Tables and figures

Table 1. Xonotlite group of silicates [91N1].

Silicate	Composition	Group
Xonotlite	$Ca_6Si_6O_{17}(OH)_2$	VIIID11
Armstrongite	$CaZrSi_6O_{15}\cdot 2.5H_2O$	VIIID11
Dalyite	$K_2ZrSi_6O_{15}$	VIIID11
Davanite	$K_2TiSi_6O_{15}$	VIIID11
Tinaksite	$K_2Na(Ca,Mn)_2TiSi_7O_{19}(OH)$	VIIID11
Tokkoite	$K_2Ca_4Si_7O_{17}(O,OH,F)_4$	VIIID11
Elpidite	$Na_2ZrSi_6O_{15}\cdot 3H_2O$	VIIID11
Sazhinite-Ce	$Na_2CeSi_6O_{14}(OH)\cdot 6H_2O$	VIIID11
Yuksporite	$(Sr,Ba)_2K_4(Ca,Na)_{14}(\square,Mn,Fe)\{(Ti,Nb)_4(O,OH)_4[Si_6O_{17}]_2[Si_2O_7]_3\}(H_2O,OH)_n$	VIIID11
$K_2CeSi_6O_{15}$		
$K_3NdSi_6O_{15}\cdot 2H_2O$		
$K_3NdSi_6O_{15}$		
$Na_3NdSi_6O_{15}\cdot 2H_2O$		
$Na_3YSi_6O_{15}$		
$Na_2LiYSi_6O_{15}$		
$Na_2Mg_2Si_6O_{15}$	See also Chap. 8.1.4.7	
$NaLiTiSi_6O_{15}$		
$NaLiSnSi_6O_{15}$		
$Li_2ZrSi_6O_{15}$		
$Cs_2TiSi_6O_{15}$		

Table 2. Atomic sites and thermal parameters.

a) Xonotlite M2a2bc (space group $P\bar{1}$); Ma2bc (space group P2/a); Ma2b2c (space group A2/a) and M2a2b2c (space group $A\bar{1}$) [01H1, 79K1]. (For composition see Table 3).

	M2a2bc			Ma2bc			Ma2b2c			M2a2b2c		
Atom	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*	*x*	*y*	*z*
Ca1	0.5000	0.5000	0.5000	0.2500	0.3750	0.5000	0.2730	0.8755	0.7523	0.5046(4)	0.0016(5)	0.7523(3)
Ca2	0.5000	0.0000	0.5000	0.2500	0.8750	0.5000						
Ca3	0.1335	0.1645	0.3368	0.0668	0.1311	0.3368	0.0668	0.1311	0.6684	0.1335(1)	0.1645(2)	0.6684(1)
Ca4	0.1385	0.6537	0.3414	0.0693	0.6191	0.3414	0.0693	0.6191	0.6707	0.1385(1)	0.6537(1)	0.6707(1)
Si1	0.2118	0.2170	0.7682	0.1059	0.1641	0.7682	0.1059	0.1641	0.3841	0.2118(2)	0.2170(2)	0.3841(1)
Si2	0.2118	0.6389	0.7686	0.1059	0.5860	0.7686	0.1059	0.5860	0.3843	0.2118(2)	0.6389(2)	0.3843(1)
Si3	0.3182	0.9547	0.0562	0.1591	0.8752	0.0562	0.1591	0.8752	0.5281	0.3182(1)	0.9547(2)	0.5281(1)
O1	0.5000	0.0000	0.0000	0.2500	0.8750	0.0000	0.2500	0.8750	0.0000	0.5000	0.0000	0.0000
O2	0.2190	0.4303	0.8422	0.1095	0.3756	0.8422	0.1095	0.3756	0.4211	0.2190(4)	0.4303(5)	0.4211(2)
O3	0.3512	0.7179	0.6192	0.1756	0.6301	0.6192	0.1756	0.6301	0.3096	0.3512(4)	0.7179(5)	0.3096(2)
O4	0.3434	0.2059	0.6174	0.1717	0.1201	0.6174	0.1717	0.1201	0.3087	0.3434(4)	0.2059(5)	0.3087(2)
O5	0.2297	0.1116	0.9720	0.1149	0.0542	0.9720	0.1149	0.0542	0.4860	0.2297(4)	0.1116(5)	0.4860(2)
O6	0.2294	0.7538	0.9716	0.1147	0.6965	0.9716	0.1147	0.6965	0.4858	0.2294(4)	0.7538(5)	0.4852(2)
O7	0.0424	0.6382	0.6652	0.0212	0.6276	0.6652	0.0212	0.6276	0.3326	0.0424(4)	0.6382(5)	0.3326(2)
O8	0.0463	0.1339	0.6740	0.0215	0.1223	0.6740	0.0215	0.1223	0.3370	0.0463(4)	0.1339(5)	0.3370(2)
O9	0.2988	0.9506	0.2780	0.1494	0.8759	0.2780	0.1494	0.8759	0.6390	0.2988(4)	0.9506(5)	0.6390(2)
O10	0.2977	0.4481	0.2694	0.1489	0.3737	0.2694	0.1489	0.3737	0.6347	0.2977(4)	0.4481(5)	0.6347(3)

