

**Tables and figures****Table 1.** Silicates from milarite group<sup>1)</sup> [91N1] (cyclosilicates group VIIC10).

Silicate	Composition
Armenite	$\text{BaCa}_2[\text{Al}_6\text{Si}_9\text{O}_{30}] \cdot 2\text{H}_2\text{O}$
Brannockite	$\text{KSn}_2[\text{Li}_3\text{Si}_2\text{O}_{30}]$
Chayesite	$\text{K}(\text{Mg}, \text{Fe}^{2+})_2[(\text{Mn}, \text{Fe}^{2+})_2\text{Fe}^{3+}\text{Si}_{12}\text{O}_{30}]$
Darapiosite	$\text{KNa}_2\text{Zr}[\text{Li}(\text{Mn}, \text{Zn})_2\text{Si}_{12}\text{O}_{30}]$
Eifelite	$\text{KNa}_3\text{Mg}[\text{Mg}_3\text{Si}_{12}\text{O}_{30}]$
Merrihueite	$(\text{K}, \text{Na})_2(\text{Fe}, \text{Mg})_2[(\text{Fe}, \text{Mg})_3\text{Si}_{12}\text{O}_{30}]$
Milarite	$\text{KCa}_2[\text{AlBe}_2\text{Si}_{12}\text{O}_{30}] \cdot \text{H}_2\text{O}$
Osumilite	$(\text{K}, \text{Na})(\text{Fe}, \text{Mg})_2[(\text{Al}, \text{Fe})_3(\text{Si}, \text{Al})_{12}\text{O}_{30}]$
Osumilite-Mg	$(\text{K}, \text{Na})(\text{Mg}, \text{Fe})_2[(\text{Al}, \text{Fe})_3(\text{Si}, \text{Al})_{12}\text{O}_{30}]$
Poudretteite	$\text{KNa}_2[\text{B}_3\text{Si}_{12}\text{O}_{30}]$
Roedderite	$(\text{Na}, \text{K})_2(\text{Mg}, \text{Fe})_2[(\text{Mg}, \text{Fe})_3\text{Si}_{12}\text{O}_{30}]$
Sogdianite [99C1]	$[\square, \text{Na}]_2\text{K}(\text{Zr}, \text{Ti}^{4+}, \text{Fe}^{3+}, \text{Al})_2[\text{Li}_3\text{Si}_2\text{O}_{30}]$
Sugilite	$(\text{Na}, \text{K})_3(\text{Fe}^{3+}, \text{Mn}, \text{Al})_2[\text{Li}_3\text{Si}_{12}\text{O}_{30}]$
Yagiite	$(\text{Na}, \text{K})_{1.5}\text{Mg}_2[(\text{Al}, \text{Mg}, \text{Fe})_3(\text{Si}, \text{Al})_{12}\text{O}_{30}]$
Synthetic silicates of milarite type	$\text{A}_x\text{M}_3\text{M}'_2\text{Si}_{12}\text{O}_{30}$ with $\text{M} = \text{Mg}^{2+}, \text{Zn}^{2+}, \text{Cu}^{2+}, \text{Li}^+$ and $\text{M}' = \text{Mg}^{2+}, \text{Cu}^{2+}, \text{Fe}^{2+}$ ; $\text{MMg}_2\text{Al}_6\text{Si}_9\text{O}_{30}$ with $\text{M} = \text{Sr}, \text{Ba}$ ; $\text{Mg}_2\text{Al}_4\text{Si}_{11}\text{O}_{30}$ ; $\text{K}_2\text{Mg}_5\text{Si}_{12}\text{O}_{30}$ etc (see Table 3)

<sup>1)</sup> In [99C1] two other members of Li-bearing members of the milarite group were mentioned: berezanskite and dusmatovite. For compositions see Table 5.

**Table 2.** Atomic sites and thermal parameters.

a) Milarite<sup>9)</sup>, having hexagonal structure (at room temperature), space group P6/mcc [80C1].

Site	Equipoint	Atomic coordinates			$B_{\text{eq}}$ [Å <sup>2</sup> ]
		$x$	$y$	$z$	
A	4c	1/3	2/3	1/4	1.90(4)
B	4d	1/3	2/3	0	1.91(2)
C	2a	0	0	1/4	1.48(5)
T1	24m	0.0819(1)	0.3359(1)	0.11244(7)	0.66(2)
T2	6f	0	1/2	1/4	0.35(6)
O1	12l	0.0951(5)	0.3828(5)	0	1.46(7)
O2	24m	0.1953(3)	0.2758(7)	0.1345(2)	1.37(5)
O3	24m	0.1153(3)	0.4722(3)	0.1808(2)	0.90(4)

<sup>9)</sup> See Table 4.

**Table 2** (cont.)b) Sugilite<sup>34)</sup>, having P6/mcc type structure [88A3].

Site	Occupation	Atomic coordinates			$B_{eq}$ [Å <sup>2</sup> ]
		$x$	$y$	$z$	
A	83% Fe, 17% Al	1/3	2/3	1/4	0.412(7)
B'	49% Na	1/2	2/3	0.0134(7)	1.7(1)
C	K	0	0	1/4	1.52(1)
T2	Li	1/2	1/2	1/4	1.44(7)
T1	Si	0.23633(5)	0.35620(5)	0.38678(3)	0.566(7)
O1		0.1383(2)	0.3972(2)	0	1.36(3)
O2		0.2232(2)	0.2774(2)	0.13775(9)	1.24(2)
O3		0.1665(1)	0.5091(1)	0.17032(8)	0.92(2)

c) Osumilite, BaMg<sub>2</sub>Al<sub>6</sub>Si<sub>9</sub>O<sub>30</sub>, having hexagonal structure (at room temperature), space group P6/mcc [95W1].

