Tables and figures

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

Silicate	Composition	Group
Tobermorite	$Ca_5Si_6O_{16}(OH)_2 \cdot xH_2O$	VIIID10
Plombierite	$Ca_5Si_6O_{16}(OH)_2 \cdot 6H_2O$	VIIID10
Riversideite	$Ca_5Si_6O_{16}(OH)_2 \cdot 2H_2O$	VIIID10
Okenite	$Ca_{10}Si_{18}O_{46} \cdot 18H_2O$	VIIID10
Oyelite	$Ca_{10}B_2Si_8O_{29} \cdot 12H_2O$	VIIID10
Nekoite	$Ca_3Si_6O_{15} \cdot 7H_2O$	VIIID10
Tacharanite	$Ca_{12}Al_2Si_{18}O_{33}(OH)_{36}$	
Calcium Silicate Hydrate (CSH)	variable composition	

Table 2. Atomic coordinates.

a) Tobermorite, $Ca_{2.25}[Si_3O_{7.5}(OH)_{1.5}] \cdot 1H_2O$, having monoclinic structure, space group $P2_1$ [81H1].

Atom	Atomic coordinates			Atom	Atomic coordinates		
	x	*Y*	*z*		*x*	*y*	*z*
Ca1	0.75	0.75	0	Ca4	0.75	0.25	0.413
Ca2	0.75	0.25	0	Ca5[a)]	0.506	0.38	0.198
Ca3	0.75	0.75	0.413	Ca6[a)]	0.506	0.88	0.198
Si1	0.25	0.287	0.056	Si4	0.25	0.207	0.373
Si2	0.25	0.707	0.056	Si5	0.084	0.417	0.282
Si3	0.068	0.909	0.141	Si6	0.25	0.787	0.373
O1	0.25	0.17	0.12	O10	0.25	0.0	0.348
O2	0.015	0.137	0.0189	O11	0.015	0.122	0.4108
O3	0.448	0.372	0.0189	O12	0.484	0.357	0.4108
O4	0.25	0.50	0.077	O13	0.25	0.335	0.31
O5	0.015	0.622	0.0189	OH/O14	0.1	0.425	0.213
O6	0.484	0.856	0.0189	O15	0.25	0.645	0.31
O7	0.25	0.83	0.12	O16	0.015	0.638	0.4108
OH/O8	0.068	0.909	0.211	O17	0.484	0.872	0.4108
O/OH9	–0.18	0.785	0.113	O/OH18	–0.175	0.288	0.306
H_2O1	0.75	0.75	0.303	H_2O2	0.75	0.25	0.11

[a)] Statistically distributed.

Table 2 (cont.)

b) Normal 11Å-tobermorite, monoclinic polytype MDO_2, space group B11m (Ural mine) [01M1].

Atom	*x*	*y*	*z*	B_{eq} [2)]·10^3
Si1	0.757(1)	0.3876(9)	0.1574(3)	7(1)
Si2	0.915(1)	0.756(1)	0.0710(3)	15(1)
Si3	0.758(1)	0.967(1)	0.1589(3)	7(1)
O1	0.754(3)	0.499(3)	0.0949(8)	18(4)
O2	0.772(4)	0.185(3)	0.1328(5)	14(2)
O3	0.992(3)	0.537(2)	0.1971(8)	11(4)
O4	0.523(3)	0.312(3)	0.1946(9)	15(4)
O5	0.898(4)	0.752(4)	0.0	17(4)
O6	0.197(3)	0.896(3)	0.0949(7)	18(4)
W6	0.237(6)	0.416(6)	0.097(1)	90(10)
O7	0.752(3)	0.853(3)	0.0972(8)	17(4)
O8	0.524(3)	0.807(3)	0.1962(8)	8(4)
O9	0.984(3)	0.045(3)	0.2002(8)	11(4)
Ca1	0.2632(9)	0.4310(9)	0.2069(3)	11(1)
Ca3	0.7519(9)	0.9228(9)	0.2945(3)	9(1)
W1 [1)]	0.42(1)	0.26(1)	–0.020(3)	130(30)
W2	0.922(7)	0.250(7)	0.0	70(1)
W3 [1)]	0.40(1)	0.76(1)	–0.019(2)	100(20)
Ca2 [1)]	0.559(4)	0.078(4)	0.044(1)	35(5)

[1)] In normal tobermorite W1 and W3 have occupancy ½, whereas Ca2 has occupancy ¼. In anomalous one, Ca2 is missing; [2)] $B_{eq} = (8/3)\pi^2 \sum_i \sum_j U_{ij} a_i^* a_j^* a_i a_j$.

c) 11Å-tobermorite, orthorhombic polytype MDO_1, space group F2dd [01M1].

