	0.229(7)
T1	x	0.2323(1)	0.0199(1)	0.2305(4)	0.0190(5)
	y	-0.1626(2)	-0.1641(2)	-0.1630(4)	-0.1622(4)
	z	-0.4505(6)	0.3018(5)	-0.436(2)	0.277(2)
T2	x	0.2282(1)	0.0268(1)	0.2265(5)	0.0230(4)
	y	-0.0759(2)	-0.0799(2)	-0.0757(4)	-0.0767(4)
	z	0.0509(6)	-0.1947(6)	0.074(2)	-0.206(2)
M1	x	0.1242(1)		0.125(1)	
	y	0.1603(1)		0.159(1)	
	z	0.3705(5)		0.401(4)	
M2	x	0.1247(1)		0.1255(5)	
	y	0.0724(2)		0.0671(3)	
	z	-0.1290(6)		-0.110(2)	
M3	x	0.1243(2)		0.125(3)	
	y	1/4		1/4	
	z	-0.1294(7)		-0.105(8)	
M4	x	0.1184(1)		0.120(1)	
	y	-0.0153(1)		0.0093(9)	
	z	0.3635(4)		0.385(7)	
A	x	0.1171(8)		-	
	y	-1/4		-	
	z	0.8480(27)		-	

Appendix C3. Site Occupancies and Annotations

Anthophyllite[23]

M1	0.960(3)Mg+0.040Fe	0.54(3) Å²
M2	0.973(3)Mg+0.027Fe	0.55(3)
M3	0.966(4)Mg+0.034Fe	0.49(4)
M4	0.349(4)Mg+0.651Fe	0.78(2)

Cation site-populations determined by constrained least-squares refinement; the equality of the M(1, 2, 3) site-equivalent isotropic temperature-factors supports the site occupancies obtained for these sites. No details of the chemical analysis are given by Finger (1967, 1970b); presumably it is taken from Rabbitt (1948) (sample #30). This anthophyllite has been re-analyzed by Seifert & Virgo (1974, 1975), giving a formula unit of $Na_{0.05}Ca_{0.09}Mg_{5.79}Fe^{2+}{}_{1.17}(Si_{7.81}Al_{0.18})O_{22}(OH)_2$ as compared with the formula $Mg_{5.53}Fe_{1.47}Si_8O_{22}(OH)_2$ used in the structure refinement. Seifert & Virgo (1974) listed p values [$p = X^{Fe}{}_{M123}\,(1-X^{Fe}{}_{M4})\,/\,X^{Fe}{}_{M4}\,(1-X^{Fe}{}_{M123})$] of 0.0186 from the site occupancies given above and 0.0201 from their Mössbauer results (Appendix F, #{76}. If allowance is made in the X-ray results for the small amount of Ca that must occur at M4, a p value of 0.0209 results, in exact agreement with the Mössbauer results. It would thus appear that the X-ray site-populations of Finger (1970b) may be adjusted to give the correct unit-formula and the following site-populations:

M1 $0.967Mg+0.033Fe^{2+}$
M2 $0.978Mg+0.022Fe^{2+}$
M3 $0.972Mg+0.028Fe^{2+}$
M4 $0.045Ca+0.444Mg+0.511Fe^{2+}$

In addition, the formula is in reasonable agreement with the relationship between alkali occupancy of the A site and tetrahedral Al demonstrated by Robinson *et al.* (1971). Mao & Seifert (1974) gave polarized optical-absorption spectra for this anthophyllite (details in text).

Holmquistite[31]

The authors give seven sets of site occupancies, all of which are reproduced here. For most sets, the only differences are between M4 occupancies:

1–3	M1	0.59Mg+0.41Fe	0.63 Å²
1–3	M2	0.92Al+0.08Fe	0.61
1–3	M3	0.44Mg+0.56Fe	0.69
1	M4	0.97Li+0.03Fe	1.50
2	M4	0.911Li+0.039Mg +0.015Na+0.015Ca+0.02□	
3	M4	0.909Li+0.046Mg +0.004Fe+0.011Na+0.03□	
4	M1	0.605Mg+0.390Fe	
4	M2	$0.920Al+0.080Fe^{3+}$	
4	M3	0.44Mg+0.56Fe	
4	M4	0.895Li+0.055Mg +0.015Na+0.015Ca+0.02□	
5	M1	0.609Mg+0.390Fe	
5	M2	$0.935Al+0.065Fe^{3+}$	
5	M3	0.44Mg+0.56Fe	
5	M4	0.910Li+0.049Mg +0.011Na+0.03□	
6	M1	0.60Mg+0.40Fe	
6	M2	$0.93Al+0.07Fe^{3+}$	
6	M3	0.44Mg+0.56Fe	
6	M4	0.91Li+0.05Mg +0.01Na+0.03□	
7	M1	$0.52Mg+0.08Al\ 0.37Fe^{2+}+0.03Fe^{3+}$	
7	M2	$0.81Al+0.07Fe^{3+}+0.12Mg$	
7	M3	$0.36Mg+0.08Al +0.04Fe^{3+}+0.52Fe^{2+}$	
7	M4	0.91Li+0.05Mg +0.01Na+0.03□	

1: occupancies from refinement (unconstrained).
2: as 1, except Na, Ca, Li and □ assigned (to M4) from original formula, such that scattering power at M4 is the same.
3: as 2, except corrected formula used.
4: assigned from original formula, assuming all Na, Ca, Li and □ are at M4, all Al and sufficient Fe^{3+} are at M2, M3 is as refinement indicates and M1 contains remaining cations.
5: as 4, except corrected formula used.
6: occupancies adjusted to correspond closely with *both* the chemical composition and the diffraction results.
7: adjustment of 6 to take account of M–O distances.

The chemical composition, which includes 3.33 wt. % Li_2O, was taken from von Knorring & Hornung (1961), who also give the composition of a coexisting hornblende. Irusteta & Whittaker (1975) suggested that some of the Na and Ca indicated by the holmquistite analysis might well be due to slight contamination by the coexisting hornblende, and corrected the composition of the holmquistite by assuming a 2% contamination; this they cited as a probable upper limit of contamination; they interpreted the diffraction results in terms of both analyses. Site occupancies were derived (set 1) by unconstrained refinement of binary site-populations;

there was some deviation from the site chemistry indicated by the chemical analysis but this was, for the most part, accounted for by the presence of small amounts of other cations present. The equivalent isotropic temperature-factors at the M1, M2 and M3 sites are similar, supporting the refined occupancies. The adjustment of the site occupancies by comparison of mean bond-lengths and ionic radii (possibility 7) is probably of little significance as the mean bond-lengths in the amphiboles do not correspond very closely with the sum of the relevant ionic radii (*e.g.*, $<Mg-^{iii}F_2^{iv}O_4>$ = 2.073 Å, <M(3)–O>, in fluor-tremolite = 2.040 Å, in protoamphibole = 2.048 Å). Examination of mean bond-lengths indicate that those from set number 6 are to be preferred, with the bulk of the excess $0.10Fe^{3+}$ atoms p.f.u. assigned to the M(1) site. This is also supported by the Mössbauer study of Law (1973); see Appendix F, #{65}. The small amount of tetrahedral Al (0.09 atoms p.f.u.) is probably ordered in the T1A site (see section on tetrahedral Al and mean bond-lengths for orthorhombic amphiboles, this study).

Gedrite[32]

T1A	0.66Si+0.34Al	0.43(4) Å²
T1B	0.62Si+0.38Al	0.42(4)
T2A	1.00Si+0.00Al	0.46(4)
T2B	0.84Si+0.16Al	0.58(4)
M1	0.12(1)Fe*+0.88Mg	0.75(7)
M2	0.04(1)Fe*+0.36Mg+0.60Al	0.34(7)
M3	0.10(2)Fe*+0.90Mg	0.47(10)
M4	0.42Fe*+0.55Mg+ 0.02Ca+0.01Na	0.63(4)
A	0.34(3)Na+0.66□	1.47(49)

Tetrahedral site-populations assigned by "method 2" of Papike *et al.* (1969), octahedral site-populations assigned by constrained least-squares refinement during structure refinement and A-site occupancy assigned by unconstrained site-population refinement. The cell contents derived from the chemical analysis (Papike & Ross 1970) indicate an A-site occupancy of 0.45 Na. However, using this value during the refinement gave an A-site isotropic temperature-factor of 2.5 Å², a value the authors felt to be anomalously high. Refinement of the A-site occupancy converged to a value of 0.34(3) Na and an isotropic temperature-factor of 1.47 Å²; this result is supported by the fact that the A-site isotropic temperature-factor is identical to the value found for gedrite[33] (Papike & Ross 1970).

If the refined A-site occupancy is taken as being correct, the remaining contents of the cell must be adjusted to maintain electro-neutrality. At first sight, the possibility of making an adequate adjustment might seem remote. However, the work of Robinson *et al.* (1971) provides a significant indication of the type of adjustment to be made. These authors suggested that the anthophyllite–gedrite series of amphiboles is a solid solution between two end-member compositions $\square\ R^{2+}{}_2R^{2+}{}_5Si_8O_{22}(OH)_2$ and $Na_{0.5}R^{2+}{}_2R^{2+}{}_{3.5}R^{3+}{}_{1.5}Si_6Al_2O_{22}(OH)_2$. This being the case, an A-site occupancy of 0.34 Na corresponds to a total cell-content $Na_{0.34}R^{2+}{}_2R^{2+}{}_{3.98}R^{3+}{}_{1.02}Si_{6.64}Al_{1.36}O_{22}(OH)_2$. The grand <T–O> distance is compatible with the contents of the tetrahedral sites derived here and not compatible with that indicated by the chemical analysis. However, a content of octahedral trivalent cations of 1.02 atoms p.f.u. is not compatible with the observed mean bond-lengths at the octahedral sites. Possibly a hydroxyl deficiency is accompanied by an increase in content of trivalent cations; without any evidence, further speculation is of questionable value. A new chemical analysis of this amphibole is desirable. Using the curves developed earlier in this study, the following tetrahedral site-populations are derived:

T1A	0.74Si+0.26Al
T2A	1.00Si
T1B	0.71Si+0.29Al
T2B	0.87Si+0.13Al

Polarized optical-absorption spectra of this gedrite are given by Mao & Seifert (1974) (details in text).

Gedrite[33]

T1A	0.73Si+0.27Al	0.56(4) Å²
T1B	0.56Si+0.44Al	0.50(4)
T2A	0.98Si+0.02Al	0.44(4)
T2B	0.71Si+0.29Al	0.59(4)
M1	0.33(1)Fe*+0.67Mg	0.71(5)
M2	0.09(1)Fe*+0.23Mg+0.68Al	0.30(6)
M3	0.39(2)Fe*+0.61Mg	0.57(7)
M4	0.65Fe*+0.32Mg +0.02Ca+0.01Na	0.62(3)
A	0.52(3)Na+0.48□	1.53(30)

Tetrahedral site-populations assigned by "method 2" of Papike *et al.* (1969), octahedral site-populations assigned by constrained least-squares refinement and A-site occupancy assigned by unconstrained site-population refinement. The grand <M–O> deviates significantly from the trend of the remaining three *Pnma* amphiboles in Figure 49, suggesting that the crystal used for the structure refinement differs somewhat from the nominal composition. The

chemical analysis (Robinson & Jaffe 1969, sample no. I34I) includes 0.011 Cr_2O_3, 0.001 NiO, 0.001 SrO, 0.001 BaO, 0.04 P_2O_5 and 0.01 Cl; cell contents include 0.005 P. The unresolved Mössbauer spectrum is presented by Seifert (1977).

Holmquistite[47]

M1 0.48Fe+0.52Mg
M2 0.92Al+0.08Mg
M3 0.54Fe+0.46Mg
M4 0.90Li+0.05 Mg
A 0.30Na+0.04(Ca, K)

Site populations were assigned on the basis of mean bond-lengths and by comparison with results of previous structure-refinements. The authors proposed that Li is positionally disordered off the 2-fold axis at the M4 site; this was not observed in the refinement of holmquistite[31] by Irusteta & Whittaker (1975).

APPENDIX C4. CATION-ANION AND CATION-CATION DISTANCES (Å)

		[23]		[31]		[32]	
		A-chain	B-chain	A-chain	B-chain	A-chain	B-chain
T1-O1		1.618(3)	1.618(3)	1.638(10)	1.630(10)	1.651(8)	1.665(9)
T1-O5		1.640(3)	1.636(3)	1.618(9)	1.613(9)	1.673(9)	1.658(8)
T1-O6		1.611(3)	1.622(3)	1.587(9)	1.610(9)	1.635(9)	1.654(10)
T1-O7		1.615(2)	1.617(2)	1.623(5)	1.620(10)	1.640(5)	1.643(6)
⟨T1-O⟩		1.621	1.623	1.616	1.618	1.650	1.655
T2-O2		1.619(3)	1.630(3)	1.630(9)	1.645(9)	1.635(9)	1.648(8)
T2-O4		1.601(3)	1.608(3)	1.589(8)	1.597(10)	1.579(8)	1.630(8)
T2-O5		1.655(3)	1.643(3)	1.657(8)	1.638(9)	1.638(9)	1.670(8)
T2-O6		1.621(3)	1.653(3)	1.644(9)	1.643(9)	1.607(9)	1.641(10)
⟨T2-O⟩		1.624	1.634	1.630	1.631	1.615	1.647
M1-O1		2.062(3)	2.053(4)	2.086(6)	2.079(9)	2.067(9)	2.054(10)
M1-O2		2.112(3)	2.133(3)	2.123(9)	2.123(9)	2.130(9)	2.158(8)
M1-O3		2.082(3)	2.063(3)	2.095(9)	2.095(8)	2.078(9)	2.061(8)
⟨M1-O⟩		2.084		2.100		2.091	
M2-O1		2.138(3)	2.121(3)	2.013(9)	2.029(9)	2.028(8)	2.005(9)
M2-O2		2.067(3)	2.082(3)	1.941(10)	1.938(10)	1.985(10)	2.021(8)
M2-O4		2.010(3)	2.037(3)	1.828(9)	1.841(10)	1.924(9)	1.951(8)
⟨M2-O⟩		2.076		1.932		1.986	
M3-O1	x2	2.075(3)	2.079(3)	2.103(9)	2.109(9)	2.055(8)	2.097(9)
M3-O3		2.055(5)	2.059(5)	2.077(14)	2.070(13)	2.017(15)	2.023(13)
⟨M3-O⟩		2.070		2.095		2.057	
M4-O2		2.156(3)	2.128(3)	2.125(19)	2.090(19)	2.217(9)	2.103(8)
M4-O4		2.044(3)	1.996(3)	2.157(21)	2.045(21)	2.123(9)	2.015(9)
M4-O5		2.387(3)	2.867(3)	2.314(19)	2.886(19)	2.222(9)	2.416(8)
M4-O6		3.481(3)	2.865(3)	3.465(19)	2.728(18)	3.864	2.923
⟨M4-O⟩	VIII	2.491		2.476		2.485	
⟨M4-O⟩	VI	2.263		2.243		2.183	
A-O6		-	-	-	-	2.65(2)	2.64(2)
A-O7		-	-	-	-	2.41(3)	2.30(3)
⟨A-O⟩		-		-		2.55	
M1-M1		3.124(2)		3.216		3.154(4)	
M1-M2		3.096	3.105	3.080	3.090	3.043(6)	3.059(6)
M1-M3		3.068(3)	3.068(3)	3.093	3.089	3.066(6)	3.053(6)
M1-M4		3.118(1)		2.962		3.114(4)	
M2-M3		3.185(1)		3.204		3.135(3)	
M2-M4		3.024	3.046	2.958	2.989	3.013(5)	3.087(5)
T1-T2		3.076(2)	3.044(2)	3.019	3.003	3.040(5)	3.001(5)
T1-T2		3.045(2)	3.055(2)	3.076	3.080	3.050(5)	3.041(5)
T1-T1		3.049(2)	3.017(2)	3.106	3.103	3.080(4)	3.032(4)

	[33]		[47]	
	A-chain	B-chain	A-chain	B-chain
T1-O1	1.653(8)	1.679(8)	1.67	1.62
T1-O5	1.660(8)	1.677(8)	1.62	1.58
T1-O6	1.641(9)	1.668(8)	1.59	1.73
T1-O7	1.649(5)	1.666(5)	1.59	1.63
⟨T1-O⟩	1.651	1.672	1.62	1.64
T2-O2	1.613(7)	1.683(8)	1.62	1.59
T2-O4	1.605(8)	1.640(8)	1.67	1.61
T2-O5	1.656(8)	1.679(8)	1.72	1.64
T2-O6	1.631(8)	1.660(8)	1.69	1.58
⟨T2-O⟩	1.626	1.666	1.68	1.61
M1-O1	2.059(8)	2.057(8)	2.20	1.98
M1-O2	2.165(8)	2.156(8)	2.07	2.16
M1-O3	2.101(8)	2.068(8)	2.08	2.09
⟨M1-O⟩	2.101		2.10	
M2-O1	2.017(8)	2.004(8)	2.00	2.04
M2-O2	1.993(8)	1.993(8)	1.97	1.95
M2-O4	1.920(8)	1.947(8)	1.79	1.79
⟨M2-O⟩	1.979		1.92	
M3-O1	2.107(8)	2.119(8)	2.04	2.18
M3-O3	2.068(12)	2.061(12)	2.16	1.99
⟨M3-O⟩	2.097		2.10	
M4-O2	2.254(8)	2.121(8)	2.05	1.97
M4-O4	2.129(8)	2.019(8)	2.10	2.12
M4-O5	2.246(7)	2.391(8)	2.41	2.97
M4-O6	3.911	2.951	3.59	2.73
⟨M4-O⟩ VIII	2.503		2.49	
⟨M4-O⟩ VI	2.193		2.23	
A-O6	2.64(1)	2.64(1)	-	-
A-O7	2.40(2)	2.35(2)	-	-
	2.54		—	
M1-M1	3.197(3)		3.22	
M1-M2	3.073(4)	3.068(4)	3.15	3.05
M1-M3	3.087(4)	3.086(4)	3.12	3.06
M1-M4	3.132(3)		2.81	
M2-M3	3.165(3)		3.23	
M2-M4	3.036(4)	3.104(4)	2.87	2.92
T1-T2	3.067(4)	3.056(4)	3.01	2.97
T1-T2	3.055(4)	3.024(4)	3.10	3.12
T1-T1	3.116(4)	3.063(4)	3.07	3.10

APPENDIX C5. ANION - ANION DISTANCES (Å)

	[23]		[31]		[32]		[33]	
	A-chain	B-chain	A-chain	B-chain	A-chain	B-chain	A-chain	B-chain
O1-O5	2.664(4)	2.667(4)	2.656	2.647	2.701(11)	2.704(12)	2.696(10)	2.715(10)
O1-O6	2.657(4)	2.648(5)	2.639	2.646	2.728(11)	2.699(13)	2.724(11)	2.725(11)
O1-O7	2.643(5)	2.635(5)	2.668	2.639	2.697(12)	2.703(14)	2.712(12)	2.743(11)
O5-O6	2.636(5)	2.659(5)	2.628	2.669	2.677(12)	2.713(13)	2.683(11)	2.749(11)
O5-O7	2.646(3)	2.649(3)	2.640	2.628	2.700(9)	2.696(8)	2.700(8)	2.725(8)
O6-O7	2.635(4)	2.632(4)	2.609	2.625	2.664(10)	2.709(14)	2.666(11)	2.736(11)
⟨O-O⟩ T1	2.647	2.648	2.640	2.642	2.694	2.704	2.697	2.732
O2-O4	2.742(4)	2.753(4)	2.728	2.764	2.747(11)	2.769(10)	2.750(10)	2.816(10)
O2-O5	2.679(4)	2.638(4)	2.660	2.647	2.683(12)	2.673(11)	2.673(10)	2.691(10)
O2-O6	2.627(4)	2.654(4)	2.647	2.650	2.641(12)	2.654(12)	2.644(11)	2.700(11)
O4-O5	2.496(4)	2.655(4)	2.559	2.645	2.460(12)	2.706(11)	2.495(11)	2.727(11)
O4-O6	2.677(4)	2.570(4)	2.675	2.589	2.643(11)	2.586(12)	2.690(11)	2.608(10)
O5-O6	2.669(5)	2.725(5)	2.690	2.668	2.633(12)	2.753(13)	2.661(11)	2.775(11)
⟨O-O⟩ T2	2.648	2.666	2.660	2.661	2.634	2.690	2.652	2.720
O1B-O2B	3.096		3.207		3.144		3.166	
O1A-O2A	3.083		3.205		3.157		3.175	
O1B-O2A	2.801		2.667		2.728		2.726	
O1A-O2B	2.838		2.669		2.782		2.738	
O1B-O3B	3.060		3.146		3.111		3.117	
O1A-O3A	3.062		3.135		3.122		3.120	
O1B-O3A	2.771		2.816		2.760		2.810	
O1A-O3B	2.763		2.807		2.743		2.773	
O2A-O2B	2.909		3.018		2.974		3.017	
O3A-O3B	2.723		2.686		2.685		2.678	
O2B-O3B	3.113		3.109		3.124		3.148	
O2A-O3A	3.104		3.104		3.130		3.159	
⟨O-O⟩ M1	2.945		2.964		2.955		2.969	
O1A-O1B	2.748		2.602		2.634		2.644	
O1B-O2B	3.035		2.820		2.903		2.897	
O1A-O2A	3.038		2.815		2.929		2.923	
O1B-O2A	2.801		2.667		2.728		2.726	
O1A-O2B	2.838		2.669		2.782		2.738	
O1B-O4B	3.064		2.740		2.893		2.885	
O1A-O4A	2.967		2.690		2.809		2.775	
O2B-O4B	3.092		2.780		2.911		2.899	
O2A-O4A	3.044		2.777		2.850		2.855	
O2B-O4A	2.807		2.652		2.746		2.710	
O2A-O4B	2.783		2.646		2.672		2.683	
O4A-O4B	2.946		2.833		2.841		2.847	
⟨O-O⟩ M2	2.930		2.724		2.808		2.799	
O1B-O1B	3.116		3.311		3.250		3.325	
O1A-O1A	3.116		3.315		3.183		3.279	
O1B-O1A x2	2.748		2.602		2.634		2.644	
O1B-O3B x2	3.072		3.086		3.063		3.127	
O1A-O3A x2	3.071		3.099		3.017		3.099	
O1B-O3A x2	2.771		2.816		2.760		2.810	
O1A-O3B x2	2.763		2.807		2.743		2.773	
⟨O-O⟩ M3	2.924		2.954		2.906		2.960	

	[23]	[31]	[32]	[33]
02B–02A	2.909	3.018	2.974	3.017
02B–04A	2.807	2.652	2.746	2.710
02B–04B	2.994	3.100	3.041	3.091
02B–05B	3.510	3.413	3.177	3.161
02A–04B	2.783	2.646	2.672	2.683
02A–04A	2.953	3.064	2.981	2.995
02A–05A	3.720	3.610	3.478	3.506
04A–05A	2.496	2.559	2.461	2.497
04A–05B	3.213	3.193	3.083	3.090
04B–05A	3.722	3.751	3.624	3.645
04B–05B	3.933	4.129	3.638	3.629
05B–05A	3.086	2.967	2.888	2.909
⟨O–O⟩ M4	3.177	3.175	3.064	3.078
07A–06B x2	3.481	3.566	3.459	3.497
07A–06A x2	2.634	2.609	2.665	2.666
07B–06B x2	4.061	4.193	3.773	3.778
07B–06A x2	4.171	4.231	4.132	4.162
06B–06A x2	3.187	3.236	3.134	3.145
06B–06B	3.956	4.117	3.724	3.707
06A–06A	4.312	4.251	4.211	4.210
⟨O–O⟩ A	3.611	3.670	3.522	3.534

[47]

	A-chain	B-chain
01-05	2.69	2.63
01-06	2.73	2.67
01-07	2.64	2.67
05-06	2.57	2.71
05-07	2.63	2.54
06-07	2.59	2.83
⟨0-0⟩ T1	2.64	2.68
02-04	2.76	2.76
02-05	2.75	2.61
02-06	2.66	2.61
04-05	2.65	2.69
04-06	2.81	2.44
05-06	2.78	2.60
⟨0-0⟩ T2	2.73	2.62

01B-02B	3.14
01A-02A	3.26
01B-02A	2.64
01A-02B	2.69
01B-03B	3.15
01A-03A	3.17
01B-03A	2.87
01A-03B	2.75
02A-02B	3.03
03A-03B	2.65
02B-03B	3.10
02A-03A	3.10
⟨0-0⟩ M1	2.96
01A-01B	2.59
01B-02B	2.83
01A-02A	2.79
01B-02A	2.64
01A-02B	2.69
01B-04B	2.67
01A-04A	2.60
02B-04B	2.72
02A-04A	2.83
02B-04A	2.62
02A-04B	2.68
04A-04B	2.86
⟨0-0⟩ M2	2.71
01B-01B	3.43
01A-01A	3.29
01B-01A x2	2.59
01B-03B x2	3.17
01A-03A x2	3.07
01B-03A x2	2.87
01A-03B x2	2.75
⟨0-0⟩ M3	2.97

[47]

02B-02A	3.03
02B-04A	2.62
02B-04B	3.18
02B-05B	3.48
02A-04B	2.68
02A-04A	2.94
02A-05A	3.58
04A-05A	2.66
04A-05B	3.33
04B-05A	3.71
04B-05B	4.20
05B-05A	2.93
⟨0-0⟩ M4	3.19
07A-06B x2	3.65
07A-06A x2	2.59
07B-06B x2	4.17
07B-06A x2	4.19
06B-06A	3.11
06B-06B	4.42
06A-06A	4.24
⟨0-0⟩ A	3.67

APPENDIX C6. INTERATOMIC ANGLES(°)

