

## Tables and figures

**Table 1.** The aenigmatite, pectolite and umbite groups of silicates [91N1].

Silicate	Composition	Group
Aenigmatite	$\text{Na}_2\text{Fe}_5\text{TiSi}_6\text{O}_{20}$	VIIID07
Serendibite	$\text{Ca}_2(\text{Mg},\text{Al})_6(\text{Si},\text{Al},\text{B})_6\text{O}_{20}$	VIIID07
Rhoenite	$\text{Ca}_2(\text{Fe},\text{Mg},\text{Ti})_6(\text{Si},\text{Al})_6\text{O}_{20}$	VIIID07
Welshite	$\text{Ca}_2\text{Mg}_4\text{Be}_2\text{FeSbSi}_4\text{O}_{20}$	VIIID07
Magbasite	$\text{KBa}(\text{Mg},\text{Fe})_6(\text{Al},\text{Sc})\text{Si}_6\text{O}_{20}\text{F}_2$	VIIID07
Dorrite	$\text{CaMgFe}_2\text{Al}_2\text{SiO}_{10}$	VIIID07
Krinovite	$\text{NaMg}_2\text{CrSi}_3\text{O}_{10}$	VIIID07
Makarochkinitite	$(\text{Ca},\text{Na})_4[(\text{Fe},\text{Mg})_7(\text{Fe}^{3+}_3\text{Ti})]\text{Si}_9\text{Be}_2\text{AlO}_{40}$	[90Y1]
Pectolite	$\text{NaCa}_2\text{Si}_3\text{O}_8(\text{OH})$	VIIID08
Pectolite-M 2abc	$\text{NaCa}_2\text{Si}_3\text{O}_8(\text{OH})$	VIIID08a
Serandite	$\text{Na}(\text{Mn},\text{Ca})_2\text{Si}_3\text{O}_8(\text{OH})$	VIIID08
Cascandite	$\text{Ca}(\text{Sc},\text{Fe})\text{Si}_3\text{O}_8(\text{OH})$	VIIID08
Foshagite	$\text{Ca}_4(\text{SiO}_3)_3(\text{OH})_2$	VIIID08
Jusite	$(\text{Ca},\text{Na},\text{K},\text{H})(\text{Si},\text{Al})\text{O}_3$	VIIID08
Trabzonite	$\text{Ca}_4\text{Si}_3\text{O}_{10}\cdot 2\text{H}_2\text{O}$	VIIID08
Wollastonite	see section 8.1.4.1.1	VIIID08
Bustamite	see section 8.1.4.1.1	VIIID08
Ferrobustamite	see section 8.1.4.1.1	VIIID08
Umbite	$\text{K}_2\text{ZrSi}_3\text{O}_9\cdot \text{H}_2\text{O}$	VIIID09
Kostylevite	$\text{K}_2\text{ZrSi}_3\text{O}_9\cdot \text{H}_2\text{O}$	VIIID09
Paraumbite	$\text{K}_3\text{Zr}_2\text{H}(\text{Si}_3\text{O}_9)_2\cdot 3\text{H}_2\text{O}$	VIIID09
Labuntsovite	$(\text{K},\text{Na})_8(\text{Ti},\text{Nb})_9(\text{SiO}_3)_{16}(\text{O},\text{OH})_{10}\cdot \text{H}_2\text{O}$ (see section 8.1.2.5, subvolume 27I2)	VIIID09
Synthetic silicate	$\text{K}_2\text{TiSi}_3\text{O}_9\cdot \text{H}_2\text{O}$	[97D1]
Kuzmenkoite	for composition see Table 3	[01R1]

**Table 2.** Atomic coordinates and isotropic temperature factors.

a) Aenigmatite<sup>1)</sup>, having triclinic structure with space group  $\text{P}\bar{1}$  [71C1].

