

Tables and figures

Table 1. Cyclosilicates from groups VIIC04, VIIC05 [91N1].

Silicate	Ideal composition	Group
Ferro-axinite	$\text{Ca}_2\text{FeAl}_2(\text{BO}_3\text{OH})(\text{SiO}_3)_4$	VIIC04
Magnesio-axinite	$\text{Ca}_2\text{MgAl}_2(\text{BO}_3\text{OH})(\text{SiO}_3)_4$	VIIC04
Mangan-axinite	$\text{Ca}_2\text{MnAl}_2(\text{BO}_3\text{OH})(\text{SiO}_3)_4$	VIIC04
Kainosite-(Y)	$\text{Ca}_2(\text{Y,Ce})_2(\text{SiO}_3)_4(\text{CO}_3) \cdot \text{H}_2\text{O}$	VIIC04
Tinzenite	$(\text{Ca,Mn,Fe}^{3+})_3\text{Al}_2\text{BSi}_4\text{O}_{15}(\text{OH})$	VIIC04
Papagoite	$\text{CaCuAlSi}_2\text{O}_6(\text{OH})_3$	VIIC04
Baotite	$\text{Ba}_4(\text{Ti,Fe,Nb})_8\text{O}_{16}(\text{SiO}_3)_4\text{Cl}$	VIIC04
Taramellite	$\text{Ba}_4(\text{Fe,Ti})_4(\text{B}_2\text{Si}_8\text{O}_{27})\text{O}_2\text{Cl}_x$	VIIC04
Titantaramellite	$\text{Ba}_4(\text{Ti,Fe,Mg})_4(\text{B}_2\text{Si}_8\text{O}_{27})\text{O}_2\text{Cl}_x$	VIIC04
Nagashimalite	$\text{Ba}_4(\text{V,Ti})_4(\text{B}_2\text{Si}_8\text{O}_{27})\text{O}_2\text{Cl}_x$	VIIC04
Muirite	$\text{Ba}_{10}\text{Ca}_2\text{MnTiSi}_{10}\text{O}_{30}(\text{OH,Cl,F})_{10}$	VIIC04
Joaquinite-(Ce)	$\text{NaBa}_2\text{FeTi}_2\text{Ce}_2(\text{SiO}_3)_8\text{O}_2(\text{OH}) \cdot \text{H}_2\text{O}$	VIIC05
Orthojoaquinite-(Ce)	$\text{NaBa}_2\text{FeTi}_2\text{Ce}_2(\text{SiO}_3)_8\text{O}_2(\text{O,OH}) \cdot \text{H}_2\text{O}$	VIIC05
Strontio-joaquinite	$(\text{Na,Fe})_2\text{Ba}_2\text{Sr}_2\text{Ti}_2(\text{SiO}_3)_8(\text{O,OH})_2 \cdot \text{H}_2\text{O}$	VIIC05
Strontio-orthojoaquinite	$\text{Na}_2\text{Ba}_2\text{Sr}_2\text{Ti}_2(\text{SiO}_3)_8(\text{O,OH})_2 \cdot \text{H}_2\text{O}$	VIIC05
Bario-orthojoaquinite	$(\text{Ba,Sr})_4\text{Fe}_2\text{Ti}_2\text{O}_2(\text{SiO}_3)_8 \cdot \text{H}_2\text{O}$	VIIC05
Baratovite	$\text{KLi}_3\text{Ca}_7(\text{Ti,Zr})_2(\text{SiO}_3)_{12}\text{F}_2$	VIIC05
Byelorussite-(Ce)	$\text{NaBa}_2\text{Ce}_2\text{MnTi}_2\text{Si}_8\text{O}_{26}(\text{F,OH}) \cdot \text{H}_2\text{O}$	VIIC05
Katayamalite	$(\text{K,Na})\text{Li}_3\text{Ca}_7\text{Ti}_2(\text{SiO}_3)_{12}(\text{OH,F})_2$	VIIC05

Table 2. Atomic parameters and temperature factors.

a) Axinite, having triclinic structure with space group $\text{P}\bar{1}$ [74T1].