	[23]		[31]		[32]		[33]	
	A-chain	B-chain	A-chain	B-chain	A-chain	B-chain	A-chain	B-chain
O1-T1-O5	109.7(2)	110.1(2)	109.3(4)	109.4(5)	108.6(4)	108.8(4)	108.8(4)	107.9(4)
O1-T1-O6	110.8(2)	109.6(2)	109.8(4)	109.6(5)	112.2(4)	108.7(5)	111.5(4)	108.9(4)
O1-T1-O7	109.7(2)	109.4(2)	109.8(5)	108.6(5)	110.0(5)	109.5(6)	110.3(5)	110.1(5)
O5-T1-O6	108.4(2)	109.4(2)	110.1(5)	111.8(5)	108.0(4)	110.0(4)	108.7(4)	110.5(4)
O5-T1-O7	108.8(2)	109.4(2)	109.0(5)	108.7(5)	109.2(5)	109.4(5)	109.3(5)	109.2(5)
O6-T1-O7	109.5(2)	109.0(2)	108.7(5)	108.7(5)	108.8(5)	110.5(6)	108.2(5)	110.2(5)
⟨O-T1-O⟩	109.5	109.5	109.5	109.5	109.5	109.5	109.5	109.5
O2-T2-O4	116.7(2)	116.5(2)	115.8(5)	117.0(5)	117.3(5)	115.2(4)	117.3(4)	115.8(4)
O2-T2-O5	109.8(2)	107.4(2)	108.1(5)	107.5(5)	110.0(5)	107.2(4)	109.6(4)	106.3(4)
O2-T2-O6	108.3(2)	107.9(2)	107.9(5)	107.5(5)	109.0(4)	107.5(5)	109.0(4)	107.6(4)
O4-T2-O5	100.1(2)	109.5(2)	104.1(5)	109.7(5)	99.6(4)	110.1(4)	99.8(4)	110.5(4)
O4-T2-O6	112.4(2)	104.0(2)	111.6(5)	106.1(5)	112.0(4)	104.4(5)	112.4(4)	104.4(4)
O5-T2-O6	109.1(2)	111.5(2)	109.1(5)	108.8(5)	108.4(4)	112.5(5)	108.0(4)	112.4(4)
⟨O-T2-O⟩	109.4	109.5	109.4	109.4	109.4	109.5	109.4	109.5
T1-O5-T2	138.0(2)	136.3(2)	134.4(5)	135.0(5)	134.2(6)	128.7(5)	134.2(5)	128.6(5)
T1-O6-T2	140.8(2)	137.8(2)	144.3(5)	142.5(5)	139.3(5)	134.8(6)	139.2(5)	133.3(5)
T1-O7-T2	141.4(3)	138.9	146.1(9)	146.6(9)	139.8(8)	134.6(9)	141.7(8)	133.6(7)
O5-O6-O5	169.2(2)	157.5(2)	166.4	163.3	162.4(4)	147.5(4)	162.5(4)	146.0(4)
O1B-M1-O2B	95.4		99.5(4)		96.5(3)		97.3(3)	
O1A-M1-O2A	95.2		99.2(3)		97.5(4)		97.4(3)	
O1B-M1-O2A	84.5		78.8(4)		81.3(4)		80.4(3)	
O1A-M1-O2B	85.2		78.7(3)		82.3(3)		80.9(3)	
O1B-M1-O3B	96.1		97.8(4)		98.1(4)		98.1(4)	
O1A-M1-O3A	95.3		97.2(4)		97.6(4)		97.0(4)	
O1B-M1-O3A	84.2		84.8(4)		83.7(5)		84.9(4)	
O1A-M1-O3B	84.1		84.3(4)		83.2(4)		84.3(4)	
O2A-M1-O2B	86.5		90.6(3)		87.7(3)		88.5(3)	
O3A-M1-O3B	82.2		79.8(3)		80.8(4)		79.8(3)	
O2B-M1-O3B	95.8		95.0(4)		95.4(4)		96.2(3)	
O2A-M1-O3A	95.5		94.8(4)		96.0(4)		95.4(3)	
⟨O-M1-O⟩	90.0		90.0		90.0		90.0	
O1A-M2-O1B	80.4		80.1		81.4(4)		82.1(3)	
O1B-M2-O2B	92.4		90.6		92.2(4)		92.8(3)	
O1A-M2-O2A	92.5		90.8(4)		93.6(4)		93.5(3)	
O1B-M2-O2A	84.0		84.3(4)		86.2(4)		86.0(3)	
O1A-M2-O2B	84.5		84.9(4)		86.7(3)		86.0(3)	
O1B-M2-O4B	94.9		90.1(4)		93.9(4)		93.7(3)	
O1A-M2-O4A	91.3		88.8(4)		90.4(4)		89.5(3)	
O2B-M2-O4B	97.3		94.7(4)		94.1(4)		94.6(3)	
O2A-M2-O4A	96.6		94.8(4)		93.5(4)		93.6(3)	
O2B-M2-O4A	86.6		89.5(4)		88.1(4)		87.6(3)	
O2A-M2-O4B	85.4		88.8(4)		85.4(4)		85.8(3)	
O4A-M2-O4B	93.4		101.1(3)		94.2(4)		94.7(3)	
⟨O-M2-O⟩	89.9		89.9		90.0		90.0	

O1B-M3-O1B		97.1	103.5(5)	101.4(4)	103.2(3)
O1A-M3-O1A		97.3	104.0(4)	101.4(4)	102.0(3)
O1B-M3-O1A	x2	82.8	76.2(3)	78.6(3)	77.4(3)
O1B-M3-O3B	x2	95.9	95.2(3)	95.9(4)	96.7(3)
O1A-M3-O3A	x2	96.1	95.7(4)	95.5(4)	95.8(3)
O1B-M3-O3A	x2	84.2	84.6(3)	84.1(4)	84.2(3)
O1A-M3-O3B	x2	83.9	84.5(3)	84.5(3)	83.3(3)
<O-M3-O>		90.0	90.0	90.0	90.0
O2B-M4-O2A		85.5	91.5	86.9(3)	87.1(3)
O2B-M4-O4A		84.6	77.3	81.0(3)	79.2(3)
O2B-M4-O4B		93.1	97.1	95.0(3)	96.5(3)
O2B-M4-O5B		88.0	85.0	88.9(3)	88.6(3)
O2A-M4-O4B		84.1	78.8	78.0(3)	77.5(3)
O2A-M4-O4A		89.3	91.4	86.7(3)	86.0(3)
O2A-M4-O5A		109.8	108.7	103.0(3)	102.2(3)
O4A-M4-O5A		68.1	69.7	68.9(3)	69.4(3)
O4A-M4-O5B		79.8	77.1	85.2(3)	85.9(3)
O4B-M4-O5A		116.0	118.6	117.3(3)	117.1(3)
O4B-M4-O5B		106.6	112.6	109.9(3)	110.3(3)
O5B-M4-O5A		71.3	68.6	76.8(3)	77.5(3)
<O-M4-O>		89.7	89.7	89.8	89.8
O7A-A-O6B	x2	-	-	86.3(7)	88.0(5)
O7A-A-O6A	x2	-	-	63.2(5)	63.5(4)
O7B-A-O6B	x2	-	-	99.4(8)	97.9(5)
O7B-A-O6A	x2	-	-	112.8(7)	112.5(4)
O6B-A-O6A	x2	-	-	72.6(4)	73.3(3)
O6B-A-O6B		-	-	89.8(8)	89.8(5)
O6A-A-O6A		-	-	104.9(8)	105.4(5)
<O-A-O>		-	-	88.6	88.8

[47]

	A-chain	B-chain
O1-T1-O5	109.8	111.3
O1-T1-O6	113.9	106.2
O1-T1-O7	108.6	110.7
O5-T1-O6	106.2	109.7
O5-T1-O7	110.0	104.9
O6-T1-O7	108.6	114.1
<O-T1-O>	109.5	109.5
O2-T2-O4	114.3	117.9
O2-T2-O5	111.6	107.8
O2-T2-O6	106.7	110.8
O4-T2-O5	102.5	111.4
O4-T2-O6	112.8	100.1
O5-T2-O6	108.8	108.0
<O-T2-O>	109.4	109.4
T1-O5-T2	129.1	135.3
T1-O6-T2	141.9	142.3
T1-O7-T1	149.1	144.9
O5-O6-O5	165.6	172.7

O1B-M1-O2B		98.0
O1A-M1-O2A		99.0
O1B-M1-O2A		81.1
O1A-M1-O2B		76.1
O1B-M1-O3B		100.6
O1A-M1-O3A		95.7
O1B-M1-O3A		90.2
O1A-M1-O3B		79.8
O2A-M1-O2B		91.0
O3A-M1-O3B		78.8
O2B-M1-O3B		93.3
O2A-M1-O3A		96.7
<O-M1-O>		90.0
O1A-M2-O1B		79.5
O1B-M2-O2B		90.4
O1A-M2-O2A		88.9
O1B-M2-O2A		82.3
O1A-M2-O2B		85.8
O1B-M2-O4B		88.3
O1A-M2-O4A		86.2
O2B-M2-O4B		93.1
O2A-M2-O4A		97.1
O2B-M2-O4A		89.0
O2A-M2-O4B		90.7
O4A-M2-O4B		106.0
<O-M2-O>		89.8
O1B-M3-O1B		102.6
O1A-M3-O1A		106.9
O1B-M3-O1A	x2	75.1
O1B-M3-O3B	x2	97.8
O1A-M3-O3A	x2	93.4
O1B-M3-O3A	x2	82.7
O1A-M3-O3B	x2	86.0
<O-M3-O>		90.0

O2B-M4-O2A		97.7
O2B-M4-O4A		80.4
O2B-M4-O4B		101.9
O2B-M4-O5B		86.8
O2A-M4-O4B		80.1
O2A-M4-O4A		89.9
O2A-M4-O5A		106.2
O4A-M4-O5A		71.8
O4A-M4-O5B		80.2
O4B-M4-O5A		109.9
O4B-M4-O5B		109.6
O5B-M4-O5A		64.9
<O-M4-O>		90.0
O7A-A-O6B	x2	-
O7A-A-O6A	x2	-
O7B-A-O6B	x2	-
O7B-A-O6A	x2	-
O6B-A-O6A	x2	-
O6B-A-O6B		-
O6A-A-O6A		-
<O-A-O>		-

APPENDIX C7. REFINEMENT DETAILS FOR *Pnma* AMPHIBOLES

	#F_o	#F_o>O	R_o	R_o^w	R_{all}	R_{all}^w	B	Abs	Wts
[23]	2656	2124	4.4	2.7	6.3	4.0	A	Yes	w
[31]	2969	1160	5.6	-	-	-	M	Yes	-
[32]	-	1417	7.6	-	-	-	I	Yes	1
[33]	-	1503	7.2	-	-	-	I	Yes	1
[47]	-	580	9.4	-	-	-	I	-	-

B: temperature-factor type, I: isotropic, A: anisotropic, 1: unit weights, w: statistical weights.

APPENDIX D. MODERN VARIETIES

[20]	Protoamphibole	Gibbs *et al.* (1960), Gibbs (1962, 1964, 1969)
(25)	Joesmithite	Moore (1968b, 1969)
(27)	Tirodite $P2_1/m$	Papike *et al.* (1968, 1969)

APPENDIX D1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	[20]	(25)	(27)
SiO_2	60.6	40.29	58.31
TiO_2	–	–	–
Al_2O_3	0.3	0.77	0.06
Fe_2O_3	–	13.04	–
FeO	–	2.70	0.13
MnO	–	2.89	8.24
MgO	33.4	12.40	27.17
CaO	–	12.40	2.46
PbO	–	6.71	–
BaO	–	1.03	–
Na_2O	0.1	–	0.22
K_2O	–	–	–
Li_2O	2.3	–	–
H_2O	0.2	6.50	–
F	5.2	–	–
	102.1	98.76	96.59
$O \equiv F$	2.2	–	–
Total	99.9	98.76	96.59
Si	7.84	6.0	8.02
Al	0.04	2.0Be	–
$\sum iv$	7.88	8.0	8.02
a(Å)	9.330(5)	9.885(15)	9.550(1)
b(Å)	17.879(8)	17.875(18)	18.007(3)
c(Å)	5.288(3)	5.227(5)	5.298(1)
β(°)	90	105.67(17)	102.65(2)
V(Å^3)	882.1	889.3	888.9(2)
Group	Pnmn	P2/a	$P2_1/m$

	[20]	(25)	(27)
Al	–	0.15	0.01
Ti^{3+}	–	–	–
Fe^{2+}	–	2.4	–
Fe	–		0.01
Mn	–	–	0.96
Mg	6.44	2.45	5.57
$\sum vi$		5.00	
Ca	–	2.0	0.36
Na	–	–	0.06
Li	0.56	–	–
$\sum M(4)$	7.00	2.0	6.97
Na	0.03	–	–
K	–	–	–
Li	0.64	–	–
Pb	–	0.4	–
Ca	–	0.6	–
$\sum A$	0.67	1.0	–
Basis	1	–	2

APPENDIX D2. ATOMIC POSITIONS

		[20]	(25)		(27)	
			A-set	B-set	A-set	B-set
O(1)	x	0.1155(4)	0.6375(12)	0.6434(14)	0.8661(7)	0.3623(6)
	y	0.0851(2)	0.1635(9)	0.3430(10)	0.3367(3)	0.8355(4)
	z	0.1659(7)	-0.2236(23)	-0.2231(26)	0.2056(10)	0.2196(10)
O(2)	x	0.1216(4)	0.6318(11)	0.6315(12)	0.8695(7)	0.3734(7)
	y	0.1726(2)	0.0795(9)	0.4253(9)	0.4232(3)	0.9206(3)
	z	0.6702(7)	0.2725(22)	0.2643(23)	0.7154(10)	0.7223(10)
O(3)	x	0.1032(5)	0.6423(13)		0.8595(10)	0.3650(11)
	y	0	0.2517(10)		1/4	3/4
	z	0.6640(9)	0.2872(24)		0.7083(15)	0.7106(15)
O(4)	x	0.1228(4)	0.3839(14)	0.3810(13)	0.1216(8)	0.6273(8)
	y	0.2511(2)	0.0037(10)	0.4977(10)	0.4982(4)	0.9972(3)
	z	0.1844(7)	0.2093(27)	0.2105(25)	0.7866(11)	0.7706(11)
O(5)	x	0.3475(5)	0.4054(13)	0.4030(13)	0.1001(7)	0.5997(7)
	y	0.1212(3)	0.1158(10)	0.3858(10)	0.3762(4)	0.8859(4)
	z	0.4292(9)	-0.1156(24)	-0.1198(25)	0.0534(11)	0.0834(10)
O(6)	x	0.3506(5)	0.4084(15)	0.4115(14)	0.1012(7)	0.5981(7)
	y	0.1308(3)	0.1363(10)	0.3630(10)	0.3743(4)	0.8682(4)
	z	0.9324(9)	0.3954(28)	0.3779(27)	0.5480(11)	0.5747(11)
O(7)	x	0.3494(6)	0.4151(15)		0.0977(10)	0.5907(11)
	y	0	0.2513(10)		1/4	3/4
	z	0.1592(11)	0.7121(28)		0.2908(17)	0.2742(17)
T(1)	x	0.2868(2)	0.4714(5)	0.4731(18)	0.0367(3)	0.5363(3)
	y	0.0847(1)	0.1691(4)	0.3315(13)	0.3348(1)	0.8340(1)
	z	0.1720(3)	0.6951(10)	0.6894(35)	0.2731(4)	0.2854(4)
T(2)	x	0.2941(2)	0.4620(5)	0.4594(5)	0.0438(3)	0.5462(3)
	y	0.1711(1)	0.0807(4)	0.4228(4)	0.4208(1)	0.9197(1)
	z	0.6694(3)	0.1896(9)	0.1799(9)	0.7805(4)	0.7915(4)
M(1)	x	0	3/4	3/4	0.7503(4)	
	y	0.0883(1)	0.1624(5)	0.3416(4)	0.3369(1)	
	z	1/2	1/2	1/2	0.4931(6)	
M(2)	x	0	3/4	3/4	0.7502(4)	
	y	0.1786(1)	0.0751(5)	0.4275(3)	0.4266(1)	
	z	0	0	0	0.9943(6)	
M(3)	x	0	3/4		0.7488(7)	
	y	0	0.2559(4)		1/4	
	z	0	0		0.9976(9)	
M(4)	x	0	1/4	1/4	0.7480(3)	
	y	0.2579(1)	0.0300(4)	0.4589(4)	0.5139(1)	
	z	1/2	1/2	1/2	0.4916(4)	
A	x	-	1/4		-	
	y	-	0.2836(1)		-	
	z	-	0		-	

APPENDIX D3. SITE POPULATIONS AND ANNOTATIONS

Protoamphibole[20]

M=M2=M3	Mg 0.53(5), 0.58(5), 0.55(5)	Å²
M4	0.25Li+0.75 Mg	0.55(6)
A	0.64Li+0.03Na	—
O3	1.0F	0.70(7)

Cation site-occupancies for the M sites established by successive difference-syntheses and supported by equality of isotropic temperature-factors. The A-site cations could not be located and were assumed to be randomly distributed around the periphery of the A-site cavity.

Joesmithite(25)

M(1)A	0.85Mg+0.15Al	0.19(9) Å²
M(1)B	0.32Mg+0.68Fe^{3+}	0.72(6)
M(2)A	0.74Mg+0.26Fe^{2+}	0.69(9)
M(2)B	1.0Fe^{3+}	0.53(5)
M(3)	0.55Mg+0.45Fe^{2+}	0.65(7)
M(4)A	1.0Ca	1.06(7)
M(4)B	1.0Ca	1.02(7)
A(2)	0.60Ca+0.40Pb	1.17(3)

Cation site-occupancies were assigned by unconstrained refinement of the total scattering-power at each site and comparison of the mean observed bond-lengths with ideal mean octahedral bond-lengths for the cation species involved. The relation between the site-nomenclature used here and that of Moore (1969) is shown in Table 71. The extremely small isotropic temperature-factor at the M(1)A site suggests that the refined total scattering-power at this site is too small. In addition, Moore (1969) indicated that these are only very approximate values because of the large standard deviations of the M–O bond lengths. The variation in mean bond-length (normalized to an anion co-ordination of $6O^{2-}$) with mean radius of the constituent cation shows considerable scatter from a linear model and also agrees poorly with Figure 44. These discrepancies are somewhat alleviated by assigning the Al and Fe^{3+} to the M(2)A site and some Fe^{2+} to the M(1)B site; however, a detailed assignment is not warranted at the present time as the chemical analysis (Moore 1968a, 1969) is of poor quality.

Tirodite $P2_1/m$(27)

M(1)	Mg	0.38 Å²
M(2)	Mg	0.37
M(3)	Mg	0.36
M(4)	0.49Mn+0.19Ca+0.01Fe +0.28Mg+0.03Na	0.95

No information given on the method of site-population assignment. The statistical equality of the isotropic temperature-factors at the M(1), M(2) and M(3) sites supports the assignment of Mg to these sites; Papike *et al.* (1969) also quoted an unpublished infrared absorption study that confirms this assignment. The structure of this sample has also been refined at 270°C, above the $P2_1/m \rightarrow C2/m$ transition; details are given in Appendix B, tirodite(41).

APPENDIX D4. CATION-ANION AND CATION-CATION DISTANCES (Å)

		[20]	(25)		(27)	
			A-set	B-set	A-set	B-set
T(1)-O(1)		1.592(4)	1.580(17)	1.632(25)	1.590(7)	1.621(6)
T(1)-O(5)		1.616(5)	1.638(17)	1.677(25)	1.607(7)	1.634(7)
T(1)-O(6)		1.623(5)	1.639(17)	1.674(25)	1.616(6)	1.636(6)
T(1)-O(7)		1.624(2)	1.582(17)	1.560(25)	1.628(4)	1.603(4)
⟨T(1)-O⟩		1.614	1.610	1.636	1.610	1.624
T(2)-O(2)		1.605(4)	1.615(17)	1.638(17)	1.624(7)	1.609(7)
T(2)-O(4)		1.592(4)	1.595(17)	1.575(17)	1.575(7)	1.610(7)
T(2)-O(5)		1.626(5)	1.671(17)	1.647(17)	1.637(6)	1.635(6)
T(2)-O(6)		1.655(5)	1.647(17)	1.644(17)	1.676(7)	1.635(7)
⟨T(2)-O⟩		1.620	1.632	1.626	1.628	1.622
M(1)-O(1)	x2	2.072(4)	2.050(17)	2.009(17)	2.069(7)	2.047(7)
M(1)-O(2)	x2	2.094(4)	2.052(17)	2.080(17)	2.123(6)	2.093(6)
M(1)-O(3)	x2	2.043(4)	2.070(17)	2.077	2.077(6)	2.075(6)
⟨M(1)-O⟩		2.070	2.075	2.055	2.082	
M(2)-O(1)	x2	2.179(4)	2.095(17)	2.025(17)	2.134(6)	2.143(6)
M(2)-O(2)	x2	2.084(4)	2.075(17)	2.040(17)	2.055(7)	2.106(8)
M(2)-O(4)	x2	1.989(4)	2.034(17)	1.975(17)	2.014(7)	2.013(6)
⟨M(2)-O⟩		2.084	2.068	2.013	2.078	
M(3)-O(1)	x4	2.062(4)	2.152(17)	2.055(17)	2.090(6)	2.070(7)
M(3)-O(3)	x2	2.021(4)	2.066(17)		2.043(11)	2.076(11)
⟨M(3)-O⟩		2.048	2.091		2.073	
M(4)-O(2)		2.107(4)	2.423(17)	2.532(17)	2.195(6)	2.208(6)
M(4)-O(4)		2.029(4)	2.313(17)	2.340(17)	2.139(8)	2.074(8)
M(4)-O(5)		3.442	2.653(17)	2.509(17)	3.209(6)	2.932(6)
M(4)-O(6)		2.453(5)	2.604(17)	2.539	2.511(8)	2.650(8)
⟨M(4)-O⟩		2.196^{VI}	2.498	2.480	2.296^{VI}	
A-O(5)	x2	3.445	3.493(17)	2.560(17)	2.733(7)	2.919(7)
A-O(6)	x2	2.746	3.453(17)	2.594(17)	3.357(7)	3.206(6)
A-O(7)		1.638 x2	2.559(17) x2		2.339(10)	2.322(11)
A-O(7)		–	–		3.720(8)	2.813(9)
⟨A-O⟩		2.377^{VI}	2.571^{VI}		3.052	
M(1)-M(1)		3.150(6)	3.203		3.129(4)	
M(1)-M(2)		3.099(3)	3.044	3.031	3.108(4)	3.097(4)
M(1)-M(3)		3.079(3)	3.102	3.029	3.100(5)	3.054(5)
M(1)-M(4)		3.035(3)	3.439	3.566	3.183(2)	
M(2)-M(3)		3.193	3.232	3.067	3.180(2)	
M(2)-M(4)		3.001(3)	3.219	3.310	3.085(3)	3.069(3)
T(1)-T(2)		3.075(3)	3.058	3.095	3.088(3)	3.075(3)
T(1)-T(2)		3.052(3)	3.052	3.073	3.046(3)	3.055(3)
T(1)-T(1)		3.029(6)	2.903		3.051(3)	3.021(3)

APPENDIX D5. ANION - ANION DISTANCES (Å)

		[20]	(25)		(27)	
			A-set	B-set	A-set	B-set
O(1)-O(5)		2.650(6)	2.647	2.686	2.634(10)	2.684(9)
O(1)-O(6)		2.642(6)	2.626	2.674	2.647(8)	2.665(8)
O(1)-O(7)		2.654(7)	2.648	2.735	2.679(10)	2.634(10)
O(5)-O(6)		2.633	2.590	2.681	2.617(9)	2.625(8)
O(5)-O(7)		2.595(8)	2.595	2.574	2.598(8)	2.655(7)
O(6)-O(7)		2.628(8)	2.629	2.647	2.615(9)	2.648(9)
⟨O-O⟩ T(1)		2.634	2.623	2.666	2.629	2.652
O(2)-O(4)		2.742(6)	2.741	2.740	2.714(10)	2.752(10)
O(2)-O(5)		2.624(6)	2.663	2.680	2.654(8)	2.628(8)
O(2)-O(6)		2.650(6)	2.662	2.649	2.704(10)	2.615(10)
O(4)-O(5)		2.661(6)	2.672	2.689	2.644(10)	2.649(9)
O(4)-O(6)		2.495(6)	2.549	2.552	2.550(10)	2.534(9)
O(5)-O(6)		2.667	2.688	2.612	2.679(9)	2.709(8)
⟨O-O⟩ T(2)		2.640	2.663	2.654	2.658	2.648
$O(1^u)$-$O(2^d)$	x2	2.851(5)	2.799	2.724	2.836	2.801
$O(1^u)$-$O(2^u)$	x2	3.092	3.019	3.031	2.771	3.054
$O(1^u)$-$O(3^d)$	x2	2.704(5)	2.779	2.765	2.817	2.712
$O(1^u)$-$O(3^u)$	x2	3.043(5)	3.015	3.033	3.100	3.018
O(2)-O(2)		2.903(1)	2.849	2.905	2.899	
O(2)-O(3)	x2	3.091(6)	3.080	3.106	3.120	3.073
O(3)-O(3)		2.597(10)	2.631	2.631	2.727	
⟨O-O⟩ M(1)		2.922	2.905	2.905	2.911	
O(1)-$O(1)_d$		2.789(1)	2.757	2.688	2.771	
$O(1^u)$-$O(2^d)$	x2	2.851(5)	2.799	2.724	2.836	2.801
$O(1^u)$-$O(2^u)$	x2	3.054(5)	3.010	2.972	3.035	3.070
O(1)-$O(4)_d$	x2	2.974(5)	2.999	2.860	2.975	3.014
$O(2^u)$-$O(4^d)$	x2	2.786	2.996	2.904	2.790	2.897
$O(2^u)$-$O(4^u)$	x2	3.059(5)	2.893	2.811	2.979	3.067
O(4)-O(4)		3.009	2.944	2.911	2.965	
⟨O-O⟩ M(2)		2.937	2.925	2.845	2.933	
$O(1^u)$-$O(1^d)$	x2	2.789(10)	2.757	2.688	2.771	
$O(1^u)$-$O(1^u)$	x2	3.039(10)	3.209		3.122	3.079
$O(1^u)$-$O(3^d)$	x4	2.704(5)	2.779	2.765	2.817	2.712
$O(1^u)$-$O(3^u)$	x4	3.061(5)	3.090	3.130	3.051	3.110
⟨O-O⟩ M(3)		2.893	2.949		2.927	
O(2)-$O(2)_d$		2.896	2.849	2.905	2.899	
$O(2^u)$-$O(4^d)$	x2	2.786	2.996	2.904	2.790	2.897
$O(2^u)$-$O(4^u)$	x2	2.927	3.130	3.103	3.030	3.000
$O(2^u)$-$O(5^u)$	x2	-	3.577	3.457	-	
$O(2^u)$-$O(6^u)$	x2	3.743	-	-	3.937	4.146
$O(4^u)$-$O(5^d)$	x2	-	3.417	3.375	-	
$O(4^u)$-$O(6^d)$	x2	3.876	-	-	4.122	4.229
$O(4^u)$-$O(6^u)$	x2	2.498	2.549	2.552	2.551	2.535
$O(5^u)$-$O(6^d)$	x2	-	3.073	3.064	-	
$O(5^u)$-$O(6^u)$	x2	-	2.590	2.681	-	
O(6)-O(6)		2.878	3.575	3.747	3.082	
⟨O-O⟩ M(4)		3.120	3.068	3.058	3.268	

APPENDIX D6. INTERATOMIC ANGLES (°)