Table 2 (cont.)

b) Synthetic $K_2TiSi_6O_{15}$, having monoclinic structure, space group $P2_1$ [01Z1].

Atom	*x*	*y*	*z*	B_{eq} [Å^2]·10^3
Ti1	0.7564(1)	0.2495(1)	0.2487(1)	8.2(2)
Si1	0.0069(2)	0.6780(1)	0.3311(2)	8.9(2)
Si2	0.4502(2)	0.6661(1)	0.4433(2)	8.5(2)
Si3	0.6714(2)	0.5090(1)	0.2924(2)	8.5(2)
Si4	0.0127(2)	0.8423(1)	0.0441(2)	8.9(2)
Si5	0.5439(2)	0.3340(1)	–0.1641(2)	9.0(2)
Si6	0.3061(2)	0.5069(1)	–0.0688(2)	8.2(2)
K1	0.1943(2)	0.4064(1)	0.4206(2)	29.6(3)
K2	0.2022(2)	0.1081(1)	0.1500(2)	26.7(3)
O1	0.2352(5)	0.8825(3)	0.1629(5)	14.1(7)
O2	0.5375(5)	0.7588(3)	0.3409(5)	13.1(6)
O3	0.7333(5)	0.3911(3)	0.3346(5)	15.0(7)
O4	0.2064(5)	0.6088(3)	–0.1702(5)	13.3(6)
O5	0.5585(5)	0.2779(3)	0.0241(5)	12.7(7)
O6	0.0235(5)	0.7927(3)	–0.1431(5)	12.5(7)
O7	–0.1330(5)	0.5755(3)	0.2778(5)	16.0(7)
O8	0.5889(5)	0.5620(3)	0.4533(5)	12.9(7)
O9	–0.1358(5)	0.9435(2)	0.0014(5)	12.6(6)
O10	0.4997(6)	0.5284(3)	0.1028(5)	16.5(7)
O11	–0.0757(5)	0.7604(3)	0.1649(5)	14.2(6)
O12	0.3861(5)	0.4318(3)	–0.2082(5)	12.2(6)
O13	0.2265(5)	0.6356(3)	0.3191(5)	14.9(7)
O14	0.4519(5)	0.7006(3)	0.6437(5)	12.3(6)
O15	0.0245(5)	0.7260(3)	0.5265(5)	13.2(7)

Table 3. Crystal structures and lattice parameters.