Atom	x	y	z	$\beta_{ij} \cdot 10^5$					
				β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Fe	0.7687	0.5904	0.1120	215	261	153	-126	-2	113
Ca1	0.7465	0.3480	0.3956	281	75	129	-27	-95	82
Ca2	0.1831	0.1006	0.0837	286	130	114	-167	-242	107
Al1	0.0529	0.8009	0.2543	115	53	17	-21	-20	40
Al2	0.3520	0.9362	0.4212	113	63	56	-124	-38	-8
Si1	0.2120	0.4502	0.2356	114	57	44	-76	-64	9
Si2	0.2189	0.2748	0.5242	91	45	41	-49	-38	6
Si3	0.6995	0.2553	0.0112	142	66	12	-28	-39	18
Si4	0.6413	0.0189	0.2304	85	68	55	-88	7	-2
B	0.6419	0.6346	0.2860	171	69	20	73	-48	-18
O1	0.0564	0.6033	0.1897	320	101	121	-59	-42	-11
O2	0.2333	0.3386	0.0982	414	115	137	-51	60	-52
O3	0.4202	0.4864	0.3135	248	129	140	-265	-200	28
O4	0.1357	0.3739	0.3713	316	288	144	-242	-111	229
O5	0.0281	0.2419	0.5638	121	188	91	-87	37	74
O6	0.3261	0.3791	0.6455	131	103	131	-72	-60	-62
O7	0.3802	0.1274	0.4956	164	59	152	-69	-15	-37
O8	0.5371	0.3433	0.8773	360	146	47	18	52	114
O9	0.8759	0.1543	0.9334	198	120	89	151	6	-7
O10	0.7693	0.3655	0.1394	431	204	112	-198	-43	-121

Table 2 (cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$\beta_{ij} \cdot 10^5$					
				β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O11	0.6037	0.1348	0.0863	404	240	123	−256	70	155
O12	0.4359	0.9817	0.2442	191	127	121	−167	20	44
O13	0.7204	0.0998	0.3842	266	186	67	−243	−62	−21
O14	0.7943	0.8735	0.1783	169	159	159	39	19	−12
O15	0.3256	0.7464	0.3545	131	75	102	−57	25	−85
O16	0.0968	0.9954	0.3232	70	133	111	−3	15	−55
H	0.0023	0.9697	0.6259	69	−744	320	−1728	−467	−1481

b) Baotite⁹⁾, having tetragonal structure, space group $I4_1/a$ [70N1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{eq} [\text{\AA}^2]$
Ba	0.02947(2)	0.09737(2)	0.62138(6)	0.42(1)
Ti	0.21264(5)	0.10787(5)	0.8699(2)	0.34(2)
(Ti,Nb,Fe)	0.22174(3)	0.11789(3)	0.3728(2)	0.39(2)
Si	0.09288(7)	0.18533(7)	0.1244(3)	0.28(2)
O1	0.0168(2)	0.1568(2)	0.1350(8)	0.60(5)
O2	0.1265(2)	0.1593(2)	0.8933(8)	0.40(5)
O3	0.1284(2)	0.1617(2)	0.3587(9)	0.48(5)
O4	0.1846(2)	0.0530(2)	0.1304(8)	0.53(5)
O5	0.1812(2)	0.0547(2)	0.6214(8)	0.59(5)
O6	0.2468(2)	0.1684(2)	0.1206(8)	0.55(5)
O7	0.2415(2)	0.1703(2)	0.6305(8)	0.50(5)
Cl	0.0000	0.2500	0.6250	0.67(4)

⁹⁾ See Table 3.

(c) Taramellite¹¹⁾, having orthorhombic symmetry, space group $Pmmn$ [80M3].