		[20]	(25)		(27)	
			A-set	B-set	A-set	B-set
O(1)-T(1)-O(5)		111.4	110.8	108.8	110.9(3)	111.0(3)
O(1)-T(1)-O(6)		110.5	109.5	107.9	111.2(4)	109.7(4)
O(1)-T(1)-O(7)		111.2	113.5	117.8	111.7(4)	109.5(4)
O(5)-T(1)-O(6)		108.8	105.1	106.5	108.6(4)	106.7(3)
O(5)-T(1)-O(7)		106.6	107.7	105.6	106.8(4)	110.2(4)
O(6)-T(1)-O(7)		108.2	109.8	109.8	107.4(4)	109.7(4)
<O-T(1)-O>		109.5	109.4	109.4	109.4	109.5
O(2)-T(2)-O(4)		118.2	117.2	116.9	116.0(4)	117.4(4)
O(2)-T(2)-O(5)		108.6	108.5	109.0	108.8(3)	108.2(3)
O(2)-T(2)-O(6)		108.8	109.0	107.6	110.0(3)	107.4(3)
O(4)-T(2)-O(5)		111.6	110.1	112.8	110.7(3)	109.4(3)
O(4)-T(2)-O(6)		100.5	103.4	104.8	103.2(4)	102.6(4)
O(5)-T(2)-O(6)		108.7	108.3	104.8	107.8(4)	111.9(3)
<O-T(2)-O>		109.4	109.4	109.3	109.4	109.5
T(1)-O(5)-T(2)		140.6	135.7	135.3	139.8(5)	138.4(4)
T(1)-O(6)-T(2)		140.9	137.3	137.7	139.4(4)	140.2(4)
T(1)-O(7)-T(1)		137.1	135.0		137.9(6)	141.0(7)
O(5)-O(6)-O(5)		172.5	164.0	161.9	178.4(4)	166.2(4)
$O(1^u)$-M(1)-$O(2^d)$	x2	86.4	86.0	83.4	85.9(3)	84.4(3)
$O(1^u)$-M(1)-$O(2^u)$	x2	96.0	94.8	95.5	95.8(3)	95.1(3)
$O(1^u)$-M(1)-$O(3^d)$	x2	82.2	85.0	85.2	85.7(3)	82.2(3)
$O(1^u)$-M(1)-$O(3^u)$	x2	95.4	94.2	95.9	96.8(3)	94.1(4)
O(2)-M(1)-O(2)		87.8	87.7	88.3	86.9(2)	
O(2)-M(1)-O(3)	x2	96.8	96.6	96.5	95.9(2)	95.0(3)
O(3)-M(1)-O(3)		78.6	79.0	78.6	82.1(2)	
<O-M(1)-O>		90.0	90.0	90.0	90.0	
O(1)-M(2)-O(1)		79.6	82.2	83.3	80.8(2)	
$O(1^u)$-M(2)-$O(2^d)$	x2	83.9	84.3	84.3	84.0(2)	83.7(2)
$O(1^u)$-M(2)-$O(2^u)$	x2	91.4	92.4	94.1	92.8(3)	92.5(3)
O(1)-M(2)-O(4)	x2	90.9	93.0	91.3	91.6(3)	92.9(3)
$O(2^u)$-M(2)-$O(4^d)$	x2	86.4	93.6	92.6	86.6(3)	89.3(3)
$O(2^u)$-M(2)-$O(4^u)$	x2	97.5	89.4	88.9	94.1(3)	96.2(3)
O(4)-M(2)-O(4)		98.5	92.5	94.9	94.8(3)	
<O-M(2)-O>		89.9	90.0	90.0	89.9	
$O(1^u)$-M(3)-$O(1^d)$	x2	85.1	79.7	81.6	83.6	
$O(1^u)$-M(3)-$O(1^u)$	x2	95.0	99.4		96.7(3)	96.1(3)
$O(1^u)$-M(3)-$O(3^d)$	x4	82.9	82.5	84.3	85.1(3)	82.5(3)
$O(1^u)$-M(3)-$O(3^u)$	x4	97.1	94.3	98.9	95.2(3)	97.2(3)
<O-M(3)-O>		90.0	90.0		90.0	
O(2)-M(4)-O(2)		87.0	72.1	70.1	82.4	
$O(2^u)$-M(4)-$O(4^d)$	x2	84.8	78.4	73.0	81.6	83.6
$O(2^u)$-M(4)-$O(4^u)$	x2	90.2	82.7	79.0	88.7	88.9
$O(2^u)$-M(4)-$O(5^u)$	x2	-	89.5	86.5	-	
$O(2^u)$-M(4)-$O(6^u)$	x2	110.1	-	-	113.4	116.9
$O(4^u)$-M(4)-$O(5^d)$	x2	-	86.4	87.9	-	
$O(4^u)$-M(4)-$O(6^d)$	x2	119.3	-	-	127.8	123.7
$O(4^u)$-M(4)-$O(6^u)$	x2	66.9	61.9	62.8	66.0	63.5
$O(5^u)$-M(4)-$O(6^d)$	x2	-	71.3	74.7	-	
$O(5^u)$-M(4)-$O(6^u)$	x2	-	58.8	64.1	-	
O(6)-M(4)-O(6)		71.7	86.7	95.1	73.3	
<O-M(4)-O>		91.8	76.0	76.3	92.5	
O(7)-O(7)-O(7)		—	—		60.4(2)	
Δ		—	—		0.329	

APPENDIX D7. REFINEMENT DETAILS FOR VARIETY STRUCTURES

	#F_o	#F_o >0	R_o	R_o^w	R_{all}	R_w	B	Abs	Wts
[20]	~640		5.3	-	-	-	I	Yes	w
(25)	·3246	1604	12.8	-	-	-	I	Yes	-
(27)	-	1860	5.5	-	-	-	A	Yes	1

I: isotropic, A: anisotropic, 1: unit weights, w: statistical weights.

APPENDIX E. PRELIMINARY DATA

(P1)	Cummingtonite	Sueno *et al.* (1972b)
(P2)	Kozulite	Kitamura & Morimoto (1972)
(P3)	Potassium-fluor-richterite	Cameron *et al.* (1973a)
(P4)	Fluor-richterite	Cameron *et al.* (1973b)
[P5]	Holmquistite	Finger & Ohashi (1974a, b)

APPENDIX E1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	(P2)	(P3)	(P4)	(P5)	
SiO_2	51.38	–	–	59.58	62.8
TiO_2	–	–	–	0.02	<0.02
Al_2O_3	1.69	–	–	7.19	8.76
Fe_2O_3	2.85	–	–	9.35	11.2
FeO	–	–	–	4.88	
MnO	27.96	–	–	0.41	0.52
MgO	2.71	–	–	11.66	12.7
CaO	1.12	–	–	0.06	<0.02
Na_2O	8.41	–	–	0.50	0.23
K_2O	1.36	–	–	0.27	<0.02
H_2O	2.16	–	–	2.26	–
F	0.08	–	–	0.21	–
	99.75			99.92	96.2
O≡F	0.03	–	–	0.10	–
Total	99.72	–	–	99.82	96.2
Si	8.00	8.00	8.00	7.95	7.98
Al	–	–	–	0.05	0.02
$\sum iv$	8.00	8.00	8.00	8.00	8.00
Al	0.31	–	–	1.08	1.29
Ti	–	–	–	–	–
Fe_{2+}^{3+}	0.33	–	–	0.94	1.19
Fe	–	–	–	0.54	
Mn	3.69	–	–	0.05	0.06
Mg	0.63	5.00	5.00	2.32	2.40
$\sum vi$	4.96	5.00	5.00	4.93	4.94
$\sum vi_{-5}$	–	–	–	–	–
Ca	0.19	1.00	1.00	0.01	–
Li	–	–	–	1.90	–
Na	1.81	1.00	1.00	0.10	0.06
$\sum M(4)$	2.00	2.00	2.00	2.00	–
Na	0.73	–	1.00	0.03	–
K	0.27	1.00	–	0.05	–
$\sum A$	1.00	1.00	1.00	0.08	–

	(P1)	(P1)	(P1)	(P2)	(P3)	(P3)
Temperature (°C)	270	400	550	24	24	400
a(Å)	9.584(2)	9.598(1)	9.615(1)	9.914	9.944(1)	9.988(1)
b(Å)	18.058(3)	18.079(2)	18.101(2)	18.111	17.972(3)	18.056(2)
c(Å)	5.303(1)	5.307(1)	5.311(1)	5.308	5.260(1)	5.272(1)
β(°)	102.64(2)	102.59(1)	102.55(1)	104.50	104.80(1)	104.70(1)
V(Å^3)	895.5	898.7	902.2	921.3	908.9(2)	919.7(2)

	(P3)	(P4)	(P4)	(P4)	(P4)	(P4)	(P5)
Temperature (°C)	600	24	400	600	800	900	24
a(Å)	10.013(1)	9.824(2)	9.855(2)	9.883(2)	9.904(1)	9.915(1)	18.321(5)
b(Å)	18.107(2)	17.952(4)	18.036(3)	18.087(2)	18.131(2)	18.149(1)	17.635(5)
c(Å)	5.278(1)	5.258(1)	5.270(1)	5.278(1)	5.284(1)	5.286(1)	5.272(3)
β(°)	104.64(1)	104.23(1)	104.10(1)	104.08(1)	104.03(1)	104.02(1)	90
V(Å^3)	925.9(2)	899.0(3)	908.4(3)	915.2(4)	920.6(2)	923.0(2)	1703(1)

APPENDIX E2. ATOMIC POSITIONS (FOR HOLMQUISTITE (P5) ONLY)

	x	y	z
01A	0.1809(4)	0.1587(4)	0.0531(12)
02A	0.1839(4)	0.0762(4)	-0.4120(13)
03A	0.1818(6)	1/4	-0.4434(17)
04A	0.1883(4)	0.0046(4)	0.0647(13)
05A	0.2025(4)	-0.1205(4)	0.3340(12)
06A	0.1955(4)	-0.1340(4)	-0.1671(12)
07A	0.2049(6)	-1/4	0.5415(18)
01B	0.0696(4)	0.1581(4)	-0.2651(12)
02B	0.0654(4)	0.0753(4)	0.2007(12)
03B	0.0686(6)	1/4	0.2350(18)
04B	0.0644(4)	0.0019(4)	-0.2728(13)
05B	0.0467(4)	-0.1160(4)	0.0494(12)
06B	0.0532(4)	-0.1369(4)	-0.4516(12)
07B	0.0440(6)	-1/4	0.2389(18)
T1A	0.2302(2)	-0.1624(2)	-0.4327(5)
T2A	0.2266(2)	-0.0768(2)	0.0725(5)
T1B	0.0194(2)	-0.1630(2)	0.2759(5)
T2B	0.0240(2)	-0.0779(1)	-0.2176(5)
M1	0.1253(2)	0.1602(1)	0.3943(6)
M2	0.1255(1)	0.0685(1)	-0.1038(4)
M3	0.1254(2)	1/4	-0.1049(8)
M4	0.1245(13)	-0.0068(9)	0.3963(42)

Appendix E3. Site Populations and Annotations

Cummingtonite(P1)

No details of chemistry or site occupancy given; the difference in cell dimensions at 270°C indicates that this cummingtonite is different from tirodite(41).

Kozulite(P2)

M(1) 0.78Mn*+0.22Mg*
M(2) 0.95Mn*+0.05Mg*
M(3) 0.58Mn*+0.42Mg*
M(4) 0.91Na+0.09Ca
A 0.73Na+0.27K
O(3) OH

where Mn* = (Mn+Fe) and Mg* = (Mg+Al). Site populations were assigned using difference-Fourier maps. The chemical composition was reported by Nambu *et al.* (1969) and includes ZnO 0.03 wt. %; space group is $C2/m$.

Potassium-fluor-richterite(P3)

In this synthetic amphibole, presumably M(1) = M(2) = M(3) = Mg, M(4) = 0.5 Ca + 0.5 Na and A = K. The K at the A site is positionally disordered in the A(m) positions. Mean bond-lengths for each of the M polyhedra increase linearly with temperature, <M(4)–O> having the greatest rate of increase. Mean Si–O bond-lengths remain constant over the temperature range 24–600°C.

Fluor-richterite(P4)

In this synthetic amphibole, presumably M(1) = M(2) = M(3) = Mg, M(4) = 0.5 Ca + 0.5 Na, A = Na by analogy with fluor-richterite (34). Note that different cell-dimensions are given by Cameron & Gibbs (1971) (see Appendix B1) and Cameron *et al.* (1973b) (see Appendix E1); these are two different structural refinements. The Na at the A site is positionally disordered in the A(1) positions. Mean bond-lengths for each of the four M sites increase linearly with increasing temperature; mean bond-lengths for the T(1) and T(2) tetrahedra remain constant over the temperature range studied (24–900°C). The cell constants given by Cameron *et al.* (1973a, b) for potassium-fluor-richterite(P3) and fluor-richterite(P4) are in the $I2/m$ orientation; values given in Appendix E1 have been transformed to the standard $C2/m$ setting.

Holmquistite[P5]

M1 0.88(1)Mg+0.12Fe*
M2 0.72(1)Al+0.28Fe*
M3 0.87(1)Mg+0.13Fe*
M4 Li

The site occupancies were derived from unconstrained site-occupancy refinement, presumably assuming that no Mg occurs at M2, and the M4 site is completely occupied by Li. During refinement, use of the cell contents calculated from the original chemical analysis (Sundius 1946a) led to unsatisfactory temperature-factors, and examination of the mineral showed inclusions of magnetite, alkali feldspar and apatite. A partial microprobe analysis gave different values but the cell contents derived from this partial analysis were not satisfactory either, resulting in high temperature-factors at M1, M3 and M4 and a low temperature-factor at M2. Note that the unconstrained refinement gives a cell content considerably different from both chemical analyses (Finger & Ohashi 1974a, b); this problem might be alleviated somewhat if the requirement that the M2 site contain only trivalent cations be relaxed. Certainly the isotropic temperature-factors for M1, M2 and M3 are rather small in the unconstrained refinement, suggesting that an increase in total Fe, as indicated by both analyses, is not unreasonable. Note that the microprobe analysis, when combined with the values of Sundius (1946a) for Li_2O, H_2O and F, gives a total of ~102%. Gravimetric analysis includes 3.52 wt. % Li_2O.

Appendix F. Mössbauer Spectral Studies of Amphiboles

The following studies are considered here:

Bancroft *et al.* (1967a)	{1} – {7}
Bancroft *et al.* (1966)	{1}, {6}, {8}, {9}
Bancroft *et al.* (1967b)	{8} – {11}
Häggström *et al.* (1969)	{12} – {14}
Bancroft & Burns (1969)	{15} – {21}
Ernst & Wai (1970)	{15}, – {22} – {31}
Burns & Greaves (1971)	{10}, {11}, {32} – {37}
Hafner & Ghose (1971)	{4} – {6}, {38} – {61}
Buckley & Wilkins (1971)	{62}
Babeshkin *et al.* (1971)	{63}
Ghose & Weidner (1972)	{1}, {60}, {61}
Virgo (1972a)	{64}
Law (1973)	{65}
Kamineni (1973)	{66}
Semet (1973)	{67}, {68}
Litvin *et al.* (1973c)	{69}
Barabanov & Tomilov (1973)	{70} - {77}
Seifert & Virgo (1974)	{78}
Borg *et al.* (1973)	{17}, {79}, {80}
Hawthorne & Grundy (1975)	{81}
Bancroft & Brown (1975)	{34}, {82} – {87}
Batievskii *et al.* (1975)	{88} – {92}
Goodman & Wilson (1976)	{93}
Litvin *et al.* (1976)	{94}, {95}
Goldman & Rossman (1977a)	{96}
Hawthorne & Grundy (1977b)	{97}
Seifert (1977, 1978)	{78}, {98} – {103}
Tripathi & Lokanathan (1978)	{104} – {114}
Goldman (1979)	{115} – {119}
Stroink *et al.* (1980)	{120} – {122}
Law & Whittaker (1981)	{65}

Early Mössbauer work on amphiboles was qualitative only and concerned with oxidation–dehydroxylation of fibrous amphiboles; the results of these studies have been superceded by more recent precise data, and are not reproduced here. Data for heated amphiboles, together with data for some synthetic amphiboles where conditions of synthesis or annealing (or both) appear to have affected cation ordering and oxidation state, are included as a separate section in each appendix. Each specific amphibole is identified by a number in curly brackets, the latter .indicating that this amphibole has been studied by Mössbauer spectroscopic methods. Additional data on the same sample, either recorded by different authors, recorded at different temperatures or recorded after heating, are indicated by lower-case letters following the sample number. All studies are at room temperature unless otherwise specified. Isomer shifts are referred to a variety of standards; in this compilation, all have been normalized to metallic iron by subtraction of the following conversion factors (stainless steel: 0.10 mm/s, sodium nitroprusside: 0.26 mm/s, ^{57}Co in Pd: –0.185 mm/s).

APPENDIX F1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	{1}	{2}	{3}	{4}	{5}	{6}	{7}	{8}	{9}
SiO_2	54.7	52.9	51.95	49.0	49.01	48.0	55.10	56.27	50.06
TiO_2	–	0.06	0.02	–	0.05	–	0.00	–	0.20
Al_2O_3	0.28	2.37	0.15	0.2	0.00	<0.1	0.10	2.07	7.28
Fe_2O_3	–	0.0	–	–	–	–	–	0.40	0.96
FeO	20.40	28.0	33.70	41.2	44.99	46.3	11.08	13.81	18.42
MnO	0.56	0.97	0.99	0.68	0.37	0.57	13.17	0.59	0.57
MgO	20.00	13.71	10.44	3.0	3.17	0.52	17.00	23.99	18.40
CaO	0.85	0.55	0.10	1.0	0.31	0.65	1.22	1.15	0.87
Na_2O	0.04	<0.1	0.08	0.02	0.04	–	0.13	–	0.76
K_2O	0.01	–	0.05	0.02	0.00	–	0.02	–	0.02
H_2O	–	1.04	2.76	–	1.59	–	2.48	1.83	2.38
F	–	–	–	–	1.00	–	0.23	–	–
	96.84	99.60	100.24	95.12	100.62	96.14	100.53	100.11	100.00
O≡F	–	–	–	–	0.42	–	0.10	–	–
Total	96.84	99.60	100.24	95.12	100.20	96.14	100.43	100.11	100.00
Si	7.95	7.83	7.92	8.11	8.00	8.07	8.02	7.86	7.20
Al	0.05	0.17	0.02	–	–	–	–	0.14	0.80
Σiv	8.00	8.00	7.94	8.11	8.00	8.07	8.02	8.00	8.00
Al	–	0.24	–	0.15	–	0.08	0.02	0.19	0.44
Ti^{3+}	–	0.01	–	–	–	–	–	–	0.03
Fe^{2+}	–	–	–	–	–	–	–	0.05	0.10
Fe	2.48	3.47	4.30	5.70	6.14	6.51	1.35	1.61	2.21
Mn	0.07	0.12	0.13	0.10	0.05	0.08	1.63	0.07	0.07
Mg	4.33	3.02	2.38	0.74	0.77	0.13	3.69	5.02	3.97
Σvi	–	–	–	–	–	–	–	–	–
Σvi-5	–	–	–	–	–	–	–	–	–
Ca	0.13	0.09	0.02	0.18	0.06	0.12	0.19	0.16	0.13
Na	–	0.01	0.02	0.01	0.01	–	0.03	–	–
$\Sigma M(4)$	7.01	6.96	6.85	6.87	7.02	6.92	6.91	7.10	7.15
Na	–	–	–	–	–	–	–	–	0.21
K_A	–	–	–	–	–	–	–	–	–
ΣA	–	–	–	–	–	–	–	–	0.21
a(Å)	–	–	9.545(4)	–	9.562(2)	9.586	9.573(3)	–	–
b(Å)	–	–	18.258(14)	–	18.380(7)	18.448	18.115(5)	–	–
c(Å)	–	–	5.320(11)	–	5.338(4)	5.344	5.304(7)	–	–
β(°)	–	–	101.96(9)	–	101.86(3)	101.95	102.35(6)	–	–
V(Å^3)	–	–	907(1)	–	918.2(7)	924.6	898.5(8)	–	–
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	Pnma	Pnma

	{10}	{11}	{12}	{13}	{14}	{15}	{16}	{17}	{18}
SiO_2	56.00	55.0	42.7	49.7	51.5	58.04	56.38	55.38	52.16
TiO_2	0.08	0.05	1.1	0.04	0.4	0.66	0.11	0.36	0.04
Al_2O_3	2.30	0.6	10.4	5.5	2.8	10.31	8.45	5.29	4.51
Fe_2O_3	1.40	1.83	–	5.30	–	2.89	4.98	9.74	10.53
FeO	4.22	19.60	15.9	4.80	6.4	6.12	9.40	13.07	18.19
MnO	0.11	0.29	–	0.12	–	0.07	0.19	0.18	0.51
MgO	20.00	11.0	11.4	18.4	20.1	11.71	9.89	6.31	3.93
CaO	11.10	10.0	11.9	12.1	11.6	1.37	1.29	1.10	1.19
Na_2O	1.10	0.24	1.6	2.2	1.8	6.97	6.77	6.40	6.27
K_2O	0.10	0.04	0.9	0.8	0.6	0.02	0.08	0.05	0.09
H_2O	–	–	–	–	–	1.98	1.90	2.08	2.30
F_2	–	–	–	–	–	–	–	–	–
	96.40	98.65	95.90	98.96	95.20	100.14	99.44	99.96	99.72
O≡F	–	–	–	–	–	–	–	–	–
Total	96.40	98.65	95.90	98.96	95.20	100.14	99.44	99.96	99.72
Si	7.85	8.05	6.53	7.02	7.47	7.92	7.94	8.00	7.84
Al	0.15	–	1.47	0.92	0.47	0.08	0.06	–	0.16
Σiv	8.00	8.05	8.00	7.94	7.94	8.00	8.00	8.00	8.00
Al	0.23	0.10	0.40	–	–	1.58	1.34	0.90	0.74
Ti^{3+}	0.02	0.01	0.11	–	0.05	0.06	0.01	0.04	0.01
Fe^{2+}	0.15	0.20	–	0.56	–	0.30	0.53	1.06	1.20
Fe	0.48	2.40	2.03	0.56	0.72	0.70	1.11	1.58	2.29
Mn	0.01	0.04	–	0.01	–	0.01	0.02	0.02	0.07
Mg	4.18	2.40	2.59	3.88	4.34	2.38	2.08	1.36	0.88
Σvi	5.07	5.15	5.13	5.01	5.11	5.03	5.09	4.96	5.19
$\Sigma vi-5$	0.07	0.15	0.13	0.01	0.11	0.03	0.09	–	0.19
Ca	1.67	1.57	1.95	1.83	1.79	0.20	0.20	0.17	0.19
Na	0.26	0.07	–	0.16	0.10	1.77	1.71	1.79	1.62
$\Sigma M(4)$	2.00	1.79	2.08	2.00	2.00	2.00	2.00	1.96	2.00
Na	0.04	–	0.45	0.43	0.40	0.07	0.14	–	0.21
K_A	0.02	0.01	0.16	0.13	0.10	–	0.01	0.01	0.01
ΣA	0.06	0.01	0.61	0.56	0.50	0.07	0.15	0.01	0.22
a(Å)	–	–	–	–	–	9.554	9.609(2)	9.647(1)	–
b(Å)	–	–	–	–	–	17.738	17.813(4)	17.905(3)	–
c(Å)	–	–	–	–	–	5.298	5.311(2)	5.316(1)	–
β(°)	–	–	–	–	–	103.72	103.61(2)	103.60(1)	–
V(Å^3)	–	–	–	–	–	872.3	883.5	892.5	–
Space group	C2/m	C2/m	C2/m	C2/m	C1/m	C2/m	C2/m	C2/m	C2/m