Site	Atomic coordinates			$B_{eq}$ [Å <sup>2</sup> ]
	$x$	$y$	$z$	
A(Mg)	1/3	2/3	1/4	0.53(5)
C(Ba)	0	0	1/4	1.847(6)
T1(Si,Al)	0.10461(6)	0.35270(6)	0.10916(3)	0.629(6)
T2(Al)	1/2	1/2	1/4	0.53(1)
O1	0.1205(3)	0.4016(3)	0	1.41(4)
O2	0.2134(2)	0.2807(2)	0.1367(1)	1.86(3)
O3	0.1386(2)	0.4951(2)	0.17939(9)	0.90(2)

d) Roedderite<sup>30)</sup>, having space group  $\overline{P}6_2c$ , at 300 K [89A1].

Site	Population	Atomic coordinates			$B_{eq}$ [Å <sup>2</sup> ]
		$x$	$y$	$z$	
A	0.95 Mg + 0.05 Fe	1/3	2/3	0.5035(2)	0.70(1)
T2		0.4969(2)	0	0	0.68(1)
B1'	0.46(1) Na	1/3	2/3	0.2713(3)	1.9(1)
B2'	0.05(1) Na	1/3	2/3	0.7713 <sup>a)</sup>	1.9 <sup>a)</sup>
C	0.94(1) K	0	0	0	1.59(1)
T1		0.2390(1)	0.3535(1)	0.64031(6)	0.436(5)
T11	Si	−0.2356(1)	−0.3513(1)	0.63996(6)	0.44 <sup>a)</sup>
O1		0.1427(5)	0.3994(5)	0.25	1.22(3)
O11		−0.1217(4)	−0.3916(5)	0.25	1.22 <sup>a)</sup>
O2		0.2147(2)	0.2713(3)	0.3862(2)	1.13(2)
O22		−0.2235(2)	−0.2819(3)	0.3807(2)	1.13 <sup>a)</sup>
O3		0.1588(3)	0.4990(2)	0.4204(2)	0.76(1)
O33		−0.1534(3)	−0.4959(3)	0.4229(2)	0.76 <sup>a)</sup>

<sup>a)</sup> Constrained parameters.<sup>30)</sup> See Table 4.

