

## Tables and figures

**Table 1.** Cyclosilicates from groups VIII C01–VIII C03 [91N1].

Silicate	Composition	Group
Wadeite	$\text{K}_2\text{ZrSi}_3\text{O}_9$	VIII C01 <sup>1)</sup>
Benitoite	$\text{BaTiSi}_3\text{O}_9$	VIII C01
Pabsite	$\text{Ba}(\text{Sn}, \text{Ti})\text{Si}_3\text{O}_9$	VIII C01
Bazirite	$\text{BaZrSi}_3\text{O}_9$	VIII C01
Walstromite	$\text{BaCa}_2\text{Si}_3\text{O}_9$	VIII C02
Margarosanite	$\text{Ca}_2\text{PbSi}_3\text{O}_9$	VIII C02
Roebblingite	$\text{Ca}_6\text{MnPb}_2(\text{Si}_3\text{O}_9)_2(\text{SO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$	VIII C02
Scawtite	$\text{Ca}_7(\text{Si}_3\text{O}_9)_2(\text{CO}_3) \cdot 2\text{H}_2\text{O}$	VIII C02
Eudialyte <sup>2)</sup>	$\text{Na}_{16}\text{Ca}_6\text{Fe}_3\text{Zr}_3(\text{Si}_3\text{O}_9)_2(\text{Si}_9\text{O}_{27})_2(\text{OH}, \text{Cl})_4$	VIII C03
Kentbrooksite	$(\text{Na}, \text{R})_{15}(\text{Ca}, \text{R})_6\text{Mn}_3\text{Zr}_3\text{NbSi}_{25}\text{O}_{74}\text{F}_2 \cdot 2\text{H}_2\text{O}$	VIII C03
Catapleiite	$\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$	VIII C03
Calcium catapleiite	$\text{CaZrSi}_3\text{O}_9 \cdot \text{H}_2\text{O}$	VIII C03
Gaidonnayite	$\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$	VIII C03
Georgechaoite	$\text{KNaZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O}$	VIII C03
Loudounite	$\text{NaCa}_9\text{Zr}_4\text{Si}_{16}\text{O}_{40}(\text{OH})_{11} \cdot 8\text{H}_2\text{O}$	VIII C03

<sup>1)</sup> The  $\text{K}_2\text{Si}_4\text{O}_9$ ,  $\text{Na}_2\text{Si}_4\text{O}_9$ ,  $\text{BaSi}_4\text{O}_9$ ,  $\text{A}_{2-x}\text{A}'_x(\text{B}_{1-z}\text{B}'_z)\text{Si}_y\text{Ge}_{3-y}\text{O}_9$  ( $\text{A}$ ,  $\text{A}' = \text{K}$ ,  $\text{Rb}$ ,  $\text{Cs}$ ,  $\text{Tl}$ ;  $\text{B}$ ,  $\text{B}' = \text{Ti}$ ,  $\text{Sn}$ ,  $\text{Ge}$ ),  $\text{K}_6\text{M}_6\text{Si}_4\text{O}_{26}$ ,  $\text{A}_3\text{M}_6\text{Si}_4\text{O}_{26}$  are also included;

<sup>2)</sup> Various eudialyte types were studied and their denominations were mentioned in text. We mention in table only kentbrooksite.

**Table 2.** Atomic positional parameters and temperature factors.

a)  $\text{K}_2\text{ZrSi}_3\text{O}_9$ , crystallizing in space group P3 [77B1].

Atom	$x$	$y$	$z$	$\beta_{ij} \cdot 10^4$					
				$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{23}$	$\beta_{13}$
Zr1	0	0	0.0000(4)	56	56	14	36	0	0
Zr2	0	0	0.4990(4)	56	56	15	37	0	0
K1	2/3	1/3	0.560(4)	96	96	36	99	0	0
K2	2/3	1/3	0.946(4)	101	101	32	93	0	0
K3	1/3	2/3	0.059(4)	99	98	34	82	0	0
K4	1/3	2/3	0.447(4)	99	98	30	77	0	0
Si1	0.386(1)	0.259(1)	0.249(4)	14	16	15	10	2	8
Si2	0.614(1)	0.741(1)	0.749(4)	30	42	8	42	−3	−7
O1	0.488(2)	0.090(2)	0.261(4)	30	40	33	42	10	12
O2	0.514(2)	0.911(2)	0.762(5)	43	51	36	62	−18	−8
O3	0.246(2)	0.236(2)	0.120(5)	63	50	19	51	−21	−26
O4	0.268(2)	0.239(2)	0.387(5)	65	56	19	41	19	39
O5	0.756(2)	0.768(2)	0.620(5)	72	88	16	90	6	22
O6	0.734(2)	0.767(3)	0.887(5)	80	100	16	10	−13	−32

**Table 2** (cont.)b)  $\text{K}_2\text{Si}_4\text{O}_9$ , crystallizing in space group  $\text{P6}_3/\text{m}$  [83S1].

Atom	$x$	$y$	$z$	$B_{\text{eq}} [\text{\AA}^2]$
K	1/3	2/3	0.05778(5)	1.139(5)
<sup>[6]</sup> Si	0	0	0	0.344(6)
<sup>[4]</sup> Si	0.36532(7)	0.23343(7)	1/4	0.323(4)
O1	0.49150(18)	0.07339(19)	1/4	0.629(12)
O2	0.23203(13)	0.20907(13)	0.10611(8)	0.619(8)

c) Walstromite,  $\text{Ca}_2\text{BaSi}_3\text{O}_9$ , crystallizing in triclinic lattice, space group  $\text{P}\bar{1}$  [68D1].