	{19}	{20}	{21}	{22}	{23}	{24}	{25}	{26}	{27}
SiO_2	51.19	56.10	53.5	55.19	55.36	54.88	54.56	55.10	55.44
TiO_2	0.03	tr	0.25	0.11	0.45	0.87	0.23	0.68	0.04
Al_2O_3	0.17	0.66	1.3	9.94	12.16	9.86	8.29	4.27	0.22
Fe_2O_3	16.55	15.60	14.5	4.63	1.56	4.35	7.94	10.61	16.77
FeO	21.27	4.06	6.99	9.21	12.11	12.02	10.31	9.78	5.23
MnO	0.32	-	0.13	0.16	0.16	0.14	0.13	0.48	0.09
MgO	1.30	14.5	12.5	9.75	7.23	7.69	8.74	8.86	12.30
CaO	0.83	0.11	2.25	1.69	1.02	1.95	0.81	1.43	2.17
Na_2O	6.14	5.45	6.42	6.57	6.75	5.62	6.71	6.38	6.76
K_2O	0.05	0.71	0.08	0.19	0.15	0.09	0.14	0.09	0.15
H_2O	2.26	-	2.57	2.51	2.63	2.35	2.25	2.02	0.60
F_2	-	-	-	-	-	-	-	-	-
	100.11	97.19	100.49	99.95	99.58	99.82	100.11	99.70	99.77
O≡F	-	-	-	-	-	-	-	-	-
Total	100.11	97.19	100.49	99.95	99.58	99.82	100.11	99.70	99.77
Si	7.94	7.94	7.71	7.74	7.79	7.76	7.75	7.93	7.90
Al	0.03	0.06	0.22	0.26	0.21	0.24	0.25	0.07	0.03
Σiv	7.97	8.00	7.93	8.00	8.00	8.00	8.00	8.00	7.93
Al	-	0.05	-	1.38	1.81	1.41	1.14	0.65	-
Ti^{3+}	-	-	0.03	0.01	0.05	0.09	0.03	0.07	0.01
Fe^{2+}	1.93	1.66	1.57	0.49	0.17	0.46	0.80	1.15	1.80
Fe	2.76	0.48	0.84	1.08	1.43	1.42	1.23	1.18	0.62
Mn	0.04	-	0.02	0.02	0.02	0.02	0.02	0.06	0.01
Mg	0.30	3.06	2.68	2.04	1.52	1.62	1.85	1.90	2.61
Σvi	5.03	5.25	5.14	5.02	4.98	5.02	5.05	5.01	5.05
$\Sigma vi-5$	0.03	0.25	0.14	0.02	-	0.02	0.05	0.01	0.05
Ca	0.14	0.17	0.35	0.25	0.15	0.30	0.12	0.22	0.34
Na	1.83	1.38	1.51	1.73	1.84	1.54	1.83	1.77	1.61
$\Sigma M(4)$	2.00	1.80	2.00	2.00	1.99	1.86	2.00	2.00	2.00
Na	0.02	-	0.28	0.06	-	-	0.02	0.01	0.26
K_A	0.01	0.13	0.02	0.03	0.03	0.02	0.02	0.02	0.03
Σ	0.03	0.13	0.30	0.09	0.03	0.02	0.04	0.03	0.29
a (Å)	-	9.72	9.742	9.591	9.551	9.592	9.617	9.673	9.727
b (Å)	-	17.95	17.955	17.814	17.781	17.834	17.862	17.923	17.958
c (Å)	-	5.31	5.287	5.306	5.310	5.308	5.312	5.316	5.306
β (°)	-	103.9	103.96	103.69	103.61	103.70	103.69	103.68	103.75
V (Å^3)	-	899	897.5	880.7	876.5	882.2	886.6	894.4	900.2
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{28}	{29}	{30}	{31}	{32}	{33}	{34}	{35}	{36}
SiO_2	49.95	51.94	51.97	52.05	56.16	52.60	43.82	50.61	52.28
TiO_2	0.11	–	0.19	0.44	–	0.08	0.68	0.09	0.05
Al_2O_3	4.23	0.20	2.01	0.40	0.20	3.13	14.85	2.42	0.18
Fe_2O_3	16.93	18.64	14.14	16.57	1.81	2.85	3.32	2.80	–
FeO	13.05	19.39	19.59	21.77	6.32	6.09	11.15	19.90	22.57
MnO	4.95	–	3.00	0.13	2.30	0.20	0.27	2.69	0.24
MgO	3.52	1.37	0.48	0.36	19.84	17.95	12.07	8.26	10.53
CaO	0.39	0.19	0.75	0.15	9.34	11.85	10.20	10.82	11.26
Na_2O	4.94	6.07	5.83	6.29	1.30	0.40	1.79	0.48	0.16
K_2O	0.32	0.04	0.34	0.20	0.14	0.25	0.12	0.14	0.07
H_2O	0.87	2.89	1.98	1.53	2.44	–	2.00	1.71	2.56
F	–	–	–	–	–	–	–	–	–
	99.26	100.73	100.28	99.89	99.87	95.40	100.27	99.89	100.20
O≡F	–	–	–	–	–	–	–	–	–
Total	99.26	100.73	100.28	99.89	99.87	95.40	100.27	99.89	100.20
Si	7.54	7.99	7.97	8.02	7.91	7.55	6.33	7.66	7.93
Al	0.46	0.01	0.03	–	0.03	0.45	1.67	0.34	0.03
Σiv	8.00	8.00	8.00	8.02	7.94	8.00	8.00	8.00	7.96
Al	0.29	0.02	0.33	0.07	–	0.08	0.86	0.09	–
Ti^{3+}	0.01	–	0.02	0.05	–	0.02	0.07	0.02	0.01
Fe^{2+}	1.92	2.15	1.63	1.92	0.19	0.31	0.36	0.32	–
Fe	1.65	2.49	2.51	2.80	0.75	0.73	1.35	2.51	2.86
Mn	0.63	–	0.39	0.02	0.27	0.01	0.03	0.34	0.03
Mg	0.79	0.32	0.11	0.08	4.18	3.83	2.60	1.86	2.38
Σvi	5.29	4.98	4.99	4.94	5.39	4.98	5.27	5.14	5.28
Σvi-5	0.29	–	–	–	0.39	–	0.27	0.14	0.28
Ca	0.06	0.04	0.12	0.03	1.44	1.82	1.58	1.75	1.83
Na	1.44	1.82	1.73	1.88	0.17	0.18	0.15	0.11	–
$\Sigma M(4)$	1.79	1.86	1.85	1.92	2.00	2.00	2.00	2.00	2.11
Na	–	–	–	–	0.19	0.21	0.37	0.03	0.05
K_A	0.06	–	0.07	0.04	0.03	0.04	0.02	0.03	0.01
ΣA	0.06	–	0.07	0.04	0.22	0.25	0.39	0.06	0.06
a (Å)	9.720	9.760	9.719	9.740	9.803(2)	–	–	9.891(1)	9.894(2)
b (Å)	18.018	18.070	18.014	18.045	18.083(5)	–	–	18.200(1)	18.198(5)
c (Å)	5.326	5.339	5.328	5.336	5.292(2)	–	–	5.305(1)	5.299(2)
β (°)	103.60	103.66	103.62	103.42	104.35(3)	–	–	104.64(1)	104.58(2)
V (Å^3)	906.6	914.9	906.5	912.5	908.9(4)	–	–	924.0(1)	923.5(4)
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{37}	{38}	{39}	{40}	{41}	{42}	{43}	{44}	{45}
SiO_2	-	52.0	49.0	51.0	48.0	49.33	50.0	48.0	54.0
TiO_2	-	<0.01	-	-	<0.01	0.02	0.02	<0.01	0.02
Al_2O_2	-	<0.1	<0.1	0.2	0.5	0.39	-	0.3	-
Fe_2O_2	-	-	-	-	-	-	-	-	-
FeO_3	-	45.6	43.8	40.5	38.6	40.94	38.6	37.3	38.6
MnO	-	1.10	0.79	0.69	0.68	0.54	0.53	0.63	0.83
MgO	-	1.40	2.30	4.3	4.4	6.65	6.0	6.40	7.3
CaO	-	0.65	0.70	1.0	1.1	0.18	0.81	0.73	0.75
Na_2O	-	0.30	-	-	-	0.12	-	-	-
K_2O	-	0.18	-	-	-	0.20	-	-	-
H_2O	-	-	-	-	-	1.54	-	-	-
F_2	-	-	-	-	-	-	-	-	-
	-	101.23	96.59	97.69	93.28	99.91	95.96	93.36	101.5
O≡F	-	-	-	-	-	-	-	-	-
Total	-	101.23	96.59	97.69	93.28	99.91	95.96	93.36	101.5
Si	8.00	8.17	8.08	8.13	8.03	7.92	8.07	7.97	8.13
Al	-	-	-	-	-	0.08	-	0.03	-
Σiv	8.00	8.17	8.08	8.13	8.03	8.00	8.07	8.00	8.13
Al	-	0.18	0.09	0.17	0.13	-	0.07	0.03	0.13
Ti_{3+}	-	-	-	-	-	-	-	-	-
Fe_{2+}	-	-	-	-	-	-	-	-	-
Fe	5.00	5.99	6.04	5.40	5.40	5.50	5.21	5.18	4.86
Mn	-	0.15	0.11	0.09	0.10	0.08	0.07	0.09	0.11
Mg	-	0.33	0.57	1.02	1.10	1.59	1.44	1.58	1.64
Σvi	5.00	-	-	-	-	-	-	-	-
$\Sigma vi-5$	-	-	-	-	-	-	-	-	-
Ca	2.00	0.11	0.12	0.17	0.20	0.03	0.14	0.13	0.12
Na	-	-	-	-	-	0.04	-	-	-
$\Sigma M(4)$	2.00	6.85	6.92	6.85	6.92	7.24	6.93	7.00	6.86
Na	-	-	-	-	-	-	-	-	-
K_A	-	0.04	-	-	-	0.04	-	-	-
Σ	-	0.04	-	-	-	0.04	-	-	-
a(Å)	9.87	9.593	9.588	9.576	9.572	9.551(1)	9.563	9.565	-
b(Å)	18.34	18.453	18.413	18.364	18.364	18.324(6)	18.333	18.332	-
c(Å)	5.30	5.343	5.340	5.335	5.342	5.328(4)	5.335	5.337	-
β(°)	104.5	101.95	101.97	102.02	102.05	101.86(2)	102.02	102.00	-
V($Å^3$)	939	925.1	922.1	917.7	921.9	912.5(6)	914.9	915.4	-
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{46}	{47}	{48}	{49}	{50}	{51}	{52}	{53}	{54}
SiO_2	50.0	53.0	51.0	51.58	51.0	54.0	52.28	51.0	46.0
TiO_2	<0.01	<0.01	–	–	–	<0.01	–	<0.01	–
Al_2O_3	0.2	<0.1	0.2	0.10	0.2	0.29	0.07	0.2	0.3
Fe_2O_3	–	–	–	–	–	–	–	–	–
FeO	36.7	36.7	34.1	34.40	34.1	32.2	31.90	28.3	28.3
MnO	1.05	0.63	1.6	0.70	0.55	0.47	0.57	0.85	1.45
MgO	7.2	8.5	8.4	10.33	10.5	10.5	12.35	11.5	12.0
CaO	0.78	0.95	0.63	0.97	1.0	0.65	0.79	1.0	2.5
Na_2O	–	–	0.05	0.02	–	0.06	0.12	–	–
K_2O	–	–	0.03	0.05	–	0.03	0.08	–	–
H_2O	–	–	–	1.99	–	–	1.62	–	–
F_2	–	–	–	–	–	–	–	–	–
	95.93	99.78	96.01	100.14	97.35	98.20	99.78	92.85	90.55
O≡F	–	–	–	–	–	–	–	–	–
Total	95.93	99.78	96.01	100.14	97.35	98.20	99.78	92.85	90.55
Si	8.01	8.07	8.06	7.95	7.92	8.16	8.00	8.09	7.67
Al	–	–	–	0.02	0.04	–	–	–	0.06
Σiv	8.01	8.07	8.06	7.97	7.96	8.16	8.00	8.09	7.73
Al	0.05	0.08	0.10	–	–	0.21	0.02	0.13	–
Ti^{3+}	–	–	–	–	–	–	–	–	–
Fe^{2+}	–	–	–	–	–	–	–	–	–
Fe	4.92	4.68	4.51	4.44	4.43	4.07	4.00	3.76	3.95
Mn	0.14	0.08	0.21	0.09	0.07	0.06	0.07	0.11	0.21
Mg	1.72	1.93	1.98	2.37	2.43	2.36	2.82	2.72	2.98
Σvi	–	–	–	–	–	–	–	–	–
Σvi_{-5}	–	–	–	–	–	–	–	–	–
Ca	0.13	0.16	0.11	0.16	0.17	0.11	0.13	0.17	0.45
Na	–	–	0.02	–	–	0.02	–	–	–
$\Sigma M(4)$	6.97	6.92	6.92	7.06	7.10	6.82	7.13	6.89	7.58
Na	–	–	–	–	–	–	0.04	–	–
K	–	–	0.01	–	–	0.01	0.02	–	–
ΣA	–	–	0.01	–	–	0.01	0.06	–	–
a(Å)	9.566	9.557	9.561	9.538(2)	9.549	9.539	9.534(2)	–	–
b(Å)	18.312	18.317	18.296	18.248(9)	18.271	18.268	18.231(5)	–	–
c(Å)	5.337	5.332	5.331	5.349(6)	5.327	5.327	5.324(4)	–	–
β(°)	102.02	101.98	102.08	101.97(3)	102.03	101.97	101.97(3)	–	–
$V(Å^3)$	914.5	913.0	911.8	910.7(9)	909.1	908.0	905.1(6)	–	–
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{55}	{56}	{57}	{58}	{59}	{60}	{61}	{62}	{63}	{65}
SiO_2	53.11	54.0	54.0	54.00	53.0	48.0	55.97	53.6	52.63	59.06
TiO_2	–	–	<0.01	–	–	<0.01	0.07	0.46	–	0.20
Al_2O_3	–	0.15	–	–	0.15	0.40	1.47	1.84	–	12.38
Fe_2O_3	–	–	–	–	–	–	0.01	1.26	–	2.36
FeO	28.17	25.7	25.7	26.53	24.4	20.0	10.5	17.4	36.74	10.84
MnO	2.59	1.40	1.40	0.59	1.7	1.35	0.37	1.29	0.70	0.25
MgO	13.26	13.5	15.0	15.52	16.0	18.5	26.14	18.8	7.36	8.82
CaO	0.88	0.45	0.53	1.34	1.0	2.2	1.25	2.25	0.61	0.21
Na_2O	–	–	–	–	–	–	0.32	0.51	0.07	0.11
K_2O	–	–	–	–	–	–	0.01	0.10	0.06	0.05
H_2O	1.99	–	–	2.02	–	–	–	2.00	1.82	2.16
F	–	–	–	–	–	–	–	0.18	–	0.18
	100.00	95.20	96.63	100.00	96.25	90.45	96.11	99.69	99.99	99.95
O≡F	–	–	–	–	–	–	–	0.08	–	0.08
Total	100.00	95.20	96.63	100.00	96.25	90.45	96.11	99.61	99.99	99.87
Si	8.00	8.20	8.09	8.00	7.97	7.64	7.83	7.74	8.16	7.89
Al	–	–	–	–	0.03	0.08	0.17	0.26	–	0.11
Σiv	8.00	8.20	8.09	8.00	8.00	7.72	8.00	8.00	8.16	8.00
Al	–	0.22	0.09	–	–	–	0.07	0.05	0.16	1.84
Ti^{3+}	–	–	–	–	–	–	0.01	0.05	–	0.02
Fe^{2+}	–	–	–	–	–	–	–	0.14	–	0.24
Fe	3.55	3.26	3.22	3.29	3.07	2.66	1.23	2.10	4.77	1.21
Mn	0.33	0.18	0.18	0.07	0.22	0.18	0.04	0.16	0.09	0.03
Mg	2.98	3.05	3.35	3.43	3.58	4.39	5.45	4.05	1.70	1.76
Σvi	–	–	–	–	–	–	–	–	–	Li=1.79
Σvi-5	–	–	–	–	–	–	–	–	–	–
Ca	0.14	0.07	0.09	0.21	0.16	0.38	0.19	0.35	0.10	0.03
Na	–	–	–	–	–	–	0.01	0.08	0.02	0.03
$\Sigma M(4)$	7.00	6.79	6.91	7.00	7.03	7.61	7.00	7.00	6.84	6.95
Na	–	–	–	–	–	–	0.08	0.06	–	–
K_A	–	–	–	–	–	–	–	0.02	0.01	0.01
Σ	–	–	–	–	–	–	0.08	0.08	0.01	0.01
a(Å)	–	9.521	–	–	9.530	9.516	9.49	–	–	18.29
b(Å)	–	18.189	–	–	18.174	18.139	18.00	–	–	17.67
c(Å)	–	5.322	–	–	5.314	5.311	5.30	–	–	5.28
β(°)	–	101.98	–	–	102.07	102.12	102.0	–	–	90
V(Å^3)	–	901.5	–	–	899.9	896.4	885.6	–	–	1706.4
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	$P2_1/m$	C2/m	C2/m	Pnma

	{66}	{67}	{67a}	{67b}	{68}	{69}	{70}	{71}	{72}
SiO_2	54.10	42.08	41.8	41.2	40.94	37.55	–	–	–
TiO_2	0.04	–	–	–	0.58	0.89	–	–	–
Al_2O_3	0.30	11.90	12.1	11.6	12.85	9.90	–	–	–
Fe_2O_3	1.66	–	–	–	–	11.89	–	–	–
FeO	25.42	8.39	8.4	8.5	10.57	21.40	–	–	–
MnO	0.78	–	–	–	0.26	1.25	–	–	–
MgO	14.71	18.82	19.1	18.5	16.01	1.31	–	–	–
CaO	0.58	13.09	13.2	12.9	12.93	7.28	–	–	–
Na_2O	0.11	3.62	3.5	3.5	2.59	4.05	–	–	–
K_2O	0.06	–	–	–	1.24	2.11	–	–	–
H_2O	1.92	(2.10)	(2.1)	(2.1)	(2.03)	1.84	–	–	–
F	–	–	–	–	–	–	–	–	–
	99.68	100.00	100.2	98.2	100.0	99.82	–	–	–
O≡F	–	–	–	–	–	–	–	–	–
Total	99.68	100.00	100.2	98.2	100.00	99.82	–	–	–
Si	8.04	6.00	–	–	5.95	6.14	7.89	7.91	7.81
Al	–	2.00	–	–	2.05	1.86	0.09	0.09	0.19
Σiv	8.04	8.00	–	–	8.00	8.00	7.98	8.00	8.00
Al	0.05	–	–	–	0.15	0.04	–	0.03	0.01
Ti^{3+}	–	–	–	–	0.06	0.11	–	–	0.03
Fe^{2+}	0.18	1.00	–	–	0.72	1.45	–	0.12	0.17
Fe	3.16	–	–	–	0.57	2.92	1.50	1.94	1.95
Mn	0.10	–	–	–	0.03	0.18	0.01	0.04	0.05
Mg	3.26	4.00	–	–	3.47	0.30	5.11	4.72	4.45
Σvi	–	5.00	–	–	5.00	5.00	–	–	–
Σvi_{-5}	–	–	–	–	–	–	–	–	–
Ca	0.09	2.00	–	–	2.01	1.27	0.31	0.14	0.30
Na	0.02	–	–	–	–	0.73	–	–	0.04
$\Sigma M(4)$	6.86	2.00	–	–	2.01	2.00	7.00	6.99	7.00
Na	–	1.00	–	–	0.73	0.55	–	–	–
K	0.01	–	–	–	0.23	0.45	–	0.01	–
ΣA	0.01	1.00	–	–	0.96	1.00	–	0.01	–
a(Å)	9.525(3)	–	9.926(5)	9.928(2)	9.940(3)	9.960(8)	–	–	–
b(Å)	18.202(4)	–	18.029(9)	18.015(9)	18.050(4)	18.177(8)	–	–	–
c(Å)	5.313(3)	–	5.297(4)	5.282(3)	5.310(4)	5.352(2)	–	–	–
β(°)	101.8(4)	–	105.46(5)	105.43(4)	105.45(4)	105.07(5)	–	–	–
V(Å^3)	901.7	–	913.7(8)	910.7(8)	918.4(4)	935(1)	–	–	–
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	Pnma	Pnma	Pnma

	{73}	{74}	{75}	{76}	{77}	{64}	{78}
SiO_2	–	–	–	–	–	–	–
TiO_2	–	–	–	–	–	–	–
Al_2O_3	–	–	–	–	–	–	–
Fe_2O_3	–	–	–	–	–	–	–
FeO	–	–	–	–	–	–	–
MnO	–	–	–	–	–	–	–
MgO	–	–	–	–	–	–	–
CaO	–	–	–	–	–	–	–
Na_2O	–	–	–	–	–	–	–
K_2O	–	–	–	–	–	–	–
H_2O	–	–	–	–	–	–	–
F	–	–	–	–	–	–	–
	–	–	–	–	–	–	–
O≡F	–	–	–	–	–	–	–
Total	–	–	–	–	–	–	–
Si	7.39	7.38	8.17	8.05	8.00	8.00	7.81
Al	0.61	0.62	–	–	–	–	0.18
Σiv	8.00	8.00	8.17	8.05	8.00	8.00	7.99
Al	0.12	0.11	0.10	0.12	0.15	–	–
Ti^{3+}	–	–	0.02	–	–	–	–
Fe^{3+}	0.22	0.23	0.08	–	0.18	–	–
Fe^{2+}	3.30	3.30	4.80	5.24	5.28	5.00	1.17
Mn	–	–	0.72	0.11	0.12	–	–
Mg	2.92	2.92	0.94	1.18	0.95	–	5.79
Σvi	–	–	–	–	–	5.00	–
$\Sigma vi-5$	–	–	–	–	–	–	–
Ca	0.27	0.27	0.13	0.27	0.30	1.00	0.09
Na	0.08	0.08	0.04	–	0.02	1.00	–
$\Sigma M(4)$	6.91	6.91	6.83	6.95	7.00	2.00	7.05
Na	–	–	–	–	–	1.00	0.05
K_A	0.09	0.09	–	–	–	–	–
ΣA	0.09	0.09	–	–	–	1.00	0.05
a(Å)	–	–	–	–	–	9.982(7)	18.560(3)
b(Å)	–	–	–	–	–	18.223(6)	18.013(2)
c(Å)	–	–	–	–	–	5.298(5)	5.282(1)
β(°)	–	–	–	–	–	103.7(1)	90
V(Å^3)	–	–	–	–	–	936(1)	1765.9
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	Pnma

	{79}	{80}	{81}	{82}	{83}	{84}	{85}	{86}	{87}
SiO_2	51.17	49.87	39.90	49.7	44.67	49.46	44.12	46.17	46.30
TiO_2	0.63	0.34	4.65	0.84	1.34	0.67	1.26	1.19	1.10
Al_2O_3	1.11	1.04	14.35	5.2	8.88	5.52	8.82	7.73	7.78
Fe_2O_3	15.18	14.25	9.60	3.2	4.67	3.69	5.53	4.58	4.78
FeO	18.48	20.19	0.04	10.0	14.76	11.08	14.77	12.97	12.09
MnO	2.85	1.22	0.08	0.55	0.47	0.58	0.50	0.60	0.58
MgO	0.32	0.03	14.52	14.4	9.67	13.61	9.19	11.23	11.84
CaO	0.80	0.44	12.14	11.9	11.79	12.12	11.74	11.77	11.90
Na_2O	6.28	7.75	1.90	0.79	1.00	0.71	1.18	1.07	0.99
K_2O	0.72	1.15	2.31	0.37	0.86	0.42	0.88	0.71	0.71
H_2O	1.61	1.00	0.50	2.40	1.82	1.82	1.80	1.85	1.73
F	0.60	2.46	0.12	–	0.10	0.15	0.14	0.12	0.12
	100.35	100.86	100.11	99.1	100.03	99.84	99.94	100.01	99.94
O≡F	0.26	1.03	0.05	–	0.04	0.06	0.06	0.05	0.05
Total	100.09	99.83	100.06	99.1	99.99	99.78	99.88	99.96	99.89
Si	7.93	7.83	5.88	7.26	6.71	7.23	6.66	6.86	6.87
Al	0.07	0.17	2.12	0.74	1.29	0.77	1.34	1.14	1.13
Σiv	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Al	0.13	0.02	0.37	0.14	0.28	0.18	0.23	0.22	0.23
Ti^{3+}	0.07	0.04	0.52	0.09	0.15	0.07	0.14	0.13	0.12
Fe^{2+}	1.77	1.68	1.06	0.35	0.53	0.41	0.63	0.51	0.53
Fe	2.39	2.65	–	1.22	1.85	1.35	1.86	1.61	1.50
Mn	0.37	0.16	0.01	0.07	0.06	0.07	0.06	0.08	0.07
Mg	0.07	0.01	3.19	3.13	2.16	2.97	2.07	2.49	2.62
Σvi	4.98	4.92	5.15	5.01	5.03	5.05	4.99	5.04	5.07
Σvi_{-5}	–	–	0.15	0.01	0.03	0.05	–	0.04	0.07
Ca	0.13	0.07	1.92	1.86	1.90	1.86	1.90	1.87	1.89
Na	1.87	1.93	–	0.13	0.07	0.09	0.10	0.09	0.04
$\Sigma M(4)$	2.00	2.00	2.07	2.00	2.00	2.00	2.00	2.00	2.00
Na	0.02	0.43	0.54	0.09	0.22	0.11	0.25	0.17	0.31
K	0.14	0.23	0.43	0.07	0.16	0.08	0.17	0.15	0.11
ΣA	0.16	0.66	0.97	0.16	0.38	0.19	0.42	0.22	0.42
a(Å)	9.769(2)	9.823(2)	9.892(1)	–	9.880	9.878	9.887	9.882	9.891
b(Å)	18.048(3)	18.021(4)	18.064(2)	–	18.179	18.129	18.174	18.126	18.169
c(Å)	5.335(1)	5.328(2)	5.312(1)	–	5.302	5.301	5.308	5.301	5.285
β(°)	103.59(1)	103.70(1)	105.39(1)	–	104.80	104.83	104.97	104.90	104.83
$V(Å^3)$	914.3	916.4	915.1(4)	–	920.7	917.7	921.4	917.6	918.1
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{88}	{89}	{90}	{91}	{92}	{94}	{95}
SiO_2	43.18	44.97	44.93	43.47	43.08	47.86	46.45
TiO_2	1.17	1.25	1.45	2.02	1.74	0.64	0.64
Al_2O_3	10.63	9.56	9.66	9.96	10.64	1.69	3.44
Fe_2O_3	6.51	3.88	3.37	3.99	3.50	17.95	16.70
FeO	10.98	13.53	12.95	16.04	16.14	19.91	19.59
MnO	0.35	0.26	0.31	0.27	0.29	0.71	0.63
MgO	11.20	10.51	11.90	8.70	8.93	0.13	-
CaO	11.50	11.32	10.96	10.84	11.24	1.64	1.63
Na_2O	1.35	0.01	1.17	1.17	1.33	6.25	5.94
K_2O	1.04	1.02	0.80	1.07	0.86	0.61	3.74
H_2O	2.09	2.47	2.08	2.15	1.99	1.67	0.95
F	0.21	0.07	0.03	0.08	0.03	1.16	1.24
	100.26	99.86	99.69	99.84	99.89	100.22	100.95
$O \equiv F$	0.09	0.03	0.01	0.03	0.01	0.49	0.52
Total	100.17	99.83	99.68	99.81	99.88	99.73	100.43
Si	6.40	6.71	6.58	6.55	6.47	7.68	7.51
Al	1.60	1.29	1.42	1.45	1.53	0.32	0.49
Σiv	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Al	0.25	0.39	0.24	0.31	0.35	-	0.16
Ti	0.14	0.14	0.17	0.23	0.20	0.08	0.08
Fe	0.79	0.43	0.37	0.45	0.40	2.17	2.02
Fe	1.36	1.69	1.59	2.02	2.02	2.68	2.65
Mn	0.05	0.03	0.03	0.04	0.04	0.10	0.09
Mg	2.47	2.32	2.60	1.95	1.99	0.03	-
Σvi	5.06	5.00	5.00	5.00	5.00	5.06	5.00
Σvi -5	0.06	-	-	-	-	0.06	-
Ca	1.82	1.80	1.72	1.74	1.80	0.28	0.28
Na	0.12	0.20	0.28	0.26	0.20	1.66	1.72
Σ M(4)	2.00	2.00	2.00	2.00	2.00	2.00	2.00
Na	0.27	0.14	0.04	0.07	0.19	0.28	0.14
K	0.22	0.28	0.16	0.21	0.17	0.17	0.77
Σ A	0.49	0.42	0.20	0.28	0.36	0.45	0.91
a (Å)	-	9.867	9.848	9.863	9.857	9.774(1)	9.935(5)
b (Å)	-	18.103	18.058	18.111	18.058	18.032(7)	18.102(2)
c (Å)	-	5.320	5.305	5.320	5.309	5.333(4)	5.339(3)
β (°)	-	105.00	105.05	104.77	104.97	103.7(1)	103.9(2)
V (Å^3)	-	918.0	911.0	918.9	913.9	913(1)	931(1)
Space Group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{96}	{97}	{98}	{99}	{100}	{101}	{102}	{103}
SiO_2	57.65	53.60	58.80	57.28	58.18	58.49	55.31	55.23
TiO_2	0.07	–	–	0.01	–	–	0.13	0.08
Al_2O_3	1.31	0.51	0.01	0.09	0.24	0.41	1.89	2.53
Fe_2O_3	–	0.35	–	–	–	–	–	–
FeO	2.06	3.50	8.11	9.99	11.41	7.89	14.08	12.73
MnO	–	12.90	0.15	0.22	0.19	0.30	0.32	0.33
MgO	23.62	16.90	28.91	28.07	27.34	29.44	23.20	24.84
CaO	13.42	1.66	0.40	0.32	0.07	0.51	0.63	0.61
Na_2O	0.61	0.75	0.03	0.01	0.03	0.06	0.15	0.22
K_2O	0.20	0.17	–	–	–	0.02	0.02	0.04
H_2O	–	2.53	–	–	–	–	–	–
F	0.21	–	–	–	–	–	–	–
	99.15	99.82	96.41	95.99	97.46	97.12	95.73	96.61
O≡F	0.09	–	–	–	–	–	–	–
Total	99.06	99.82	96.41	95.99	97.46	97.12	95.73	96.61
Si	7.81	7.87	8.05	7.96	7.95	7.96	7.88	7.74
Al	0.19	0.09	–	0.02	0.05	0.04	0.12	0.26
Σiv	8.00	7.94	8.05	7.98	8.00	8.00	8.00	8.00
Al	0.02	–	–	–	0.01	0.02	0.19	0.16
Ti_{3+}	0.01	–	–	–	–	–	–	0.01
Fe_{2+}	–	0.07	–	–	–	–	–	–
Fe	0.23	0.42	0.93	1.16	1.29	0.90	1.68	1.49
Mn	–	1.60	0.02	0.03	0.02	0.03	0.03	0.04
Mg	4.77	3.70	5.90	5.82	5.69	5.97	4.92	5.19
Σvi	5.03	Zn 0.75	–	–	–	–	–	–
Σvi_{-5}	0.03	–	–	–	–	–	–	–
Ca	1.95	0.26	0.06	0.05	0.01	0.07	0.10	0.09
Na	0.02	0.21	0.01	–	–	0.01	0.04	0.02
$\Sigma M(4)$	2.00	6.97	6.92	7.06	7.02	7.00	6.96	7.00
Na	0.14	–	–	–	0.01	0.01	–	0.04
K_A	0.03	0.02	–	–	–	–	–	0.01
ΣA	0.17	0.02	–	–	0.01	0.01	–	0.05
a(Å)	–	9.606(1)	18.544(3)	18.541(4)	18.541(7)	18.544(8)	18.570(3)	18.560(3)
b(Å)	–	18.126(1)	18.014(3)	18.020(5)	18.027(7)	18.011(7)	18.024(3)	18.017(3)
c(Å)	–	5.317(1)	5.286(2)	5.287(2)	5.274(3)	5.281(5)	5.285(1)	5.287(2)
β(°)	–	102.63(1)	90	90	90	90	90	90
V(Å^3)	–	903.4	1765.8	1766.4	1762.8	1763.8	1768.9	1767.9
Space group	C2/m	C2/m	Pnma	Pnma	Pnma	Pnma	Pnma	Pnma

