Tables and figures

Table 1. Silicates from groups VIIIC11-VIIIC13 [91N1].

Silicate	Composition	Group
Hyalotekite	$Ba_2Ca_2Pb_2(B,Si,Al)_2(Si,Be)_{10}O_{28}F$	VIIIC11
Hilairite	$Na_2ZrSi_3O_9 \cdot 3H_2O$	VIIIC12
Calciohilairite	$CaZrSi_3O_9 \cdot 3H_2O$	VIIIC12
Komkovite	$BaZrSi_3O_9 \cdot 3H_2O$	[91S1]
Clinophosinaite	$Na_3Ca(SiO_3)(PO_4)$	VIIIC13
Phosinaite	$Na_{11}(Na,Ca)_2Ca_2Ce(SiO_3)_4(PO_4)_4$	VIIIC13
Nagelschmidtite	$Ca_7(SiO_4)_2(PO_4)_2$	VIIIC13

Table 2. Atomic sites and thermal parameters.

a) Hyalotekite[1)] [82M1].

$I\bar{1}$ refinement					I2/m refinement				
Atom	Multiplicity	*x*	*y*	*z*	*x*	*y*	*z*	Atom	Equipoint
Pb1	0.290(7)	0.1543(2)	0.1726(2)	0.0043(2)	0.173	0.183	0.008	Pb	
Ba1	0.710	0.1878(4)	0.1924(3)	0.0109(2)					
Pb2	0.291(7)	0.8460(3)	0.1719(2)	0.0046(2)	0.827	0.183	0.008	Pb	$\bar{x}$, *y*, *z*
Ba2	0.709	0.8097(3)	0.1927(2)	0.0105(2)					
Ca	1.000	0.9996(1)	0.0031(1)	0.2289(1)	0	0.002	0.229	Ca	
Si1	0.81(1)	0.3172(2)	0.4995(2)	0.0001(2)	0.317	½	0	Si1	
Be	0.19								
Si2	1.00	0.1936(2)	0.5267(2)	0.2482(2)	0.194	0.527	0.248	Si2	
Si3	1.00	0.8061(2)	0.5274(2)	0.2480(2)	0.806	0.527	0.248	Si2	$\bar{x}$, *y*, *z*
Si4	1.00	0.9994(2)	0.3222(2)	0.2626(2)	0	0.324	0.263	Si4	
Si5	1.00	0.0002(2)	0.7224(1)	0.2825(2)	0	0.724	0.283	Si5	
B	1.00	0.4999(7)	0.3367(6)	0.0305(7)	½	0.337	0.031	B	
O1	1.00	0.8845(4)	0.6385(4)	0.3068(4)	0.884	0.640	0.308	O1	
O2	1.00	0.8833(5)	0.4043(4)	0.2314(5)	0.882	0.400	0.228	O2	
O3	1.00	0.1159(5)	0.4031(5)	0.2325(5)	0.118	0.400	0.228	O2	$\bar{x}$, *y*, *z*
O4	1.00	0.1158(4)	0.6385(4)	0.3062(4)	0.116	0.640	0.308	O1	$\bar{x}$, *y*, *z*
O5	1.00	0.2328(4)	0.5685(4)	0.1035(4)	0.232	0.568	0.102	O5	
O6	1.00	0.7666(4)	0.5700(4)	0.1031(4)	0.768	0.568	0.102	O5	$\bar{x}$, *y*, *z*
O7	1.00	0.6078(4)	0.4054(4)	0.0791(4)	0.609	0.403	0.079	O7	
O8	1.00	0.3935(4)	0.4044(4)	0.0796(4)	0.391	0.403	0.079	O7	$\bar{x}$, *y*, *z*
O9	1.00	0.5020(5)	0.2126(4)	0.0868(5)	½	0.216	0.084	O9	
O10	1.00	0.4994(4)	0.6660(4)	0.1133(4)	½	0.664	0.110	O10	
O11	1.00	0.0007(4)	0.7836(4)	0.1428(4)	0	0.781	0.143	O11	
O12	1.00	0.9988(4)	0.2082(4)	0.1657(4)	0	0.210	0.167	O12	
O13	1.00	0.3020(4)	0.5075(4)	0.3424(4)	0.301	0.509	0.342	O13	
O14	1.00	0.6973(4)	0.5083(4)	0.3422(4)	0.699	0.509	0.342	O13	$\bar{x}$, *y*, *z*
F	1.00	0.0000	0.0000	0.0000	0	0	0	F	

Table 2 (cont.)

b) R analog of hilairite[6], having orthorhombic structure, space group R32 [92R1].