Atom	Multiplicity	Point symmetry	<i>x</i>	<i>y</i>	<i>z</i>	$B_{eq} [\text{\AA}^2]$
Ba1	2	mm	0.75	0.25	0.2394(1)	1.10
Ba2	2	mm	0.25	0.25	0.4659(2)	1.94
Ba3	4	m	0.25	0.4749(0)	0.0070(1)	0.81
M	8 ^{a)}	1	0.6295(1)	0.5020(1)	0.4765(1)	0.75
Si1	8	1	0.4894(1)	0.3662(1)	0.2048(3)	0.52
Si2	8	1	0.4736(2)	0.6441(4)	0.2073(2)	0.45
B	4	m	0.25	0.6593(7)	0.2773(15)	0.64
O1	4	m	0.5062(6)	0.25	0.2212(10)	0.81
O2	4	m	0.5207(5)	0.75	0.2684(10)	0.76
O3	4	m	0.25	0.5767(4)	0.4088(9)	0.72
O4	4	m	0.75	0.5715(4)	0.3623(10)	1.24
O5	8	1	0.5388(4)	0.6092(3)	0.0167(7)	0.86
O6	8	1	0.3798(4)	0.4001(3)	0.3135(6)	0.83
O7	8	1	0.6073(3)	0.4110(3)	0.2617(7)	0.78
O8	8	1	0.3456(4)	0.6482(3)	0.1479(6)	0.74
O9	8	1	0.4946(4)	0.5722(3)	0.3763(7)	0.95
O10	2	mm	0.25	0.75	0.3803(11)	0.65
Cl	2 ^{b)}	mm	0.25	0.25	−0.0088(9)	2.24

^{a)} Site population 0.75Fe + 0.25Ti; ^{b)} site occupancy 0.89; ¹¹⁾ see Table 3.

Table 2 (cont.)(d) Joaquinite²³⁾, having monoclinic structure, space group C2 [75D1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> _{eq} [Å ²]
Ba	0.2366(1)	0.0	0.0058(1)	0.94(2)
R	0.1667(1)	0.7467(1)	0.4518(1)	1.17(2)
Ti	0.0490(3)	0.7369(5)	0.1276(3)	0.36(4)
Fe ^{a)}	0.0	0.3694(6)	0.5	0.6(1)
Na ^{a)}	0.0	0.054(3)	0.5	5.9(8)
Si1	0.3773(5)	0.7343(7)	0.2426(4)	0.66(8)
Si2	0.3085(5)	0.2674(7)	0.2432(5)	0.91(9)
Si3	0.1206(6)	0.0375(7)	0.2917(5)	0.80(9)
Si4	0.0929(6)	0.4365(6)	0.2709(6)	0.68(9)
O1 ^{b)}	0.0	0.867(2)	0.0	0.6(3)
O2 ^{b)}	0.0	0.606(2)	0.0	0.8(3)
O3	0.116(2)	0.881(2)	0.251(1)	1.2(2)
O4	0.188(1)	0.385(2)	0.191(1)	0.9(2)
O5	0.226(2)	0.115(2)	0.237(1)	1.3(3)
O6	0.233(1)	0.715(1)	0.133(1)	0.7(2)
O7	0.472(2)	0.605(2)	0.229(2)	1.6(3)
O8	0.086(2)	0.604(2)	0.268(1)	1.0(2)
O9	0.371(1)	0.737(2)	0.375(1)	1.0(2)
O10	0.412(1)	0.303(2)	0.372(1)	1.5(3)
O11	0.144(2)	0.368(2)	0.403(1)	1.4(3)
O12	0.173(2)	0.044(2)	0.443(1)	1.7(3)
O13	0.367(1)	0.254(2)	0.133(1)	0.8(2)
O14	0.439(2)	0.880(2)	0.203(2)	1.7(3)
OH ^{b)}	0.0	0.576(4)	0.5	5.0(9)
H ₂ O ^{b)}	0.0	0.199(3)	0.0	2.6(5)