Cell dimensions of heat-treated amphiboles

	{15a}	{15b}	{15c}	{15d}	{27}	{27a}	{27b}
a	9.554(8)	9.550(8)	9.524(8)	9.827(8)	9.727(8)	9.683(8)	9.680(8)
b	17.738(19)	17.758(19)	17.716(19)	17.903(19)	17.958(19)	17.912(19)	17.913(19)
c	5.298(7)	5.293(7)	5.269(7)	5.294(7)	5.306(7)	5.287(7)	5.292(7)
β	103.7(1)	103.7(1)	103.6(1)	103.8(1)	103.8(1)	103.6(1)	103.6(1)
V	872.3	872.1	863.9	904.6	900.2	891.2	891.7
Space group	C2/m	C2/m	C2/m	-	C2/m	C2/m	C2/m

	{29}	{29a}	{29b}	{31}	{31a}	{67a}	{67b}
a	9.760(8)	9.619(8)	9.635(8)	9.740(8)	9.618(8)	9.928(2)	9.930(5)
b	18.070(19)	17.946(19)	17.953(19)	18.045(19)	17.902(19)	18.015(9)	18.025(8)
c	5.339(7)	5.295(7)	5.286(7)	5.336(7)	5.286(7)	5.282(3)	5.290(4)
β	103.7(1)	103.2(1)	103.3(1)	103.4(1)	103.4(1)	105.43(4)	105.43(4)
V	914.9	889.8	889.9	912.5	885.3	910.7(8)	912.0(10)
Space group	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

	{67c}	{67d}	{67e}	{67f}
a	9.933(2)	9.932(2)	9.933(1)	9.926(5)
b	18.029(4)	18.015(4)	18.028(3)	18.029(9)
c	5.293(1)	5.289(1)	5.297(1)	5.297(4)
β	105.43(1)	105.43(2)	105.44(2)	105.46(5)
V	913.0(5)	912.2(3)	914.3(3)	913.7(8)
Space group	C2/m	C2/m	C2/m	C2/m

PRESSURE-TEMPERATURE CONDITIONS FOR HEAT-TREATED AMPHIBOLES

	P(bars)	buffer	T(°C)	time(hrs)		P(bars)	buffer	T(°C)	time(hrs)
{15a}		unheated			{98n}	1000	-	600	882
{15b}	1	air	705	1	{98o}	1000	-	600	286
{15c}	1	air	705	95	{99}		unheated		
{15d}	2000	NNO	513	15667	{99a}	1000	-	800	3
{27}		unheated			{99b}	1000	-	730	20
{27a}	1	air	706	94	{99c}	1000	-	690	168
{27b}	1	air	704	1	{99d}	1000	-	650	121
{29}		unheated			{99e}	1000	-	600	481
{29a}	1	air	706	94	{99f}	1000	-	550	1339
{29b}	1	air	704	1	{100}		unheated		
{31}		unheated			{100a}	1000	-	780	24
{31a}	1	air	707	95	{100b}	1000	-	760	43
{1a}		unheated			{100c}	1000	-	750	45
{1b}	2000	*	398	672	{100d}	1000	-	730	45
{1c}	2000	*	500	305	{100e}	1000	-	700	74
{1d}	2000	*	600	302	{100f}	1000	-	680	142
{1e}	2000	*	700	146	{100g}	1000	-	660	427
{60b}		unheated			{100h}	1000	-	620	882
{60c}	2000	*	500	305	{100i}	1000	-	600	682
{60d}	2000	*	602	302	{100j}	1000	-	550	1339
{60e}	2000	*	700	146	{101}		unheated		
{61b}		unheated			{101a}	1000	-	800	3
{61c}+	2000	*	600	144	{101b}	1000	-	760	43
{67a}+	2000	IQF	850	50	{101c}	1000	-	730	20
{67b}+	2000	WM	850	-	{101d}	1000	-	690	168
{67c}+	2000	FMQ	850	46	{101e}	1000	-	650	121
{67d}+	2000	NNO	850	50	{101f}	1000	-	600	481
{67e}+	2000	HM	850	50	{101g}	1000	-	550	1339
{67f}+	2000	CT	850	26	{102}		unheated		
{67g}	2000	CCO	707	150	{102a}	1000	-	800	3
{67h}	2000	CT	850	10	{102b}	1000	-	760	4
{67i}	2000	IQF	850	10	{102c}	1000	-	730	45
{78}		unheated			{102d}	1000	-	700	96
{78a}	2000	QFM	720	96	{102e}	1000	-	680	142
{78b}	2000	QFM	670	216	{102f}	1000	-	650	121
{78c}d	2000	QFM	600	360	{102g}	1000	-	600	481
{78d}d	2000	QFM	600	168	{102h}	1000	-	550	1339
{78e}d	2000	QFM	550	445	{103}		unheated		
{78f}d	2000	QFM	550	576	{103a}	1000	-	800	3
{98}		unheated			{103b}	1000	-	780	14
{98a}	1000	-	800	3	{103c}	1000	-	760	43
{98b}	1000	-	780	24	{103d}	1000	-	750	45
{98c}	1000	-	760	43	{103e}	1000	-	730	33
{98d}	1000	-	750	45	{103f}	1000	-	700	96
{98e}	1000	-	730	45	{103g}	1000	-	690	168
{98f}	1000	-	700	96	{103h}	1000	-	680	142
{98g}	1000	-	690	168	{103i}	1000	-	660	427
{98h}	1000	-	680	142	{103j}	1000	-	650	882
{98i}	1000	-	660	427	{103k}	1000	-	620	882
{98j}d	1000	-	650	882	{103l}	1000	-	600	219
{98k}	1000	-	650	391	{103m}d	1000	-	600	219
{98l}	1000	-	630	768	{103n}d	1000	-	550	1053
{98m}	1000	-	620	882	{103o}d	1000	-	550	1053

*starting material was disordered by prior heating at 780°C{98} and {103} and 720°C {78}.
+Fe kept in reduced condition by using 8 vol.% hydrogen-92 vol.% argon pressure medium.
Conditions indicated are those of synthesis.

APPENDIX F2. MÖSSBAUER PARAMETERS FOR AMPHIBOLES

(a) Natural amphiboles

	Isomer shift (mm/sec)					Quadrupole splitting (mm/sec)					Half-width (mm/sec)				
	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}
{1}	←	1.14	→	1.08	–	←	2.76	→	1.64	–	←	0.38	→	0.38	–
{2}	←	1.17	→	1.10	–	←	2.90	→	1.62	–	←	0.42	→	0.39	–
{3}	←	1.15	→	1.06	–	←	2.75	→	1.55	–	←	0.39	→	0.37	–
{4}	←	1.14	→	1.04	–	←	2.72	→	1.51	–	←	0.39	→	0.35	–
{5}	←	1.14	→	1.05	–	←	2.78	→	1.53	–	←	0.39	→	0.40	–
{6}	←	1.15	→	1.05	–	←	2.78	→	1.50	–	←	0.40	→	0.35	–
{7}	←	1.13	→	1.04	–	←	2.76	→	1.68	–	←	0.40	→	0.36	–
{8}	←	1.11	→	1.10	–	←	2.61	→	1.81	–	←	0.37	→	0.28	–
{9}	←	1.12	→	1.08	–	←	2.58	→	1.80	–	←	0.36	→	0.31	–
{10}	1.14	1.12	1.14	–	–	2.82	1.89	2.82	–	–	0.29	0.44	0.29	–	–
{11}	1.14	1.14	1.14	–	–	2.81	1.98	2.81	–	–	0.28	0.46	0.28	–	–
{15}	1.12	–	1.10	–	0.35	2.82	–	2.33	–	0.48	0.30	–	0.33	–	0.33
{16}	1.13	–	1.12	–	0.37	2.82	–	2.27	–	0.42	0.36	–	0.40	–	0.35
{17}	1.13	–	1.13	–	0.37	2.82	–	2.32	–	0.42	0.31	–	0.38	–	0.30
{18}	1.13	–	1.11	–	0.38	2.85	–	2.36	–	0.47	0.31	–	0.41	–	0.34
{19}	1.13	–	1.10	–	0.37	2.83	–	2.32	–	0.43	0.29	–	0.29	–	0.29
{20}	1.15	–	1.15	–	0.36	2.82	–	2.39	–	0.41	0.38	–	0.31	–	0.44
{21a}	1.12	–	1.04	–	0.39	2.75	–	2.15	–	0.49	0.32	–	0.42	–	0.34
{21b}	1.13	1.02	1.10	–	0.39	2.79	2.00	2.41	–	0.48	0.31	0.34	0.34	–	0.34
{15a}	1.13	–	1.10	–	0.34	2.81	–	2.30	–	0.48	0.25	–	0.25	–	0.25
{22}	1.13	–	1.12	–	0.38	2.79	–	2.24	–	0.46	–	–	–	–	–
{23}	1.13	–	1.11	–	0.36	2.82	–	2.22	–	0.47	–	–	–	–	–
{24}	1.14	–	1.11	–	0.38	2.82	–	2.23	–	0.47	–	–	–	–	–
{25}	1.14	–	1.12	–	0.37	2.82	–	2.25	–	0.46	–	–	–	–	–
{26}	1.14	–	1.07	–	0.37	2.82	–	2.27	–	0.47	–	–	–	–	–
{27}	1.14	–	1.12	–	0.39	2.79	–	2.48	–	0.44	0.29	–	0.29	–	0.29
{21c}	1.14	–	1.04	–	0.40	2.75	–	2.01	–	0.50	–	–	–	–	–
{28}	1.14	–	1.07	–	0.37	2.83	–	2.33	–	0.45	–	–	–	–	–
{29}	1.14	–	1.12	–	0.40	2.87	–	2.36	–	0.44	0.26	–	0.26	–	0.26
{30}	1.14	–	1.09	–	0.37	2.86	–	2.38	–	0.44	–	–	–	–	–
{31}	1.14	–	1.11	–	0.37	2.88	–	2.33	–	0.42	–	–	–	–	–
{10a}	1.14	1.14	1.12	–	0.28	2.89	1.91	2.57	–	0.53	←	0.26	→	–	0.68
{32}	1.13	←	1.07	→	–	0.44	2.89	←	2.04	→	–	0.45	←	0.31	→	–	0.40
{33}	1.13	1.20	1.11	–	0.41	2.88	1.80	2.44	–	0.63	←	0.28	→	–	0.35
{34}	1.11	1.10	1.07	–	0.38	2.71	1.72	2.30	–	0.65	←	0.32	→	–	0.41
{11a}	1.13	1.12	1.14	–	–	2.86	1.77	2.19	–	–	←	0.28	→	–	–
{11b}	1.25	1.29	1.27	–	0.48	3.18	1.99	2.64	–	0.67	←	0.30	→	–	0.41
{35}	1.15	1.14	1.14	–	0.40	2.89	1.85	2.32	–	0.57	←	0.29	→	–	0.46
{35a}	1.23	1.11	1.20	–	0.52	3.10	2.10	2.65	–	0.53	←	0.29	→	–	0.45
{36}	1.11	1.11	1.12	–	–	2.81	1.73	2.13	–	–	←	0.29	→	–	–
{37}	1.12	←	1.14	→	1.08	–	2.72	←	2.16	→	1.37	–	←	0.34	→	–	–
{5a}	←	1.16	→	1.07	–	←	2.79	→	1.55	–	←	0.29	→	0.27	–
{5b}	←	1.28	→	1.18	–	←	3.10	→	1.54	–	←	0.34	→	0.30	–
{60}	←	1.16	→	1.11	–	←	2.81	→	1.67	–	←	0.28	→	0.27	–

	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}
{60a}	←	1.27	→	1.23	–	←	3.08	→	1.75	–	←	0.31	→	0.31	–
{61}	←	1.15	→	1.12	–	←	2.74	→	1.80	–	←	0.32	→	0.27	–
{61a}	←	1.26	→	1.24	–	←	2.99	→	1.85	–	←	0.36	→	0.27	–
{62}					–	←	2.77	→	1.71	–	←	0.34	→	0.33	–
{62a}					–	←	3.03	→	1.81	–	←	0.45	→	0.45	–
{63}	–	–	–	–	–	←	2.78	→	1.48	–	–	–	–	–	–
{1a}	←	1.26	→	1.22	–	←	3.08	→	1.77	–	←	0.27	→	0.27	–
{60b}	←	1.28	→	1.24	–	←	3.09	→	1.75	–	←	0.34	→	0.34	–
{61b}	←	1.26	→	1.26	–	←	3.05	→	1.87	–	←	0.31	→	0.30	–
{64}	1.25	?	1.25	–	0.51	3.09	?	3.09	–	0.51	?	?	?	–	0.28
{65}	1.13	–	1.11	–	0.49	2.81	–	2.03	–	0.33	0.30	–	0.38	–	0.40
{66a}	←	1.17	→	1.11	–	←	2.87	→	1.67	–	←	0.39	→	0.37	–
{66b}	←	1.28	→	1.23	–	←	3.16	→	1.82	–	←	0.55	→	0.61	–
{68}	1.12	1.10	1.12	–	0.39	2.64	2.01	2.64	–	0.80	←	0.21	→	–	0.25
{69}	1.14	1.00	1.12	–	0.42	2.78	2.06	2.40	–	0.60	←	0.33	→	–	0.40
{78}	←	1.24	→	1.23	–	←	2.99	→	1.86	–	←	0.33	→	0.27	–
{82}	1.14	1.05	1.11	–	0.49	2.81	1.99	2.39	–	0.53	←	0.33	→	–	0.38
{83}	1.13	1.00	1.12	–	0.46	2.76	2.02	2.35	–	0.57	←	0.32	→	–	0.38
{84}	1.12	1.03	1.09	–	0.46	2.79	2.01	2.40	–	0.54	←	0.32	→	–	0.37
{85}	1.13	1.02	1.11	–	0.46	2.76	2.01	2.37	–	0.56	←	0.32	→	–	0.37
{86}	1.13	1.04	1.11	–	0.45	2.79	2.01	2.39	–	0.57	←	0.32	→	–	0.38
{87}	1.13	1.02	1.10	–	0.45	2.79	2.04	2.41	–	0.58	←	0.32	→	–	0.38
{34a}	1.10	1.09	1.06	–	0.37	2.71	1.72	2.30	–	0.65	←	0.32	→	–	0.41
{88}	1.15	1.01	1.13	–	0.44	2.79	2.18	2.39	–	0.63	0.34	0.34	0.34	–	0.44
{89}	1.16	1.03	1.13	–	0.46	2.77	1.99	2.36	–	0.61	0.33	0.33	0.33	–	0.44
{90}	1.12	1.00	1.09	–	0.44	2.85	2.06	2.44	–	0.54	0.38	0.38	0.38	–	0.52
{91}	1.16	1.06	1.15	–	0.51	2.82	1.96	2.46	–	0.49	0.37	0.37	0.37	–	0.46
{92}	1.15	1.04	1.12	–	0.50	2.79	1.95	2.39	–	0.50	0.36	0.36	0.36	–	0.45
{93a}	1.13	1.12	1.11	–	0.36	2.85	1.92	2.52	–	0.73	0.27	0.35	0.35	–	0.48
{93b}	1.13	1.13	1.11	1.11	0.35	2.84	2.02	2.56	1.71	0.75	0.25	0.30	0.32	0.24	0.48
{93c}	1.13	1.13	1.12	–	0.36	2.87	1.94	2.58	–	0.78	0.27	0.42	0.35	–	0.53
{93d}	1.13	1.14	1.12	1.12	0.34	2.88	2.06	2.60	1.71	0.80	0.27	0.36	0.31	0.30	0.54
{93e}	1.13	1.14	1.09	–	0.34	2.85	1.92	2.49	–	0.79	0.27	0.35	0.35	–	0.61
{93f}	1.13	1.15	1.12	1.13	0.32	2.88	2.02	2.58	1.75	0.84	0.26	0.31	0.30	0.25	0.59
{94}	–	–	–	–	–	2.95	–	2.46	–	0.50	0.35	–	0.35	–	0.36
{95}	–	–	–	–	–	2.90	1.88	2.56	–	0.57	0.36	0.36	0.36	–	0.41
{96}	←	1.14	→	1.17	0.48	←	2.82	→	1.84	0.74	←	0.32	→	0.34	0.53
{97a}	←	1.13	→	1.14	0.45	←	2.81	→	1.78	0.51	←	←	0.33	→	→
{97b}	←	1.23	→	1.15	0.45	←	3.08	→	1.74	0.64	←	←	0.36	→	→
{98a}	←	1.15	→	1.13	–	←	2.78	→	1.82	–	←	0.26	→	0.28	–
{98b}	←	1.27	→	1.26	–	←	3.11	→	1.87	–	←	0.27	→	0.28	–
{99a}	←	1.15	→	1.13	–	←	2.80	→	1.82	–	←	0.25	→	0.28	–
{99b}	←	1.27	→	1.26	–	←	3.13	→	1.89	–	←	0.29	→	0.29	–
{100a}	←	1.16	→	1.13	–	←	2.76	→	1.81	–	←	0.28	→	0.30	–
{100b}	←	1.28	→	1.26	–	←	3.10	→	1.87	–	←	0.28	→	0.30	–

	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}	M(1)	M(2)	M(3)	M(4)	Fe^{3+}
{101a}	←	1.15	→	1.13	–	←	2.78	→	1.83	–	←	0.27	→	0.29	–
{101b}	←	1.28	→	1.26	–	←	3.09	→	1.88	–	←	0.29	→	0.29	–
{102a}	←	1.15	→	1.13	–	←	2.74	→	1.84	–	←	0.34	→	0.31	–
{102b}	←	1.27	→	1.26	–	←	3.02	→	1.90	–	←	0.36	→	0.32	–
{103a}	←	1.15	→	1.13	–	←	2.70	→	1.85	–	←	0.36	→	0.30	–
{103b}	←	1.26	→	1.26	–	←	2.96	→	1.90	–	←	0.42	→	0.31	–
{78g}	←	1.16	→	1.13	–	←	2.74	→	1.84	–	←	0.30	→	0.32	–
{78h}	←	1.27	→	1.26	–	←	3.05	→	1.89	–	←	0.34	→	0.30	–
{104}	1.15	1.15	1.15	–	0.27	2.96	1.95	1.95	–	0.91	0.27	0.41	0.41	–	0.72
{105}	1.15	1.16	1.16	–	–	2.93	1.87	1.87	–	–	0.30	0.60	0.60	–	–
{106}	1.12	1.12	1.12	–	–	2.75	1.79	1.79	–	–	0.40	0.40	0.40	–	–
{107}	1.14	1.25	1.25	–	–	2.73	2.04	2.04	–	–	0.32	0.64	0.64	–	–
{108}	1.18	1.07	1.07	–	0.50	2.68	1.89	1.89	–	0.47	0.40	0.45	0.45	–	0.41
{109}	1.16	1.16	1.16	–	–	2.58	1.94	1.94	–	–	0.28	0.62	0.62	–	–
{110}	1.15	1.11	1.11	–	0.47	2.83	2.00	2.00	–	0.50	0.35	0.52	0.52	–	0.34
{111}	1.13	1.12	1.12	–	0.27	2.70	2.17	2.17	–	1.04	0.29	0.64	0.64	–	0.52
{112}	1.15	0.88	0.88	–	0.42	2.48	2.21	2.21	–	0.66	0.52	0.31	0.31	–	0.56
{118}	1.26	1.26	1.26	1.23	0.64	3.10	2.50	3.10	1.86	0.41	0.36	0.36	0.36	0.36	0.46
{119}	1.15	1.14	1.15	1.10	0.61	2.59	2.26	2.59	1.88	0.55	0.31	0.31	0.31	0.31	0.49
{120}	←	1.11	→	1.10	–	←	2.64	→	1.82	–	←	0.48	→	0.32	–
{121}	←	1.14	→	1.07	0.37	←	2.80	→	1.58	1.06	←	0.38	→	0.52	0.68
{122}	1.12	–	1.13	–	0.38	2.90	–	2.42	–	0.42	0.34	–	0.34	–	0.31

(b) Heat-treated amphiboles

		M(1)		M(2)		M(3)		M(4)		M(1)+M(3)		M(1)+M(2)+M(3)	
		I.S.	Q.S.	I.S.	Q.S.	I.S.	Q.S.	I.S.	Q.S.	I.S.	Q.S.	I.S.	Q.S.
{15a}	Fe^{2+}	1.13	2.81	–	–	1.10	2.30	–	–	–	–	–	–
	Fe^{3+}	–	–	0.34	0.48	–	–	–	–	–	–	–	–
{15b}	Fe^{2+}	1.11	2.82	–	–	1.13	2.14	–	–	–	–	–	–
	Fe^{3+}	–	–	0.31	0.59	–	–	–	–	0.43	1.22	–	–
{15c}	Fe^{3+}	–	–	0.31	0.71	–	–	–	–	0.39	1.30	–	–
{15d}	Fe^{2+}	–	–	–	–	–	–	–	–	–	–	1.15	2.74
	Fe^{3+}	–	–	–	–	–	–	–	–	–	–	0.39	0.54
{27}	Fe^{2+}	1.14	2.79	–	–	1.12	2.48	–	–	–	–	–	–
	Fe^{3+}	–	–	0.39	0.44	–	–	–	–	–	–	–	–
{27a}	Fe^{3+}	0.38	1.18	0.38	0.57	0.45	0.84	–	–	–	–	–	–
{27b}	Fe^{3+}	0.37	1.23	0.35	0.60	0.47	0.87	–	–	–	–	–	–
{29}	Fe^{2+}	1.14	2.87	–	–	1.12	2.36	–	–	–	–	–	–
	Fe^{3+}	–	–	0.40	0.44	–	–	–	–	–	–	–	–
{29a}	Fe^{2+}	0.95	2.08	–	–	1.10	2.70	–	–	–	–	–	–
	Fe^{3+}	–	–	0.36	0.61	–	–	–	–	0.32	0.98	–	–
{29b}	Fe^{2+}	–	–	–	–	–	–	–	–	–	–	1.05	2.13
	Fe^{3+}	–	–	0.42	0.58	–	–	–	–	0.41	1.02	–	–
{63a}	Fe^{2+}	–	–	–	–	–	–	–	1.48	–	–	–	2.78
{63b}	Fe^{2+}	–	–	–	–	–	–	–	1.48	–	–	–	2.76
{63c}	Fe^{2+}	–	–	–	–	–	–	–	–	–	–	–	2.72
{63d}	Fe^{2+}	–	–	–	–	–	–	–	–	–	–	–	2.72
{1a}	Fe^{2+}	–	–	–	–	–	–	1.22	1.77	–	–	1.26	3.08
{1b}	Fe^{2+}	–	–	–	–	–	–	1.22	1.76	–	–	1.26	3.07
{1c}	Fe^{2+}	–	–	–	–	–	–	1.25	1.82	–	–	1.29	3.16
{1d}	Fe^{2+}	–	–	–	–	–	–	1.25	1.82	–	–	1.29	3.17
{1e}	Fe^{2+}	–	–	–	–	–	–	1.25	1.82	–	–	1.29	3.17
{60b}	Fe^{2+}	–	–	–	–	–	–	1.24	1.75	–	–	1.28	3.09
{60c}	Fe^{2+}	–	–	–	–	–	–	1.20	1.73	–	–	1.26	3.04
{60d}	Fe^{2+}	–	–	–	–	–	–	1.21	1.74	–	–	1.26	3.05
{60e}	Fe^{2+}	–	–	–	–	–	–	1.24	1.75	–	–	1.28	3.09
{61b}	Fe^{2+}	–	–	–	–	–	–	1.26	1.87	–	–	1.26	3.05
{61c}	Fe^{2+}	–	–	–	–	–	–	1.25	1.84	–	–	1.28	3.06
{67a}	Fe^{2+}	–	–	1.14	2.11	–	–	–	–	1.13	2.73	–	–
	Fe^{3+}	–	–	0.26	0.79	–	–	–	–	–	–	–	–
{67c}	Fe^{2+}	–	–	1.15	1.92	–	–	–	–	1.10	2.74	–	–
	Fe^{3+}	–	–	0.36	0.84	–	–	–	–	–	–	–	–
{67f}	Fe^{3+}	–	–	0.36	0.73	–	–	–	–	0.35	1.28	–	–
{67g}	Fe^{2+}	–	–	1.13	1.87	–	–	–	–	1.12	2.67	–	–
	Fe^{3+}	–	–	0.39	0.79	–	–	–	–	0.37	1.39	–	–
{67h}	Fe^{3+}	–	–	0.37	0.79	–	–	–	–	0.37	1.23	–	–
{67i}	Fe^{2+}	–	–	1.17	2.01	–	–	–	–	1.12	2.71	–	–
	Fe^{3+}	–	–	0.37	0.85	–	–	–	–	–	–	–	–
{78}	Fe^{2+}	–	–	–	–	–	–	1.23	1.86	–	–	1.24	2.99
{78a}	Fe^{2+}	–	–	–	–	–	–	1.22	1.84	–	–	1.24	3.00
{78b}	Fe^{2+}	–	–	–	–	–	–	1.23	1.85	–	–	1.25	3.01
{78c}	Fe^{2+}	–	–	–	–	–	–	1.23	1.85	–	–	1.25	3.01