Atom	$x$	$y$	$z$	$B_{\text{eq}} [\text{\AA}^2]$	Occupation
M1	0	0	$\frac{1}{2}$	0.76(7)	$\text{Fe}_{0.89}^{2+}\text{Ti}_{0.11}^{4+}$
M2	0	$\frac{1}{2}$	0	0.73(7)	$\text{Fe}_{0.87}^{2+}\text{Ti}_{0.13}^{4+}$
M3	0.3214(3)	0.8528(3)	0.1779(3)	0.92(5)	$\text{Fe}_{0.95}^{2+}\text{Ti}_{0.05}^{4+}$
M4	0.7655(3)	0.8199(3)	0.1511(3)	0.93(5)	$\text{Fe}_{0.76}^{2+}\text{Ti}_{0.24}^{4+}$
M5	0.0961(4)	0.9392(3)	0.0530(3)	1.01(5)	$\text{Fe}_{0.90}^{2+}\text{Ti}_{0.10}^{4+}$
M6	0.5959(3)	0.9432(3)	0.0661(3)	0.92(5)	$\text{Fe}_{1.00}^{2+}$
M7	0.9970(4)	0.7434(4)	0.2577(3)	0.70(5)	$\text{Fe}_{0.41}^{2+}\text{Ti}_{0.59}^{4+}$

**Table 2a** (cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>eq</sub> [Å <sup>2</sup> ]	Occupation
Na1	0.2089(8)	0.6298(8)	0.3893(7)	0.55(11)	Na <sup>+</sup>
Na2	0.6607(8)	0.6117(9)	0.3741(8)	1.06(13)	Na <sup>+</sup>
T1	0.4768(5)	0.2345(5)	0.3313(5)	0.41(8)	Si <sub>1.0</sub> <sup>4+</sup>
T2	0.9864(5)	0.2363(5)	0.3466(5)	0.39(7)	Si <sub>1.0</sub> <sup>4+</sup>
T3	0.7921(5)	0.3435(5)	0.2416(4)	0.40(7)	Si <sub>0.90</sub> <sup>4+</sup> Fe <sub>0.10</sub> <sup>3+</sup>
T4	0.2772(5)	0.3382(5)	0.2252(5)	0.62(8)	Si <sub>0.95</sub> <sup>4+</sup> Fe <sub>0.05</sub> <sup>3+</sup>
T5	0.6487(5)	0.9448(5)	0.4447(5)	0.50(8)	Si <sub>0.94</sub> <sup>4+</sup> Fe <sub>0.06</sub> <sup>3+</sup>
T6	0.3528(5)	0.5588(5)	0.0501(5)	0.51(8)	Si <sub>0.95</sub> <sup>4+</sup> Fe <sub>0.05</sub> <sup>3+</sup>
O1	0.3542(14)	0.0641(14)	0.1621(13)	0.64(21)	
O2	0.8611(14)	0.0666(13)	0.1807(12)	0.43(20)	
O3	0.5540(15)	0.9534(15)	0.2958(13)	0.75(21)	
O4	0.0151(15)	0.9258(15)	0.2670(13)	0.83(21)	
O5	0.2353(15)	0.8747(14)	0.3933(13)	0.65(20)	
O6	0.7541(15)	0.8843(14)	0.3902(13)	0.63(21)	
O7	0.4929(15)	0.1948(15)	0.4973(13)	0.75(22)	
O8	0.9575(14)	0.7755(14)	0.4871(12)	0.58(20)	
O9	0.8996(15)	0.3230(14)	0.3735(13)	0.76(20)	
O10	0.4034(15)	0.3364(15)	0.3529(13)	0.93(22)	
O11	0.6653(14)	0.1744(14)	0.0709(12)	0.57(20)	
O12	0.1570(14)	0.1688(14)	0.0612(12)	0.57(20)	
O13	0.5233(15)	0.7108(14)	0.0393(12)	0.56(20)	
O14	0.0673(13)	0.7340(13)	0.0757(12)	0.37(19)	
O15	0.2417(15)	0.6060(16)	0.1120(13)	0.89(23)	
O16	0.7510(14)	0.6018(15)	0.1275(13)	0.64(21)	
O17	0.4002(14)	0.5015(14)	0.1883(12)	0.52(20)	
O18	0.9363(16)	0.5147(16)	0.2264(14)	1.09(23)	
O19	0.1648(14)	0.3649(14)	0.3183(12)	0.62(20)	
O20	0.6731(15)	0.3626(15)	0.3366(13)	0.99(21)	

<sup>1)</sup> Composition according to Table 3.