Atom	$x$	$y$	$z$
Ca1	0.272	0.507	0.763
Ca2	0.435	0.831	0.935
Ba	0.049	0.848	0.323
Si1	0.096	0.222	0.145
Si2	0.235	0.484	0.284
Si3	0.442	0.196	0.511
O1	0.236	0.251	−0.027
O2	−0.098	0.114	0.102
O3	0.042	0.366	0.212
O4	0.366	0.556	0.089
O5	0.125	0.580	0.389
O6	0.352	0.365	0.494
O7	0.613	0.238	0.368
O8	0.517	0.084	0.765
O9	0.238	0.130	0.389

d) Roeblingite, having monoclinic structure of space group  $\text{C2}/\text{m}$  [84M2].

Atom	$x$	$y$	$z$	$\beta_{ij} \cdot 10^3$					
				$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
Pb	0.1010(1)	0.0000	0.1450(1)	13.4(3)	11.5(3)	14.5(3)	0	3.0(2)	0
Mn	0.0000	0.5000	0.5000	10(2)	10(2)	16(2)	0	3(1)	0
Ca1	0.0549(3)	0.5000	0.2371(3)	12(1)	11(1)	15(1)	0	4(1)	0
Ca2	0.3042(2)	0.2306(3)	0.3307(2)	9(1)	9(1)	15(9)	2(1)		2(1)
Si1	0.2632(4)	0.5000	0.4846(4)	8(2)	7(2)	13(2)	0	3(1)	0
O1	0.2217(10)	0.5000	0.3592(10)	9(4)	18(6)	14(5)	0	5(4)	0
O2 <sup>a)</sup>	0.3224(10)	0.0000	0.4472(11)	6(5)	29(7)	22(6)	0	12(4)	0
O3	0.1552(7)	0.1580(10)	0.4802(7)	12(3)	5(3)	17(3)	−4(3)	3(3)	10(3)
Si2	0.0612(2)	0.1732(4)	0.3690(3)	8(1)	5(1)	15(1)	2(1)	4(1)	1(1)
O4	0.1173(7)	0.1938(12)	0.2742(7)	14(4)	17(4)	13(3)	−3(3)	8(3)	−7(3)
O5	0.4870(7)	0.1768(11)	0.3708(7)	12(3)	3(3)	23(4)	−4(3)	3(3)	−4(3)
O6	−0.0011(10)	0.0000	0.3571(12)	10(5)	2(4)	31(6)	0	11(4)	0
S	0.2626(4)	0.5000	0.1123(3)	15(2)	11(2)	14(2)	0	7(1)	0
O7	0.2851(13)	0.5000	0.0088(12)	29(7)	25(7)	20(6)	0	15(5)	0
O8	0.1475(3)	0.5000	0.1018(14)	22(7)	38(8)	26(7)	0	5(6)	0
O9	0.3101(9)	0.3581(13)	0.1728(9)	34(5)	16(4)	25(4)	10(4)	17(4)	8(4)
OW1	0.2754(10)	0.0000	0.2143(11)	9(5)	17(6)	16(5)	0	4(4)	0
OW2	0.4460(9)	0.1742(15)	0.0967(9)	19(4)	26(5)	30(5)	2(4)	1(4)	−2(4)

<sup>a)</sup> Non-positive definite thermal parameter.

**Table 2** (cont.)e) Scawtite,  $\text{Ca}_7(\text{Si}_6\text{O}_{18})(\text{CO}_3) \cdot 2\text{H}_2\text{O}$ , having monoclinic structure, space group I2/m [73P1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$
Ca1	0.2120(1)	0.1402(1)	0.1996(2)	1.00(2)
Ca2	1/2	0.2495(1)	0	0.66(3)
Ca3	1/2	1/2	0	1.39(5)
Si1	0.7729(1)	0.3957(1)	0.2059(2)	0.45(3)
Si2	0	0.3233(1)	0	0.46(4)
O1	0.9028(4)	0.3933(3)	0.0901(6)	1.13(8)
O2	0.0879(4)	0.2683(3)	0.1837(6)	0.89(8)
O3	0.6447(4)	0.3756(3)	0.0322(6)	0.84(7)
O4	0.6980(4)	0.1619(2)	0.0918(6)	0.74(7)
O5	0.7409(6)	0	0.2268(8)	0.83(10)
O6 [H <sub>2</sub> O]	0.3452(7)	0	0.2033(9)	1.66(13)
C	0	0	0	1.46(24)
O7 <sup>a)</sup>	0.0152(12)	0.0699(9)	0.1024(20)	4.04(33)
O8 <sup>a)</sup>	0.0665(13)	0	0.1777(18)	1.47(25)

<sup>a)</sup> O7 and O8 were assigned to an occupancy of 0.5.f) Eudialyte<sup>17)</sup> (footnote see Table 3), having trigonal structure, space group R3m [99R2].

1) Framework of Ti-rich eudialyte.

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$	Site occupation
M1	0.1637(1)	0.3274(1)	0.0833(1)	1.21(2)	2.33 Zr + 0.67 Ti
M2	−0.0034(2)	0.4983(1)	0.2496(1)	1.27(3)	1.7 Ti + 1.3 Zr
M3	0.0743(1)	0.6668(2)	0.1662(1)	1.26(3)	4.77 Ca + 1.23 Mn
M4	−0.0007(2)	0.2606(1)	−0.0007(1)	1.24(2)	3.73 Ca + 1.87 Na + 0.4 Ce
Si1	0.3209(2)	0.0514(2)	0.1183(1)	1.65(5)	
Si2	0.2464(3)	0.1232(2)	0.2955(1)	1.24(6)	
Si3	0.0627(3)	0.3446(3)	0.2843(1)	1.37(5)	
Si4	0.5981(2)	0.4019(2)	0.2924(1)	1.71(7)	
Si5	0.0717(2)	0.1434(3)	0.0405(1)	1.49(7)	
Si6	0.4054(2)	0.5946(2)	0.2068(1)	1.44(7)	
Si7	0.5398(1)	0.4602(1)	0.1269(1)	1.35(6)	
Si8	0.2632(2)	0.5264(3)	0.1249(1)	1.54(8)	
Si9	0.0029(2)	0.6064(2)	0.0487(1)	0.97(4)	
Si10	0.1246(2)	0.2492(3)	0.2042(1)	1.50(7)	
Si11	0.4172(4)	0.2086(3)	0.0374(1)	1.37(7)	
Si12	0.3399(3)	0.0651(3)	0.2146(1)	1.33(5)	
O1	0.3558(8)	0.1779(5)	0.1105(1)	0.9(3)	
O2	0.3110(8)	0.1555(6)	0.3188(1)	2.2(2)	
O3	0.5136(3)	0.0272(5)	0.1521(1)	0.8(3)	
O4	0.3794(9)	0.2783(6)	0.0542(1)	2.1(2)	
O5	0.0714(5)	0.3715(5)	0.3092(1)	1.0(2)	
O6	0.0261(6)	0.2478(6)	0.1033(1)	1.6(2)	
O7	0.3024(11)	0.1512(9)	0.2246(2)	2.5(3)	
O8	0.1007(6)	0.3969(7)	0.0641(1)	2.5(2)	
O9	0.0614(5)	0.1228(7)	0.2047(3)	5.3(5)	
O10	0.5709(8)	0.1418(10)	0.2678(4)	4.6(4)	
O11	0.2357(6)	0.4714(9)	0.1016(2)	2.5(4)	