^{a)} Refined occupancy for the Fe site is (0.79Fe, 0.21Na), and that for the Na site is (0.75Na, 0.25Fe). Other sites are assumed to be fully occupied;

^{b)} Atoms O1, O2 and H₂O are in 2a sites and atoms Fe, Na and OH are in 2b. All others are in the general positions 4c of space group C2;

The approximate coordinates of atoms in the orthorhombic form of joaquinite²³⁾ (subscript o) can be derived from those in the monoclinic cell (subscript c). The general equations are: $z_0 = (1/2)z_c + 1/4$; $x_0 = (1/2 - z_c)$

$\cos \beta \frac{c_c}{a_c}$. The *y* coordinate is unchanged;

²³⁾ See Table 3.

Table 3. Crystal structures and lattice parameters at RT.

Silicate	Space group	Lattice parameters				Refs.
		<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	α, β, γ	
Ferro-axinite ¹⁾	$P\bar{1}$	7.1479(4)	9.1962(5)	8.9576(4)	$\alpha = 91.857(4)^\circ$ $\beta = 98.177(4)^\circ$ $\gamma = 77.359(4)^\circ$	00S1
Ferro-axinite ²⁾	$P\bar{1}$	7.148	9.156	8.960	$\alpha = 88^\circ 04'$ $\beta = 81.36'$ $\gamma = 77^\circ 42'$	52I1
Ferro-axinite ³⁾	$P\bar{1}$	7.1437(4)	9.1898(6)	8.9529(4)	$\alpha = 91.857(6)^\circ$ $\beta = 98.188(5)^\circ$ $\gamma = 77.359(4)^\circ$	81S1
Axinite ⁴⁾	$P\bar{1}$	7.1566(15)	9.1995(20)	8.959(2)	$\alpha = 91.8(8)^\circ$ $\beta = 98.14(02)^\circ$ $\gamma = 77.30(2)^\circ$	74T1
Magnesio-axinite ⁵⁾	$P\bar{1}$	7.1381(3)	9.1626(4)	8.9421(4)	$\alpha = 91.903(4)^\circ$ $\beta = 98.105(3)^\circ$ $\gamma = 77.468(4)^\circ$	00S1
Mangan-axinite ⁶⁾	$P\bar{1}$	7.1849(4)	9.2152(5)	8.9765(4)	$\alpha = 91.761(4)^\circ$ $\beta = 98.153(4)^\circ$ $\gamma = 77.150(4)^\circ$	00S1
Mangan-axinite ⁷⁾	$P\bar{1}$	7.161(2)	9.190(3)	8.978(3)	$\alpha = 88.26(3)^\circ$ $\beta = 81.80(3)^\circ$ $\gamma = 77.26(2)^\circ$	72F1
Kainosite (natural)		13.01	14.27	6.75		50B1
Kainosite (natural)	Pmnb	12.93(3)	14.33(3)	6.73(3)		61R1
Kainosite-(Y) ⁸⁾	Pmnb	13.05(1)	14.33(1)	6.73(1)		64P1
Baotite ⁹⁾	$I4_1/a$	19.99(1)		5.908(2)		70N1
Taramellite ¹⁰⁾	Pmmn	13.95	12.21	7.15		65M1
Taramellite ^{11),a)}	Pmmn	12.150(3)	13.946(3)	7.129(2)		80M3
Taramellite ^{11),a)}	Pmmn	12.125(6)	13.929(6)	7.136(5)		84A1
Taramellite ¹²⁾		7.05	13.95	12.01		57M1, 65M1
Ti-taramellite ^{13),a)}	Pmmn	12.200(2)	13.952(2)	7.128(1)		80M3
Ti-taramellite ^{13),a)}	Pmmn	12.184(4)	13.938(6)	7.127(3)		84A1
Ti-taramellite ^{14),a)}	Pmmn	12.217(6)	13.954(8)	7.130(4)		84A1
Ti-taramellite ^{15),a)}	Pmmn	12.202(4)	13.981(5)	7.134(3)		84A1
Ti-taramellite ^{16),a)}	Pmmn	12.220(5)	14.005(9)	7.141(3)		84A1
Ti-taramellite ^{17),a)}	Pmmn	12.199(7)	13.962(8)	7.140(4)		84A1
Ti-taramellite ^{18),a)}	Pmmn	12.213(4)	13.980(3)	7.136(2)		84A1
Ti-taramellite ^{19),a)}	Pmmn	12.149(7)	13.904(12)	7.12(2)		84A1
Ti-taramellite ^{20),a)}	Pmmn	12.053(5)	13.93(2)	7.138(3)		84A1
Nagashimalite ²¹⁾	Pmmn	12.122(3)	13.937(3)	7.116(2)		80M1,2
Muirite ²²⁾	$P4/mmm, P4mm,$ $P422$ or $P42m$	13.942		5.590		65A2
Joaquinite-(Ce) ²³⁾	C2	10.516(3)	9.686(3)	11.833(4)	$\beta = 109.670(3)^\circ$	75D1
Joaquinite-(Ce) ²⁴⁾	C2, Cm, or C2/m	10.51(2)	9.66(2)	11.82(2)	$\beta = 109.5(2)^\circ$	72L1
Orthojoaquinite ²³⁾	Cc2m, Ccm2 ₁ or Ccmm	10.48	9.66	22.26		75D1
Orthojoaquinite ²⁴⁾		10.48(2)	9.66(2)	22.26(2)		72L1