**Table 2** (cont.)b) Serandite<sup>16)</sup>, having triclinic lattice with space group  $P\bar{1}$  [00J1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> [Å <sup>2</sup> ]	Occupation
Na	0.5557(2)	0.2553(3)	0.3529(3)	1.45(6)	
Mn1	0.8531(2)	0.5945(2)	0.1349(3)	0.81(6)	0.941(9)
Mn2	0.8491(2)	0.0840(2)	0.1329(2)	0.74(6)	0.983(9)
Si1	0.2151(2)	0.4017(2)	0.3424(2)	0.53(4)	
Si2	0.2059(2)	0.9511(2)	0.3512(2)	0.49(4)	
Si3	0.4543(2)	0.7370(2)	0.1428(2)	0.50(4)	
O1	0.6643(1)	0.7943(1)	0.1138(2)	0.87(3)	
O2	0.3226(1)	0.7065(1)	0.9435(2)	0.86(3)	
O3	0.1788(1)	0.4926(1)	0.5554(2)	0.84(3)	
O4	0.1598(1)	0.8443(1)	0.5572(2)	0.87(4)	
O5	0.0614(1)	0.3912(1)	0.1671(2)	0.79(3)	
O6	0.0519(1)	0.8912(1)	0.1724(2)	0.78(3)	
O7	0.4071(1)	0.5335(1)	0.2772(2)	0.93(3)	
O8	0.3972(1)	0.9067(1)	0.2866(2)	0.92(3)	
O9	0.2593(1)	0.1888(1)	0.3931(2)	0.86(3)	
H1	0.1482(4)	0.6374(4)	0.5498(5)	2.06(10)	0.842(6)
H2	0.1518(17)	0.6872(18)	0.5483(22)	1.5(2)	0.158(6)

<sup>16)</sup> Determined by neutron diffraction; composition (Mn<sub>2.00</sub>Ca<sub>0.03</sub>)NaHSi<sub>3</sub>O<sub>9</sub>.c) Cascandite, CaScSi<sub>3</sub>O<sub>8</sub>(OH), having  $C\bar{1}$ -type structure [82M1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>
M1	0.0027(1)	0.6629(1)	0.9128(1)
M2	−0.0019(1)	0.6421(1)	0.4062(1)
Si1	0.2163(1)	0.0402(1)	0.0886(2)
Si2	0.2102(1)	0.0666(1)	0.5229(2)
Si3	0.2055(1)	0.8366(1)	0.7399(2)
OA1	0.1160(3)	0.4490(3)	0.8729(5)
OA2	0.1176(3)	0.4462(3)	0.4203(5)
OA3	0.1279(4)	0.6930(4)	0.2416(5)
OB1	0.1295(4)	0.1568(3)	−0.0262(5)
OB2	0.1479(4)	0.2006(3)	0.6291(5)
OB3	0.1113(4)	0.7139(3)	0.6736(5)
OC1	0.1571(4)	0.0538(4)	0.2871(5)
OC2	0.1507(4)	0.9458(3)	0.5940(5)
OC3	0.1815(4)	0.8981(3)	0.9601(5)
H	0.13	0.18	0.86
A	0.03	0.89	0.28

**Table 2** (cont.)d)  $\text{K}_2\text{TiSi}_3\text{O}_9 \cdot \text{H}_2\text{O}$ , having orthorhombic structure with space group  $\text{P}2_12_12_1$  [97D1].

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> [Å <sup>2</sup> ]
Ti	4a	0.7417(7)	0.0450(4)	0.2890(3)	1.73(9)
K1	4a	0.7943(7)	0.4314(5)	0.5804(3)	3.9(2)
K2	4a	0.3466(6)	0.2062(5)	0.1354(3)	4.8(2)
Si1	4a	0.7729(10)	0.0410(6)	0.5472(4)	1.33(6)
Si2	4a	0.9919(9)	0.3216(6)	0.3271(5)	1.33(6)
Si3	4a	0.5758(9)	0.3566(6)	0.3296(6)	1.33(6)
O1	4a	0.9486(13)	0.1655(11)	0.3034(9)	1.82(9)
O2	4a	0.7981(14)	0.3982(9)	0.3466(7)	1.82(9)
O3	4a	0.5768(11)	0.1986(11)	0.3145(8)	1.82(9)
O4	4a	0.6276(16)	0.1600(10)	0.5743(7)	1.82(9)
O5	4a	0.5185(14)	0.9413(1)	0.2609(8)	1.82(9)
O6	4a	0.7445(13)	0.9263(9)	0.6323(7)	1.82(9)
O7	4a	0.9861(15)	0.1030(10)	0.5601(9)	1.82(9)
O8	4a	0.8993(14)	0.8914(9)	0.2685(9)	1.82(9)
O9	4a	0.7302(16)	0.9873(7)	0.4337(7)	1.82(9)
OW	4a	0.3804(16)	0.1863(10)	0.9274(7)	6.4(5)