**Table 2** (cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$	Site occupation
O12	0.2962(7)	0.2533(6)	0.1436(1)	1.3(2)	
O13	0.5500(4)	0.4500(4)	0.3103(1)	1.5(3)	
O14	0.2717(5)	0.5434(7)	0.2059(2)	2.1(3)	
O15	0.0328(9)	0.6219(7)	0.0225(1)	2.6(2)	
O16	0.3756(11)	0.3026(9)	0.1894(1)	3.2(2)	
O17	0.1238(8)	0.0619(5)	0.0391(2)	2.4(4)	
O18	0.5444(1)	0.2722(8)	0.2952(2)	2.1(4)	
O19	0.0570(4)	0.2981(4)	0.2196(1)	1.0(1)	
O20	0.5112(3)	0.0224(5)	0.0565(1)	1.1(3)	
O21	0.3970(6)	0.6030(6)	0.1262(2)	2.6(4)	
O22	0.0939(3)	0.1878(5)	0.0642(1)	1.1(3)	
O23	0.0706(6)	0.6357(7)	0.2686(1)	1.6(2)	
O24	0.1640(6)	0.3280(9)	0.2746(2)	3.0(3)	
O25	0.4370(9)	0.3596(9)	0.2315(1)	2.9(3)	
O26	0.5490(13)	0.2745(9)	0.0320(2)	5.8(4)	
O27	0.1135(6)	0.2270(8)	0.0204(2)	2.8(4)	
O28	0.2247(6)	0.4494(8)	0.1452(2)	2.4(3)	
O29	0.1100(13)	0.5550(9)	0.1871(1)	3.2(5)	
O30	0.2720(9)	0.2235(7)	0.2797(1)	2.6(2)	
O31	0.6069(5)	0.2137(7)	0.1251(2)	2.5(5)	
O32	0.4384(9)	0.3856(9)	0.1121(1)	3.4(3)	
O33	0.1146(14)	0.0573(9)	0.2975(3)	6.0(6)	
O34	0.1476(5)	0.2952(8)	0.1818(2)	1.8(4)	
O35	0.4351(6)	0.5649(6)	0.2316(2)	3.5(5)	
O36	0.3618(9)	0.1809(7)	0.0144(1)	1.6(4)	

## 2) extra framework positions

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{eq}} [\text{\AA}^2]$	Site occupation
T1a	2/3	1/3	0.0195(8)	1.7(9)	0.2 Si
T1b	2/3	1/3	0.0438(1)	0.8(7)	0.8 Si
T2a	2/3	1/3	0.1165(1)	3.0(9)	0.16 Si
TM	2/3	1/3	0.1366(1)	1.8(1)	0.42 Si + 0.42 Al
T3a	0	0	0.1861(1)	2.6(1)	0.9 Mn
T3b	0	0	0.2160(1)	2.9(9)	0.1 Si
T4a	0	0	0.2884(1)	0.6(1)	0.8 Si
T4b	0	0	0.3051(4)	1.0(8)	0.2 Si
Ti	0.3734(9)	0.1867(6)	0.1641(1)	2.1(1)	
Fe1	0.3142(5)	0.1571(4)	0.1674(1)	1.5(1)	
Fe2	−0.0136(20)	0.4932(16)	0.0005(4)	1.1(4)	
M5	0.2228(5)	0.4456(9)	0.3348(2)	2.3(2)	0.67 Na + 0.23 Ce
M6	0.0973(2)	0.1946(3)	0.1429(1)	3.3(1)	2.6 Na + 0.4 Sr
M7	0.2227(4)	0.4454(5)	0.2434(1)	4.9(1)	1.83 Na + 0.27 Ce
M8	0.4459(9)	0.2228(7)	0.2573(1)	3.3(2)	0.94 Na + 0.23 Ce
M9	0.4416(6)	0.5584(6)	−0.0019(2)	2.1(2)	1.46 Na + 0.37 Sr
Na1	0.1032(8)	0.5516(6)	0.3039(1)	2.9(2)	
Na2	0.2176(9)	0.1088(6)	0.0768(1)	3.1(3)	
Na3	0.2132(3)	0.4264(5)	0.0280(2)	3.8(2)	
Na4	0.4450(5)	0.5550(5)	0.0898(1)	4.7(3)	