**Table 2** (cont.)e) Armenite<sup>2)</sup>, refined in space group Pnc2 [99A1].

Site	Atomic coordinates			$B_{\text{eq}}$
	$x$	$y$	$z$	[Å <sup>2</sup> ]
Ba	0.25003(7)	0.75472(3)	0.06890(6)	1.165(6)
Ca1	0.4182(1)	0.2475(2)	0.0516(3)	1.11(1)
Ca2	0.0825(1)	0.2536(2)	0.0931(2)	1.11(1)
T <sub>d</sub> 1Si	0.2956(1)	0.4581(3)	0.2070(2)	0.36(5) <sup>b)</sup>
T <sub>d</sub> 2Al	0.1302(2)	−0.0512(3)	−0.2970(2)	0.70(5) <sup>b)</sup>
T <sub>d</sub> 3Si	0.5830(2)	0.3321(3)	0.2066(2)	0.49(5) <sup>b)</sup>
T <sub>d</sub> 4Si	0.2081(2)	0.0460(3)	0.2103(3)	0.77(5) <sup>b)</sup>
T <sub>d</sub> 5Al	0.3722(2)	0.9560(2)	0.2081(2)	0.49(5) <sup>b)</sup>
T <sub>d</sub> 6Si	0.0857(2)	0.6609(3)	−0.2940(2)	0.54(5) <sup>b)</sup>
T <sub>d</sub> 7Al	0.5889(2)	0.3328(3)	0.4352(3)	0.62(5) <sup>b)</sup>
T <sub>d</sub> 8Al	0.0851(2)	0.6725(3)	−0.0662(3)	0.64(5) <sup>b)</sup>
T <sub>d</sub> 9Si	0.2890(2)	0.4547(3)	0.4313(3)	0.42(5) <sup>b)</sup>
T <sub>d</sub> ASi	0.1252(2)	0.5325(3)	0.4324(2)	0.61(5) <sup>b)</sup>
T <sub>d</sub> BSi	0.3721(1)	0.9602(2)	0.4370(2)	0.44(4) <sup>b)</sup>
T <sub>d</sub> CSi	0.2090(2)	0.4597(3)	−0.0622(3)	0.72(5) <sup>b)</sup>
T <sub>c</sub> 1Al	0.2511(3)	0.2530(1)	0.0719(3)	0.48(2) <sup>b)</sup>
T <sub>c</sub> 2Al	0	0	0.0659(4)	0.33(7) <sup>b)</sup>
T <sub>c</sub> 3Si	0	1/2	0.0674(4)	0.34(7) <sup>b)</sup>
T <sub>c</sub> 4Si	1/2	0	0.0747(4)	0.82(8) <sup>b)</sup>
T <sub>c</sub> 5Al	1/2	1/2	0.0746(4)	0.78(8) <sup>b)</sup>
O11	0.3851(4)	0.9925(8)	0.3276(4)	1.0(2) <sup>b)</sup>
O12	0.2941(5)	0.4229(9)	0.3191(5)	1.3(2) <sup>b)</sup>
O13	0.1077(4)	−0.0104(7)	−0.1780(4)	1.0(2) <sup>b)</sup>
O14	0.4415(4)	0.6622(8)	0.3188(5)	1.1(2) <sup>b)</sup>
O15	0.2049(5)	0.0820(8)	0.3245(5)	1.1(2) <sup>b)</sup>
O16	0.9397(5)	0.1609(8)	0.3166(5)	1.2(2) <sup>b)</sup>
O21	0.2079(3)	0.4973(5)	0.4604(5)	1.0(1) <sup>b)</sup>
O22	0.1249(1)	0.7918(6)	−0.3221(5)	1.3(1) <sup>b)</sup>
O23	0.1152(3)	0.8234(6)	−0.0376(5)	1.1(1) <sup>b)</sup>
O24	0.3564(3)	0.5622(5)	0.1863(4)	1.1(1) <sup>b)</sup>
O25	0.3380(3)	0.9270(5)	−0.0399(4)	1.0(1) <sup>b)</sup>
O26	0.1464(3)	0.9455(5)	0.1867(4)	1.1(1) <sup>b)</sup>
O27	0.3807(3)	0.7995(5)	0.1792(5)	0.8(1) <sup>b)</sup>
O28	0.2195(3)	0.5204(5)	0.1741(5)	0.8(1) <sup>b)</sup>
O29	0.2907(3)	0.4994(6)	−0.0353(5)	1.2(1) <sup>b)</sup>
O210	0.2831(3)	0.9818(6)	0.1796(5)	1.2(1) <sup>b)</sup>
O211	0.3784(3)	0.6875(6)	−0.0349(5)	1.0(1) <sup>b)</sup>
O212	0.1604(3)	0.5806(5)	−0.0386(4)	0.77(9) <sup>b)</sup>
O31	0.0700(4)	0.4677(7)	0.1324(5)	0.9(1) <sup>b)</sup>
O32	0.0718(3)	0.4439(6)	−0.5030(5)	0.7(1) <sup>b)</sup>
O33	0.1925(4)	0.1708(7)	0.1470(6)	0.7(1) <sup>b)</sup>
O34	−0.0183(4)	0.1294(7)	0.1362(6)	1.2(2) <sup>b)</sup>
O35	0.1876(4)	0.3388(7)	0.0042(6)	0.8(1) <sup>b)</sup>
O36	−0.0113(4)	0.3736(7)	0.0046(6)	1.3(2) <sup>b)</sup>
O37	0.4832(3)	0.8764(6)	0.0086(5)	0.4(1) <sup>b)</sup>
O38	0.4871(3)	0.6373(6)	0.1404(5)	0.2(1) <sup>b)</sup>
O39	0.3119(4)	0.3350(7)	0.1419(6)	0.8(1) <sup>b)</sup>

**Table 2** (cont.)

Site	Atomic coordinates			$B_{\text{eq}}$ [Å <sup>2</sup> ]
	$x$	$y$	$z$	
O310	0.3069(4)	0.3352(7)	0.4989(6)	0.8(1) <sup>b)</sup>
O311	0.4311(3)	0.0444(6)	0.1370(5)	0.9(1) <sup>b)</sup>
O312	0.4258(4)	0.0405(7)	0.5061(5)	0.9(1) <sup>b)</sup>
W1	0.4252(5)	0.2516(7)	0.3738(6)	2.0(2) <sup>b)</sup>
W2	0.0725(5)	0.2635(8)	0.2683(8)	2.8(2) <sup>b)</sup>
CC <sup>c)</sup>	0.255(3)	0.753(7)	−0.195(4)	1.58 <sup>b)</sup>

<sup>b)</sup> Atoms refined isotropically. T<sub>c</sub> represents ring-connecting tetrahedra. T<sub>d</sub> are double-ring tetrahedra;

<sup>c)</sup> The CC site is occupied by 0.11(1) O.

For footnotes <sup>2),9),30),34)</sup> see Table 4.

**Table 3.** Site occupancies in some milarite group silicates [80C1, 91H1].

Site	Equipoint	Site symmetry	CN <sup>a)</sup>	Occupancies
T1	24m	1	4	Si, Al
T2	6f	222	4	Li, Be, B, Mg, Al, Si, Mn <sup>2+</sup> , Zn
A	4c	32	6	Al, Fe <sup>3+</sup> , Sn <sup>4+</sup> , Mg, Zr, Fe <sup>2+</sup> , Ca, Na, Y, R <sup>b)</sup>
B	4d	$\bar{6}$	9	Na, H <sub>2</sub> O, □, Ca (?), K (?)
C <sup>c)</sup>	2a	62	12	K, Na, Ba, □, Ca (?)
D	2b	6/m	18	□, ?

<sup>a)</sup> Coordination;

<sup>b)</sup> Rare-earth element;

<sup>c)</sup> In [95W1] osumilites were prepared with C site occupied by M = Ba, Sr in MMg<sub>2</sub>Al<sub>6</sub>Si<sub>9</sub>O<sub>30</sub> osumilites and empty in Mg<sub>2</sub>Al<sub>4</sub>Si<sub>11</sub>O<sub>30</sub> osumilites.