APPENDIX F3. SITE POPULATIONS OF AMPHIBOLES

(a) Natural amphiboles

	M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)	Fe^{3+}/Fe^{2+}
{1}	–	0.06	–	0.83	0.24	–	–
{2}	–	0.33	–	0.74	0.50	–	–
{3}	–	0.36	–	0.87	0.65	–	–
{4}	–	0.83	–	0.84	0.87	–	–
{5}	–	0.81	–	0.98	0.85	–	–
{6}	–	0.96	–	0.90	0.98	–	–
{7}	–	0.29	–	0.19	0.15	–	–
{8}	–	0.00	–	0.70	0.08	–	–
{9}	–	0.09	–	0.71	0.21	–	–
{10}	–	–	–	–	–	–	–
{11}	–	–	–	–	–	–	–
{12}	–	–	–	–	–	–	0.50
{13}	–	–	–	–	–	–	0.78
{14}	–	–	–	–	–	–	0.61
{15}	0.19	–	0.32	–	–	–	0.43
{16}	0.31	–	0.50	–	–	–	0.48
{17}	0.48	–	0.57	–	–	–	0.67
{18}	0.67	0.08	0.81	–	–	–	0.52
{19}	0.89	0.12	0.75	–	–	–	0.70
{20}	0.17	0.03	0.09	–	–	–	3.46
{21a}	0.28	–	0.28	–	–	–	1.87
{21b}	0.26	0.08	0.18	–	–	–	1.87
{15a}	0.22	–	0.31	–	–	–	0.30
{22}	0.36	–	0.39	–	–	–	0.41
{23}	0.40	–	0.52	–	–	–	0.20
{24}	0.46	–	0.46	–	–	–	0.38
{25}	0.42	–	0.38	–	–	–	0.66
{26}	0.44	–	0.31	–	–	–	0.96
{27}	0.26	–	0.22	–	–	–	2.16
{21c}	0.42	–	0.27	–	–	–	1.18
{28}	0.59	–	0.56	–	–	–	1.04
{29}	0.84	–	0.88	–	–	–	0.81
{30}	0.75	–	0.78	–	–	–	0.82
{31}	0.86	–	0.89	–	–	–	0.80
{10a}	0.14	0.07	0.07	–	–	–	0.31
{32}	0.19	–	–	–	M(2)+M(3)=0.12	–	0.34
{33}	0.22	0.08	0.14	–	–	–	0.38
{34}	0.36	0.19	0.26	–	–	–	0.33
{11a}	0.74	0.23	0.46	–	–	–	–
{11b}	0.79	0.16	0.50	–	–	–	0.09
{35}	0.77	0.20	0.58	–	–	–	0.13
{35a}	0.83	0.17	0.50	–	–	–	0.14
{36}	0.84	0.28	0.62	–	–	–	–
{37}	–	–	–	–	–	–	–
{6a}	–	–	–	0.94	–	0.96	–
{38}	–	–	–	0.90	–	0.91	–
{39}	–	–	–	0.93	–	0.86	–
{5a}	–	–	–	0.96	–	0.84	–
{4a}	–	–	–	0.88	–	0.83	–

	M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)	Fe^{3+}/Fe^{2+}
{40}	–	–	–	0.89	–	0.77	–
{41}	–	–	–	0.90	–	0.75	–
{42}	–	–	–	0.95	–	0.68	–
{43}	–	–	–	0.86	–	0.72	–
{44}	–	–	–	0.87	–	0.68	–
{45}	–	–	–	0.85	–	0.67	–
{46}	–	–	–	0.86	–	0.65	–
{47}	–	–	–	0.87	–	0.61	–
{48}	–	–	–	0.85	–	0.58	–
{49}	–	–	–	0.89	–	0.52	–
{50}	–	–	–	0.89	–	0.52	–
{51}	–	–	–	0.87	–	0.51	–
{52}	–	–	–	0.84	–	0.44	–
{53}	–	–	–	0.87	–	0.43	–
{54}	–	–	–	0.85	–	0.39	–
{55}	–	–	–	0.79	–	0.39	–
{56}	–	–	–	0.87	–	0.35	–
{57}	–	–	–	0.84	–	0.32	–
{58}	–	–	–	0.85	–	0.32	–
{59}	–	–	–	0.79	–	0.30	–
{60}	–	–	–	0.73	–	0.20	–
{61}	–	–	–	0.53	–	0.04	–
{62}	0.27	–	0.27	0.65	–	–	0.07
{1a}	–	–	–	0.88	–	0.16	–
{60b}	–	–	–	0.78	–	0.22	–
{61b}	–	–	–	0.57	–	0.03	–
{64}	–	0.75	–	–	1.00	–	0.11
{65}	0.38	–	0.57	–	–	–	0.10
{66}	–	–	–	0.81	–	0.30	–
{68}	–	0.07	–	–	0.14	–	1.27
{69}	0.85	0.18	0.85	–	–	–	0.50
{78}	–	–	–	0.53	–	0.02	–
{17a}	–	–	–	–	–	–	0.67
{79}	–	–	–	–	–	–	0.72
{80}	–	–	–	–	–	–	0.59
{82}	0.39	0.14	0.39	–	–	–	0.28
{83}	0.53	0.15	0.51	–	–	–	0.34
{84}	0.38	0.13	0.34	–	–	–	0.33
{85}	0.51	0.16	0.54	–	–	–	0.38
{86}	0.45	0.13	0.44	–	–	–	0.36
{87}	0.41	0.14	0.41	–	–	–	0.39
{88}	0.43	0.10	0.41	–	–	–	0.48
{89}	0.47	0.11	0.35	–	–	–	0.42
{90}	0.42	0.15	0.39	–	–	–	0.29
{91}	0.57	0.20	0.50	–	–	–	0.22
{92}	0.51	0.20	0.58	–	–	–	0.22
{94}	0.92	–	0.97	–	–	–	0.73
{95}	0.97	0.19	1.00	–	–	–	0.41

	M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)	Fe^{3+}/Fe^{2+}
{96}	–	–	–	0.05	–	0.07	–
{97}	–	–	–	0.048	–	0.024	0.08
{78a}	–	–	–	0.53	–	0.022	–
{98}	–	–	–	0.42	–	0.016	–
{99}	–	–	–	0.54	–	0.015	–
{100}	–	–	–	0.60	–	0.019	–
{101}	–	–	–	0.41	–	0.014	–
{102}	–	–	–	0.68	–	0.063	–
{103}	–	–	–	0.61	–	0.056	–
{118}	–	0.07	–	0.07	0.12	–	0.08
{119}	–	0.13	–	0.07	0.11	–	0.34

(b) Heat-treated amphiboles

		M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)
{15a}	Fe^{2+}	0.22	–	0.31	–	–	–
	Fe^{3+}	–	0.11	–	–	–	–
{15b}	Fe^{2+}	0.16	–	0.15	–	–	–
	Fe^{3+}	–	0.13	–	–	0.09	–
{15c}	Fe^{3+}	–	0.16	–	–	0.22	–
{15d}	Fe^{2+}	–	–	–	–	–	0.05
	Fe^{3+}	–	–	–	–	–	0.15
{27}	Fe^{2+}	0.26	–	0.22	–	–	–
	Fe^{3+}	–	0.80	–	–	–	–
{27a}	Fe^{3+}	0.35	0.67	0.31	–	–	–
{27b}	Fe^{3+}	0.48	0.47	0.45	–	–	–
{29}	Fe^{2+}	0.84	–	0.88	–	–	–
	Fe^{3+}	–	1.03	–	–	–	–
{29a}	Fe^{2+}	0.49	–	0.53	–	–	–
	Fe^{3+}	–	0.99	–	–	0.38	–
{29b}	Fe^{2+}	–	–	–	–	–	0.17
	Fe^{3+}	–	0.81	–	–	0.72	–
{1a}	Fe^{2+}	–	–	–	0.88	–	0.16
{1b}	Fe^{2+}	–	–	–	0.87	–	0.16
{1c}	Fe^{2+}	–	–	–	0.79	–	0.19
{1d}	Fe^{2+}	–	–	–	0.74	–	0.21
{1e}	Fe^{2+}	–	–	–	0.71	–	0.22
{60}	Fe^{2+}	–	–	–	0.78	–	0.22
{60a}	Fe^{2+}	–	–	–	0.74	–	0.23
{60b}	Fe^{2+}	–	–	–	0.73	–	0.24
{60c}	Fe^{2+}	–	–	–	0.69	–	0.25

		M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)
{61b}	Fe^{2+}	–	–	–	0.57	–	0.03
{61c}	Fe^{2+}	–	–	–	0.44	–	0.08
{67a}	Fe^{2+}	–	0.12	–	–	0.21	–
	Fe^{3+}	–	0.07	–	–	–	–
{67c}	Fe^{2+}	–	0.09	–	–	0.12	–
	Fe^{3+}	–	0.23	–	–	–	–
{67f}	Fe^{3+}	–	0.27	–	–	0.15	–
{67g}	Fe^{2+}	–	0.03	–	–	0.06	–
	Fe^{3+}	–	0.27	–	–	0.07	–
{67h}	Fe^{3+}	–	0.17	–	–	0.22	–
{67i}	Fe^{2+}	–	0.09	–	–	0.16	–
	Fe^{3+}	–	0.17	–	–	–	–
{78}	Fe^{2+}	–	–	–	0.53	–	0.02
{78a}	Fe^{2+}	–	–	–	0.40	–	0.07
{78b}	Fe^{2+}	–	–	–	0.41	–	0.07
{78c}	Fe^{2+}	–	–	–	0.43	–	0.06
{78d}	Fe^{2+}	–	–	–	0.43	–	0.06
{78e}	Fe^{2+}	–	–	–	0.47	–	0.04
{78f}	Fe^{2+}	–	–	–	0.45	–	0.06
{98}	Fe^{2+}	–	–	–	0.42	–	0.02
{98a}	Fe^{2+}	–	–	–	0.31	–	0.06
{98b}	Fe^{2+}	–	–	–	0.33	–	0.06
{98c}	Fe^{2+}	–	–	–	0.32	–	0.06
{98d}	Fe^{2+}	–	–	–	0.33	–	0.05
{98e}	Fe^{2+}	–	–	–	0.33	–	0.05
{98f}	Fe^{2+}	–	–	–	0.33	–	0.05
{98g}	Fe^{2+}	–	–	–	0.34	–	0.05
{98h}	Fe^{2+}	–	–	–	0.34	–	0.05
{98i}	Fe^{2+}	–	–	–	0.36	–	0.04
{98j}	Fe^{2+}	–	–	–	0.35	–	0.04
{98k}	Fe^{2+}	–	–	–	0.35	–	0.05
{98l}	Fe^{2+}	–	–	–	0.36	–	0.04
{98m}	Fe^{2+}	–	–	–	0.36	–	0.04
{98n}	Fe^{2+}	–	–	–	0.37	–	0.04
{98o}	Fe^{2+}	–	–	–	0.35	–	0.04
{99}	Fe^{2+}	–	–	–	0.54	–	0.01
{99a}	Fe^{2+}	–	–	–	0.39	–	0.08
{99b}	Fe^{2+}	–	–	–	0.41	–	0.07
{99c}	Fe^{2+}	–	–	–	0.42	–	0.06
{99d}	Fe^{2+}	–	–	–	0.43	–	0.06
{99e}	Fe^{2+}	–	–	–	0.45	–	0.05
{99f}	Fe^{2+}	–	–	–	0.50	–	0.03
{100}	Fe^{2+}	–	–	–	0.60	–	0.02
{100a}	Fe^{2+}	–	–	–	0.45	–	0.08

		M(1)	M(2)	M(3)	M(4)	M(1)+M(3)	M(1)+M(2)+M(3)
{100b}	Fe^{2+}	–	–	–	0.46	–	0.07
{100c}	Fe^{2+}	–	–	–	0.47	–	0.07
{100d}	Fe^{2+}	–	–	–	0.47	–	0.07
{100e}	Fe^{2+}	–	–	–	0.48	–	0.07
{100f}	Fe^{2+}	–	–	–	0.48	–	0.07
{100g}	Fe^{2+}	–	–	–	0.49	–	0.06
{100h}	Fe^{2+}	–	–	–	0.51	–	0.05
{100i}	Fe^{2+}	–	–	–	0.51	–	0.05
{100j}	Fe^{2+}	–	–	–	0.51	–	0.05
{101}	Fe^{2+}	–	–	–	0.41	–	0.01
{101a}	Fe^{2+}	–	–	–	0.30	–	0.06
{101b}	Fe^{2+}	–	–	–	0.32	–	0.05
{101c}	Fe^{2+}	–	–	–	0.32	–	0.05
{101d}	Fe^{2+}	–	–	–	0.34	–	0.05
{101e}	Fe^{2+}	–	–	–	0.34	–	0.05
{101f}	Fe^{2+}	–	–	–	0.35	–	0.04
{101g}	Fe^{2+}	–	–	–	0.36	–	0.03
{102}	Fe^{2+}	–	–	–	0.68	–	0.06
{102a}	Fe^{2+}	–	–	–	0.52	–	0.13
{102b}	Fe^{2+}	–	–	–	0.53	–	0.12
{102c}	Fe^{2+}	–	–	–	0.54	–	0.12
{102d}	Fe^{2+}	–	–	–	0.55	–	0.12
{102e}	Fe^{2+}	–	–	–	0.56	–	0.11
{102f}	Fe^{2+}	–	–	–	0.56	–	0.11
{102g}	Fe^{2+}	–	–	–	0.58	–	0.10
{102h}	Fe^{2+}	–	–	–	0.59	–	0.10
{103}	Fe^{2+}	–	–	–	0.61	–	0.06
{103a}	Fe^{2+}	–	–	–	0.46	–	0.12
{103b}	Fe^{2+}	–	–	–	0.46	–	0.11
{103c}	Fe^{2+}	–	–	–	0.47	–	0.11
{103d}	Fe^{2+}	–	–	–	0.48	–	0.11
{103e}	Fe^{2+}	–	–	–	0.47	–	0.11
{103f}	Fe^{2+}	–	–	–	0.47	–	0.11
{103g}	Fe^{2+}	–	–	–	0.50	–	0.10
{103h}	Fe^{2+}	–	–	–	0.50	–	0.10
{103i}	Fe^{2+}	–	–	–	0.50	–	0.10
{103j}	Fe^{2+}	–	–	–	0.51	–	0.10
{103k}	Fe^{2+}	–	–	–	0.52	–	0.09
{103l}	Fe^{2+}	–	–	–	0.51	–	0.10
{103m}	Fe^{2+}	–	–	–	0.51	–	0.09
{103n}	Fe^{2+}	–	–	–	0.53	–	0.09
{103o}	Fe^{2+}	–	–	–	0.53	–	0.09

Appendix F4. Miscellaneous Information and Comments

Bancroft et al. (1967a), Bancroft et al. (1968)

Combined Mössbauer – infrared spectroscopic examination of cummingtonite{1} – {3}, grunerite{4} – {6} and tirodite{7}; complete site-populations derived by application of both methods (note misprint in tirodite{7} values, correct values given in this appendix). Chemical analyses and cell dimensions are from: {1} Ghose & Weidner (1972), who give further spectroscopic data on this specimen; {2} Mason (1953); {3}, {5}, {7}, Klein (1964, 1966); {4}, {6} Mueller (1960), Viswanathan & Ghose (1965).

Grunerite{5} is grunerite(22), the structure of which is reported by Finger (1969a). Burns (1969, 1970a) gave optical absorption spectra for grunerite{6}.

Bancroft et al. (1966)

Combined Mössbauer and infrared spectroscopic study of anthophyllite{8} and {9}, cummingtonite{1} and grunerite{6}; same data in Bancroft *et al.* (1967a, b). Adams *et al.* (1972) gave a X-ray photoelectron spectrum for anthophyllite{8}.

Bancroft et al. (1967b)

Mössbauer examination of anthophyllite{8} and {9} and actinolite{10} and {11}; there was incomplete resolution for both amphibole types, with two Fe^{2+} doublets in anthophyllite (M1+M2+M3 and M4) and two Fe^{2+} doublets in actinolite [M(1)+M(3) and M(2)]. Chemical analyses are from: {8} Rabbitt (1948); {9} Tilley (1957); {10} Burns & Greaves (1971), who gave further spectroscopic data on this sample; {11} Mueller (1960). Burns (1969, 1970a) gave optical absorption spectra for actinolite{10} and {11}.

Häggström et al. (1969)

Mössbauer spectroscopic study of edenitic hornblende {12}, edenite {13} and edenite {14}; there was incomplete resolution, with two doublets due to Fe^{2+} at M(1)+M(3) and M(2), and one doublet due to Fe^{3+} at M(2). Chemical analyses are from Annersten (1968).

Bancroft & Burns (1969)

Combined Mössbauer – infrared spectroscopic examination of glaucophane{15} and {16}, crossite{17} and {18} riebeckite{19} and magnesio-riebeckite{20} and {21}; fairly complete site-populations were derived. For magnesio-riebeckite{21}, the spectrum wat fitted to three quadrupole doublets (magnesio-riebeckite {21a}) and four quadrupole doublets (magnesio-riebeckite{21b}), respectively. Chemical analyses and cell parameters are from: {15} Ernst & Wai (1970) who give additional spectroscopic data on this sample; also note that this is glaucophane(26), the structure of which was refined by Papike & Clark (1968), with detailed structural data being listed in Appendix B; {16}, {17} Borg (1967b); {18}, {19} this reference; {20} Whittaker (1949), who reported the structure of this amphibole, magnesio-riebeckite (3) that is listed in Appendix A; {21} Ernst (1963), Ernst & Wai (1970). For {21}, the large discrepancy between the chemical analysis and Mössbauer results for the Fe^{3+}/Fe^{2+} ratio prompted a new partial chemical analysis of this amphibole. The results (Fe_2O_3 9.91, FeO 7.07 wt. %) agreed with the Mössbauer results; additional spectroscopic results are given by Ernst & Wai (1970), who noted that with the newly determined Fe_2O_3 and FeO values, the oxide sum for {21} is unrealistically low at 95.98 wt. %.

Ernst & Wai (1970)

Combined Mössbauer – infrared spectroscopic examination of glaucophane{15a} and {22} – {24}, crossite{25} and {26}, magnesio-riebeckite {27} and {21c}, riebeckite{28} – {31}; fairly complete site-populations were derived. Cell dimensions from this study, chemical analyses from: {15a}, {22} and {23} this study; {24} and {25} Banno (1959); {26} Borg (1967b); {27} Ernst (1960); {21} Whittaker (1949); {28} Switzer (1951); {29} Peacock (1928); {30} and {31} Onuki & Ernst (1969). Extensive heating experiments were performed, and the products were examined spectroscopically (samples {15b} – {15d}, {27a}, {27b}, {29a}, {29b}, {31a}).

Greaves et al. (1971)

See following reference.

Burns & Greaves (1971)

Combined Mössbauer – infrared spectroscopic examination of actinolite{10a}, {11a}, {33}, manganoan actinolite{32}, tschermakitic hornblende{34}, manganoan ferro-actinolite{35},

ferro-actinolite{36} and pure ferro-actinolite {37}; complete site-populations were assigned. Chemical analyses and cell dimensions are from: {10a}, {33} this study; {11a} Mueller (1960); {32}, {36} Klein (1966); {34} Tilley (1957); {35} Mitchell *et al.* (1971); {37} Ernst (1963). Manganoan ferro-actinolite {35} is the same sample as manganoan ferro-actinolite(37), the structure of which is reported by Mitchell *et al.* (1971). A detailed comparison of results from Mössbauer and infrared methods is given, together with the advantage and disadvantages of both methods for site-population characterization.

Hafner & Ghose (1971)

Mössbauer spectroscopic examination of grunerite{4a}, {5a}, {6a}, {38} – {47}, cummingtonite{48} – {54} and {56} – {60}, manganoan cummingtonite{55} and magnesio-cummingtonite{61}; there was incomplete resolution, with two Fe^{2+} doublets [M(1)+M(2)+M(3) and M(4)] resolved.

Spectra were recorded at room temperature and liquid-nitrogen temperature; {5a}, {60} and {61} are at room temperature, {56}, {60a} and {61a} are at low temperature (77 K). Chemical analyses and cell dimensions are from: {4a}, {6a,} {38} – {42}, {44} – {48}, {50}, {51}, {53}, {54}, {56}, {57}, {59}, {60} Mueller (1960), Viswanathan & Ghose (1965); {5a}, {43}, {49}, {52}, Klein (1964, 1966); {55}, {58} Butler (1969); {61} Kisch (1969). Grunerite{5a}, is grunerite(22), the structure of which is reported by Finger (1969a). Cummingtonite{60} is cummingtonite(21), the structure of which is reported by Ghose (1961) with additional modifications by Fischer (1966) and Mitchell *et al.* (1971), with preferred parameters being given in Appendix B.

Buckley & Wilkins (1971)

Combined Mössbauer and infrared spectroscopic study of cummingtonite{62} at room temperature and 77 K; cimplete cation site-populations were assigned from combined results. Also reported is a magnetic hyperfine spectrum recorded at 4.2 K.

Babeshkin et al. (1971)

A Mössbauer spectroscopic examination of a grunerite{63} (called cummingtonite) after heat treatment at several different temperatures. With increasing temperature, increasing Fe^{3+} is formed at the M(1, 2, 3) sites, whereas the Fe^{2+} content of the M(4) site remains the same. The ratio of the recoil-free fraction at the M(1, 2, 3) and M(4) sites was determined "semi-empirically" to be 0.9 (*cf.* Bancroft *et al.* 1967a). The isomer shifts are not listed in Appendix F2, as it is not clear to what referent they are referred; the relevant values are: M(4): {63a} 1.09 mm/s, {63b} 1.14 mm/s, no other values quoted. M(1)+M(2)+M(3): {63a} 1.26 mm/s, {63b} 1.28 mm/s, {63c} 1.25 mm/s, {63d} 1.24 mm/s, {63d} 1.26 mm/s. Heat-treatment conditions are: {63a} 600°C, {63b} 700°C, {63c} 800°C, {63d} 900°C.

Ghose & Weidner (1972)

Mössbauer spectroscopic examination of cummingtonite{1a} – {1e}, {60a}, {60b} and magnesio-cummingtonite{61a}, {61b} at low temperatures (77 K); there was incomplete resolution, with two Fe^{2+} doublets [M(1)+M(2)+M(3) and M(4)] resolved. Chemical analyses and cell dimensions are from: {1a} – {1e} this study; {60a}, {60b} Mueller (1960), Viswanathan & Ghose (1965); {61a}, {61b} Kisch (1969). This study concentrates primarily on ordering as a function of equilibration temperature.

Singh & Bonardi (1972)

Mössbauer spectroscopic examination of an arfvedsonite; the analysis of the spectrum is incompatible with the amphibole structure, and the results are not reproduced here.

Virgo (1972a)

Mössbauer spectroscopic study of "pure" ferro-richterite{64} at low temperature showed the presence of Fe^{3+} in the structure. However, there was incomplete resolution, and the data are incomplete.

Law (1973)

Mössbauer spectroscopic examination of a holmquistite{65} that is holmquistite[31], the structure of which is reported by Irusteta & Whittaker (1975). An excellent discussion of spectrum fitting is also given.

Kamineni (1973)

A Mössbauer spectral study of grunerite{66} (called cummingtonite) at both room (298 K) and low temperature (77 K). Site populations

were calculated assuming the ratio of the recoil-free fractions at the M(1, 2,3) and M(4) sites to be 0.9 (*cf.* Bancroft *et al.* 1967a). Note that the peak widths are extremely large.

Khristoforov et al. (1973)

A Mössbauer spectroscopic examination of a variety of apparently uncharacterized calcic amphiboles. Virtually no numerical data are given, quadrupole splitting and site populations are presented graphically. However, the two spectra reproduced show off-resonance counts of $\sim 1.6 \times 10^3$ and $\sim 3.8 \times 10^3$, respectively, together with excessive absorption.

Semet (1973)

A combined Mössbauer and infrared spectroscopic examination of "pure" magnesio-hastingsite{67} and natural magnesio-hastingsite{68}. The "pure' magnesio-hastingsite was synthesized (and further equilibrated) on a variety of oxygen buffers; the Mössbauer studies showed that Fe occurs as both Fe^{3+} and Fe^{2+}, the oxidation ratio being a function of the oxygen fugacity of synthesis. The ideal chemical composition (with Fe_2O_3 expressed as FeO) is given Appendix F1, together with two microprobe analyses of amphiboles synthesized at 850°C and 2 kbar on the cuprite–tenorite and iron–quartz–fayalite buffers, with $Fe^{3+}/(Fe^{3+}+Fe^{2+})$ ratios of 1.0 and 0.13, respectively.

Litvin et al. (1973c)

Combined Mössbauer spectroscopic and X-ray diffraction study of potassian ferri-taramite {69}, which is the same specimen as potassian ferri-taramite(51), the structure of which is also reported in this paper.

Barabanov & Tomilov (1973)

Mössbauer spectroscopic study of anthophyllite{70} – {72}, cummungtonite{73} and {74}, dannemorite{75} and grunerite{76} and {77}; incomplete resolution obtained, with two Fe^{2+} doublets due to occupancy of M(1) +M(2)+M(3) and M(4) sites, respectively. Cell contents are the only numerical data given; a discussion of variation in hyperfine parameters and Fe^{2+} ordering in the Fe–Mg–Mn amphiboles is given.