**Table 2** (cont.)

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>B</i> <sub>eq</sub> [Å <sup>2</sup> ]	Site occupation
Na5a	0.5731(3)	0.1462(4)	0.1878(2)	2.4(2)	1.33 Na + 1.0 OH
Na5b	0.5395(11)	0.4605(11)	0.1939(15)	2(1) <sup>a)</sup>	
Na6	0.2634(25)	0.5268(36)	0.2499(6)	4(1) <sup>a)</sup>	
Na7	0.5072(20)	0.2536(15)	0.2476(3)	4.9(2)	
Na8a	0.1478(10)	0.0739(7)	0.2403(3)	5.0(3)	
Na8b	0.1115(40)	0.1616(50)	0.2528(9)	7.4(9) <sup>a)</sup>	
Na9a	0.5040(15)	0.2620(9)	0.0865(3)	3.7(3)	
Na9b	0.5087(30)	0.2087(30)	0.0863(5)	3.7(5) <sup>a)</sup>	
Na10	0.2002(47)	0.1001(33)	0.1721(8)	3.1(9)	
Cl1	1/3	2/3	0.3131(1)	0.9(2)	
Cl2	0	0	0.1165(9)	2.7(7)	
OH1	1/3	2/3	0.3250(9)	3(2) <sup>a)</sup>	
OH2	2/3	1/3	0.0678(2)	1.0(4)	
OH3	2/3	1/3	0.0928(50)	5(4) <sup>a)</sup>	
OH4	0.5462(47)	0.2731(33)	0.1721(11)	4.9(9)	
OH5	2/3	1/3	0.1637(9)	1.0(7)	
OH6	0	0	0.1463(12)	7.8(7)	
OH7	0	0	0.2410(11)	2.1(5) <sup>a)</sup>	
OH8	0	0	0.2597(12)	0.4(4)	
OH9	0	0	0.3333(11)	3.4(4) <sup>a)</sup>	
H <sub>2</sub> O1	1/3	2/3	0.2683(5)	3(2) <sup>a)</sup>	
H <sub>2</sub> O2	2/3	1/3	0.2241(15)	7(4) <sup>a)</sup>	
H <sub>2</sub> O3	1/3	2/3	0.0228(2)	2.8(1)	
H <sub>2</sub> O4	0	0	0.0026(9)	7(1) <sup>a)</sup>	

<sup>a)</sup> Isotropic thermal parameters.

g) Gaidonnayite, Na<sub>2</sub>ZrSi<sub>3</sub>O<sub>9</sub> · 2H<sub>2</sub>O, having monoclinic structure, space group I2/m [85C1].

Atom	<i>x</i>	<i>y</i>	<i>z</i>	<i>β</i> <sub>ij</sub> · 10 <sup>4</sup>					
				<i>β</i> <sub>11</sub>	<i>β</i> <sub>22</sub>	<i>β</i> <sub>33</sub>	<i>β</i> <sub>12</sub>	<i>β</i> <sub>13</sub>	<i>β</i> <sub>23</sub>
Na1	0.7466(3)	0.1567(2)	0.4307(4)	51(2)	45(2)	162(8)	7(4)	−19(8)	−5(6)
Na2	−0.0041(3)	0.3876(3)	0.3316(5)	47(2)	37(2)	180(10)	6(4)	−10(6)	−49(6)
Zr	0.2500	0.0531(1)	0.1510(1)	24(1)	15(1)	63(1)	0(1)	−4(1)	0(1)
Si1	0.2809(1)	0.2883(1)	0.3927(2)	21(1)	7(1)	59(4)	−1(1)	−4(3)	0(2)
Si2	0.4981(1)	0.4180(1)	0.3911(2)	20(1)	15(1)	58(4)	−1(1)	−5(3)	−1(3)
Si3	0.7144(1)	0.3918(1)	0.1501(2)	20(1)	15(1)	51(4)	1(1)	4(3)	−8(2)
O1	0.2116(5)	0.3952(3)	0.3644(7)	25(3)	8(2)	90(10)	7(5)	−3(9)	−21(7)
O2	0.4173(4)	0.3155(3)	0.4186(7)	22(3)	9(2)	103(11)	−12(4)	−16(10)	15(8)
O3	0.7417(5)	0.2699(3)	0.1017(6)	29(3)	14(2)	56(8)	18(5)	21(11)	12(7)
O4	0.2654(5)	0.2096(3)	0.2065(7)	39(4)	17(2)	78(9)	−18(5)	36(12)	3(8)
O5	0.4225(4)	0.1940(4)	0.1562(7)	23(3)	14(3)	107(12)	12(5)	−16(9)	−23(8)
O6	0.5759(4)	0.3940(4)	0.1960(7)	22(3)	35(3)	60(9)	−1(5)	10(9)	−29(9)
O7	0.0743(4)	0.0706(4)	0.0898(7)	15(3)	23(2)	67(10)	2(4)	−5(9)	−3(9)
O8	0.2398(5)	0.0361(3)	0.4583(7)	27(3)	12(2)	6(8)	3(5)	11(10)	−6(6)
O9	0.7817(5)	0.4258(4)	0.3474(6)	31(3)	19(2)	47(10)	−11(5)	−20(9)	−18(7)
H <sub>2</sub> O1	0.5397(5)	0.1326(4)	0.4739(10)	48(5)	32(3)	186(17)	11(6)	−30(15)	−32(12)
H <sub>2</sub> O2	0.9558(7)	0.1991(5)	0.3821(10)	60(6)	35(4)	118(14)	26(7)	−18(14)	23(11)