**Table 4.** Crystal structures and lattice parameters.

Silicate	$T$ [K]	Space group	Lattice parameters [Å]			Refs.
			$a$	$b$	$c$	
Armenite <sup>1)</sup> pseudo-hexagonal (average structure)	RT	P6/mcc	10.69		13.90	60T1,75B1
Armenite <sup>2)</sup>	RT	Pnna	13.874(2)	18.660(2)	10.697(1)	92A1
Armenite <sup>2)</sup>	RT	Pnc2	18.660(2)	10.697(1)	13.874(2)	99A1
Brannockite <sup>3)</sup>	RT	P6/mcc	10.002(2)		14.263(3)	88A1,88A3
Chayesite <sup>4)</sup>	RT	P6/mcc	10.153(4)		14.388(6)	89V1
Darapiosite <sup>5)</sup>	RT	P6/mcc	10.32		14.39	75S1
Eifelite <sup>6)</sup>	RT	P6/mcc	10.137(5)		14.223(6)	83A1
Merrhueite <sup>7)</sup>	RT	P6/mcc	10.222(2)		14.152(2)	72K1
Merrhueite <sup>8)</sup>	RT	P6/mcc	10.16(6)		14.32(6)	65D1
Milarite <sup>9)</sup>	RT	P6/mcc	10.420(2)		13.810(9)	80C1
Milarite <sup>10)</sup>	RT	P6/mcc	10.428(6)		13.675(9)	80C1

**Table 4** (cont.)

Silicate	<i>T</i> [K]	Space group	Lattice parameters [Å]			Refs.
			<i>a</i>	<i>b</i>	<i>c</i>	
Milarite <sup>11)</sup>	RT	P6/mcc	10.417(5)		13.688(7)	80C1
Milarite <sup>12)</sup>	RT	P6/mcc	10.40		13.80	64C1, 75B1
Milarite <sup>13)</sup>	RT	P6/mcc	10.410(1)		13.845(3)	91H1
Milarite <sup>14)</sup>	RT	P6/mcc	10.404(4)		13.825(5)	91H1
Milarite <sup>15)</sup>	RT	P6/mcc	10.415(3)		13.763(5)	91H1
Milarite <sup>16)</sup>	RT	P6/mcc	10.396(1)		13.781(4)	91H1
Milarite <sup>17)</sup>	RT	P6/mcc	10.342(2)		13.777(6)	91H1
Milarite <sup>18)</sup>	RT	P6/mcc	10.340(1)		13.758(2)	91H1
Osumilite <sup>19)</sup>	RT	P6/mcc	10.086		14.325	88A3
Osumilite <sup>20)</sup>	RT	P6/mcc	10.150(2)		14.286(2)	88A3
Osumilite <sup>21)</sup>	RT	P6/mcc	10.071(2)		14.303(2)	88A3
Osumilite <sup>22)</sup>	RT	P6/mcc	10.155(1)		14.284(4)	69B1
Osumilite <sup>23)</sup>	RT	P6/mcc	10.17		14.34	53M1, 56M1
Osumilite <sup>24)</sup>	RT	P6/mcc	10.078(2)		14.317(6)	62S1
Osumilite <sup>25)</sup>	RT	P6/mcc	10.0912(5)		14.336(1)	82G1
Osumilite <sup>26)</sup>	RT	P6/mcc	10.1037(8)		14.329(2)	82G1
Osumilite <sup>27)</sup>	RT	P6/mcc	10.087(2)		14.333(5)	81O1
Osumilite (synthetic) (BaMg <sub>2</sub> Al <sub>6</sub> Si <sub>9</sub> O <sub>30</sub> )	RT	P6/mcc	10.129(2)		14.340(2)	95W1
Osumilite (synthetic) (SrMg <sub>2</sub> Al <sub>6</sub> Si <sub>9</sub> O <sub>30</sub> )	RT	P6/mcc	10.1273(5)		14.2274(8)	95W1
Osumilite (synthetic) (Mg <sub>2</sub> Al <sub>4</sub> Si <sub>11</sub> O <sub>30</sub> )	RT	P6/mcc	10.058(2)		14.336(3)	95W1
Osumilite-Mg <sup>28)</sup>	RT	P6/mcc	10.078(2)		14.319(2)	88A2
Poudretteite <sup>29)</sup>	RT	P6/mcc	10.239(1)		13.485(3)	87G1
Roedderite <sup>30)</sup>	100	P6 <sub>2</sub> c	10.139(3)		14.269(4)	89A1
Roedderite <sup>30)</sup>	300	P6 <sub>2</sub> c	10.141(2)		14.286(3)	89A1
Sogdianite <sup>31)</sup>	RT	P6/mcc	10.09		13.98	68D1
Sogdianite <sup>32)</sup>	RT	P6/mcc	10.083(5)		14.24(1)	75B1
Sogdianite <sup>33)</sup>	RT	P6/mcc	10.053(1)		14.211(2)	99C1
Sugilite <sup>34)</sup>	RT	P6/mcc	10.009(2)		14.006(3)	88A3
Sugilite <sup>35)</sup>	RT	P6/mcc	10.007		14.000	76K1
Yagiite <sup>36)</sup>	RT	P6/mcc	10.09(1)		14.29(3)	69B2
K <sub>2</sub> Mg <sub>5</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.21 <sub>1</sub>		14.15 <sub>2</sub>	80N1
K <sub>2</sub> Mg <sub>3</sub> Mg <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.222(2)		14.152(2)	72K1
K <sub>2</sub> Mg <sub>3</sub> Cu <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.16 <sub>9</sub>		14.18 <sub>2</sub>	80N1
K <sub>2</sub> Mg <sub>3</sub> Fe <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.22 <sub>0</sub>		14.17 <sub>6</sub>	80N1
K <sub>2</sub> Mg <sub>3</sub> Zn <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.19 <sub>9</sub>		14.14 <sub>5</sub>	80N1
Na <sub>2</sub> Mg <sub>5</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.15 <sub>1</sub>		14.22 <sub>8</sub>	80N1
Na <sub>2</sub> Mg <sub>3</sub> Cu <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.09 <sub>6</sub>		14.25 <sub>0</sub>	80N1
Na <sub>2</sub> Mg <sub>3</sub> Fe <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.15 <sub>5</sub>		14.25 <sub>9</sub>	80N1
Na <sub>2</sub> Mg <sub>3</sub> Zn <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.14 <sub>5</sub>		14.21 <sub>6</sub>	80N1
NaKMg <sub>5</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.15 <sub>2</sub>		14.28 <sub>0</sub>	80N1
NaKMg <sub>3</sub> Cu <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.08 <sub>8</sub>		14.30 <sub>2</sub>	80N1
RbNaMg <sub>5</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.13 <sub>5</sub>		14.37 <sub>6</sub>	80N1
RbNaMg <sub>3</sub> Cu <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.07 <sub>2</sub>		14.42 <sub>6</sub>	80N1
RbNaMg <sub>3</sub> Fe <sub>2</sub> Si <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.13 <sub>1</sub>		14.40 <sub>8</sub>	80N1
K <sub>3</sub> Mg <sub>4</sub> LiSi <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.25 <sub>3</sub>		14.04 <sub>0</sub>	80N1
Na <sub>3</sub> Mg <sub>4</sub> LiSi <sub>12</sub> O <sub>30</sub>	RT	P6/mcc	10.15 <sub>5</sub>		14.15 <sub>8</sub>	80N1