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
Na1	0	0	0.1955(4)	2.2(1)
Na2	0.359(1)	0	0.5	4.1(2)
M1	0	0	0	0.68(3)
M2	0.3333	0.6667	0.1663(1)	0.66(2)
Si	0.4216(2)	0.4094(2)	0.2472(1)	0.52(3)
O1	0.096(1)	0.176(1)	0.0795(3)	1.0(1)
O2	0.104(1)	0.207(1)	0.5732(3)	1.2(1)
O3	0.659(1)	0	0	0.9(1)
O4	0.641(1)	0	0.5	1.3(2)
H_2O	0.501(1)	0.140(1)	0.0593(4)	1.7(1)
H1	0.53(2)	0.43(2)	0.04(1)	
H2	0.48(2)	0.68(2)	0.00(1)	

M1 = $(Zr_{0.7}Nb_{0.1}Ti_{0.2})$; M2 = $(Y_{0.8}R_{0.2})$; Na2 = $Na_{2.4}K_{0.6}$.

c) Komkovite[7], having orthorhombic structure, space group R32 [91S1].

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
Ba	0	0	0.2565(7)	4.0(1)
Zr1	0	0	0	2.3(2)
Zr2	0	0	0.5	0.1(1)
Si	0.343(2)	0.256(2)	0.427(2)	1.0(3)
O1	0.178(5)	0.095(5)	0.417(6)	1.8(5)
O2	0.479(5)	0.234(5)	0.404(6)	2.3(5)
O3	0.644(6)	0	0	2.4(5)
O4	0.748(4)	0	0.5	1.3(5)
O5(H_2O)[a]	0.281(7)	0.002(7)	0.283(7)	3.0(6)

[a] H_2O molecules randomly occupy 81(9) % of the O5 positions.

d) Phosinaite[10], having orthorhombic structure, space group $P2_12_12$ [81K2].

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
Ce	0	0.5	0.1394(2)	0.82(4)
Ca	0.0205(9)	0.2506(5)	0.5026(3)	1.99(8)
Ca+Na	0.0183(14)	0.2659(4)	0.1876(6)	3.85(15)
Si1	0.3104(9)	0.3889(4)	0.3203(6)	2.19(13)
Si2	0.2552(9)	0.5885(4)	0.3642(5)	1.85(10)
P1	0.2342(9)	–0.1179(3)	0.3061(4)	1.49(10)
P2	0.2690(10)	0.1250(4)	0.0250(5)	1.99(11)
Na1	0	0	0.451(1)	3.58(28)
Na2	0	0	0.160(1)	4.43(32)
Na3	0.5	0.5	0.127(1)	3.06(25)
Na4	0.5	0	0.172(1)	3.25(26)
Na5	0.5	0	0.458(1)	3.19(27)
Na6	0.539(2)	0.259(1)	0.183(1)	4.37(26)
Na7	0.265(1)	0.141(1)	0.330(1)	1.93(16)
Na8	0.226(2)	-0.150(1)	0.002(1)	5.41(32)

Table 2 (cont.)

Atom	*x*	*y*	*z*	B_{eq} [Å^2]
O1	0.256(2)	0.405(1)	0.196(1)	2.98(31)
O2	0.236(2)	0.297(1)	0.374(1)	2.88(29)
O3	0.537(3)	0.385(1)	0.326(1)	5.78(50)
O4	0.249(2)	0.479(1)	0.359(1)	3.03(21)
O5	0.787(2)	0.358(1)	0.471(1)	3.02(33)
O6	0.873(2)	0.396(1)	0.268(1)	4.18(40)
O7	0.585(2)	0.159(1)	0.353(1)	2.81(31)
O8	0.792(2)	0.149(1)	0.186(1)	3.11(33)
O9	0.756(2)	0.014(1)	0.314(1)	2.82(29)
O10	0.938(2)	0.150(1)	0.370(1)	3.05(34)
O11	0.955(3)	0.356(1)	0.035(1)	4.94(46)
O12	0.283(3)	0.158(1)	0.145(1)	4.11(38)
O13	0.743(3)	-0.023(1)	0.014(1)	5.00(43)
O14	0.602(3)	0.339(1)	0.027(2)	6.51(55)

Table 3. Crystal structures and lattice parameters, at RT.