**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]	$\alpha, \beta, \gamma$	
Aenigmatite <sup>1)</sup>	$\text{P}\bar{1}$	10.406(13)	10.813(14)	8.926(6)	$\alpha = 104^\circ 56(9)'$ $\beta = 96^\circ 52(11)'$ $\gamma = 125^\circ 19(6)'$	71C1
Serendibite <sup>2)</sup>	triclinic	9.513(2)	10.001(3)	8.622(3)	$\alpha = 95.85(2)^\circ$ $\beta = 114.70(2)^\circ$ $\gamma = 64.28(2)^\circ$	77H1
Serendibite <sup>3)</sup>	triclinic	8.630	9.826	10.393	$\alpha = 103.58^\circ$ $\beta = 106.36^\circ$ $\gamma = 118.21^\circ$	68S1
Serendibite <sup>4)</sup>	P1	8.630	9.532	10.019	$\alpha = 64.17^\circ$ $\beta = 83.94^\circ$ $\gamma = 65.29^\circ$	74B1
Rhoenite <sup>5)</sup>	triclinic	10.415	11.207	9.0118	$\alpha = 102^\circ 03'$ $\beta = 100^\circ 31'$ $\gamma = 127^\circ 42'$	69W1
Dorrite <sup>6)</sup>	$\text{P}\bar{1}$ or P1	10.505(3)	10.897(3)	9.019(1)	$\alpha = 106.26(2)^\circ$ $\beta = 95.16(2)^\circ$ $\gamma = 124.75(2)^\circ$	88C1
Krinovite <sup>7)</sup>	monoclinic	19.48(4)	29.18(6)	10.25(2)	$\beta = 103(2)^\circ$	68O1

**Table 3** (cont.)

Silicate	Space group	Lattice parameters				Refs.
		$a$ [Å]	$b$ [Å]	$c$ [Å]	$\alpha, \beta, \gamma$	
Krinovite <sup>8)</sup>	triclinic	10.22	10.67	8.80	$\alpha = 105.1^\circ$ $\beta = 96.6^\circ$ $\gamma = 125.0^\circ$	72M1
Krinovite <sup>9)</sup>	$P\bar{1}$	10.238(4)	10.642(4)	8.780(3)	$\alpha = 105.13(3)^\circ$ $\beta = 96.50(4)^\circ$ $\gamma = 125.15(3)^\circ$	89B1
Makarochkinitite <sup>10)</sup>	$P\bar{1}$	10.352(5)	10.744(3)	8.864(4)	$\alpha = 105.73(3)^\circ$ $\beta = 96.16(3)^\circ$ $\gamma = 124.91(3)^\circ$	90Y1
Pectolite <sup>11)</sup>	triclinic	7.99	7.04	7.02	$\alpha = 90.52^\circ$ $\beta = 95.18^\circ$ $\gamma = 102.47^\circ$	56B1
Pectolite <sup>12)</sup>	$P\bar{1}$	7.988	7.040	7.025	$\alpha = 90.52^\circ$ $\beta = 95.18^\circ$ $\gamma = 102.47^\circ$	67P1
Pectolite <sup>13)</sup>	$P\bar{1}$	7.980(1)	7.023(1)	7.018(1)	$\alpha = 90.54(1)^\circ$ $\beta = 95.14(1)^\circ$ $\gamma = 102.55(1)^\circ$	77T1
Pectolite <sup>14)</sup> (Schizolite)	$C\bar{1}$	10.059(4)	10.880(8)	6.978(6)	$\alpha = 98.84(7)^\circ$ $\beta = 100.58(5)^\circ$ $\gamma = 82.64(5)^\circ$	78O1
Serandite <sup>15)</sup>	$C\bar{1}$	9.909(9)	10.667(9)	6.913(4)	$\alpha = 99.10(6)^\circ$ $\beta = 100.51(6)^\circ$ $\gamma = 82.49(7)^\circ$	78O1
Serandite <sup>16)</sup>	$P\bar{1}$	7.7185(4)	6.9064(5)	6.7624(5)	$\alpha = 90.492(5)^\circ$ $\beta = 90.085(5)^\circ$ $\gamma = 102.775(6)^\circ$	00J1
Serandite <sup>17)</sup>	$P\bar{1}$	7.7163(7)	6.9116(7)	6.7368(5)	$\alpha = 90.465(7)^\circ$ $\beta = 94.037(7)^\circ$ $\gamma = 102.844(7)^\circ$	00J1
Serandite <sup>18)</sup>	$P\bar{1}$	7.683(1)	6.889(1)	6.747(1)	$\alpha = 90.53(5)^\circ$ $\beta = 94.12(2)^\circ$ $\gamma = 102.75(2)^\circ$	76T1
Cascandite <sup>19)</sup>	$P\bar{1}$	7.529(11)	7.051(12)	6.755(9)	$\alpha = 92^\circ 7(5)'$ $\beta = 93^\circ 40(5)'$ $\gamma = 104^\circ 39(5)'$	82M2
Cascandite <sup>19)</sup>	$P\bar{1}$	7.503(6)	7.076(6)	6.777(6)	$\alpha = 92.23(8)^\circ$ $\beta = 93.58(8)^\circ$ $\gamma = 104.49(8)^\circ$	82M1