- 1) Natural sample corresponding to formula  $\text{BaCa}_2\text{Al}_6\text{Si}_9\text{O}_{30}(\text{H}_2\text{O})_2$ ;
- 2) Natural sample, Rémigny, Quebec, Canada;
- 3) Natural sample from Foot Mine, North Carolina, having the end-member composition  $\text{KSn}_2\text{Li}_3\text{Si}_{12}\text{O}_{30}$  [73W1];
- 4)  $(\text{K}_{1.14}\text{Na}_{0.10})(\text{Mg}_{3.29}\text{Fe}^{2+}_{0.67}\text{Mn}_{0.04})(\text{Fe}^{3+}_{0.64}\text{Fe}^{2+}_{0.29}\text{Al}_{0.04}\text{Ti}_{0.03})\text{Si}_{12.00}\text{O}_{30.00}$ ;
- 5)  $(\text{K}_{1.23}\text{Na}_{1.08}\text{Ca}_{0.11}\text{Li}_{0.58})\text{Li}_{0.73}(\text{Zn}_{1.10}\text{Mn}_{1.31})(\text{Zr}_{0.46}\text{Fe}_{0.26}\text{Nb}_{0.07})\text{Si}_{12}(\text{O},\text{OH})_{30}$ ;
- 6)  $\text{KNa}_2\text{Mg}_{4.5}\text{Si}_{12}\text{O}_{30}$ ;
- 7) Natural sample;
- 8)  $(\text{K}_{0.94}\text{Na}_{0.76}\text{Ca}_{0.06})(\text{Fe}_{3.85}\text{Mg}_{1.27}\text{Mn}_{0.08}\text{Al}_{0.04})\text{Si}_{12}\text{O}_{30.11}$ ;
- 9) Natural sample, King Mountain;  $\text{Ca}_{4.00}\text{K}_{2.00}(\text{Na}_{0.12}\text{Ca}_{0.15}\text{H}_2\text{O}_{1.85})\text{Si}_{23.88}\text{Al}_{1.86}\text{Be}_{4.23}\text{O}_{30}$ ;
- 10) Natural sample, Vezna,  $\text{Ca}_{4.00}\text{K}_{2.00}(\text{Na}_{0.49}\text{K}_{0.33}\text{Ca}_{0.03}\text{H}_2\text{O}_{2.24})\text{Si}_{24.07}\text{Al}_{0.89}\text{Be}_{5.08}\text{O}_{30}$ ;
- 11) Natural sample, Vezna; composition not mentioned;
- 12)  $\text{Ca}_2\text{K}(\text{Be}_{2.3}\text{Al}_{0.7})\text{Si}_{12}\text{O}_{29.7}(\text{OH})_{0.3}(\text{H}_2\text{O})_{0.70}$ ;
- 13)  $\text{Ca}_{2.03}\text{K}_{1.05}\text{Na}_{0.06}\text{Mn}_{0.04}\text{Al}_{1.11}\text{Be}_{2.06}\text{Si}_{11.83}\text{O}_{30}(\text{H}_2\text{O})_{1.20}$ ;
- 14)  $\text{Ca}_{1.96}\text{K}_{1.07}\text{Na}_{0.17}\text{Y}_{0.03}\text{Al}_{0.87}\text{Be}_{2.19}\text{Si}_{11.95}\text{O}_{30}(\text{H}_2\text{O})_{1.29}$ ;
- 15)  $\text{Ca}_{1.67}\text{K}_{0.86}\text{Na}_{0.62}\text{Al}_{1.38}\text{Be}_{1.72}\text{Si}_{11.90}\text{O}_{30}(\text{H}_2\text{O})_{1.65}$ ;
- 16)  $\text{Ca}_{2.08}\text{K}_{0.96}\text{Na}_{0.16}\text{Mn}_{0.02}\text{Al}_{0.67}\text{Be}_{2.33}\text{Si}_{12.00}\text{O}_{30}(\text{H}_2\text{O})_{1.68}$ ;
- 17)  $\text{Ca}_{1.42}\text{K}_{1.05}\text{Na}_{0.05}\text{Y}_{0.47}\text{Al}_{0.30}\text{Be}_{2.61}\text{Si}_{12.09}\text{O}_{30}$ ;
- 18)  $\text{Ca}_{1.15}\text{K}_{1.06}\text{Na}_{0.02}\text{Y}_{0.62}\text{Al}_{0.05}\text{Be}_{2.82}\text{Si}_{12.13}\text{O}_{30}$ ;
- 19) Natural sample, Antarctica;
- 20) Natural sample, Hayasaki;
- 21) Natural sample, Eifel B93;
- 22)  $(\text{Ca}_{0.005}\text{Na}_{0.31}\text{K}_{0.78})(\text{Mg}_{0.92}\text{Fe}_{0.92}\text{Mn}_{0.16})(\text{Si}_{10.22}\text{Al}_{4.41}\text{Fe}^{3+}_{0.37})\text{O}_{30} \cdot \text{H}_2\text{O}$ ;
- 23) Natural sample, Osumi province:  $(\text{K},\text{Na},\text{Ca})_{0.98}(\text{Fe},\text{Mg})_{2.00}(\text{Mg},\text{Al},\text{Mn})_{2.95}(\text{Si},\text{Al})_{12}\text{O}_{30}$ ;
- 24) Natural sample;
- 25)  $\text{Na}_{0.01}\text{Ca}_{0.01}\text{Mg}_{1.725}\text{Mn}_{0.003}\text{Fe}_{0.136}\text{Al}_{0.272}\text{Ti}_{0.002}\text{Si}_{1.861}\text{O}_6$ ;