Atom	*x*	*y*	*z*	B_{eq}·10^3
Si1	0.2500(6)	0.2900(8)	0.0790(2)	6(1)
Si2	0.1760(6)	-0.001(1)	0.0356(1)	8(1)
Si3	0.2518(6)	0.7077(8)	0.0789(2)	4(1)
O1	0.136(1)	0.263(2)	0.1006(3)	3(3)
O1b	0.138(1)	0.757(3)	0.0975(4)	7(3)
O2	0.620(2)	0.505(3)	0.1511(4)	11(3)
O2b	0.620(2)	0.003(3)	0.1541(4)	7(3)
O3	0.183(2)	0.0	0.0	17(4)
O5	0.251(2)	0.499(3)	0.0667(3)	10(2)
O6	0.248(2)	0.179(3)	0.0475(6)	19(4)
O6b	0.244(2)	0.824(3)	0.0476(5)	11(4)
O7	0.034(2)	0.007(3)	0.0457(5)	24(4)
O7b	0.996(3)	0.508(4)	0.0478(6)	44(6)
Ca1	0.0048(3)	0.9977(8)	0.1034(1)	78(9)
Ca3	0.9984(3)	0.5009(8)	0.1026(1)	74(9)
W2	0.692(4)	0.0	0.0	60(10
W3	0.416(6)	0.298(8)	0.001(2)	60(20)

Table 2 (cont.)

d) Clinotobermorite, having triclinic structure, space group C1 [00M1] [1)]

Atom	Atomic coordinates			$B_{eq}\cdot10^3$	Atom	Atomic coordinates			$B_{eq}\cdot10^3$
	x	*y*	*z*			*x*	*y*	*z*	
Ca1	0.3640(3)	0.1072(4)	0.9228(3)	23(4)	Ca3	0.8679(3)	0.0998(4)	0.8981(3)	24(4)
Ca1A	–0.3634(3)	–0.1042(4)	–0.9134(3)	23(4)	Ca3A	–0.8711(3)	–0.1001(4)	–0.9069(3)	24(4)
Ca2	0.3113(5)	–0.0177(7)	0.4289(5)	24(4)					
Si1	0.8931(5)	0.2046(7)	0.1839(4)	14(5)	Si2A	–0.9950(6)	0.0383(8)	–0.3608(5)	56(5)
Si1A	–0.8941(5)	–0.2096(7)	–0.1841(4)	14(5)	Si3	0.8949(5)	–0.3726(7)	0.1869(4)	18(5)
Si2	0.9963(6)	–0.0362(8)	0.3553(5)	56(5)	Si3A	–0.8946(5)	0.3688(7)	–0.1859(4)	18(5)
O1	0.913(2)	0.124(2)	0.310(1)	13(1)	O4	0.891(1)	0.431(2)	0.237(1)	9(1)
O1A	–0.916(2)	–0.128(2)	0.309(1)	13(1)	O4A	–0.895(1)	–0.432(2)	–0.238(1)	9(1)
O11	0.919(1)	–0.229(2)	0.316(1)	10(1)	O5	0.009(2)	–0.002(3)	0.497(2)	14(2)
O11A	–0.912(1)	0.227(2)	–0.309(1)	10(1)	W5	0.514(2)	0.009(3)	0.511(2)	23(3)
O2	0.771(1)	–0.343(2)	0.115(1)	4(1)	O6	0.127(1)	–0.041(2)	0.311(1)	14(2)
O2A	–0.767(1)	0.349(2)	–0.108(1)	4(1)	O6A	–0.124(1)	0.053(2)	–0.319(1)	10(2)
O21	0.765(2)	0.149(2)	0.106(1)	8(1)	W6	–0.335(4)	–0.051(5)	–0.683(4)	92(7)
O21A	–0.767(2)	–0.151(2)	–0.111(1)	8(1)	W6A	0.342(4)	0.043(5)	0.699(4)	92(7)
O3	0.005(1)	–0.355(2)	0.111(1)	5(1)	W7	0.260(3)	–0.238(4)	0.537(2)	54(6)
O3A	0.003(1)	0.357(2)	–0.106(1)	5(1)	W8	0.260(2)	0.257(4)	0.535(2)	57(7)
O31	0.002(1)	0.155(2)	0.099(1)	4(1)					
O31A	0.005(1)	–0.161(2)	–0.105(1)	4(1)					

[1)] The atoms related by the pseudo-center of inversion are differentiate by the letter A.