**Table 3** (cont.)

Silicate	Space group	Lattice parameters				Refs.
		<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	$\alpha, \beta, \gamma$	
Cascandite <sup>19)</sup>	C $\bar{1}$	9.791(8)	10.420(9)	7.076(6)	$\alpha = 98.91(8)^\circ$ $\beta = 102.63(8)^\circ$ $\gamma = 84.17(8)^\circ$	82M1
Foshagite <sup>20)</sup>	triclinic	10.32	7.36	7.94	$\alpha = 117.6^\circ$ $\beta = 104.5^\circ$ $\gamma = 90^\circ$	60G1
Trabzonite <sup>21)</sup>	P2 <sub>1</sub> or P2 <sub>1</sub> /m	6.895(2)	20.640(3)	6.920(2)	$\beta = 98^\circ$	87S1, 88J1
Umbite <sup>22)</sup>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	10.208(2)	13.241(4)	7.174(1)		81I1, 93I1
Umbite <sup>22)</sup>	P2 <sub>1</sub>	10.207	13.241	7.174	$\gamma = 90.07(2)^\circ$	93I1
Paraumbite <sup>23)</sup>	orthorhombic	10.34(4)	13.29(5)	14.55(6)		81I1, 83K1
Labuntsovit <sup>24)</sup>	I2/m	14.18	15.48	13.70	$\gamma = 117^\circ$	74G1
Mn-labuntsovit <sup>25)</sup>	C2/m	14.369(3)	13.906(3)	7.212(1)	$\beta = 117.09(2)^\circ$	98G1
Labuntsovit, Ca analog <sup>26)</sup>	Cm	14.365(7)	13.887(7)	7.814(2)	$\beta = 117.36(5)^\circ$	01R1
Ca-Nb labuntsovit <sup>27)</sup>	C2/m	14.641(1)	14.214(1)	7.9148(2)	$\beta = 117.36(1)^\circ$	00Y1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub> ·H <sub>2</sub> O	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	7.1543(7)	9.9408(11)	12.9460(10)		00Z1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub> ·H <sub>2</sub> O	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	7.1362(2)	9.9084(3)	12.9414(4)		97D1
K <sub>2</sub> Zr <sub>0.8</sub> Ti <sub>0.2</sub> Si <sub>3</sub> O <sub>9</sub> ·H <sub>2</sub> O		7.174	10.208	13.241		97D1
Kostylevit <sup>28)</sup>	P2 <sub>1</sub> /a	13.171(4)	11.717(4)	6.565(2)	$\beta = 105.26^\circ$	81I2, 83K2
Kuzmenkoite <sup>29)</sup>	Cm	14.369(3)	13.906(3)	7.812(1)	$\beta = 117.09(2)^\circ$	00R1

1) (Na<sub>3.97</sub>Ca<sub>0.03</sub>)(Fe<sup>2+</sup><sub>8.06</sub>Ti<sup>4+</sup><sub>2.07</sub>Fe<sup>3+</sup><sub>0.47</sub>Mg<sup>2+</sup><sub>0.70</sub>Mn<sup>2+</sup><sub>0.59</sub>Ca<sup>2+</sup><sub>0.11</sub>)(Si<sup>4+</sup><sub>11.26</sub>Fe<sup>3+</sup><sub>0.53</sub>Al<sup>3+</sup><sub>0.21</sub>)O<sub>40</sub>;

2) Composition [wt %]: SiO<sub>2</sub> – 20.85, Al<sub>2</sub>O<sub>3</sub> – 40.20, FeO – 3.48 (total iron), MgO – 12.17, CaO – 17.11, Na<sub>2</sub>O – 0.02, TiO<sub>2</sub> – 0.06;