Seifert & Virgo (1974)

Low-temperature (77 K) Mössbauer spectroscopic study of anthophyllite{78} after heat-treatment at various temperatures; incomplete resolution attained, with two Fe^{2+} doublets due to occupancy of M1+M2+M3 and M4, respectively. This is anthophyllite[23], the structure of which is reported by Finger (1970a, b).

Borg et al. (1973)

Mössbauer spectroscopic study of crossite {17a} manganoan riebeckite{79} and arfvedsonite{80}; chemical analyses and cell dimensions from Borg (1967b). Manganoan riebeckite {79} includes Li_2O 0.14, ZnO 0.29, CuO 0.13 to give Li 0.09, Zn 0.03, Cu 0.02 p.f.u.; arfvedsonite{80} includes Li_2O 0.44, ZnO 0.67, CuO 0.01 to give Li 0.28, Zn 0.08 p.f.u. This study demonstrates the utility of using magnetic hyperfine spectra at very low temperatures (4 – 30 K) to achieve increased resolution, particularly with regard to the determination of accurate Fe^{3+}/Fe^{2+} ratios; see also Borg & Borg (1980).

Hawthorne & Grundy (1975)

Room- and low-temperature (77 K) Mössbauer spectroscopic study of potassian oxykaersutite{81}, the structure of which is reported by Hawthorne & Grundy (1973b). Only Fe^{3+} is present, and an attempt was made to resolve Fe^{3+} in all three M(1), M(2) and M(3) sites using area constraints derived from the site occupancies from the X-ray study. However, the X-ray site-occupancies are probably not correct (see Appendix B). The spectrum is not adequately represented by a single quadrupole-split Fe^{3+} doublet ($\chi^2 - 874$), and the half-width (0.68 mm/s) is high. Either the spectrum is the result of overlap of Fe^{3+} in more than one site (but with occupancies different from the ones given) or there is broadening due to next-nearest-neighbor occupancy, or both of these factors are operative simultaneously.

Bancroft & Brown (1975)

Mössbauer spectroscopic study of actinoyltic hornblende{82}, magnesio-hornblende{83} – {87} and tschermakitic hornblende{34a}; complete resolution was obtained (three Fe^{2+} doublets and one Fe^{3+} doublet). Chemical analyses and cell dimensions are from Dodge *et al.* (1968), with the exception of {34a}, which is from Burns & Greaves (1971). A fairly extended discussion and justification of the spectrum resolution and peak assignment are given.

Andersen et al. (1975)

Mössbauer spectroscopic study of a series of uncharacterized samples of arfvedsonite at a series of temperatures between 100 and 550 K, carried out in order to determine Fe^{2+}/Fe^{3+} ratios and compare them with results of conventional wet-chemical analysis. These authors suggest that there is a difference in the recoil-free fraction of Fe^{2+} and Fe^{3+} in the amphibole structure, it being necessary to correct for this to obtain accurate Fe^{2+}/Fe^{3+} ratios by Mössbauer spectroscopy.

Batievskii et al. (1975)

Mössbauer spectroscopic study of magnesio-hastingstitic hornblende{88}, potassian magnesio-hornblende{89}, magnesio-hornblende{90}, ferro-hornblende{91} and ferro-tschermakitic hornblende{92}. Chemical analyses include P_2O_5: 0.01, 0.03, 0.02, 0.02, 0.03 wt. %; Cr_2O_3: 0.024, 0.04, 0.013, 0.04, 0.09 wt. %; NiO: 0.02, 0.04, 0.05, 0.02,–, respectively. Complete site-population assignments are given assuming that all octahedrally co-ordinated trivalent cations are confined to the M(2) site.

Goodman & Wilson (1976)

Mössbauer spectroscopic examination of virtually uncharacterized amphibole designated "hornblende" {93} that was sampled at various levels through a soil profile to examine the effects of weathering [see also Wilson & Farmer (1970) for a similar infrared spectroscopic study]. In the data quoted in Appendix F2, {93a}, {93c} and {93e} refer to hornblende from various horizons, whose spectra are fitted to four quadrupole split doublets, whereas samples {93b}, {93d} and {93f} refer to the same samples fitted to five quadrupole split doublets. Up to six doublets were fitted to the spectra; however, the six-doublet fits are not justified (Law 1973). The five-doublet fits were assigned as Fe^{2+} in M(1), M(2), M(3) and M(4), with an additional wide doublet for Fe^{3+} in the M(1), M(2) and M(3) sites.

Litvin et al. (1976)

Combined X-ray structure and Mössbauer spectroscopic studies of arfvedsonite{94} and potassium-arfvedsonite{95}; these two amphiboles are identical to arfvedsonite(64) and potassium-arfvedsonite(65), details of which are given in Appendix B. Isomer shifts are not listed in Appendix F2a because it is not evident to which referent they are referred; the relevant values for Fe^{2+} at M(1), M(2) and M(3) and Fe^{3+} are: 1.31, –, 1.32, 0.57 and 1.35, 1.39, 1.37, 0.60 for {94} and {95}, respectively.

Goldman & Rossman (1977a)

A combined Mössbauer and optical-absorption spectroscopic study of tremolite{96}; incomplete resolution obtained, with two Fe^{2+} doublets [M(1)+M(2)+M(3) and M(4)] and one Fe^{3+} doublet being resolved. Strong evidence from the optical-absorption spectra of tremolite {96}, actinolite and a pargasite is provided to support the Mössbauer assignment of peaks.

Hawthorne & Grundy (1977b)

A combined Mössbauer spectroscopic and X-ray difraction study of zincian tirodite{97} that is identical to zincian tirodite(57); incomplete resolution obtained, with two Fe^{2+} doublets due to Fe^{2+} in M(1)+M(2)+M(3) and M(4), and two Fe^{3+} doublets due to Fe^{3+} in T(2) and M(2). Spectra at both room-temperature {97a} and liquid-nitrogen temperature {97b}. Parameters obtained for tetrahedrally co-ordinated Fe^{3+} are: I.S. = 0.11(0.12), Q.S. = 0.49(0.52), H.W. = 0.33(0.36) mm/s for the room-temperature (low-temperature) spectrum. Chemical analysis is from Klein & Ito (1968).

Seifert (1977)

See following paper.

Seifert (1978)

Mössbauer spectroscopic study of anthophyllite{78} and {98} – {103}; incomplete resolution obtained, with two Fe^{2+} doublets due to Fe^{2+} in M1+M2+M3 and M4. Spectra recorded at room and liquid-nitrogen temperatures (indicated by a and b respectively). Note that anthophyllite{78} is anthophyllite[23], the structure of which was refined by Finger (1970b). Site occupancies were calculated for the amphiboles equilibrated at various temperatures up to 800°C and a pressure of 1 kbar.

Tripathi & Lokanathan (1978)

Mössbauer spectroscopic study of actinolite {104} – {109}, hornblende{110} – {112} and winchite{113} and {114}. The amphiboles are apparently completely uncharacterized. The winchite spectra are characterized by two Fe^{3+} doublets and no Fe^{2+} doublets.

Goldman (1979)

Combined Mössbauer and electronic-absorption spectroscopic study of grunerite{115}, actinolite{116}, ferrotremolite{117}, actinolite {118} and pargasite{119}. This paper also presents a review of some previous Mössbauer studies on calcic amphiboles together with a re-assessment of the peak assignments, suggesting that Fe^{2+} prefers to enter the M(4) site prior to the M(1) and M(3) sites and that a doublet due to this occupancy is an important feature in the spectra of Fe^{2+}–poor amphiboles. Only limited Mössbauer data are presented; the spectrum of {118} was recorded at 77 K, and the spectrum of {119} was recorded at room temperature.

Stroink et al. (1980)

Mössbauer spectroscopic examination of anthophyllite{120}, cummingtonite{121} and magnesio-riebeckite{122}. Compositional and X-ray data are given by Rendall (1970) and Timbrell (1970). There was incomplete resolution for the Fe–Mg–Mn amphiboles, with two doublets due to Fe^{2+} at M(4) and M(1)+M(2) +M(3), and a small Fe^{3+} shoulder detectable. Magnesio-riebeckite{122} was resolved into two Fe^{2+} doublets, M(1) and M(3), and an Fe^{3+} doublet, M(2), and shows minor peaks due to admixture of magnetite. Note that the Q.S. value for Fe^{3+} in cummingtonite{121} must be wrong.

Law & Whittaker (1981)

Combined Mössbauer and infrared absorption spectroscopic study of holmquistite{65}, that is the same as holmquistite[31]; see also Law (1973). A comparison of these results with the results of X-ray structure-refinement is given.

Appendix G. Infrared Spectral Studies of Amphiboles

This technique has found considerable application in cation-ordering studies on amphiboles, although its use has tailed off in recent years as realization of the problems encountered with this technique has become apparent. Despite these drawbacks, considerable information concerning cation ordering has been derived, and a brief outline of these results is given here. The majority of amphiboles examined by this technique have also been studied using Mössbauer spectroscopy; these amphiboles are identified in this appendix using the numbers (in curly brackets) of Appendix F where the cell data are given. Amphiboles examined solely by this method are identified by numbers in angular brackets. Cation site-populations for both { } and < > samples are given here; for the { } data, site populations are given just from the infrared method, as the site populations derived by a combination of both methods are given in Appendix F.

Many vibrational spectroscopic studies are in the near-infrared region. The following studies are considered here:

Kukovskii & Litvin (1970)	*1 – 14*
Barabanov *et al.* (1974)	*15 – 53*
Liese (1975)	*54 – 60*

The data are given in Appendices G4 and G5 and Figures 97 and 98. Amphiboles *8*, *9* and *10* are magnesio-hornblende(46), hastingsite(44) and potassian ferri-taramite(51), respectively.

APPENDIX G1. CHEMICAL COMPOSITIONS AND UNIT-CELL DATA

	<1>	<2>	<3>	<4>	<5>	<6>	<7>	<8>	<9>	<10>	<11>	<12>
SiO_2	–	59.44	48.75	52.0	53.0	55.0	52.0	55.0	56.0	49.0	56.16	52.28
TiO_2	–	0.04	0.57	0.05	<0.01	<0.01	<0.01	<0.01	–	<0.01	–	0.05
Al_2O_3	–	12.78	9.67	~1.0	~0.2	–	~0.3	~0.2	0.22	~0.4	0.20	0.18
Fe_2O_3	–	1.48	1.74	–	–	–	–	–	–	–	1.81	–
FeO	–	9.20	11.49	20.0	18.0	16.1	14.2	12.1	8.2	5.5	6.32	22.57
MnO	–	0.10	0.28	0.37	0.29	0.26	0.71	0.60	0.11	0.27	2.30	0.24
MgO	–	10.22	12.78	11.5	13.5	14.0	15.0	17.5	22.0	21.0	19.84	10.53
CaO	–	0.71	11.91	11.0	10.0	10.0	10.5	12.0	11.0	11.0	9.34	11.26
Na_2O	–	0.18	0.77	–	–	–	0.08	0.60	–	–	1.30	0.16
K_2O	–	0.32	0.17	–	–	–	0.04	0.08	–	–	0.14	0.07
H_2O	–	2.08	1.81	–	–	–	–	–	–	–	2.46	2.56
F	–	0.12	0.12	–	–	–	–	–	–	–	0.79	–
	–	100.43	100.24	95.92	95.00	95.37	92.84	98.09	97.53	87.18	100.66	100.20
O ≡ F	–	0.06	0.06	–	–	–	–	–	–	–	0.33	–
Total	–	100.37	100.18	95.92	95.00	95.37	92.84	98.09	97.53	87.18	100.33	100.20
Si	7.94	7.82	7.00	7.88	7.99	8.15	7.94	7.88	7.86	7.69	7.90	7.86
Al	0.03	0.18	1.00	0.12	0.01	–	0.05	0.03	0.04	0.07	0.03	0.04
$\sum iv$	7.97	8.00	8.00	8.00	8.00	8.15	7.99	7.91	7.90	7.76	7.93	7.90
Al	–	1.80	0.64	0.06	0.03	–	–	–	–	–	–	–
Ti	–	–	0.06	0.01	–	–	–	–	–	–	–	0.01
Fe^{3+}	2.10	0.15	0.19	–	–	–	–	–	–	–	0.22	–
Fe^{2+}	1.88	1.01	1.38	2.53	2.27	1.99	1.81	1.45	0.96	0.72	0.74	2.82
Mn	–	0.01	0.03	0.05	0.04	0.03	0.09	0.07	0.01	0.04	0.27	0.03
Mg	1.04	2.00	2.73	2.60	3.03	3.09	3.41	3.74	4.60	4.91	4.16	2.34
$\sum vi$	5.02	4.97	5.03	5.25	5.37	5.11	5.31	5.26	5.57	5.67	5.39	5.20
$\sum vi-5$	0.02	Li=1.99	0.03	0.25	0.37	0.11	0.31	0.26	0.57	0.67	0.39	0.20
Ca	0.17	0.10	1.83	1.79	1.62	1.59	1.72	1.84	1.65	1.85	1.40	1.81
Na	1.75	–	0.04	–	–	–	–	–	–	–	0.21	–
$\sum$ M(4)	1.94	2.09	2.00	2.04	1.99	1.70	2.03	2.10	2.22	2.52	2.00	2.01
Na	–	0.05	0.17	–	–	–	–	0.17	–	–	0.14	0.05
K	–	0.05	0.03	–	–	–	–	0.02	–	–	0.02	0.02
$\sum$ A	–	0.10	0.10	–	–	–	–	0.10	–	–	0.16	0.07
a (Å)	–	–	–	–	–	–	–	–	–	–	9.803(2)	9.894(2)
b (Å)	–	–	–	–	–	–	–	–	–	–	18.083(5)	18.198(5)
c (Å)	–	–	–	–	–	–	–	–	–	–	5.292(2)	5.299(2)
β (°)	–	–	–	–	–	–	–	–	–	–	104.35(3)	104.58(2)
V ($Å^3$)	–	–	–	–	–	–	–	–	–	–	909.0(4)	923.5(4)
Space Group	C2/m	Pnma	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m	C2/m

APPENDIX G2. SITE OCCUPANCIES IN AMPHIBOLES BY INFRARED SPECTROSCOPY

	M(1)+M(3) per site	M(2) per site
⟨1⟩	$0.28Mg+0.67Fe^{2+}+0.05Fe^{2+}$	$0.03Mg+0.97Fe^{3+}$
⟨4⟩	$0.54(Fe^{2+}+Mn)$	$0.44(Fe^{2+}+Mn)$
⟨5⟩	$0.47(Fe^{2+}+Mn)$	$0.37(Fe^{2+}+Mn)$
⟨6⟩	$0.45(Fe^{2+}+Mn)$	$0.33(Fe^{2+}+Mn)$
⟨7⟩	$0.40(Fe^{2+}+Mn)$	$0.30(Fe^{2+}+Mn)$
⟨8⟩	$0.33(Fe^{2+}+Mn)$	$0.23(Fe^{2+}+Mn)$
⟨9⟩	$0.19(Fe^{2+}+Mn)$	$0.14(Fe^{2+}+Mn)$
⟨10⟩	$0.13(Fe^{2+}+Mn)$	$0.13(Fe^{2+}+Mn)$
⟨11⟩	$0.21(Fe^{2+}+Mn)$	$0.16(Fe^{2+}+Mn)$
⟨12⟩	$0.57(Fe^{2+}+Mn)$	$0.52(Fe^{2+}+Mn)$
⟨13⟩	$0.17(Fe^{2+}+Mn)$	$0.02(Fe^{2+}+Mn)$
⟨14⟩	$0.26(Fe^{2+}+Mn)$	$0.11(Fe^{2+}+Mn)$
⟨15⟩	$0.23(Fe^{2+}+Mn)$	$0.06(Fe^{2+}+Mn)$
⟨16⟩	$0.23(Fe^{2+}+Mn)$	$0.03(Fe^{2+}+Mn)$
⟨17⟩	$0.23(Fe^{2+}+Mn)$	$0.03(Fe^{2+}+Mn)$
⟨18⟩	$0.23(Fe^{2+}+Mn)$	$0.01(Fe^{2+}+Mn)$
⟨19⟩	$(0.77Mg+)0.23Al$	$(0.84Mg+)0.16Al$

	M(1) per site	M(2) per site	M(3) per site
⟨20⟩	$0.88Mg+0.12Fe^{2+}$	$0.90Mg+0.01Fe^{2+}$	$0.61Mg+0.38Fe^{2+}$
⟨21⟩	$0.85Mg+0.22Fe^{2+}$	$0.30Mg+0.03Fe^{2+}$	$0.59Mg+0.39Fe^{2+}$
⟨22⟩	$0.94Mg+0.07Fe^{2+}$	$0.83Mg+0.16Fe^{2+}$	$0.62Mg+0.38Fe^{2+}$
⟨23⟩	$0.84Mg+0.17Fe^{2+}$	$0.75Mg+0.16Fe^{2+}$	$0.62Mg+0.40Fe^{2+}$
⟨24⟩	$0.74Mg+0.26Fe^{2+}$	$Mg+0.11Fe^{2+}$	$0.55Mg+0.45Fe^{2+}$
⟨25⟩	$0.72Mg+0.29Fe^{2+}$	$0.54Mg+0.10Fe^{2+}$	$0.58Mg+0.42Fe^{2+}$
⟨26⟩	$0.78Mg+0.22Fe^{2+}$	$0.67Mg+0.21Fe^{2+}$	$0.59Mg+0.41Fe^{2+}$
⟨27⟩	$0.66Mg+0.33Fe^{2+}$	$0.56Mg+0.16Fe^{2+}$	$0.55Mg+0.45Fe^{2+}$
⟨28⟩	$0.69Mg+0.31Fe^{2+}$	$0.46Mg+0.29Fe^{2+}$	$0.54Mg+0.46Fe^{2+}$
⟨29⟩	$0.56Mg+0.42Fe^{2+}$	$0.27Mg+0.24Fe^{2+}$	$0.53Mg+0.47Fe^{2+}$
⟨30⟩	$0.50Mg+0.48Fe^{2+}$	$0.46Mg+0.29Fe^{2+}$	$0.59Mg+0.41Fe^{2+}$
⟨31⟩	$0.55Mg+0.44Fe^{2+}$	$0.50Mg+0.33Fe^{2+}$	$0.58Mg+0.47Fe^{2+}$
⟨32⟩	$0.55Mg+0.46Fe^{2+}$	$0.23Mg+0.69Fe^{2+}$	$0.59Mg+0.39Fe^{2+}$
⟨33⟩	$0.70Mg+0.30Fe^{2+}$	$0.83Mg+0.04Fe^{2+}$	$0.58Mg+0.42Fe^{2+}$
⟨34⟩	$0.75Mg+0.25Fe^{2+}$	$0.75Mg+0.02Fe^{2+}$	$0.58Mg+0.42Fe^{2+}$
⟨35⟩	$0.78Mg+0.22Fe^{2+}$	$0.65Mg+0.02Fe^{2+}$	$0.53Mg+0.48Fe^{2+}$

	M(1)+M(3) per site	M(2)+M(4) per site
{1}	$0.24Fe^{2+}$	$0.44Fe^{2+}$
{2}	$0.50Fe^{2+}$	$0.53Fe^{2+}$
{3}	$0.65Fe^{2+}$	$0.61Fe^{2+}$
{4}	$0.87Fe^{2+}$	$0.83Fe^{2+}$
{5}	$0.85Fe^{2+}$	$0.89Fe^{2+}$
{6}	$0.98Fe^{2+}$	$0.93Fe^{2+}$
{7}	$0.15Fe^{2+}$	$0.24Fe^{2+}$
{8}	$0.08Fe^{2+}$	$0.34Fe^{2+}$
{9}	$0.21Fe^{2+}$	$0.40Fe^{2+}$
{10a}	$0.83Mg+0.17(Fe+Mn)$	$0.85Mg+0.08(Fe+Mn)$
{11} *	$0.47Mg+0.49(Fe^{2+}+Mn)+0.04Fe^{3+}$	$0.50Mg+0.49(Fe^{2+}+Mn)+0.04Fe^{3+}$
{19} *	$0.09Mg+0.84Fe^{2+}+0.07Fe^{3+}$	$0.02Mg+0.12Fe^{2+}+0.86Fe^{3+}$
{20} *	$0.82Mg+0.14Fe^{2+}+0.04Fe^{3+}$	$0.20Mg+0.03Fe^{2+}+0.77Fe^{3+}$
{32}	$0.81Mg+0.19(Fe+Mn)$	$0.88Mg+0.32(Fe+Mn)$
{33}	$0.80Mg+0.20(Fe+Mn)$	$0.72Mg+0.23(Fe+Mn)$
{35}	$0.43Mg+0.52(Fe^{2+}+Mn)+0.05Fe^{3+}$	$0.29Mg+0.65(Fe^{2+}+Mn)+0.09Fe^{3+}$
{36}	$0.45Mg+0.49(Fe^{2+}+Mn)+0.07Fe^{3+}$	$0.52Mg+0.63(Fe+Mn)$

Appendix G3. Miscellaneous Information and Comments

Burns & Strens (1966)

Examination of actinolite{10}, {11} and {33}, cummingtonite{1} – {3} and grunerite {4} and {5}, in which partial site-populations were derived.

Strens (1966)

Infrared study of several amphibole series (holmquistite, glaucophane, riebeckite, tremolite, anthophyllite, cummingtonite – grunerite); no quantitative results are given. However, it is noted that Fe^{2+} "definitely" prefers the M(1) site in glaucophane, with a slight preference in riebeckite; this is not in accord with the X-ray results of Papike & Clark (1968) or the Mössbauer results of Bancroft & Burns (1969) and Ernst & Wai (1970). In addition, cation clustering (the occurrence of FeFeFe and MgMgMg arrangements in adjacent 2M(1)+ M(3) sites, in amounts greater than that expected for random mixing) was reported to occur in all series except the cummingtonite – grunerite amphiboles.

Bancroft et al. (1966)

Combined Mössbauer and infrared spectroscopic study of anthophyllite{8} and {9}, cummingtonite{1} and grunerite{6}.

Bancroft et al. (1967a)

Combined Mössbauer – infrared spectroscopic examination of cummingtonite{1} – {3}, grunerite{4} – {6} and tirodite{7}.

Burns & Prentice (1968)

Infrared spectroscopic study of riebeckite {19}, magnesio-riebeckite{20} and crocidolite <1>. Site occupancies are derived for the M(1)+M(3) and M(2) positions; using the criteria of Strens (1966), it is noted that the M(1) positions are favored in preference to M(3) positions in the order $Fe^{3+} > Fe^{2+} > Mg$, and that significant clustering of cations occurs.

Bancroft & Burns (1969)

Combined Mössbauer and infrared spectroscopic study of glaucophane{15} and {16}, crossite{17} and {18}, riebeckite{19} and magnesio-riebeckite{20} and {21}. The spectra indicate that the majority of the Al^{3+} and Fe^{3+} cations occupy the M(2) positions, although additional inflections in the spectra occur that could be due to trivalent cations at the M(1) or M(3) positions (or both).

Wilkins et al. (1970)

Infrared spectroscopic study of holmquistite <2> and magnesio-hornblende <3>; chemical analyses include Li_2O 3.76 and 0.18 wt. % for <2> and <3>, respectively. Holmquistite shows four bands, the intensities of which indicate a nearly random distribution of Mg and Fe^{2+} over the M(1) and M(3) sites; no minor bands occur, indicating that no univalent or trivalent cations occur at M(1) and M(3). The hornblende shows four main bands, due to Mg and Fe^{2+} configurations, a high-frequency band at $\sim$3690 cm^{-1} and at least two broad bands around 3600 cm^{-1}; the high-frequency band was assigned to configurations involving a filled A-site, and the low-frequency bands were assigned to "various combinations of trivalent and divalent ions"; no exact site-populations were assigned. ΣM(4) for magnesio-hornblende <3> includes 0.10 Li.

Wilkins (1970)

Infrared spectroscopic study of actinolite <4>–<13>, {33}, <14>–<18>; site populations are given as occupancies of M(1)+M(3) and M(2), assuming negligible occupancy of M(4). Chemical analyses are from: <4> – <10>, Mueller (1960); <11> and <12>, Klein (1966); {33}, see Appendix F. Actinolite <13>–<18> are only characterized by $(Fe^{2+}+Mn^{2+})/(Fe^{2+}+Mn^{2+}+Mg)$ ratios that were derived by analysis for Fe^{2+} assuming an "ideal actinolite formula"; these ratios are not listed in Appendix G1, but are retrievable by summing the $(Fe^{2+}+Mn^{2+})$ site-populations and dividing by 5.0. Note that actinolite<5> coexists with cummingtonite{53}.

Burns & Law (1970)

A discussion of the problems associated with estimating site populations in anthophyllite and gedrite by the infrared method, with cummingtonite{1} and anthophyllite{9} as illustrations.

Ernst & Wai (1970)

Combined Mössbauer and infrared spectroscopic study of glaucophane{15a}, magnesio-riebeckite{27} and riebeckite{29}, as well as the heated products {15b} – {15d}, {27b} and {27c}, and {29b} and {29c}, the heating conditions being given in Appendix F1.

Burns & Greaves (1971)

Combined Mössbauer and infrared spectroscopic study of actinolite{10a}, {11} and {33}, manganoan actinolite {32}, manganoan

ferro-actinolite{35} and ferro-actinolite{36}; further details are given in Appendix F4.

Buckley & Wilkins (1971)

Combined Mössbauer and infrared spectroscopic study of cummingtonite{62}; complete site-populations assigned.

Rowbotham & Farmer (1973)

Examination of the variation of principal stretching frequency in synthetic richterite – tremolite amphiboles, together with a comparison with natural amphiboles. The samples of pure richterite appear to be nonstoichiometric.

Semet (1973)

Combined Mössbauer and infrared spectroscopic study of "pure" magnesio-hastingsite{67}, natural magnesio-hastingsite{68} and pure pargasite<19>. Semet 1973 suggested that the "broad absorption band in the infrared spectra of the Fe^{2+}-rich synthetic magnesio-hastingsites in the OH-stretching region may be attributed to extra hydroxyl ions". The spectrum of pure pargasite<19> is interpreted as indicating random distribution of Mg and Al over the M(1), M(2) and M(3) sites.

Nikitina et al. (1973)

Infrared spectroscopic study of sixteen apparently uncharacterized calcic amphiboles <20>–<35> (the sequence followed is that of Table 4, this reference); <20>, <22>, <24> and <27> have also been examined by Mössbauer spectroscopy (Khristoforov *et al.* 1973), and a comparison of results is given here.