**Table 3.** Crystal structures and lattice parameters.

Silicate	Space group	Lattice parameters						Refs.
		$a$ [Å]	$b$ [Å]	$c$ [Å]	$\alpha$	$\beta$	$\gamma$	
Wadeite <sup>1)</sup>	$P\bar{6}$	6.926(1)		10.177(1)				77B1
Wadeite <sup>1)</sup>		6.893(4)		10.172(2)				55H1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub>		6.772		9.927				71A1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub>		6.774		9.922				71C1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub>		6.79(3)		9.87(4)				73S1
K <sub>2</sub> <sup>[6]</sup> Si <sup>[4]</sup> Si <sub>3</sub> O <sub>9</sub>	P6 <sub>3</sub> /m	6.6124(9)		9.5102(8)				83S1
Na <sub>2</sub> SiSi <sub>3</sub> O <sub>9</sub>	P2 <sub>1</sub> /n	10.875(2)	9.326(1)	19.224(7)		90.18(2) <sup>o</sup>		96F1
Benitoite <sup>2)</sup>		6.61		9.73				30Z1
Benitoite <sup>2)</sup>	$P\bar{6}$ c2	6.6410(7)		9.7597(10)				65G1, 69F1
Benitoite <sup>3)</sup>	$P\bar{6}$ c2	6.63(1)		9.73(1)				72L1
Pabsite <sup>4)</sup>	$P\bar{6}$ c2	6.706(2)		9.829(2)				65G1
BaSnSi <sub>3</sub> O <sub>9</sub>		6.724(2)		9.854(2)				65G1
BaSiSi <sub>3</sub> O <sub>9</sub>	P3	11.2469(11)		4.4851(6)				99H1
Ba <sub>3</sub> Nb <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	9.00(1)		7.89(1)				70S1
Ba <sub>3</sub> Nb <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	8.98 <sub>1</sub>		7.84 <sub>0</sub>				76C1
Ba <sub>3</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	9.00 <sub>1</sub>		7.73 <sub>4</sub>				76C1
Sr <sub>3</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	8.91 <sub>3</sub>		7.63 <sub>3</sub>				76C1
K <sub>6</sub> Ta <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	9.06 <sub>6</sub>		7.87 <sub>3</sub>				76C1
K <sub>6</sub> Nb <sub>6</sub> Si <sub>4</sub> O <sub>26</sub>	$P\bar{6}$ 2m	9.03 <sub>2</sub>		8.04 <sub>1</sub>				76C1
BaSn(Ge <sub>3-x</sub> Si <sub>x</sub> )O <sub>9</sub>								72C1
x = 0.0		6.89 <sub>4</sub>		10.23 <sub>3</sub>				
0.5		6.87 <sub>1</sub>		10.17 <sub>2</sub>				
1.0		6.83 <sub>8</sub>		10.12 <sub>0</sub>				
1.5		6.79 <sub>8</sub>		10.01 <sub>3</sub>				
2.0		6.77 <sub>5</sub>		9.97 <sub>1</sub>				
2.5		6.75 <sub>1</sub>		9.89 <sub>0</sub>				
3.0		6.72 <sub>8</sub>		9.83 <sub>8</sub>				
KTa(Ge <sub>3-x</sub> Si <sub>x</sub> )O <sub>9</sub>								72C1
x = 0.0		6.97 <sub>2</sub>		10.14 <sub>4</sub>				
0.5		6.94 <sub>1</sub>		10.09 <sub>4</sub>				
1.0		6.90 <sub>3</sub>		10.03 <sub>2</sub>				
1.5		6.87 <sub>6</sub>		9.97 <sub>0</sub>				
RbTa(Ge <sub>3-x</sub> Si <sub>x</sub> )O <sub>9</sub>								72C1
x = 0.0		7.04 <sub>1</sub>		10.11 <sub>6</sub>				
0.5		7.01 <sub>5</sub>		10.07 <sub>4</sub>				
1.0		6.98 <sub>0</sub>		10.02 <sub>4</sub>				
1.5		6.92 <sub>9</sub>		9.95 <sub>4</sub>				
TlTa(Ge <sub>3-x</sub> Si <sub>x</sub> )O <sub>9</sub>								72C1
x = 0.0		7.03 <sub>6</sub>		10.12 <sub>4</sub>				
0.5		7.01 <sub>3</sub>		10.08 <sub>8</sub>				
1.0		6.99 <sub>1</sub>		10.04 <sub>6</sub>				
Walstromite <sup>5)</sup>	$P\bar{1}$ or P1	6.734(5)	9.607(5)	6.687(5)	69°51′	102°14′	97°6.5′	65A1
Walstromite <sup>6)</sup>	$P\bar{1}$	6.73 <sub>3</sub>	9.61 <sub>6</sub>	6.72 <sub>3</sub>	69°37′	102°20′	96°54′	68D1
Margarosane <sup>7)</sup>	$P\bar{1}$	6.768(4)	9.575(4)	6.718(5)	110.36(3) <sup>o</sup>	102.98(4) <sup>o</sup>	83.02(5) <sup>o</sup>	69F2
Roebelingite <sup>8)</sup>	C2/m	13.208(4)	8.287(2)	13.089(9)		106.65(6) <sup>o</sup>		84M2
Scawtite <sup>9)</sup>	A-centered	6.61	15.22	10.98		115°24′		55M1
Scawtite <sup>9)</sup>	I2/m	10.118(3)	15.187(4)	6.626(1)		100°40(1)′		73P1
Scawtite <sup>9)</sup>	I2/m	10.22	15.42	6.70		100°29′		55M2

**Table 3** (cont.)

Silicate	Space group	Lattice parameters					Refs.
		<i>a</i> [Å]	<i>b</i> [Å]	<i>c</i> [Å]	$\alpha$	$\beta$	$\gamma$
Eudialyte <sup>10)</sup>	R3m	14.252		30.018			71G2
Eucolite <sup>11)</sup>		14.255(2)		29.915(5)			88R2
Eudialyte <sup>12)</sup>		14.250		30.083			91P1
Eudialyte <sup>13)</sup>		14.257		30.05			87R1
Eudialyte <sup>14)</sup>		14.275		29.996			91P1
Eudialyte <sup>15)</sup>	R3m	14.249		29.997			91P1
Low-Fe eudialyte <sup>16)</sup>		14.170(4)		35.35(2)			98R1
Ti-rich eudialyte <sup>17)</sup>	R3m	14.153(9)		60.72(5)			99R2
Kentbrooks site <sup>18)</sup>	R3m	14.1686(2)		30.0847(4)			98J1
Mn-Na ordered eudialyte <sup>19)</sup>	R3	14.205(7)		30.265(15)			00R1
Eudialyte <sup>25)</sup> (Barnasovite)	C2/m C2 or Cm	21.6	14.4	13.0			118° 53D1
Catapleiite <sup>20)</sup>	B2/b	23.917	20.148	7.432			147.46° 88I1
Catapleiite <sup>26)</sup>	I2/c	12.770(9)	7.419(5)	20.158(8)			90.41(4)° 74C1
Gaidonnayite <sup>21)</sup>	P2 <sub>1</sub> nb	11.740(3)	12.820(3)	6.691(1)			74C1, 85C1
Georgechaoite <sup>22)</sup>	P2 <sub>1</sub> nb	11.836(4)	12.940(6)	6.735(4)			85B1, 85G1