3) Natural sample. The cell is related to that of [77H1] by the transformation matrices 001/101/1  $\bar{1}$  0;

4) Natural sample. The cell is related to that of [77H1] by the transformation matrices; 001/100/010

5) (Na<sub>0.35</sub>K<sub>0.22</sub>Ca<sub>3.56</sub>)(Fe<sup>2+</sup><sub>2.55</sub>Ti<sup>4+</sup><sub>1.91</sub>Fe<sup>3+</sup><sub>2.34</sub>Mg<sup>2+</sup><sub>5.03</sub>)(Si<sup>4+</sup><sub>6.54</sub>Al<sup>3+</sup><sub>5.44</sub>Fe<sup>3+</sup><sub>0.02</sub>)O<sub>40</sub>;

6) (Ca<sub>1.92</sub>Na<sub>0.07</sub>K<sub>0.01</sub>)(Ca<sub>0.05</sub>Mg<sub>1.05</sub>Mn<sub>0.03</sub>Fe<sup>2+</sup><sub>0.44</sub>Ti<sub>0.05</sub>Fe<sup>3+</sup><sub>4.38</sub>)(Fe<sup>3+</sup><sub>2.00</sub>Al<sub>2.40</sub>Si<sub>1.60</sub>)O<sub>20</sub>;

7) NaMg<sub>2</sub>CrSi<sub>3</sub>O<sub>10</sub>;

8) Na<sub>4</sub>(Mg<sub>2</sub>Cr<sub>4</sub>)Si<sub>12</sub>O<sub>40</sub>;

9) Na<sub>2</sub>Mg<sub>4</sub>Cr<sub>2</sub>(Si<sub>6</sub>O<sub>18</sub>)O<sub>2</sub>;

10) (Ca<sub>1.75</sub>Na<sub>0.25</sub>)(Fe<sup>2+</sup><sub>3.80</sub>Fe<sup>3+</sup><sub>1.35</sub>Ti<sup>4+</sup><sub>0.06</sub>Mg<sup>2+</sup><sub>0.85</sub>)O<sub>2</sub>(Si<sub>4.4</sub>Al<sub>0.6</sub>Be<sub>1.0</sub>)O<sub>18</sub>;

11) Natural sample;

12) Composition [wt %]: CaO – 33.20, MgO – 0.12, FeO – 1.00, Na<sub>2</sub>O – 9.01, SiO<sub>2</sub> – 53.80, H<sub>2</sub>O – 2.94;

13) HNaCa<sub>1.969</sub>Mn<sub>0.045</sub>Fe<sub>0.014</sub>Si<sub>3</sub>O<sub>9</sub>;

14) (Mn<sub>1.26</sub>Fe<sub>0.27</sub>Ca<sub>2.42</sub>)Na<sub>2.15</sub>Si<sub>5.99</sub>O<sub>17</sub>H<sub>2</sub>O;

15) (Mn<sub>3.23</sub>Fe<sub>0.13</sub>Ca<sub>0.65</sub>)Na<sub>1.98</sub>Si<sub>5.99</sub>O<sub>17</sub>H<sub>2</sub>O;

16) (Mn<sub>2.0</sub>Ca<sub>0.03</sub>)NaHSi<sub>3</sub>O<sub>9</sub> including H<sub>2</sub>O by difference; X-ray data;

17) Similar composition as above; neutron diffraction data;