Silicate	*T* [K]	Space group	Lattice parameters				Refs.
			a [Å]	*b* [Å]	*c* [Å]	α, β, γ	
Xonotlite[1)] (pseudo-cell)	RT	C2/m	16.53	3.66	7.04	$\alpha = 90^o$ $\beta = 90^o$ $\gamma = 90^o$	55M1
Xonotlite[2)] (pseudo-cell)	RT	C2/m	17.029(1)	3.676(0)	7.005(1)	$\alpha = 90^o$ $\beta = 90.33(2)^o$ $\gamma = 90^o$	77K2
Xonotlite[3)] (pseudo-cell)	RT	C2/m	17.03	3.678	7.003	$\beta = 90.32^o$	81E1
Xonotlite[4)] (cell of hypothetical protoxonotlite)	RT	C2/m	17.031(4)	7.682(1)	7.012(2)	$\alpha = 90^o$ $\beta = 90.37(2)^o$ $\gamma = 90^o$	79K1

Table 3 (cont.)

Silicate	*T* [K]	Space group	Lattice parameters				Refs.
			a [Å]	*b* [Å]	*c* [Å]	α, β, γ	
Xonotlite[4] M2a2b2c	RT	A $\bar{1}$	8.712(2)	7.363(2)	14.023(4)	α= 89.99(2)° β= 90.36(2)° γ= 102.18(2)°	79K1
Xonotlite M2a2bc	RT	P $\bar{1}$	8.712	7.363	7.012	α= 89.99° β= 90.36° γ= 102.18°	01H1
Xonotlite Ma2bc	RT	P2/a	17.032	7.363	7.012	α= 90.0° β= 90.36° γ= 90.0°	01H1
Xonotlite Ma2b2c	RT	A2/a	17.032	7.363	14.023	α= 90.0° β= 90.36° γ= 90.0°	01H1
Armstrongite[5]	RT	C2	14.04	14.16	7.81	β= 109°33’	78K1
Dalyite[6]	RT	P $\bar{1}$	7.00	7.51	7.73	α= 106° β= 113.5° γ= 80.5°	80S1
Davanite[7]	RT	tricl.	7.14(3)	7.53(3)	6.93(2)	α= 103.35° β= 114.48° γ= 93.80°	84L1
Davanite[8]	RT		7.250(2)	7.474(2)	6.909(3)	α= 105.59(5)° β= 112.81(5)° γ= 99.28(5)°	87R1
Davanite[9]	RT		7.26(1)	7.51(2)	6.92(1)	α= 105.6(2)° β= 112.9(1)° γ= 99.4(2)°	87R1
Davanite[10]	RT		7.272(3)	7.480(4)	6.910(2)	α= 105.55(3)° β= 112.83(3)° γ= 99.42(3)°	87R1
$K_2TiSi_6O_{15}$	RT	$P2_1$	6.916(3)	12.812(3)	7.661(2)	β= 106.25(4)°	01Z1
Tinaksite[11]	RT	P $\bar{1}$	10.377(3)	12.166(3)	7.059(1)	α= 90.91(1)° β= 99.3(1)° γ= 92.76(3)°	80B1
Tinaksite[12]	RT	P1 or P $\bar{1}$	10.35(5)	12.17(5)	7.05(3)	α= 91°00(30)’ β= 99°20(30)’ γ= 92°30(30)’	65R1, 71P1
Tokkoite[13]	RT	tricl.	10.37(3)	25.39(5)	7.27(1)	α= 91.67(1)° β= 100.66(1)° γ= 92.09(1)°	86L1
Tokkoite[13]	RT	P $\bar{1}$	10.438(3)	12.511(3)	7.112(2)	α= 89.92(2)° β= 99.75(2)° γ= 92.89(2)°	89R1
Elpidite[14]	RT	Pbcm	7.14(2)	14.68(1)	14.65(1)		73C1
Elpidite[15]	RT		7.14	14.68	14.58		67C1

Table 3 (cont.)