Silicate	Space group	Lattice parameters						Refs.
		a [Å]	*b* [Å]	*c* [Å]	α	β	γ	
Hyalotekite[1)]	$I\bar{1}$	11.310(2)	10.955(2)	10.317(3)	90.43(2)°	90.02(2)°	90.16(2)°	82M1
Hilairite[2)]	R32	10.556(1)		15.855(2)				81I1
Hilairite[3)]	R32	10.556(1)		15.851(2)				74C1
Hilairite[4)]	R32	8.064			81.64°			88I1
Calciohilairite[5)]	R32	20.870(4)		16.002(4)				88B1
R-analog of hilairite[6)]	R32	10.825(5)		15.809(4)				92R1
Komkovite[7)]	R32	10.526(6)		15.736(9)			120°	91S1
Clinophosinaite[8)]	P2/c	7.303	12.201	14.715		91°56'		81K1
Clinophosinaite[9)]	P2/c	7.30	12.21	14.81		≅ 92°		81K1
Phosinaite[10)]	$P2_12_12$	7.234(3)	14.670(4)	12.231(4)				81K2

1) $(K_{0.280}B_{1.942}Pb_{1.669}Ca_{2.068}Na_{0.082})(Mn^{2+}_{0.061}Mg_{0.033}Cu^{2+}_{0.016}Fe^{3+}_{0.012}Al_{0.052}Si_{0.191}B_{1.598})(Si_{1.555}Be_{0.445})Si_8O_{28}(F_{0.775}Cl_{0.025})$;
2) $Na_2ZrSi_3O_9 \cdot 3H_2O$;
3) $Na_{1.85}K_{0.05}Ca_{0.02}Zr_{1.03}Si_{2.99}O_9 \cdot 3.21H_2O$;
4) $Na_2ZrSi_3O_9 \cdot 3H_2O$;
5) $(Ca_{0.89}Zr_{0.15}Na_{0.03}Cu_{0.03})(Zr_{0.99}Fe_{0.01})(Si_{2.82}Al_{0.09})O_9 \cdot 3.3H_2O$;
6) $Na_2(Na_{2.4}K_{0.6})[(Zr_{0.7}Ti_{0.2}Nb_{0.1})(Y_{0.8}R_{0.2})(Si_6O_{18})] \cdot 6H_2O$;
7) $BaZrSi_3O_9 \cdot 2.4H_2O$;
8) Composition [wt %]: P_2O_5-25.53; SiO_2-20.1; R_2O_3-0.18; CaO-15.65; SrO-3.08; MnO-0.60; Na_2O-32.55; K_2O-0.09;
9) Composition [wt %]: P_2O_5-25.5; SiO_2-20.1; R_2O_3-0.44; CaO-16.45; SrO-1.91; MnO-0.54; Na_2O-32.7; K_2O-0.05;
10) $Na_{11}(Na,Ca)_2Ca_2Ce_{0.67}[Si_4O_{12}][PO_4]$;
11) $(Ca_{3.78}Na_{0.06}K_{0.06})(Si_{1.58}P_{0.40})O_8$.

Table 4. Refractive indices.

Silicate	n_α	n_β	n_γ	$2V$°		Refs.
Hilairite[3)]	1.596(1) (ε)		1.609(1) (ω)		uniaxial, negative	74C1
Calciohilairite[5)]	1.619(1) (ε)		1.622(1) (ω)		uniaxial, negative	88B1
Clinophosinaite[8)]	1.557	1.561	1.567	80°	biaxial, positive	81K1
Clinophosinaite[9)]	1.566	1.559	1.563	75°	biaxial, positive	81K1
Nagelschmidtite[11,a)] (transparent)	1.680		1.698	≅ 0		77G1, 78F1
Nagelschmidtite[11,a)] (slightly yellow)	1.638		1.652			77G1, 78F1
Nagelschmidtite (synthetic)	1.642…1.680	1.642…1.675	1.661…1.690	0°…20°		77G1, 78F1

[a)] Usually uniaxial positive, rarely biaxial positive with $2V^o \cong 0$.

For other footnotes see Table 3.