Table 3 (cont.)

Silicate	Space group	Lattice parameters				Refs.
		<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	α, β, γ	
Strontio-joaquinite ²⁵⁾	P2, Pm or P2/m	10.516(6)	9.764(5)	11.87(1)	$\beta = 109^\circ 17(4)'$	82W1
Strontio-orthojoaquinite ²⁶⁾	Pcam, Pca2 ₁	10.517	9.777	22.392		74C1
Bario-orthojoaquinite ²⁷⁾	Ccmm, Ccm2 ₁ , or Cc2m	10.477(6)	9.599(1)	22.59(1)		82W1
Baratovite ²⁸⁾	C2/c	16.941(3)	9.746(2)	20.907(3)	$\beta = 112.50(10)^\circ$	79M1
Katayamalite ²⁹⁾	C1	9.721	16.923	19.942	$\alpha = 91.43^\circ$ $\beta = 104.15^\circ$ $\gamma = 89.94^\circ$	83M1
Katayamalite ²⁹⁾	P1	9.763	9.721	19.942	$\alpha = 104.15^\circ$ $\beta = 81.76^\circ$ $\gamma = 119.92^\circ$	83M1

1) $\text{Ca}_{3.94}\text{Mn}_{0.06}\text{Fe}^{2+}_{1.68}\text{Mg}_{0.30}\text{Al}_{3.95}\text{B}_{2.07}\text{Si}_{7.99}\text{O}_{30.0}(\text{OH})_2$;

2) $\text{Ca}_2\text{Mn}_{0.3}\text{Fe}_{0.7}\text{Al}_2\text{BSi}_4\text{O}_{16}\text{H}$;

3) $\text{Ca}_{3.90}(\text{Ti}_{0.01}\text{K}_{0.044}\text{Na}_{0.13}\text{Mn}_{0.26}\text{Fe}_{1.10}\text{Mg}_{0.37})(\text{Al}_{3.56}\text{Fe}_{0.18})(\text{OH})_{1.96}\text{B}_{1.96}\text{Si}_8\text{O}_{29.34}$;

4) $\text{Ca}_2(\text{Fe}, \text{Mn})\text{Al}_2\text{BSi}_4\text{O}_{16}\text{H}$ with Fe: Mn ratio close to 1 : 1;

5) $\text{Ca}_{3.96}\text{Mn}_{0.07}\text{Mg}_{1.92}\text{Al}_{4.00}\text{B}_{2.00}\text{Si}_{8.04}\text{O}_{30.1}(\text{OH})_{1.9}$;