- 26)  $\text{Na}_{0.09}\text{K}_{0.925}\text{Ca}_{0.018}\text{Ba}_{0.010}\text{Mg}_{1.882}\text{Mn}_{0.003}\text{Fe}_{0.380}\text{Ti}_{0.013}\text{Al}_{2.743}\text{Si}_{10.120}\text{Al}_{1.880}\text{O}_{30}$ ;
- 27)  $\text{KMg}_2(\text{Al}_{2.75}\text{Mg}_{0.25})(\text{Al}_{1.75}\text{Si}_{10.25})\text{O}_{30}$ ;
- 28) Natural sample,  $(\text{K},\text{Na})(\text{Mg},\text{Fe})_2[(\text{Al},\text{Fe})_3(\text{Si},\text{Al})_{12}\text{O}_{30}]$ ;
- 29)  $\text{K}_{1.00}(\text{Na}_{1.87}\text{K}_{0.04})\text{B}_{3.05}\text{Si}_{12.14}\text{O}_{30}$ ;
- 30)  $\text{Na}_{1.15}\text{K}_{1.0}(\text{Mg}_{4.66}\text{Fe}_{0.12}\text{Mn}_{0.10}\text{Ti}_{0.01})\text{Si}_{12}\text{O}_{30}$ ;
- 31)  $\text{K}_{1.1}\text{Na}_{0.9}\text{Li}_{2.6}\text{Fe}^{2+}_{0.2}\text{Fe}^{3+}_{0.2}\text{Al}_{0.2}\text{Ti}_{0.4}\text{Zr}_{0.8}\text{Si}_{12}\text{O}_{30}$ ;
- 32)  $\text{K}(\text{Na}_{0.95}\text{K}_{0.05})(\text{Zr}_{0.8}\text{Fe}^{3+}_{0.6}\text{Ti}_{0.4}\text{Fe}^{2+}_{0.2})(\text{Li}_{2.55}\text{Al}_{0.15}\square_{0.30})\text{Si}_{12}\text{O}_{30}$ ;
- 33)  $\text{K}(\square_{1.15}\text{Na}_{0.85})(\text{Zr}_{0.76}\text{Ti}^{4+}_{0.38}\text{Fe}^{3+}_{0.73}\text{Al}_{0.13})[\text{Li}_3\text{Si}_{12}\text{O}_{30}]$ ;
- 34)  $\text{K}_{1.00}\text{Na}_{1.96}(\text{Fe},\text{Mn})_{1.66}\text{Al}_{0.34}\text{Li}_{3.00}\text{Si}_{12}\text{O}_{30}$ ;
- 35)  ${}^{\text{C}}(\text{K}_{0.81}\text{Na}_{0.19}){}^{\text{B}}(\text{H}_2\text{O}_{0.91}\text{Na}_{0.64})_2{}^{\text{A}}(\text{Fe}^{3+}_{1.32}\text{Na}_{0.59}\text{Ti}_{0.06}\text{Fe}^{2+}_{0.03})_2{}^{\text{T}2}(\text{Li}_{2.12}\text{Al}_{0.59}\text{Fe}^{3+}_{0.29})_3\text{Si}_{12}\text{O}_{30}$ ;
- 36)  $\text{K}_{0.30}\text{Na}_{1.20}\text{Mg}_{2.00}(\text{Mg}_{0.60}\text{Fe}_{0.34}\text{Ti}_{0.10}\text{Al}_{1.96})(\text{Si}_{10.22}\text{Al}_{1.78})\text{O}_{30}$ ;
- 37)  ${}^{[12]}(\text{Na}_{0.10}\text{K}_{0.89}\text{Fe}^{2+}_{0.37}){}^{[6]}(\text{Mg}_{1.43}\text{Fe}^{2+}_{0.53}\text{Mn}_{0.01}){}^{[4]}(\text{Al}_{2.66}){}^{[4]}(\text{Si}_{10.3}\text{Al}_{1.70})\text{O}_{30}$ ;
- 38) Osumilite<sup>37</sup> heated at 813°C, 15 h;
- 39)  ${}^{[12]}(\text{Na}_{0.06}\text{K}_{0.69}\text{Fe}^{2+}_{0.10}){}^{[6]}(\text{Mg}_{0.75}\text{Fe}^{2+}_{1.01}\text{Fe}^{3+}_{0.06}\text{Ti}_{0.01}\text{Mn}_{0.17}){}^{[4]}(\text{Al}_{2.66}\text{Fe}^{3+}_{0.23}){}^{[4]}(\text{Si}_{10.3}\text{Al}_{1.70})\text{O}_{30}$ ;
- 40)  $\text{K}_{1.15}\text{Na}_{0.05}\text{Ca}_{2.09}\text{Al}_{0.63}\text{Be}_{2.37}\text{Si}_{12}\text{O}_{30} \cdot 0.6\text{H}_2\text{O}$ ;
- 41)  $\text{K}_{1.10}\text{Na}_{0.16}\text{Ca}_{2.00}\text{Mn}_{0.02}\text{Al}_{0.66}\text{Be}_{2.34}\text{Si}_{12}\text{O}_{30} \cdot 0.77\text{H}_2\text{O}$ ;
- 42) Natural sample, Wasenalp, Valais, Switzerland;
- 43) Natural sample, Rémigny, Quebec, Canada;
- 44)  $\text{Na}_2\text{Mg}_5\text{Si}_{12}\text{O}_{30}$ ;
- 45)  $\text{K}_{0.93}\text{Na}_{0.09}\text{Ca}_{0.02}\text{Ba}_{0.01}\text{Mg}_{1.88}\text{Fe}_{0.38}\text{Ti}_{0.01}\text{Al}_{4.62}\text{Si}_{10.12}\text{O}_{30}$ ;
- 46) Composition [wt %]: 60.6-SiO<sub>2</sub>; 22.0-Al<sub>2</sub>O<sub>3</sub>; 3-MgO; 9.4-FeO; 1.0-MgO; 0.7-Na<sub>2</sub>O; 3.2-K<sub>2</sub>O (total iron was reported as FeO);
- 47) Natural sample, Foot Mine;
- 48) Natural crystal; composition close to sample<sup>6)</sup>.