Table 3. Crystal structures and lattice parameters.

Silicate	*T* [K]	Space group	Lattice parameters				Refs.
			a [Å]	*b* [Å]	*c* [Å]	α, β, γ	
9Å-Tobermorite[1)]	RT		11.17	7.38	18.7		88H1
9Å-Tobermorite[2)] (MDO_1)	RT		11.161(5)	7.303(4)	18.771(9)	$\beta = 92.91(5)^o$	00M1
9 Å-Tobermorite[2)] (MDO_2)	RT	C $\bar{1}$	11.156(5)	7.303(3)	9.566(5)	$\alpha = 101.08(4)^o$ $\beta = 92.83(5)^o$ $\gamma = 89.98(4)^o$	99M1, 00M1
11Å-Tobermorite[3)]	RT	$P2_1$	11.17	7.38	22.6	β not mentioned	88H1
11Å-Tobermorite[4)]	RT	B11m	6.735	7.385	22.847	$\beta = 123.25^o$	99M1
11Å- Tobermorite (normal) [5)] (MDO_2) (Ural mine)	RT	B11m	6.732(2)	7.369(1)	22.680(4)	$\gamma = 123.18(1)^o$	01M1
11Å- Tobermorite (anomalous) [6)] MDO_2 (Wessels mine)	RT	B11m	6.735(2)	7.385(1)	22.487(4)	$\gamma = 123.25(1)^o$	01M1
11Å-Tobermorite (anomalous)[7)] MDO_1 (Wessels mine)	RT	F2dd	11.265(2)	7.386(1)	44.970(9)		01M1
14Å-Tobermorite[8)]	RT	$P2_1$	11.17	7.38	27.94	β not mentioned	88H1

Table 3 (cont.)

Silicate	*T* [K]	Space group	Lattice parameters				Refs.
			a [Å]	*b* [Å]	*c* [Å]	α, β, γ	
Tobermorite[9,10)]	RT	Imm2	5.586(4)	3.696(2)	22.779(7)		81H1
Tobermorite[10,11)]	RT	$P2_1$	6.69	7.39	22.779	$\gamma = 123.49^o$	81H1
Tobermorite with 15.47 wt % Fe	RT	orth.	11.34	7.36	22.42		91L1
Clinotobermorite[12)]	RT		11.19	7.29	22.46	$\beta = 96.97^o$	97H1
Clinotobermorite[13)]	RT	Cc or C2/c	11.331(9)	7.353(7)	22.67(2)	$\beta = 96.59(7)^o$	89H1
Clinotobermorite[14)] (MDO_1)	RT	Cc	11.276(2)	7.3427(8)	22.642(4)	$\beta = 97.28(1)^o$	99M1, 00M1
Clinotobermorite[15)] (MDO_2)	RT	C1	11.274(2)	7.3439(7)	11.468(2)	$\alpha = 99.18(1)^o$ $\beta = 97.19(1)^o$ $\gamma = 90.09(1)^o$	99M1, 00M1
Okenite[16)] (subcell) (substructure)	RT	$P\bar{1}$	9.69(1)	7.28(1)	22.02(4)	$\alpha = 92.7(2)^o$ $\beta = 100.1(3)^o$ $\gamma = 110.9(1)^o$	83M1
Okenite[16)]	RT	triclinic	9.84	7.20	21.33	$\alpha = 90.0^o$ $\beta = 103.9^o$ $\gamma = 111.5^o$	56G1
Okenite[16)]	RT	$C\bar{1}$	19.38(2)	14.56(2)	22.02(4)	$\alpha = 97.7(2)^o$ $\beta = 100.1(3)^o$ $\gamma = 110.9(1)^o$	83M1
Okenite[17)]	RT	$P\bar{1}$	9.81(1)	14.56(2)	22.02(4)	$\alpha = 87.3(2)^o$ $\beta = 106.0(3)^o$ $\gamma = 112.8(1)^o$	83M1
Oyelite[18)]	RT	Orth.	11.25	7.25	5.911		84K1, 86D1
Nekoite[19)]	RT	P1	9.793(5)	7.339(5)	7.558(3)	$\alpha = 103.50(5)^o$ $\beta = 86.53(8)^o$ $\gamma = 111.77(7)^o$	83M1
Nekoite[20)]	RT	P1	7.588(3)	9.793(5)	7.339(5)	$\alpha = 111.77(7)^o$ $\beta = 103.50(5)^o$ $\gamma = 86.53(3)^o$	80A1
Tacharanite[21)]	RT	monocl.	17.07	3.65	27.9	$\beta = 114.1^o$	75C1