6) $\text{Ca}_{3.87}\text{Mn}_{2.02}\text{Al}_{3.76}\text{Fe}^{3+}_{0.31}\text{Fe}^{2+}_{0.07}\text{B}_{1.99}\text{Si}_{8.02}\text{O}_{30.2}(\text{OH})_{1.8}$;

7) $(\text{Ca}_{1.85}\text{Mg}_{0.04}\text{Fe}^{2+}_{0.26}\text{Mn}^{2+}_{0.94})(\text{Al}_{2.03}\text{Fe}^{3+}_{0.01})\text{B}_{0.99}\text{Si}_{3.98}\text{O}_{16}\text{H}_{0.83}$;

8) Composition [mol %]: CaO -0.2992; Na_2O -0.0006; K_2O -0.0001; Ce_2O_3 -0.0012; Nd_2O_3 -0.0006; Sm_2O_3 -0.0008; Y_2O_3 -0.1119; Gd_2O_3 -0.0067; Dy_2O_3 -0.0083; Er_2O_3 -0.0092; Yb_2O_3 -0.0069; Fe_2O_3 -0.0036; Al_2O_3 -0.0118; SiO_2 -0.5867; TiO_2 -0.0003; ThO_2 -0.0001; CO_2 -0.1045; H_2O^+ -0.1437; No. of atoms in the cell determined from above include 4H_2 ;

9) $\text{Ba}_4\text{Ti}_4(\text{Ti}_{0.48}\text{Nb}_{0.36}\text{Fe}_{0.16})_4\text{ClO}_{16}[\text{Si}_4\text{O}_{12}]$;

10) Natural sample, Candoglia, Italy. Composition close to ¹¹⁾;

11), a) $\text{Si}_{15.74}\text{Al}_{0.26}\text{Ti}_{2.61}\text{Fe}_{4.72}\text{Mg}_{0.04}\text{V}_{0.04}\text{Ba}_{7.50}\text{Cl}_{1.20}$; (O content not mentioned);

12) Natural sample, Rush Creek, California;

13), a) $\text{Si}_{15.85}\text{Al}_{0.15}\text{Ti}_{3.91}\text{Fe}_{2.61}\text{Mg}_{0.91}\text{Mn}_{0.12}\text{V}_{0.14}\text{Cr}_{0.01}\text{Ba}_{7.71}\text{Cl}_{1.72}$;

14), a) $\text{Si}_{15.89}\text{Al}_{0.11}\text{Ti}_{3.34}\text{Fe}_{3.21}\text{Mg}_{0.53}\text{Cr}_{0.09}\text{Ba}_{7.47}\text{Cl}_{1.89}$;

15), a) $\text{Si}_{15.91}\text{Al}_{0.09}\text{Ti}_{3.58}\text{Fe}_{1.30}\text{Mg}_{2.29}\text{Mn}_{0.03}\text{V}_{0.18}\text{Cr}_{0.04}\text{Ba}_{7.34}\text{Cl}_{1.38}$;

16), a) $\text{Si}_{15.87}\text{Al}_{0.13}\text{Ti}_{3.75}\text{Fe}_{2.37}\text{Mg}_{1.0}\text{Mn}_{0.02}\text{V}_{0.12}\text{Cr}_{0.05}\text{Ba}_{7.52}\text{Cl}_{1.68}$;

17), a) $\text{Si}_{15.86}\text{Al}_{0.14}\text{Ti}_{3.98}\text{Fe}_{1.20}\text{Mg}_{1.54}\text{Mn}_{0.48}\text{V}_{0.31}\text{Ba}_{7.45}\text{Cl}_{1.68}$;

18), a) $\text{Si}_{15.87}\text{Al}_{0.13}\text{Ti}_{3.32}\text{Fe}_{1.64}\text{Mg}_{1.63}\text{Mn}_{0.08}\text{V}_{0.82}\text{Cr}_{0.25}\text{Ba}_{7.40}\text{Cl}_{1.48}$;