**Table 3** (cont.)

- 18)  $(\text{Mn}_{1.88}\text{Ca}_{0.17}\text{Mg}_{0.01})\text{Na}_{1.0}\text{HSi}_{2.97}\text{O}_9$ ;  
 19)  $\text{Ca}(\text{Sc}_{0.74}\text{Mg}_{0.02}\text{Al}_{0.01}\text{Fe}^{2+}_{0.22})(\text{Na}_{0.01}\text{Ca}_{0.04}\text{Mn}_{0.10}\square_{0.85})\text{Si}_3\text{O}_{8.02}(\text{OH})$  ;  
 20)  $\text{Ca}_4(\text{Si}_3\text{O}_9)(\text{OH})_2$ ;  
 21)  $(\text{Ca}_{3.99}\text{Na}_{0.05}\text{Mg}_{0.01})\text{Si}_{3.07}\text{O}_{12}\text{H}_{3.66}$ ;  
 22)  $(\text{K}_{2.02}\text{Na}_{0.02})(\text{Zr}_{0.77}\text{Ti}_{0.18}\text{Hf}_{0.01}\text{Fe}_{0.01})\text{Si}_{3.00}\text{H}_{2.38}\text{F}_{0.45}\text{O}_{9.92}$ ;  
 23)  $(\text{K}_{2.92}\text{Na}_{0.03})(\text{Zr}_{2.02}\text{Hf}_{0.01}\text{Ti}_{0.10}\text{Fe}_{0.01})\text{H}_{0.94}\text{Si}_{5.89}\text{O}_{18.00}\cdot 7.34\text{H}_2\text{O}$ ;  
 24)  $(\text{K}_{0.43}\text{Na}_{0.29}\text{Ba}_{0.16}\text{Ca}_{0.06}\text{Mn}_{0.09})(\text{Ti}_{0.89}\text{Nb}_{0.03}\text{Fe}_{0.05}\text{Mg}_{0.03})[\text{Si}_{1.83}\text{Al}_{0.07}\text{O}_{5.79}(\text{OH})_{1.21}]\cdot 0.6\text{H}_2\text{O}$ ;  
 25)  $\text{Na}_{0.3}\text{K}_{3.2}\text{Ba}_{0.2}\text{Ti}_{6.8}\text{Nb}_{1.0}\text{Fe}_{0.35}\text{Mn}_{1.3}\text{Mg}_{0.2}(\text{Si}_4\text{O}_{12})_4\text{O}_8\cdot n\text{H}_2\text{O}$ ,  $n = 11.3$ ;  
 26)  $\text{K}_{3.2}\text{Ca}_{1.2}\text{Ba}_{0.2}[\text{Mn}_{1.7}\text{Fe}_{0.1}(\text{H}_2\text{O})_{3.6}][\text{Ti}_4(\text{Ti}_{3.8}\text{Nb}_{0.2})(\text{O},\text{OH})_8]\{\text{Si}_4\text{O}_{12}\}_4\cdot 6.1\text{H}_2\text{O}$ ;  
 27)  $\square_4(\text{K}_{1.0}\text{Na}_{0.9})(\text{Ca}_{0.6}\text{Na}_{0.3})\{\text{Ca}_{1.4}(\text{Nb}_{2.7}\text{Ti}_{1.2}\text{Fe}_{0.05})(\text{Nb}_{2.65}\text{Ti}_{1.3}\text{Fe}_{0.05})[\text{Si}_6\text{O}_{48}](\text{OH}_{4.75}\text{O}_{3.25})\}\cdot 11\text{H}_2\text{O}$ ;  
 28)  $\text{K}_{2.03}(\text{Zr}_{0.87}\text{Ti}_{0.12}\text{Hf}_{0.01})\text{Si}_{3.01}\text{O}_9\cdot \text{H}_2\text{O}$ ;  
 29)  $[\text{K}_{3.2}(\text{H}_3\text{O})_{1.5}\text{Na}_{0.35}\text{Ba}_{0.1}(\text{Mn}_{1.12}\text{Nb}_{0.28})\cdot 8.5\text{H}_2\text{O}]\{[(\text{Ti}_{3.2}\text{Fe}^{3+}_{0.8})(\text{Ti}_{3.6}\text{Nb}_{0.4})](\text{OH}_{7.6}\text{O}_{0.4})(\text{Si}_4\text{O}_{12})_4\}$ .

**Table 4.** Refractive indices.

Silicate	$n_\alpha$	$n_\beta$	$n_\gamma$	$2 V^\circ$		Refs.
				Obs.	Calc.	
Aenigmatite <sup>1)</sup>	1.800(5)	1.813(5)	1.88(1)	52°	49°	74Y1
Rhoenite <sup>2)</sup>	1.808(5)		1.840(5)	>70°		69W1
Magbasite <sup>3)</sup>	1.597	1.609	1.615	70°		65S1
Dorrite <sup>4)</sup>	1.82(1)	1.84(1)	1.86(1)	90°		88C1
Krinovite <sup>5)</sup>	1.712(2)	1.725(2)	1.760(5)	61(2)°	64°	68O1
Serendibite <sup>6)</sup>	1.700	1.703	1.706	81°		77H1
Trabzonite <sup>7)</sup>	1.632(2)	1.634(2)	1.640(2)	55(5)°	60	87S1
Umbite <sup>8)</sup>	1.596(2)	1.619(2)		80°		81I1, 83K1
Paraumbite <sup>9)</sup>	1.588(2)	1.601(2)	1.610(2)	82°		81I1, 83K1
Labuntsovite <sup>11)</sup>	1.689	1.702	1.795	41°		55S2
Kostylevite <sup>10)</sup>	1.595(2)	1.598(2)	1.610(2)	48°		81I2, 83K2