	Fe^{2+} (infrared)			Fe^{2+} Mössbauer		
	M(1)	M(2)	M(3)	M(1)	M(2)	M(3)
<20>	0.12	0.01	0.38	0.10	0.03	0.39
<22>	0.07	0.16	0.38	0.12	0.15	0.30
<24>	0.26	0.11	0.45	0.27	0.08	0.47
<27>	0.33	0.16	0.45	0.39	0.12	0.42

Spectra were fitted using Lorentzian line-shape, and the site populations were calculated from the "normalized intensities of the bands at their peaks"; this presumably refers to peak heights, as the authors indicate that site populations assigned on the basis of "integral intensities" are inconsistent with the chemistry of the samples. The authors offer a rather peculiar argument to arrive at the conclusion that the B and C bands are due to the configurations $MgMgFe^{2+}$ and $Fe^{2+}Fe^{2+}Mg$, respectively, at M(1)M(1)M(3), presumably with configurations involving both Mg and Fe^{2+} at M(1)M(1) not in evidence. With this assumption, complete site-populations were derived. The occurrence of prominent clustering of cations was also noted.

Strens (1974)

A review of infrared spectroscopic work on chain, ribbon and ring silicates, with special emphasis on the hydroxyl-stretching region in the spectra of alkali amphiboles.

Law (1976)

A discussion of the peak-intensity criteria for cation ordering and clustering in amphiboles.

Maresch & Langer (1976)

Synthesis and infrared study of three synthetic amphiboles $Li_{0.27}(Li_{1.11}Mg_{0.89})Mg_5(Si_{8.01}O_{21.20}OH_{0.80})(OH)_2$ <36>, $Na_2Mg_6Si_8O_{22}(OH)_2$ <37> and $Na_3Mg_5(Si_8O_{21}OH)(OH)_2$ <38>; cell data for <37> and <38> are from Witte *et al.* (1969). The fine structure in the hydroxyl-stretching region of <36> could not be completely interpreted; however, a band at 3727 cm^{-1} was assigned to hydroxyl in an Si–OH configuration.

Law & Whittaker (1981)

Combined Mössbauer and infrared-absorption spectroscopic study of holmquistite{65}, which is equivalent to holmquistite[31].

APPENDIX G4. CHEMICAL ANALYSES AND UNIT-CELL DATA FOR AMPHIBOLES EXAMINED BY VIBRATIONAL SPECTROSCOPY

	1	2	3	4	5	6	7	8	9
SiO_2	56.30	55.73	50.00	46.11	42.28	48.10	41.91	44.61	37.93
TiO_2	-	0.35	0.47	0.87	0.57	0.10	0.69	1.79	3.30
Al_2O_3	0.51	3.75	4.92	8.21	11.66	11.05	15.15	8.70	7.96
Fe_2O_3	0.83	0.67	3.47	5.21	3.74	0.67	6.22	3.46	3.96
FeO	2.73	5.03	9.91	9.05	9.69	1.65	8.38	16.09	28.32
MnO	0.34	0.10	0.28	0.48	0.39	-	0.14	0.29	0.57
MgO	23.10	19.44	16.27	14.12	13.22	20.60	13.40	10.45	2.56
CaO	12.94	12.14	11.13	11.76	12.67	12.50	9.74	10.36	9.66
Na_2O	0.34	0.43	1.14	1.33	2.00	2.54	1.05	1.47	1.71
K_2O	0.12	0.04	0.17	0.82	1.05	1.24	0.55	0.39	1.55
P_2O_5	-	0.11	0.14	0.11	0.51	-	1.22	0.11	0.11
SO_3	0.21	0.13	0.12	0.12	0.34	-	0.39	0.12	0.33
H_2O	0.22	0.01	0.08	0.08	0.26	0.11	0.14	0.06	0.08
	2.62	2.36	2.19	2.14	1.45	0.71	0.96	2.04	2.42
F	-	-	-	-	-	1.90	-	-	-
	100.21	100.29	100.29	100.41	99.85	101.17	99.86	99.84	100.36
$O \equiv F$	-	-	-	-	-	0.80	-	-	-
$\sum$	100.21	100.29	100.29	100.41	99.85	100.37	99.86	99.84	100.36
Si	7.82	7.73	7.10	6.69	6.29	6.66	5.91	6.59	6.11
Al	0.09	0.27	0.82	1.31	1.71	1.34	2.09	1.41	1.51
$\sum iv$	7.91	8.00	7.92	8.00	8.00	8.00	8.00	8.00	8.00
Al	-	0.35	-	0.09	0.35	0.47	0.44	0.10	-
Ti	-	0.04	0.05	0.10	0.08	0.01	0.08	0.19	0.40
Fe^{3+}	0.09	0.07	0.31	0.58	0.41	0.08	0.66	0.39	0.10
Fe^{2+}	0.30	0.58	1.18	1.10	1.21	0.19	0.99	1.99	3.80
Mn	0.03	0.01	0.03	0.06	0.05	-	0.02	0.04	0.08
Mg	4.67	3.93	3.43	3.07	2.92	4.25	2.81	2.30	0.62
$\sum vi$	5.09	4.98	5.00	5.00	5.02	5.00	5.00	5.01	5.00
$\sum vi - 5$	0.09	-	-	-	0.02	-	-	0.01	-
Ca	1.92	1.81	1.70	1.84	2.02	1.85	1.55	1.64	1.68
Na	-	0.10	0.30	0.16	-	0.15	0.30	0.35	0.32
$\sum$ M(4)	2.01	1.91	2.00	2.00	2.04	2.00	1.85	2.00	2.00
Na	0.08	-	0.01	0.23	0.57	0.53	-	0.06	0.20
K	0.02	-	0.03	0.16	0.21	0.12	0.12	0.07	0.33
$\sum$ A	0.10	-	0.04	0.39	0.78	0.65	0.12	0.13	0.53
a(Å)	9.839	9.831	9.842	9.862	9.865	9.887	9.818	9.843	9.952
b(Å)	18.063	18.063	18.076	18.080	18.060	17.991	18.004	18.113	18.243
c(Å)	5.278	5.284	5.296	5.309	5.316	5.299	5.281	5.316	5.339
β(°)	104.7	104.6	104.8	104.9	105.2	105.4	104.5	105.0	105.0
V(Å^3)	907.3	908.0	911.0	914.3	913.7	908.6	909.1	915.4	936.0

	10	11	12	13	14	15	16	17	18
SiO_2	37.55	48.76	48.66	49.48	62.09	56.74	56.68	55.12	46.50
TiO_2	0.89	1.82	0.38	0.08	–	–	–	0.29	0.36
Al_2O_3	9.90	3.43	0.04	1.26	0.68	0.27	0.72	1.22	14.21
Fe_2O_3	11.98	10.05	0.25	0.21	0.09	0.47	1.16	1.63	2.15
FeO	21.40	14.66	39.63	22.62	1.00	12.90	16.37	16.42	17.24
MnO	1.25	2.18	1.30	15.62	0.02	0.49	0.37	0.42	0.20
MgO	1.31	5.81	6.13	9.00	32.52	24.67	22.24	21.06	16.17
CaO	7.28	1.51	0.69	–	0.52	2.27	0.90	1.99	0.48
Na_2O	4.05	8.00	0.05	0.05	0.10	–	0.03	0.15	1.12
K_2O	2.11	1.80	–	0.04	0.02	0.05	0.02	0.02	0.06
P_2O_5	0.14	0.07	0.03	–	0.12	–	–	–	–
SO_3	0.12	–	0.37	–	–	–	–	–	–
H_2O	0.04	0.04	0.04	0.16	–	1.87	1.76	1.43	1.32
	1.80	1.87	2.71	1.56	3.24	–	–	–	–
F	–	–	–	–	–	0.14	0.20	0.07	0.03
	99.82	100.01	100.34	100.10	100.39	99.87	100.45	99.82	99.84
$O \equiv F$	–	–	–	–	–	0.06	0.08	0.03	0.01
$\sum$	99.82	100.01	100.34	100.10	100.39	99.81	100.37	99.79	99.83
Si	6.14	7.50	8.00	7.78	8.00	7.91	7.94	7.81	6.63
Al	1.86	0.50	–	0.22	–	0.04	0.06	0.19	1.37
$\sum iv$	8.00	8.00	8.00	8.00	8.00	7.95	8.00	8.00	8.00
Al	0.04	0.12	0.04	–	0.10	–	0.06	0.01	1.01
Ti	0.11	0.21	0.05	0.01	–	–	–	0.03	0.04
Fe^{3+}	1.45	1.16	0.04	0.02	0.01	0.05	0.12	0.17	0.23
Fe^{2+}	2.92	1.90	5.54	2.96	0.11	1.51	1.92	1.94	2.05
Mn	0.18	0.28	0.18	2.06	–	0.06	0.04	0.05	0.02
Mg	0.30	1.33	1.43	2.11	6.24	5.13	4.65	4.44	3.43
$\sum vi$	5.00	5.00	–	–	–	–	–	–	–
$\sum vi-5$	–	–	–	–	–	–	–	–	–
Ca	1.27	0.25	0.09	–	0.07	0.34	0.14	0.30	0.07
Na	0.73	1.75	–	–	0.02	–	0.01	0.04	0.13
$\sum$ M(4)	2.00	2.00	7.37	7.16	6.53	7.08	6.94	7.00	7.00
Na	0.56	1.05	–	–	–	–	–	–	0.18
K	0.45	0.35	–	–	–	0.01	–	–	0.01
$\sum$ A	1.01	1.40	–	–	–	0.01	–	–	0.19
a(Å)	9.951	9.903	–	9.575	18.50	–	–	–	–
b(Å)	18.166	18.066	–	18.27	17.94	–	–	–	–
c(Å)	5.354	5.332	–	5.343	5.37	–	–	–	–
β(°)	105.0	104.0	–	102.2	90	90	90	90	90
V($Å^3$)	934.4	925.6	–	914.2	1782	–	–	–	–

	20	21	22	24	25	29	32	33	34
SiO_2	48.55	50.19	50.51	50.95	50.77	51.47	49.65	54.15	53.69
TiO_2	0.02	–	–	0.21	–	0.04	0.07	–	0.03
Al_2O_3	0.72	0.80	0.62	0.54	0.86	1.10	4.14	0.65	2.47
Fe_2O_3	0.96	1.46	0.24	0.71	0.62	0.44	2.01	0.99	2.85
FeO	43.47	39.35	39.32	35.79	35.40	33.37	26.55	23.90	5.75
MnO	0.35	0.87	0.86	5.34	2.01	1.85	0.01	0.18	0.16
MgO	2.39	3.97	4.95	3.94	6.69	9.25	13.14	16.63	18.92
CaO	1.80	1.69	1.57	0.76	2.28	0.50	1.72	0.78	11.93
Na_2O	0.08	0.03	0.03	0.13	0.03	0.08	0.29	0.03	0.57
K_2O	0.01	0.03	0.04	–	–	0.01	0.48	0.02	0.18
P_2O_5	–	–	–	–	–	–	–	–	–
SO_3	–	–	–	–	–	–	–	–	–
H_2O	2.06	1.81	1.03	1.91	0.56	1.76	1.46	1.00	2.28
	–	–	–	–	–	–	–	–	–
F	–	–	–	–	0.10	0.04	–	–	–
	100.41	100.20	99.17	100.28	99.32	99.91	99.52	98.33	98.83
$0 \equiv F$	–	–	–	–	0.04	0.02	–	–	–
$\sum$	100.41	100.20	99.17	100.28	99.28	99.89	99.52	98.33	98.83
Si	7.88	7.97	8.01	8.07	7.92	7.93	7.45	7.97	7.64
Al	0.12	0.03	–	–	0.08	0.07	0.55	0.03	0.36
$\sum iv$	8.00	8.00	8.01	8.07	8.00	8.00	8.00	8.00	8.00
Al	0.02	0.12	0.12	0.17	0.07	0.13	0.19	0.08	0.06
Ti	–	–	–	0.03	–	0.01	0.01	–	–
Fe^{3+}	0.12	0.17	0.03	0.09	0.07	0.05	0.23	0.11	0.31
Fe^{2+}	5.90	5.23	5.21	4.74	4.62	4.30	3.33	2.94	0.68
Mn	0.05	0.12	0.12	0.72	0.27	0.24	–	0.02	0.02
Mg	0.58	0.94	1.17	0.93	1.56	2.12	2.94	3.65	4.01
$\sum vi$	–	–	–	–	–	–	–	–	5.08
$\sum vi-5$	–	–	–	–	–	–	–	–	0.08
Ca	0.31	0.29	0.27	0.13	0.38	0.08	0.28	0.12	1.82
Na	0.02	0.01	0.01	0.04	0.01	0.02	0.03	0.01	0.10
$\sum$ M(4)	7.00	6.87	6.92	6.83	6.97	6.95	7.00	6.93	2.00
Na	–	–	–	–	–	–	0.06	–	0.06
K	–	0.01	0.01	–	–	–	0.09	–	0.03
$\sum$ A	–	0.01	0.01	–	–	–	0.15	–	0.09
a(Å)	–	–	–	–	–	–	–	–	–
b(Å)	–	–	–	–	–	–	–	–	–
c(Å)	–	–	–	–	–	–	–	–	–
β(°)	–	–	–	–	–	–	–	–	–
V(Å^3)	–	–	–	–	–	–	–	–	–

	35	36	37	38	40	43	44	45	50
SiO_2	55.45	56.93	56.04	57.28	46.28	45.18	45.20	45.22	49.84
TiO_2	0.02	0.01	0.01	–	0.84	0.69	0.89	0.91	–
Al_2O_3	1.07	0.72	2.19	0.62	12.09	13.51	11.61	11.08	4.15
Fe_2O_3	3.01	1.69	3.74	1.69	3.04	3.85	4.54	4.11	2.99
FeO	4.67	4.62	4.21	4.00	11.15	14.27	11.00	11.30	15.67
MnO	0.09	0.04	0.07	0.10	0.23	0.41	0.30	0.26	0.14
MgO	19.98	20.58	19.92	21.46	11.59	7.30	11.35	11.62	12.45
CaO	11.68	12.18	11.15	11.76	11.40	11.50	11.32	12.20	11.90
Na_2O	0.64	0.20	0.84	0.29	1.24	1.09	1.35	1.13	0.38
K_2O	0.09	0.05	0.05	0.02	0.46	1.21	0.53	0.50	0.22
P_2O_5	–	–	–	–	–	–	–	–	–
SO_3	–	–	–	–	–	–	–	–	–
H_2O	2.04	1.92	1.71	1.79	1.85	0.79	1.74	1.52	2.45
	–	–	–	–	–	–	–	–	–
F	0.07	0.03	–	0.04	–	0.05	–	0.04	0.08
	98.81	98.94	99.83	99.05	100.17	99.85	99.83	99.89	100.27
$O \equiv F$	0.03	0.01	–	0.02	–	0.02	–	0.02	0.03
$\sum$	98.78	98.93	99.83	99.03	100.17	99.83	99.83	99.87	100.24
Si	7.82	7.94	7.75	7.94	6.69	6.62	6.60	6.60	7.38
Al	0.18	0.06	0.25	0.06	1.31	1.38	1.40	1.40	0.62
$\sum iv$	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00	8.00
Al	–	0.06	0.11	0.04	0.75	0.96	0.60	0.51	0.10
Ti	–	–	–	–	0.09	0.08	0.10	0.10	–
Fe^{3+}	0.32	0.18	0.39	0.18	0.33	0.43	0.50	0.45	0.33
Fe^{2+}	0.55	0.54	0.49	0.46	1.35	1.75	1.34	1.38	1.94
Mn	0.01	0.01	0.01	0.01	0.03	0.05	0.04	0.03	0.02
Mg	4.20	4.28	4.11	4.44	2.50	1.59	2.47	2.53	2.75
$\sum vi$	5.08	5.06	5.10	5.13	5.04	4.85	5.04	5.00	5.13
$\sum vi-5$	0.08	0.06	0.10	0.13	0.04	–	0.04	–	0.13
Ca	1.76	1.82	1.65	1.75	1.77	1.81	1.77	1.91	1.89
Na	0.16	0.05	0.23	0.08	0.19	0.19	0.19	0.09	–
$\sum M(4)$	2.00	1.93	1.98	1.96	2.00	2.00	2.00	2.00	2.02
Na	0.02	–	–	–	0.16	0.12	0.20	0.23	0.11
K	0.02	0.01	0.01	–	0.09	0.23	0.10	0.09	0.04
$\sum A$	0.04	0.01	0.01	–	0.25	0.34	0.30	0.32	0.15
a(Å)	–	–	–	–	–	–	–	–	–
b(Å)	–	–	–	–	–	–	–	–	–
c(Å)	–	–	–	–	–	–	–	–	–
β(°)	–	–	–	–	–	–	–	–	–
V(Å^3)	–	–	–	–	–	–	–	–	–

APPENDIX G5. INFRARED ABSORPTION FREQUENCIES (cm^{-1}) FOR AMPHIBOLES

15	16	17	18	19	20	21	22	23	24	25	26	27	28
1132	1133	1135	–	1130	1130	1132	1134	1135	1135	1135	1135	1135	1136
1112	–	1110	1110	1110	–	–	–	–	–	–	–	–	–
1097	1092	1093	1093	1100	1082	1083	1085	1088	1083	1085	1088	1090	1092
–	–	–	–	–	–	–	–	–	–	–	–	–	–
1000	1000	–	–	1010	1000	1000	1000	1002	1005	997	1003	1005	1000
982	980	982	980	983	975	975	975	975	975	975	977	975	980
–	–	–	–	–	–	–	–	–	–	–	–	–	–
912	–	–	–	913	–	–	–	–	–	–	–	–	–
900	901	903	910	–	890	895	890	900	895	900	900	900	899
–	–	–	–	–	–	–	–	–	–	–	–	–	–
782	782	780	780	784	775	774	775	778	772	775	778	780	778
755	755	–	755	758	–	–	–	–	–	–	–	–	–
737	–	740	–	–	730	730	731	735	732	732	733	734	732
710	700	–	708	712	703	704	703	708	702	708	708	710	707
691	692	697	695	692	–	–	–	–	–	–	–	–	–
672	672	668	–	–	–	–	–	–	–	–	–	–	–
659	657	655	660	660	655	655	652	653	651	655	655	652	650
–	–	–	–	–	632	635	635	635	635	638	638	640	640
537	–	–	–	535	532	532	531	528	530	530	535	532	530
522	523	525	525	–	507	508	508	508	509	509	510	512	516
500	495	495	498	500	478	480	481	480	482	480	483	483	489
470	465	465	465	468	–	–	–	–	–	–	–	–	–
440	442	440	–	447	–	–	–	–	–	452	452	–	–
–	–	–	–	–	423	425	426	426	427	427	429	432	433
415	412	410	–	417	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–

29	30	31	32	33	34	35	36	37	38	39	40	41	42
1137	1133	1138	1135	1134	–	–	–	–	–	–	1130	–	1130
–	–	–	–	–	1110	1112	1110	1110	1111	1120	–	–	–
1083	1088	1090	1090	1090	–	–	–	–	–	–	1090	1100	1090
–	–	–	–	–	1060	1070	–	–	–	–	1040	1050	1050
1000	1000	1005	1005	1000	992	1000	995	995	998	1000	–	–	–
975	978	975	975	975	–	–	–	–	–	–	–	–	–
–	–	–	–	–	955	958	952	960	955	965	955	960	960
–	–	–	–	–	922	920	920	920	920	928	–	–	–
898	900	905	898	899	–	–	–	–	–	–	–	–	–
–	–	–	–	–	800	800	800	800	800	805	800	–	–
777	778	780	777	778	–	–	–	–	–	–	–	–	–
–	–	–	–	–	757	760	758	760	760	762	755	752	755
732	733	–	735	740	–	–	–	–	–	–	–	–	–
703	708	708	700	698	–	–	–	–	–	–	–	–	–
–	–	–	–	–	687	688	687	687	687	692	697	700	710
–	–	–	–	–	–	–	–	–	–	–	–	–	–
657	655	655	657	657	662	662	662	662	661	665	660	640	650
641	642	643	647	649	645	644	643	645	645	645	–	–	–
532	527	532	–	–	–	–	–	–	–	–	–	–	–
516	512	518	520	520	512	512	512	512	512	515	512	507	510
490	482	488	495	493	–	–	–	–	–	–	–	–	–
–	–	–	–	–	470	465	468	470	470	475	462	465	465
452	–	453	455	457	450	450	450	450	450	453	–	–	–
432	430	435	437	437	425	425	425	425	423	425	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–	–	–	–	–	–

43	44	45	46	47	48	49	50	51
–	1130	1125	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
1080	1090	1090	1100	–	1105	–	1110	1112
1050	1040	1040	1062	1068	–	1062	1065	1065
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
950	955	955	955	955	965	965	960	960
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
798	797	800	–	802	803	–	–	800
–	–	–	–	–	–	–	–	–
755	752	754	755	753	753	755	760	760
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
695	695	695	700	697	700	698	695	693
–	–	–	–	–	–	–	–	–
655	655	657	648	648	645	645	655	655
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
515	515	515	507	505	508	505	512	517
–	–	–	–	–	–	–	–	–
465	465	465	466	467	467	468	468	470
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–	–

52	53	54	55	56	57	58	59	60
–	1130	–	1126	–	–	–	–	1125
–	–	1010	–	–	–	–	1105	–
1085	1105	–	1085	1093	1098	–	–	1077
1050	–	–	1026	1043	1050	1060	1050	–
–	–	–	1000	994	993	–	–	–
–	–	–	978	–	–	–	980	–
962	–	–	–	956	950	965	–	969
–	–	–	–	918	920	–	–	–
–	–	880	900	–	–	–	900	900
803	–	–	–	–	–	–	789	–
–	–	780	778	–	–	–	–	–
758	762	–	–	760	758	745	–	750
–	–	–	740	–	720	–	730	–
–	–	–	–	–	–	–	–	700
700	710	–	690	682	683	–	–	–
–	–	667	–	–	–	–	–	–
660	642	–	648	–	660	661	–	–
–	–	–	–	–	640	–	–	644
–	–	530	–	530	540	–	555	538
520	500	500	519	504	508	510	–	490
–	–	–	492	–	–	–	–	–
470	475	462	–	465	461	–	475	–
–	–	448	455	445	–	450	450	453
–	–	423	433	422	420	–	–	–
–	–	392	–	400	400	–	–	398
–	–	–	–	388	389	–	368	–
–	–	340	–	357	356	–	330	–
–	–	–	–	310	312	315	–	314

APPENDIX H. MAGNETIC SUSCEPTIBILITY OF AMPHIBOLES

CHEMICAL COMPOSITIONS* OF AMPHIBOLES FOR WHICH MAGNETIC SUSCEPTIBILITY DATA ARE AVAILABLE

	1	2	3	4	5	6	7	8	9	10	11
SiO_2	52.41	43.20	44.07	54.09	56.61	45	–	–	–	–	–
TiO_2	0.45	1.65	1.70	3.54	1.04	0	–	–	–	–	–
Al_2O_3	0.61	12.44	12.37	0.22	0.24	4	–	–	–	–	–
Fe_2O_3	14.37	3.21	0.18	0.66	1.10	10	1.00	1.82	2.52	7.13	5.29
FeO	14.82	10.10	10.23	4.69	3.90	26	4.90	8.93	3.14	8.13	8.47
MnO	1.46	0.21	0.18	0.26	0.29	0	0.14	0.16	0.12	0.14	0.19
MgO	5.07	13.27	14.20	21.29	22.27	0	–	–	–	–	–
CaO	1.33	11.36	12.42	12.14	12.33	2	–	–	–	–	–
Na_2O	4.94	2.72	1.00	0.21	0.06	7	–	–	–	–	–
K_2O	2.10	0.40	0.30	0.16	0.18	3	–	–	–	–	–
H_2O	2.12	1.45	2.88	2.90	2.45	1	–	–	–	–	–
F	0.30	–	–	–	–	–	–	–	–	–	–
	99.98	100.08	99.53	100.16	100.57	98					
O≡F	0.13	–	–	–	–	–	–	–	–	–	–
	99.85	100.08	99.53	100.16	100.57	98					

	12	13	14	15	16	17	18	19	20
Fe_2O_3	–	1.93	1.95	1.62	10.50	6.27	1.26	–	–
FeO	4.24	7.79	5.45	2.78	2.26	9.27	10.46	–	–
MnO	0.08	0.16	0.16	0.03	0.17	0.09	0.02	–	–

	21	22	23	24	25	26	27	28	29
Fe^{3+}	550	560	–	–	643	787	1830	1345	3000
Fe^{2+}	221	730	–	–	900	1168	522	820	–
Mn	85	50	–	–	10	182	38	530	40

	30	31	32	33	34	35	36	37	38
Fe^{3+}	1540	1710	1697	–	1440	1480	1726	510	1216
Fe^{2+}	1060	790	1179	–	1935	1960	1781	3123	3002
Mn	185	460	127	230	189	1510	49	86	69

	39	40	41	42	43	44	45
Fe^{3+}	670	875	730	1204	1200	–	–
Fe^{2+}	3280	3230	3603	3427	3295	–	–
Mn	110	492	113	155	97	–	–

*For samples 19 – 45, the magnetic ion contents are given as cation contents (×100?).

AMPHIBOLE NAMES ASSIGNED TO ABOVE AMPHIBOLES BY AUTHORS

1	Riebeckite	29	Hornblende
2	Hornblende	30	Arfvedsonite
3	Hornblende	31	Riebeckite
4	Actinolite	32	Riebeckite
5	Actinolite	33	Arfvedsonite
6	Arfvedsonite	34	Arfvedsonite
19	Tremolite	35	Arfvedsonite
20	Pargasite	36	Riebeckite
21	Richterite	37	Hastingsite
22	Hornblende	38	Riebeckite
23	Pargasite	39	Hastingsite
24	Hornblende	40	Hastingsite
25	Hornblende	41	Hastingsite
26	Katophorite	42	Hastingsite
27	Magnesioriebeckite	43	Hastingsite
28	Arfvedsonite	44	Hastingsite
		45	Hastingsite

MAGNETIC SUSCEPTIBILITY ($\times 10^6$ emu/g) OF AMPHIBOLES

	1	2	3	4	5	6	7	8	9	10	11	12	13
R.T.	75	22	33	13	13	80	11	18	9	28	24	7	16
95 K	–	–	–	–	–	–	29	44	29	82	71	24	43
90 K	330	130	120	30	30	420	–	–	–	–	–	–	–

	14	15	16	17	18	19	20	21	22	23	24	25	26
R.T.	13	6	21	29	20	2	5	12	13	17	20	25	32
95 K	35	18	62	69	63	–	–	–	–	–	–	–	–
90 K	–	–	–	–	–	–	–	–	–	–	–	–	–

	27	28	29	30	31	32	33	34	35	36	37	38	39
R.T.	33	34	37	38	38	41	41	47	47	53	54	60	62

	40	41	42	43	44	45
R.T.	63	64	68	65	69	70

1 – 16 Syono (1960), 7 – 18 Babkine *et al.* (1968),

19 – 45 Efimov *et al.* (1972).