**Table 5.** Endmember formulae for the Li-bearing members of the milarite group [99C1].

Silicate	A <sup>a)</sup>	B <sup>a)</sup>	C	T2 <sup>b)</sup>	T1 <sup>c)</sup>
Brannockite	Sn <sup>4+</sup>	□	K	Li	Si
Berezanskite	Ti <sup>4+</sup>	□	K	Li	Si
Sogdianite	Zr <sup>4+</sup>	□	K	Li	Si
Sugilite	Fe <sup>3+</sup>	Na	K	Li	Si
Darapiosite	Mn <sup>2+</sup>	Na	K	Zn <sub>2</sub> Li <sub>1</sub>	Si
Dusmatovite	Mn <sup>2+</sup>	K	K	Zn <sub>2</sub> Li <sub>1</sub>	Si

<sup>a)</sup> Multiplicity of 2; <sup>b)</sup> Multiplicity of 3; <sup>c)</sup> Multiplicity of 12.

**Table 6.** Data obtained from <sup>57</sup>Fe NGR spectra.

Sample <sup>02)</sup>	<i>T</i> [K]	Site	$\delta^{1)}$ [mm/s]	$\Delta Q$ [mm/s]	<i>DH</i> [mm/s]	<i>A</i> [%]	Refs.
Osumilite <sup>37)</sup>	RT	Fe <sup>2+</sup>	1.20	2.35	0.42	68	78G1, 82G1
		Fe <sup>2+</sup>	1.14	1.86	0.42	32	
Osumilite <sup>37)</sup>	RT	Fe <sup>2+</sup>	1.21	2.41	0.38	53	78G1
		Fe <sup>2+</sup>	1.16	2.03	0.38	35	
		Fe <sup>2+</sup>	1.17	1.48	0.38	12	
Osumilite <sup>38)</sup>	RT	Fe <sup>2+</sup>	1.22	2.34	0.34	51	78G1
		Fe <sup>2+</sup>	1.19	1.88	0.34	30	
		Fe <sup>2+</sup>	1.26	1.41	0.34	19	
Osumilite <sup>39)</sup>	RT	Fe <sup>2+</sup>	1.19	2.33	0.33	45	78G1
		Fe <sup>2+</sup>	1.20	1.86	0.33	20	
		Fe <sup>2+</sup>	1.21	1.40	0.33	15	
		Fe <sup>3+</sup> (tetr.)	0.25	1.71	0.33	16	
		Fe <sup>3+</sup> (oct)	0.40	0.60	0.33	4	
Osumilite <sup>26)</sup>	RT	Fe <sup>2+</sup>	1.19(3)	2.33(3)	0.45(2)	61(5)	82G1
		Fe <sup>2+</sup>	1.13(3)	1.70(3)	0.45(2)	34(2)	
		Fe <sup>3+</sup>	0.42(4)	0.73(4)	0.45(2)	5(2)	

<sup>1)</sup> Relative to  $\alpha$ -Fe; <sup>2)</sup> For footnotes (composition) of the samples see Table 4.