19), a) $\text{Si}_{15.75}\text{Al}_{0.25}\text{Ti}_{3.88}\text{Fe}_{1.40}\text{Mg}_{1.04}\text{V}_{1.21}\text{Cr}_{0.03}\text{Ba}_{7.37}\text{Cl}_{1.71}$;

20), a) $\text{Si}_{15.92}\text{Al}_{0.08}\text{Ti}_{4.58}\text{Fe}_{3.08}\text{Mg}_{0.10}\text{V}_{0.03}\text{Ba}_{7.47}\text{Cl}_{0.03}$. For samples ^{11, 13-20)} O content not mentioned;

a) For samples ^{11, 13-20)} O and B content not mentioned. The B content was suggested to be close to that given by $(\text{Si}_{16}\text{B}_4\text{O}_{54})$

21) $\text{Ba}_{4.01}(\text{V}^{3+}_{3.30}\text{Ti}_{0.51}\text{Mn}_{0.10})\text{B}_{1.71}\text{Si}_8\text{O}_{27.64}(\text{OH})_{1.28}\text{Cl}_{0.72}$;

22) $(\text{Ba}_{9.82}\text{K}_{0.05}\text{Sr}_{0.03})\text{Ca}_{2.10}(\text{Mn}_{0.73}\text{Fe}_{0.14}\text{Mg}_{0.07})\text{Ti}_{1.32}(\text{Si}_{9.31}\text{Al}_{0.26})\text{O}_{29.52}(\text{OH}_{5.05}\text{Cl}_{3.21}\text{F}_{1.86})$;

23) Natural sample, San Benito country; ideal composition $\text{NaFe}^{2+}\text{Ba}_2\text{R}_2\text{Ti}_2\text{Si}_8\text{O}_{26}\text{OH} \cdot \text{H}_2\text{O}$;

24) $\text{Ba}_{8.1}(\text{Sr}_{1.7}\text{R}_{6.5}\text{Ti}_{0.1})(\text{Ca}_{0.2}\text{Na}_{3.3}\text{Fe}_{3.1}\text{Li}_{0.8}\text{Mg}_{0.1})\text{Ti}_{8.1}\text{Si}_{32}\text{O}_{98.7}(\text{OH})_{18.3}$;

25) $(\text{Na}_{2.28}\text{Li}_{0.11}\text{Fe}^{2+}_{1.44}\square_{0.17})\square_2\text{Ba}_{4.09}\text{Ti}_{4.00}[\text{O}_{1.27}(\text{OH})_{2.73}]\text{Sr}_{4.01}\text{R}_{0.01}[\text{Si}_4\text{O}_{12}]_4 \cdot 1.62\text{H}_2\text{O}$;

26) Natural sample;

27) $(\text{Na}_{0.11}\text{Fe}_{3.61}\text{Mn}_{0.24}\square_{0.05})\square_2\text{Ba}_4(\text{Ti}_{3.88}\text{Al}_{0.12})(\text{Ba}_{2.88}\text{Sr}_{0.88}\text{Ca}_{0.08}\text{Al}_{0.19})\text{O}_4[\text{Si}_4\text{O}_{12}]_4 \cdot 2.0\text{H}_2\text{O}$;

28) $\text{KLi}_3\text{Ca}_7(\text{Ti}_{0.87}\text{Zr}_{0.13})_2[\text{Si}_6\text{O}_{18}]_2\text{F}_2$;

Table 3 (cont.)