1)  $\text{K}_2\text{ZrSi}_3\text{O}_9$ ;2)  $\text{BaTiSi}_3\text{O}_9$ ;3)  $\text{Ba}_{0.01}\text{Na}_{0.02}\text{Ti}_{1.01}\text{Si}_{2.98}\text{O}_9$ ;4)  $\text{BaSn}_{0.77}\text{Ti}_{0.23}\text{Si}_3\text{O}_9$ ;5)  $\text{BaCa}_2\text{Si}_3\text{O}_9$ ;6)  $\text{BaCa}_2\text{Si}_3\text{O}_9$  synthetic;7)  $\text{Pb}_{2.04}\text{Ca}_{4.06}\text{Mn}_{0.17}\text{Si}_{5.87}\text{O}_{18.01}$ ;8)  $\text{Ca}_6\text{MnPb}_2(\text{Si}_3\text{O}_9)_2(\text{SO}_4)_2(\text{OH})_2 \cdot 4\text{H}_2\text{O}$ ;

9) Natural samples, composition not mentioned;

10) Composition [wt %]:  $\text{SiO}_2$  – 50.14;  $\text{TiO}_2$  – 0.46;  $\text{ZrO}_2$  – 11.83;  $\text{Al}_2\text{O}_3$  – 0.07;  $\text{Fe}_2\text{O}_3$  – 0.50;  $\text{FeO}$  – 5.32;  $\text{MgO}$  – 0.24;  $\text{CaO}$  – 11.18;  $\text{Na}_2\text{O}$  – 14.06;  $\text{K}_2\text{O}$  – 1.39;  $\text{MnO}$  – 0.60;  $\text{SrO}$  – 0.47;  $\text{R}_2\text{O}_3$  – 0.37;  $(\text{Ta},\text{Nb})_2\text{O}_5$  – 0.11;  $\text{H}_2\text{O}^-$  – 0.12;  $\text{H}_2\text{O}^+$  – 1.07;  $\text{S}$  – 0.04;  $\text{Cl}$  – 1.82;  $\text{O} = \text{Cl}_2$  – 0.41;11) Composition [wt %]:  $\text{SiO}_2$  – 45.51;  $\text{ZrO}_2$  – 11.86;  $\text{CaO}$  – 10.78;  $\text{FeO}$  – 4.52;  $\text{Fe}_2\text{O}_3$  – 0.73;  $\text{R}_2\text{O}_3$  – 5.62;  $\text{TiO}_2$  – 0.39;  $\text{Nb}_2\text{O}_5$  – 1.72;  $\text{Al}_2\text{O}_3$  – 0.44;  $\text{MnO}$  – 1.70;  $\text{MgO}$  – 1.17;  $\text{SrO}$  – 1.43;  $\text{Na}_2\text{O}$  – 12.38;  $\text{K}_2\text{O}$  – 0.59;  $\text{H}_2\text{O}$  – 0.56;  $\text{Cl}$  – 1.28;12) Composition [wt %]:  $\text{SiO}_2$  – 50.69;  $\text{ZrO}_2$  – 11.39;  $\text{TiO}_2$  – 0.55;  $\text{Nb}_2\text{O}_5$  – 0.49;  $\text{Ta}_2\text{O}_5$  – 0.03;  $\text{R}_2\text{O}_3$  – 0.37;  $\text{Al}_2\text{O}_3$  – 0.17;  $\text{Fe}_2\text{O}_3$  – 0.40;  $\text{FeO}$  – 4.99;  $\text{MnO}$  – 0.55;  $\text{CaO}$  – 10.62;  $\text{SrO}$  – 0.79;  $\text{BaO}$  – (n.d.);  $\text{Na}_2\text{O}$  – 14.49;  $\text{K}_2\text{O}$  – 2.07;  $\text{H}_2\text{O}^-$  – 0.61;  $\text{Cl}$  – 1.91;13) Composition [wt %]:  $\text{SiO}_2$  – 49.93;  $\text{ZrO}_2$  – 12.23;  $\text{TiO}_2$  – 0.78;  $\text{Nb}_2\text{O}_5$  – 0.16;  $\text{R}_2\text{O}_3$  – 0.39;  $\text{Al}_2\text{O}_3$  – 0.16;  $\text{Fe}_2\text{O}_3$  – 0.67;  $\text{FeO}$  – 4.35;  $\text{MnO}$  – 0.46;  $\text{MgO}$  – 0.03;  $\text{CaO}$  – 11.08;  $\text{SrO}$  – 0.90;  $\text{BaO}$  – 0.20;  $\text{Na}_2\text{O}$  – 15.02;  $\text{K}_2\text{O}$  – 2.13;  $\text{H}_2\text{O}^-$  – 0.50;  $\text{Cl}$  – 2.06;14) Composition [wt %]:  $\text{SiO}_2$  – 45.96;  $\text{ZrO}_2$  – 13.58;  $\text{TiO}_2$  – 0.25;  $\text{Nb}_2\text{O}_5$  – 2.48;  $\text{Ta}_2\text{O}_5$  – 0.08;  $\text{R}_2\text{O}_3$  – 4.13;  $\text{Al}_2\text{O}_3$  – 0.35;  $\text{Fe}_2\text{O}_3$  – 0.97;  $\text{FeO}$  – 5.11;  $\text{MnO}$  – 2.29;  $\text{MgO}$  – 0.58;  $\text{CaO}$  – 9.55;  $\text{SrO}$  – 0.68;  $\text{BaO}$  – (n.d.);  $\text{Na}_2\text{O}$  – 11.92;  $\text{K}_2\text{O}$  – 0.60;  $\text{H}_2\text{O}^-$  – 0.60;  $\text{Cl}$  – 0.99;15) Composition [wt %]:  $\text{SiO}_2$  – 48.46;  $\text{ZrO}_2$  – 11.61;  $\text{TiO}_2$  – 0.23;  $\text{Nb}_2\text{O}_5$  – 1.56;  $\text{Ta}_2\text{O}_5$  – 0.16;  $\text{R}_2\text{O}_3$  – 3.33;  $\text{Al}_2\text{O}_3$  – 0.31;  $\text{Fe}_2\text{O}_3$  – 0.32;  $\text{FeO}$  – 5.30;  $\text{MnO}$  – 1.98;  $\text{CaO}$  – 9.79;  $\text{SrO}$  – 0.59;  $\text{BaO}$  – (n.d.);  $\text{Na}_2\text{O}$  – 13.69;  $\text{K}_2\text{O}$  – 0.54;  $\text{H}_2\text{O}^-$  – 0.84;  $\text{Cl}$  – 1.33;16)  $\text{Na}_{16.83}\text{K}_{0.29}\text{Sr}_{0.61}\text{Ba}_{0.04}\text{Ca}_{4.33}\text{Mn}_{1.62}\text{Fe}_{0.15}\text{R}_{0.41}\text{Zr}_{2.88}\text{Ti}_{0.19}\text{Si}_{25.29}\text{Nb}_{0.35}\text{O}_{73.3}\text{Cl}_{0.61} \cdot n\text{H}_2\text{O}$ ;17)  $\text{Zr}_{3.63}\text{Ti}_{3.37}\text{Ca}_{8.5}\text{Mn}_{2.13}\text{Si}_{50.68}\text{Al}_{0.42}\text{Fe}_{0.94}\text{Na}_{34.43}\text{Sr}_{0.77}\text{Ce}_{1.13}\text{O}_{144}\text{Cl}_{0.9}(\text{OH})_{5.7} \cdot 1.5\text{H}_2\text{O}$ ;