1)  $(\text{Na}_{4.01}\text{K}_{0.01})(\text{Ca}_{0.15}\text{Mn}_{0.21}\text{Ti}_{1.79}\text{Fe}^{2+}_{9.00}\text{Mg}_{0.05}\text{Fe}^{2+}_{0.77})(\text{Si}_{11.67}\text{Al}_{0.24}\text{Fe}^{3+}_{0.09})\text{O}_{40}$ ;

2)  $(\text{Na}_{0.35}\text{K}_{0.22}\text{Ca}_{3.56})(\text{Fe}^{2+}_{2.55}\text{Ti}^{4+}_{1.91}\text{Fe}^{3+}_{2.34}\text{Mg}^{2+}_{5.03})(\text{Si}^{4+}_{6.54}\text{Al}^{3+}_{5.44}\text{Fe}^{3+}_{0.02})\text{O}_{40}$ ;

3)  $\text{KBa}(\text{Al},\text{Sc})(\text{Mg},\text{Fe}^{2+})_6\text{Si}_6\text{O}_{20}\text{F}_2$ ;

4)  $(\text{Ca}_{1.92}\text{Na}_{0.07}\text{K}_{0.01})(\text{Ca}_{0.05}\text{Mg}_{1.05}\text{Mn}_{0.03}\text{Fe}^{2+}_{0.44}\text{Ti}_{0.05}\text{Fe}^{3+}_{4.38})(\text{Fe}^{3+}_{2.00}\text{Al}_{2.40}\text{Si}_{1.60})\text{O}_{20}$ ;

5)  $\text{NaMg}_2\text{CrSi}_3\text{O}_{10}$ ;

6) Natural sample:  $\text{SiO}_2 - 20.85$ ;  $\text{Al}_2\text{O}_3 - 40.20$ ;  $\text{FeO}(\text{total iron}) - 3.48$ ;  $\text{MgO} - 12.71$ ;  $\text{CaO} - 17.11$ ;  $\text{Na}_2\text{O} - 0.02$ ;  $\text{TiO}_2 - 0.06$  ( $\text{B}_2\text{O}_3$  not determined);

7)  $(\text{Ca}_{3.99}\text{Na}_{0.05}\text{Mg}_{0.01})\text{Si}_{3.07}\text{O}_{12}\text{H}_{3.66}$ ;

8)  $(\text{K}_{2.02}\text{Na}_{0.02})(\text{Zr}_{0.77}\text{Ti}_{0.18}\text{Hf}_{0.01}\text{Fe}_{0.01})\text{Si}_{3.00}\text{H}_{2.38}\text{F}_{0.45}\text{O}_{9.92}$ ;

9)  $(\text{K}_{2.92}\text{Na}_{0.03})(\text{Zr}_{2.02}\text{Hf}_{0.01}\text{Ti}_{0.10}\text{Fe}_{0.01})\text{H}_{0.94}\text{Si}_{5.89}\text{O}_{18}\cdot 7.34\text{H}_2\text{O}$ ;

10)  $\text{K}_{2.03}(\text{Zr}_{0.87}\text{Ti}_{0.12}\text{Hf}_{0.01})\text{Si}_{3.01}\text{O}_9\cdot \text{H}_2\text{O}$ ;

11) Natural sample:  $\text{SiO}_2 - 39.59$ ;  $\text{Al}_2\text{O}_3 - 1.30$ ;  $\text{Fe}_2\text{O}_3 - 1.56$ ;  $\text{Nb}_2\text{O}_5 - 1.45$ ;  $\text{TiO}_2 - 25.49$ ;  $\text{MgO} - 0.42$ ;  $\text{MnO} - 2.34$ ;  $\text{CaO} - 1.19$ ;  $\text{BaO} - 6.61$ ;  $\text{K}_2\text{O} - 7.23$ ;  $\text{K}_2\text{O} - 7.23$ ;  $\text{Na}_2\text{O} - 3.18$ ;  $\text{H}_2\text{O} - 7.91$ .