- ²⁹⁾ $(\text{K}_{0.85}\text{Na}_{0.10})\text{Li}_{3.00}(\text{Ca}_{6.94}\text{Mn}_{0.04})(\text{Ti}_{1.90}\text{Fe}^{3+}_{0.05})\text{Si}_{12.00}\text{O}_{35.78}(\text{OH})_{1.85}\text{F}_{0.25}$;
³⁰⁾ $(\text{Ba}_{3.872}\text{Na}_{0.089}\text{Ca}_{0.040}\text{K}_{0.041})(\text{Ti}_{5.822}\text{Nb}_{1.322}\text{Fe}^{2+}_{0.408}\text{Fe}^{3+}_{0.201}\text{Al}_{0.233}\text{Cr}_{0.009})(\text{Si}_{3.739}\text{Al}_{0.261})\text{O}_{12}(\text{O}_{15.186}\text{OH}_{0.814})$
 $(\text{Cl}_{0.897}\text{OH}_{0.103})$;
³¹⁾ Natural sample, 2.87 % Fe;
³²⁾ Composition [wt %]: BaO-39.3; FeO-6.70; MgO-1.13; MnO-0.40; TiO-11.6; SiO₂-33.0 Cl-1.95.

Table 4. Hyperfine parameters determined by NGR method at ⁵⁷Fe.

Sample	<i>T</i> [K]	Site	δ^1 [mm/s]	ΔQ [mm/s]	<i>DH</i> [mm/s]	<i>A</i> [%]	Refs.
Baotite ³⁰⁾	95	Fe ²⁺ (Ti)	1.15(1)	2.65(2)	0.37(2)	69	98S1
		Fe ³⁺ (Ti)	0.46(5)	0.61(6)	0.51(6)	31	
	298	Fe ²⁺ (Ti)	1.02(1)	2.64(1)	0.34(1)	67	
		Fe ³⁺ (Ti)	0.37(3)	0.61(1)	0.50(3)	33	
Baotite ³¹⁾	298	Fe ²⁺	1.029	2.632	0.318	43.1	92Q1
		Fe ³⁺	0.389	0.636	0.602	56.9	

¹⁾ Relative to α -Fe.

^{30), 31)} See Table 3.

Table 5. Refractive indices.

Sample	<i>n</i> _α	<i>n</i> _β	<i>n</i> _γ	<i>2V</i> [°]			Refs.
				exp.	calc.		
Mangan-axinite ⁷⁾	1.678(3)	1.687(3)	1.692(3)	75(5)		biaxial negative	72F1
Kainosite-(Y) ⁸⁾	1.665(1)	1.685(1)	1.689(1)	40	49.5	biaxial negative	64P1
Ti-Taramellite ¹³⁾	1.753(2)	1.757(2)	1.782(3)	45(5)			84A1
Ti-Taramellite ¹⁴⁾	1.752(2)	1.760(1)	1.770(6)	77(3)		biaxial positive	84A1
Ti-Taramellite ¹⁵⁾	1.747(1)	1.758(1)					84A1
Ti-Taramellite ¹⁶⁾	1.751(2)	1.761(2)		59(5)			84A1
Ti-Taramellite ¹⁷⁾	1.751(3)	1.757(2)	1.780(6)	51(2)			84A1
Ti-Taramellite ¹⁸⁾	1.739(1)	1.749(2)					84A1
Ti-Taramellite ¹⁹⁾	1.748(2)	1.752(2)					84A1
Nagashimalite ²¹⁾	1.750(2)	1.753(2)	1.780(5)	≈30		biaxial positive	80M1, 80M2
Muirite ²²⁾	1.697(ω)		1.704(ε)			uniaxial positive	65A2
Joaquinite ²⁴⁾	1.753(1)	1.767(1)	1.822(2)	30...55		biaxial positive	72L1
Joaquinite ²⁶⁾	1.748	1.767	1.823	50			32P1
Strontio-joaquinite ²⁵⁾	1.710(2)	1.718(2)	1.780(3)	35...45		biaxial positive	82W1
Bario-orthojoaquinite ²⁷⁾	1.735(2)	1.737(2)	1.80(1)	10...15		biaxial positive	82W1
Katayamalite ²⁹⁾	1.670	1.671	1.677	32		biaxial positive	83M1

For footnotes see Table 3.