**Table 7.** <sup>29</sup>Si chemical shifts<sup>a)</sup> obtained from MAS NMR spectra.

Sample <sup>c)</sup>	Tetra- hedron	Chemical shifts [ppm] and intensities				Refs.
		4Al	3Al 1Si	2Al 2Si	1Al 3Si	
Milarite <sup>40)</sup>	T <sub>d</sub>				−104.8 (1Be,Al)3Si	99A1
Milarite <sup>41,b)</sup>	T <sub>d</sub>				−104.3 (1Be,Al)3Si	
Armenite <sup>42)</sup>	T <sub>c</sub>	−82.3 (~ 12 %)				99A1
	T <sub>d</sub>		−95.0 (~ 44 %)	−101.8 (≅ 44 %)		
Armenite <sup>43)</sup>	T <sub>c</sub>	−82.5 (6 %)				99A1
	T <sub>d</sub>		−95.0 (59 %)	−101.8 (35 %)		
Roedderite <sup>44)</sup>	T <sub>d</sub>				−100.6 (1Mg 3Si)	90H1

<sup>a)</sup> As compared to <sup>29</sup>Si in Si(CH<sub>3</sub>)<sub>4</sub>; <sup>b)</sup> After 24 h heat treatment at 800°C the bands remain broad and centered at −104.5 ppm. <sup>c)</sup> For footnotes (composition) of the samples see Table 4.

**Table 8.** H<sub>2</sub>O vibrations in armenite and milarite determined from FTIR data [99A1].

Peak positions [cm <sup>-1</sup> ]	⊥ <i>c</i>	∥ <i>c</i>	Assignment
<i>Armenite</i> <sup>42)</sup>			
5105	weak	weak, broad	$\nu_2 \nu_3$
≅3620	strong, shoulder	weak, shoulder	$\nu_3/\nu_1$
≅3420	very strong, broad <sup>a)</sup>	very strong, narrow <sup>a)</sup>	$\nu_1/\nu_3$
3250	very weak	weak, narrow	$2\nu_2$
1645	weak, narrow	strong, narrow	$\nu_2$
<i>Milarite</i> <sup>40)</sup>			
5195	weak	—	$\nu_2 \nu_3$
≅3600	strong, shoulder	weak, shoulder	$\nu_3 \nu_1$
≅3520	very strong <sup>a)</sup>	strong, narrow	$\nu_1 \nu_3$
3220	very weak	weak	$2\nu_2$
1625	medium, narrow	very strong, narrow <sup>a)</sup>	$\nu_2$

<sup>a)</sup> Peaks are off scale;<sup>40)</sup>, <sup>42)</sup> See Table 4 for composition.**Table 9.** Refractive indices.

Sample <sup>c)</sup>	Refractive indices		2 <i>V</i> <sup>o</sup>	Refs.
	<i>n</i> (ε)	<i>n</i> (ω)		
Armenite				biaxial negative
Chayesite <sup>4)</sup>	1.578(1)	1.575(1)		uniaxial positive
Darapiosite <sup>5)</sup>	1.575(2)	1.580(2)		uniaxial negative
Eifelite <sup>6)</sup>	1.5458(5)	1.5445(5)		uniaxial positive
Eifelite <sup>48)</sup>	1.5443(5)	1.5430(5)		uniaxial positive
Merrihueite <sup>8)</sup>	$n_s = 1.559...1.592$		5...10°	uniaxial or biaxial <sup>a)</sup>
Milarite (natural)	1.529	1.532	small	biaxial negative <sup>b)</sup>
Milarite <sup>9)</sup>	1.537	1.5385		sector zoning
Milarite <sup>10)</sup>	1.546	1.549		uniaxial
Milarite <sup>11)</sup>	1.552	1.555		uniaxial
Osumilite <sup>22)</sup>	1.546	1.550		
Osumilite <sup>7)</sup>	1.549...1.551	1.545...1.547		uniaxial positive
BaMg <sub>2</sub> Al <sub>6</sub> Si <sub>9</sub> O <sub>30</sub>	1.5500(10)	1.5575(10)		
(synthetic osumilite)	( <i>n</i> <sub>o</sub> )	( <i>n</i> <sub>e</sub> )		
SrMg <sub>2</sub> Al <sub>6</sub> Si <sub>9</sub> O <sub>30</sub>	1.5379(10)	1.5466(10)		
(synthetic osumilite)	( <i>n</i> <sub>o</sub> )	( <i>n</i> <sub>e</sub> )		
Poudretteite <sup>29)</sup>	1.532(1)	1.516(1)		
Roedderite	1.548	1.534		
Roedderite(natural)	1.542	1.537		
Yagiite <sup>36)</sup>	1.544(2)	1.536(2)		uniaxial positive

<sup>a)</sup> Variable Fe content;<sup>b)</sup> Becomes uniaxial negative at high temperatures;<sup>c)</sup> For footnotes (composition) of the samples see Table 4.