Silicate	*T* [K]	Space group	Lattice parameters				Refs.
			a [Å]	*b* [Å]	*c* [Å]	α, β, γ	
Sazhinite[16)]	RT	Pmnm, Pmm2, P222	7.35(3)	7.50(3)	15.62(6)		74E1
Sazhinite[17)]	RT	Pmm2	7.50(3)	15.62(6)	7.35(3)		80S1
Yuksporite[18)]	RT	$P2_1/m$	7.126(3)	24.913(6)	17.075(7)	$\beta = 101.89(3)^o$	04K1
Yuksporite[19)]	RT	Orth.	24.869(8)	16.756(6)	7.057(3)		85K2
Yuksporite[20)]	RT	triclinic	16.50(5)	25.21(4)	21.11(3)	$\alpha = 100.4(3)^o$ $\beta = 110.0(4)^o$ $\gamma = 90.4(1)^o$	03M1
$K_2CeSi_6O_{15}$	RT	monocl.	13.059(6)	11.854(4)	8.698(2)	$\beta = 90^o9'$	77K1
$K_3NdSi_6O_{15}$	RT	Pbam	7.276	16.011	14.984		77P1
α-$K_3NdSi_6O_{15}\cdot 2H_2O$	RT	Pbam	16.008(2)	15.004(2)	7.2794(7)		00H1
α'-$K_3NdSi_6O_{15}\cdot 2H_2O$	RT	Pnnm	16.008(2)	15.004(2)	14.56		00H1
β-$K_3NdSi_6O_{15}$	RT	$Bb2_1m$	14.370(2)	15.518(2)	14.265(2)		00H2
$Na_3NdSi_6O_{15}\cdot 2H_2O$	RT	Cmm2	7.385(2)	30.831(7)	7.1168(3)		97H2
α-$Na_3YSi_6O_{15}$	RT	Ibmm	10.468(2)	15.2467(3)	8.3855(6)		95H1
$Cs_2TiSi_6O_{15}$	RT	C2/c	13.386(5)	7.423(3)	15.134(5)	$\beta = 107.71(3)^o$	97G1

1) Natural sample;
2) San Francisco, Ca natural sample;
3) Composition not mentioned;
4) Composition [wt %]: SiO_2 – 49.99; Fe_2O_3 – 0.48; MnO – 0.16; CaO – 46.19; Na_2O – 0.17; K_2O – 0.02; $H_2O(+)$ – 2.95; $H_2O(-)$ – 0.10; natural sample, Chiba, Japan;
5) $CaZr(Si_6O_{15})\cdot 2.5H_2O$;
6) $K_2ZrSi_6O_{15}$;
7) $K_{1.98}Ti_{1.01}Si_{6.01}O_{15.03}$ with not determined Mg, Fe and Na content;
8) $K_2TiSi_6O_{15}$ synthetic; lattice parameters recalculated from data of [83G1];
9) Natural sample, Murmanskii, lattice parameters recalculated from data of [84L1];
10) Natural sample, Smoky Butte, lattice parameters recalculated from data of [86W1];
11) $Ca_2K_2NaTiO[Si_7O_{18}(OH)]$;
12) $NaK_2(Ca,Fe^{2+})_2(Ti,Fe^{3+})Si_7O_{19}(OH)$;
13) $K_{1.85}(Ca_{0.87}Ti_{0.13})(Ca_{0.85}Na_{0.15})(Ca_{1.71}Fe_{0.15}Mn_{0.08}Mg_{0.06}[Si_7O_{18}(OH)](F_{0.61}OH_{0.39})$;
14) $Na_2ZrSi_6O_{15}\cdot 3H_2O$;
15) Natural sample, Mt St Hilaire, Canada;
16) $Na_3CeSi_6O_{15}\cdot 6H_2O$;
17) $Na_2HCeSi_6O_{15}\cdot 1.5H_2O$;
18) $Sr_{1.40}Ba_{0.65}K_{3.75}Ca_{8.50}Na_{5.50}Mn_{0.15}Fe_{0.10}\{(Ti,Nb)_4(O,OH)_4[Si_6O_{17}]_2(Si_2O_7)_3\}(H_2O,OH)_3$;
19) $(Na_{3.48}K_{3.67}Ba_{1.58})(Ca_{9.47}Sr_{1.59})(Ti_{3.88}Mn_{0.11}Fe_{0.26})Si_{17.96}Al_{0.04}O_{60.39}F_{4.51}Cl_{0.63}\cdot nH_2O$;
20) $(Ca,K,Na,Sr,Ba)_{48}[(Ti,Nb,Fe,Mn)_{12}(OH)_{12}Si_{48}O_{144}]$ $(F,OH,Cl)_{14}$; in original paper denoted eveslogite.