1) $Ca_5[Si_6O_{16}(OH)_2]$-MDO_1;
2) $Ca_5Si_6O_{16}(OH)_2$ – MDO_2 – structure obtained by dehydration of clinotobermorite at 225°C;
3) $Ca_5[Si_6O_{16}(OH)_2]\cdot 2H_2O$;
4) Composition not mentioned;
5) $Ca_{4.5}Si_6O_{16}(OH)\cdot 5H_2O$;
6) $Ca_4Si_6O_{15}(OH)_2\cdot 5H_2O$;
7) $Ca_4Si_6O_{15}(OH)_2\cdot 5H_2O$;
8) $Ca_5[Si_6O_{16}(OH)_2]\cdot xH_2O$;
9) Crystal data for the subcell;
10) $Ca_{2.25}[Si_3O_{7.5}(OH)_{1.5}]\cdot 1H_2O$;
11) Possible ordered structure;
12) $Cs_5[Si_3O_8(OH)_2\cdot 4H_2O$ – $Ca_5[Si_6O_{17}]\cdot 5H_2O$. The subcell parameters (space group I2/m) a = 5.593(6) Å, b = 3.645(4) Å, c = 22.456(27) Å, $\beta = 96.97(2)^o$;
13) $Ca_5Si_6(O,OH)_{18}\cdot 5H_2O$;

Table 3 (cont.)

14) $Ca_5Si_6O_{17}\cdot 5H_2O$ – MDO_1-type structure;
15) Composition not given; MDO_2-type structure;
16) $Ca_{10}Si_{18}O_{46}\cdot 18H_2O$;
17) $Ca_9Si_{18}O_{45}\cdot 18H_2O$;
18) $0.99CaO\cdot 0.10B_2O_3\cdot 0.80SiO_2\cdot 1.25H_2O$;
19) Composition not mentioned;
20) $Ca_3Si_6O_{15}\cdot 7H_2O$;
21) $Ca_{12}Al_2Si_{18}O_{33}(OH)_{36}$, *b* is certainly, *a* and *c* probably doubled in the true cell [97H1].

Table 4. Magnetic properties.

Silicate	*T* [K]	M_0 [emu/cm^3]	T_m [K]	$\mu_o H_c$ [T]	Θ [K]	Ref.
Fe-substituted CSH[1)]	1.8	10	≅ 10	0.17	–1.6	97L1

1) CSH; composition of lyophilised solid yields: (Fe+Ca)/(Al+Si) = 1, Fe/Ca = 4 and Al/Si = 0.2.

Table 5. Data obtained by ^{57}Fe NGR method.

Silicate	*T* [K]	Site	δ[1)] [mm/s]	ΔQ [mm/s]	B_{hf} [T]	*DH* [mm/s]	*A* [%]	Refs.
Fe-Tobermorite[2)]	RT	$^{[4]}Fe^{3+}$	0.3668	0.7338		0.4090	100	85P1
Fe-Tobermorite[3)]	RT	$^{[4]}Fe^{3+}$	0.3649	0.6431		0.5102	75	85P1
		$^{[6]}Fe^{3+}$	0.5591	0.9012		0.5450	25	
CSH[4)]	RT	Fe^{3+}	0.36(2)	0.50(2)		0.31(2)	29(5)	91L1
		Fe^{3+}	0.35(2)	0.85(2)		0.47(2)	71(5)	
Fe-substituted CSH[5)]	RT	Fe^{3+}	0.35	0.94			40	97L1
		Fe^{3+}	0.35	0.56			60	
	4.2	Fe^{3+}			48.9		40	97L1
		Fe^{3+}			45.6		60	

1) Relative to α-Fe.
2) Starting materials: 0.420 g $Na_2SiO_3\cdot 9H_2O$ + 0.0444 g $FeCl_3\cdot 6H_2O$ + 0.0768 g CaO at 180°C saturated steam, 2 days;
3) Starting materials: 4.2 g $Na_2SiO_3\cdot 9H_2O$ + 0. 444 g $FeCl_3\cdot 6H_2O$ + 0.768 g CaO at 175°C saturated steam, 14 days;
4) $Ca_{2.35}Fe_{2.02}Si_6O_{18}H_2\cdot 4H_2O$ obtained from CSH identical to 11Å-tobermorite by Ca ↔ Fe exchange reaction;
5) CSH; composition of lyophilised solid yields: (Fe+Ca)/(Al+Si) = 1, Fe/Ca = 4 and Al/Si = 0.2. The phase is not well crystallized.