**Table 3** (cont.)

- <sup>18)</sup>  $(\text{Na}_{14.93}\text{R}_{0.44}\text{Y}_{0.42}\text{K}_{0.30}\text{Sr}_{0.15})(\text{Ca}_{3.27}\text{Mn}_{1.78}\text{R}_{0.62}\text{Na}_{0.30})(\text{Mn}_{1.90}\text{Fe}_{0.72}\text{Al}_{0.13}\text{Mg}_{0.05})(\text{Nb}_{0.55}\text{Zr}_{0.12}\text{Ti}_{0.10})\text{Si}_{0.60}$   
 $(\text{Zr}_{2.81}\text{Hf}_{0.06}\text{Ti}_{0.13})[(\text{Si}_3\text{O}_9)_2(\text{Si}_9\text{O}_{27})_2\text{O}_2](\text{F}_{1.51}\text{Cl}_{0.27}\text{OH}_{0.22}) \cdot 2.3\text{H}_2\text{O};$   
<sup>19)</sup>  $\text{Zr}_3[(\text{Mn}_{2.1}\text{Ca}_{0.72}\text{Ce}_{0.18})(\text{Na}_{1.35}\text{Ca}_{1.05}\text{Ce}_{0.45}\text{Sr}_{0.15})][\text{Si}_3\text{O}_9]_2[\text{Si}_9\text{O}_{27}]_2[{}^{[4]}\text{Fe}_{1.51}({}^{[4]}\text{Zr}_{0.6}{}^{[6]}\text{Na}_{0.58})$   
 $({}^{[5]}\text{Ti}_{0.15}\text{Nb}_{0.12}){}^{[6]}\text{Si}_{1.9}\text{Al}_{0.1}](\text{Na}_{14}\text{Sr}_{0.4}\text{K}_{0.2})(\text{OH},\text{O})_4(\text{F},\text{Cl})_{0.7} \cdot 1.1\text{H}_2\text{O};$   
<sup>20)</sup>  $\text{Na}_2\text{ZrSi}_3\text{O}_9 \cdot 2\text{H}_2\text{O};$   
<sup>21)</sup>  $(\text{Na}_{1.72}\text{K}_{0.19})(\text{Zr}_{1.00}\text{Nb}_{0.09}\text{Ti}_{0.02})\text{Si}_{2.88}\text{O}_9 \cdot 10\text{H}_2\text{O};$   
<sup>22)</sup>  $\text{Na}_{1.02}\text{K}_{0.96}(\text{Zr}_{0.99}\text{Ti}_{0.01}\text{Fe}_{0.01})(\text{Si}_{3.01}\text{O}_9) \cdot 2.14\text{H}_2\text{O};$   
<sup>23)</sup>  $(\text{Na}_{0.85}\text{K}_{0.09}\text{Ca}_{0.06})(\text{Ca}_{4.31}\text{Fe}_{0.56}\text{Mg}_{0.15})\text{Zr}_{4.22}(\text{Si}_{15.44}\text{Al}_{0.32})\text{O}_{40}(\text{OH})_{10.70} \cdot 7.92\text{H}_2\text{O};$   
<sup>24)</sup>  $(\text{Ca}_{0.98}\text{Na}_{0.04})\text{Zr}_{1.00}(\text{Si}_{2.94}\text{Al}_{0.04})\text{O}_9 \cdot 2.01\text{H}_2\text{O};$   
<sup>25)</sup>  $(\text{Na}_{5.45}\text{Ca}_{3.06}\text{Sr}_{0.38}\text{R}_{0.28})(\text{Fe}_{1.15}\text{Mn}_{0.82})(\text{Zr}_{1.62}\text{Nb}_{0.30}\text{Ti}_{0.06})\text{Si}_{12}(\text{O}_{36.33}\text{Cl}_{0.67});$   
<sup>26)</sup> Natural sample, Mont St. Hilaire, Quebec.