Table 4. Data obtained by NMR studies.

Sample	Nucleus	Site	Chemical[1] shift [ppm]	Related area (%)		Refs.
				Natural[2]	Synthetic[3]	
Xonotlite	^{29}Si	Q^2	–86.6		67	87E1
		Q^3	–97.8		33	
	^{29}Si	Q^1	–79.6	0	3	98N1
		Q^2_H	–86.3	38	37	
		Q^2_L	–87.1	30	30	
		Q^3	–97.5	32	30	
Xonotlite	^{1}H	Ca-OH	2.19	73	65	98N1
		Si-OH	1.86	18	24	
		molecular water	5.26	9	11	

1) The ^{29}Si chemical shift of 3-(trimethylsilyl)-propane sulfonic acid sodium salt (DSS) was 1.534 ppm and the ^{1}H shift of water was 4.877 ppm;
2) Composition [wt %]: SiO_2 – 50.80; Al_2O_3 – 0.38; Fe_2O_3- 0.05; CaO – 44.70; Na_2O – 0.78; K_2O – 0.02; MnO – 0.01, Ig. loss – 3.18;
3) Hydrothermally synthesized at 250°C for 60 h from CaO and silica acid [98N1].

Table 5. Activation energies and conductivities. Electrode material: Pt and Ag.

Sample	σ	Activation energy, E_a [eV]		σ(873 K)·10^5 [Ω^{-1}cm^{-1}]	Ref.
		High temperature	Low temperature		
α_{II}-$K_3NdSi_6O_{15}$	σ_{11}(Pt)	1.1	0.3	3.4	00H1
	σ_{22}(Ag)		0.6	5.8	
	σ_{22}(Pt)	1.3	0.7	6.9	
	σ_{33}(Pt)	1.3	0.8	17	

Table 6. Refractive indices.

Silicate	n_α	n_β	n_γ	$2V^o$		Refs.
Oyelite[1]	1.602	1.606	1.613			84K1, 86D1
Davanite[2]	1.623(2)		1.668(2)		Optically biaxial positive	84L1
Tinaksite[3]	1.593	1.621	1.666	74°…78°	Optically biaxial positive	65R1, 71P1
Tokkoite[4]	1.570(2)		1.577(2)	38(5)°		86L1
Sazhinite[5]	1.525(2)	1.528(2)	1.544(2)	47°	Optically biaxial positive	74E1
$K_2ZrSi_3O_9·H_2O$	1.596	1.610	1.619	80°	Optically biaxial negative	81I1

1) Composition: 0.99 CaO·0.10 B_2O_3·0.80 SiO_2·1.25 H_2O (see chapter 8.1.4.5);
2) $K_{1.98}Ti_{1.01}Si_{6.01}O_{15.3}$ with not determined Mg, Fe and Na content; 3) $NaK_2(Ca,Fe^{2+})_2(Ti,Fe^{3+})Si_7O_{19}(OH)$;
4) $(K_{1.85}Na_{0.15})(Ca_{3.43}Mg_{0.06}Mn_{0.08}Fe_{0.15}Ti_{0.13})Si_{7.13}O_{17}(O_{1.63}OH_{2.02}F_{0.61})$; 5) $Na_3CeSi_6O_{15}·6\ H_2O$.