Table 6. Data obtained by ^{27}Al and ^{29}Si MAS NMR spectroscopy.

Silicate	Si/Al ratio	^{27}Al chemical shift[1] [ppm]		^{29}Si chemical shift[2, 3] [ppm]						Refs.
				Q^1	$Q^2(0Al)$	$Q^2(1Al)$	$Q^3(0Al)$	$Q^3(1Al)$	Q^4	
11Å-Tobermorite A[4, 6]	No[5]	60	64.1		–85.7		–95.7			85K3[4]
11Å-Tobermorite A[4, 7]	No[5]	58.8	64.5		–85.7		–96.3			
11Å-Tobermorite A[4, 8]	20	59.1	64.5		–84.6			–91.5		
11Å-Tobermorite A[4, 9]	9	57.5	65.4		–84.6	–82.0	–95.9	–92.0		
11Å-Tobermorite A[4, 10]	20	57.3	64.2		–85.2	–82.0	–96.0	–92.0		
11Å-Tobermorite N[4, 11]	5		62.0		–84.7	–80.2				
Tobermorite A[12]			65.2		–87.1		–96.6			91T1
Tobermorite A[13]			63.4		–86.9		–96.6			
Tobermorite A[14]			61.2		–85.0	–81.9	–97.0	–93.0		
Tobermorite A[15]			57.3		–86.4	–83.3	–96.4	–94.5		
Tobermorite A[16]			57.3(15)		–85.2	–82.1	–96.9	–90.9		
14Å-Tobermorite					–85.2					80L1
Jennite (synthesized 80° C) [80H1]				–81.4	–85.2					87K2
Calcium silicate hydrates										89G1
Ca/Si = 1.31				–80.4	–86.6					
Ca/Si = 1.07				–79.2	–85.8					
Ca/Si = 0.91					–86.8					
Ca/Si = 0.71					–85.0					
Ca/Si = 0.12					–85.0		–100.7		–114.7	
Ca/Si = 0.02							–100.7		–114.5	

1) Relative to $[Al(H_2O)_6]^{3+}$;
2) Relative to tetramethylsilane (TMS);
3) Q represents the SiO_4 tetrahedron while the superscript refers to the number of other tetrahedra to which it is linked. The shift ranges of aluminosilicates are designated as Q(nAl);
4) A ratio Ca/(Si+Al) ≅ 0.83 was used in all tobermorites synthesized by [85K3]. Anomalous (A) tobermorites were denoted those for which the 11.3 Å reflection did not collapse to the 9 Å one upon heating at 573 K for 20 h. By N is denoted a normal tobermorite;
5) No added Al. Trace amounts of Al present as impurity in the reactants;
6) Obtained from quartz + CaO, 175°C, 18 h;
7) Obtained from Na_2SiO_3 + $FeCl_3$ + CaO, 175°C, 14 days; impurities: calcite, goethite;
8) Obtained from amorphous SiO_2 + kaolinite + KOH, 175°C, 7 days; impurity:calcite;
9) Obtained from Na_2SiO_3+ $AlCl_3$ + CaO; 180°C, 7 days; impurity: calcite;
10) Obtained from amorphous SiO_2 + kaolinite + CaO + NaOH; 175°C, 7 days; impurity: calcite;
11) Obtained from fumed silica + γ-Al_2O_3 + CaO; 80°C, 120 days;
12) $Ca_{5.0}Na_{0.036}Al_{0.060}Si_{5.93}O_{16}(OH)_2 \cdot 4.91H_2O$;
13) $Ca_{5.0}Na_{0.218}Al_{0.30}Si_{5.72}O_{16}(OH)_2 \cdot 5.00H_2O$;
14) $Ca_{5.0}Na_{0.284}Al_{0.60}Si_{5.41}O_{16}(OH)_2 \cdot 5.50H_2O$;
15) $Ca_{5.0}Na_{0.520}Al_{0.90}Si_{5.10}O_{16}(OH)_2 \cdot 5.79H_2O$;
16) $Ca_{5.0}Na_{0.680}Al_{1.20}Si_{4.81}O_{16}(OH)_2 \cdot 6.42H_2O$.