**Table 4.** Hyperfine parameters determined by <sup>57</sup>Fe NGR method [91P1].

	<i>T</i> [K]	Site	$\delta^{1)}$ [mm/s]	$\Delta Q$ [mm/s]	<i>DH</i> [mm/s]	$DH_L^{2)}$ [mm/s]	$DH_H^{2)}$ [mm/s]	<i>A</i> [%]
Eudialyte <sup>12)</sup>	77	Fe1 <sup>2+</sup>	1.195 <sub>7</sub>	0.375 <sub>7</sub>		0.429 <sub>6</sub>	0.640 <sub>7</sub>	76 <sub>1</sub>
		Fe2 <sup>2+</sup>	1.45 <sub>2</sub>	2.72 <sub>2</sub>	0.55 <sub>2</sub>			12 <sub>1</sub>
		Fe <sup>3+</sup>	0.69	0.53 <sub>2</sub>	0.65 <sub>3</sub>			12 <sub>1</sub>
	300	Fe1 <sup>2+</sup>	1.079 <sub>7</sub>	0.345 <sub>8</sub>		0.39 <sub>1</sub>	0.50 <sub>1</sub>	81 <sub>4</sub>
		Fe2 <sup>2+</sup>	1.34 <sub>1</sub>	2.46 <sub>1</sub>	0.46 <sub>1</sub>			8 <sub>1</sub>
		Fe <sup>3+</sup>	0.58 <sub>3</sub>	0.53 <sub>3</sub>	0.60 <sub>3</sub>			11 <sub>1</sub>

<sup>1)</sup> Relative to  $\alpha$ -Fe; <sup>2)</sup> H and L are the high-velocity and low-velocity components of the Fe1<sup>2+</sup> doublet;

<sup>12)</sup> See Table 3 for composition

**Table 5.** Data obtained by NMR studies.

Sample	Nucleus	Site	$\eta$	$e^2qQ/h$ [MHz]	$\delta^{1)}$ [ppm]	Relative intensity	Refs.
K <sub>2</sub> Si <sub>4</sub> O <sub>9</sub>	<sup>17</sup> O	O1	0.35(5)	4.45(5)	62.5(1)	1	94X1
		O2	0.20(5)	4.90(5)	97(1)	2	
K <sub>2</sub> Si <sub>4</sub> O <sub>9</sub>	<sup>17</sup> O	BO <sup>2)</sup>	0	4.9(2)	52(4)	7	94X1
glass		NBO <sup>3)</sup>	0	2.3(1)	76(2)	2	
Na <sub>2</sub> Si <sub>4</sub> O <sub>9</sub>	<sup>17</sup> O	BO	0	5.0(2)	50(4)	7	94X1
glass		NBO	0	2.3(1)	36(3)	2	
Na <sub>2</sub> Si <sub>4</sub> O <sub>9</sub>	<sup>29</sup> Si	Q <sup>3</sup>			−92.6 <sup>4)</sup>		91X1
glass (1atm)		Q <sup>4</sup>			−105.5 <sup>4)</sup>		
BaTiSi <sub>3</sub> O <sub>9</sub>	<sup>29</sup> Si	Si(2Ti)			−94.2		84M1
BaTiSi <sub>3</sub> O <sub>9</sub>	<sup>29</sup> Si	Si(2Ti)			−94.3		97B1
K <sub>2</sub> TiSi <sub>3</sub> O <sub>9</sub>	<sup>29</sup> Si	Si(2Ti)			−94.4		97B1

<sup>1)</sup> Relative to deionized H<sub>2</sub>O; <sup>2)</sup> BO-bridging oxygen atom; <sup>3)</sup> NBO-nonbridging oxygen atom;

<sup>4)</sup> Relative to tetrametylsilane.



**Table 6.** Refractive indices.

Sample	$n_\alpha$	$n_\beta$	$n_\gamma$	$2V$		Refs.
				exp.	calc.	
Benitoite <sup>3)</sup>	1.756(1) ( $\omega$ )		1.800(1) ( $\epsilon$ )			uniaxial, positive 72L1
BaTiSi <sub>3</sub> O <sub>9</sub>	1.757		1.804			uniaxial, positive 65G1
Pabsite <sup>4)</sup>	1.685(2) ( $\omega$ )		1.674(2) ( $\epsilon$ )			uniaxial, negative 65G1
Scawtite <sup>9)</sup>	1.595	1.605	1.662	+75°		55M1
Walstromite <sup>5)</sup>	1.668	1.684	1.685	30°		biaxial negative 65A2
Eudialyte <sup>11)</sup>	1.624...1.626		1.620...1.622			88R2
Eudialyte- yellowish- green <sup>25)</sup>	1.633	1.639	1.639	13°...17°		biaxial negative 53D1
(Barnasovite)						
Eudialyte- reddish-brown <sup>25)</sup>	1.624	1.628	1.628	12°		biaxial negative 53D1
(Barnasovite)						
Kentbrooksite <sup>18)</sup>	1.628(2) ( $\omega$ )		1.623(2) ( $\epsilon$ )			uniaxial, negative 98J1
Calcium catapleiite <sup>24)</sup>	1.603		1.639			uniaxial, positive 64P1
Catapleiite <sup>26)</sup>	1.588(1)	1.591(1)	1.624(1)	40(1)°	34°	74C1
Gaidonnayite <sup>21)</sup>	1.573(1)	1.592(1)	1.599(1)	121(1)°	119.5°	biaxial 74C1
Georgechaoite <sup>22)</sup>	1.578(1)	1.597(1)	1.606(1)	67°	68°	biaxial negative 85B1, 85G1
Loudounite <sup>23)</sup>	1.536(4)		1.554(4)			biaxial 83D1

For footnotes (compositions) see Table 3.