Tables and figures

Table 1. Inosilicates from groups VIIID03 and VIIID04 [91N1].

Silicate	Composition	Group
Carpholite	$MnAl_2Si_2O_6(OH)_4$	VIIID03
Ferrocarpholite	$(Fe,Mg)Al_2Si_2O_6(OH)_4$	VIIID03
Magnesiocarpholite	$(Mg,Fe)(Al,Fe)_2Si_2O_6(OH)_4$	VIIID03
Balipholite	$LiBaMg_2Al_3(Si_2O_6)_2(OH)_4F_4$	VIIID03
Shattuckite	$Cu_5(SiO_3)_4(OH)_2$	VIIID04
Plancheite	$Cu_8(Si_4O_{11})_2(OH)_4 \cdot H_2O$	VIIID04
Gilalite	$Cu_5Si_6O_{17} \cdot 7H_2O$	VIIID04
Apachite	$Cu_9Si_{10}O_{29} \cdot 11H_2O$	VIIID04
Chrysocolla	$(Cu,Al)_2H_2Si_2O_5(OH)_4 \cdot nH_2O$	VIIID04

Table 2. Atomic coordinates and isotropic temperature factors.

a) Magnesiocarpholite[4)], having orthorhombic structure [01F1].

Atom	*x*	*y*	*z*	B_{eq} [Å^2]·10^2
K[1)]	0	0.75	0.25	1.0
M1	0	0.87500(2)	0.75	0.84(2)
Al1	0.19088(4)	0.75	0.75	0.60(2)
Al2	0	0.96131(3)	0.25	0.66(2)
Si	0.19355(3)	0.87981(2)	0.4167(1)	0.59(1)
O1	0.20599(7)	0.79991(5)	0.4310(2)	0.81(2)
O2	0.08047(7)	0.89933(5)	0.4085(2)	0.84(2)
O3	0.24801(8)	0.91275(5)	0.6711(2)	0.91(2)
OH1	0.09973(9)	0.80978(6)	0.8791(2)	1.13(2)
OH2	0.06810(8)	0.96589(5)	0.9273(2)	0.83(2)
H1	–0.093(3)	0.801(2)	0.506(9)	6.10(1.30)
H2	0.134(2)	0.963(1)	0.916(5)	2.40(70)

1) Partial occupancy.

b) Shattuckite, having orthorhombic structure, space group Pcab [77E1].

Atom	Equipoint	*x*	*y*	*z*
Cu1	4a	0.5	0	0.5
Cu2	8c	0.33090(8)	0.02547(7).	0.03970(16)
Cu3	8c	0.25205(10)	0.28125(3)	0.46765(16)
Si1	8c	0.54485(17)	0.13502(8)	0.2173(4)
Si2	8c	0.39742(17)	0.15706(8)	0.7265(4)
O1	8c	0.5054(4)	0.0554(2)	0.1996(9)
O2	8c	0.3426(4)	0.0805(2)	0.7439(9)
O3	8c	0.7076(4)	0.1512(2)	0.2203(9)
O4	8c	0.4913(5)	0.1735(2)	0.9708(9)

Table 2b (cont.)

Atom	Equipoint	*x*	*y*	*z*
O5	8c	0.4907(5)	0.1670(2)	0.4777(9)
O6	8c	0.2836(4)	0.2163(2)	0.7193(9)
O7(OH)	8c	0.6779(4)	0.0243(2)	0.6426(8)
H	8c	0.71	0.435	0.63

Table 3. Crystal structures and lattice parameters at RT.

Silicate	Space group	Lattice parameters				Refs.
		a [Å]	*b* [Å]	*c* [Å]	β	
Carpholite[1)]	Ccca	13.831	20.296	5.121		75N1
Ferrocarpholite[2)]		13.77	20.18	5.10		51D1
Mg-rich carpholite[3)]	Ccca	13.714(2)	20.079(2)	5.105(1)		81V1
Magnesiocarpholite[4)]	Ccca	13.726	20.099	5.112		01F1
Magnesiocarpholite[5)]	Ccca	13.716	20.084	5.110		01F1
K-, Li and F-bearing carpholite[6)]	Ccca	13.715(5)	20.302(7)	5.138(3)		89G1
Balipholite[7)]	Ccca	13.60	20.24	5.16		75W1, 76F1
Shattuckite[8)]	Pcab	9.885(1)	19.832(2)	5.3825(8)		77E1
Shattuckite (natural)	Pcab	9.881(3)	19.82(2)	5.398(3)		64N1
Plancheite[9)]	Pcnb	19.043(3)	20.129(5)	5.269(1)		77E1
Gilalite[10)]	monoclinic	13.38	19.16	9.026	$\cong 90^o$	80C1
Apachite[11)]	monoclinic	12.89	6.055	19.11	90.42^o	80C1
Chrysocolla[12)]		5.7	8.85	6.7		68C1, 69F1

1) Composition [%]: SiO_2 – 35.00; Al_2O_3 – 32.66; Fe_2O_3 – 2.46; MnO – 18.51, H_2O^+ - 10.60;
2) Composition [%]: SiO_2 – 37.38; TiO_2 – 0.22; Al_2O_3 – 29.23; Fe_2O_3 – 2.06; FeO – 17.88, MnO – 0.14; MgO – 2.51; CaO – 0.13; Na_2O – 0.14; K_2O – 0.09; H_2O^+ - 10.02; H_2O^- - 0.34; SO_3 – 0.12;
3) $(Mg_{0.795}Fe^{2+}_{0.203}Mn_{0.002})Al_2Si_2O_6(OH)_4$;
4) $K_{0.002}(Mg_{0.65}Fe^{2+}_{0.32}Fe^{3+}_{0.03})Al_{1.97}Si_{2.00}O_{5.90}(OH)_{3.95}F_{0.15}$;
5) $K_{0.002}(Mg_{0.65}Fe^{2+}_{0.34}Fe^{3+}_{0.01})Al_{1.98}Si_{2.00}O_{5.92}(OH)_{3.96}F_{0.12}$;
6) $K_{0.70}(Mn_{1.25}Li_{0.52}Na_{0.15}Fe_{0.05}Mg_{0.01})Al_{3.95}Si_{3.99}O_{11.75}(OH)_{5.06}F_{3.19}$;
7) $(Ba_{0.88}K_{0.07}Na_{0.06}Ca_{0.03})(Mg_{1.69}Al_{0.17}Fe^{2+}_{0.06}Fe^{3+}_{0.03})Li_{0.95}Al_{3.00}(Si_{3.93}Al_{0.07})O_{11.96}(OH)_{8.07}$;
8) $Cu_5(SiO_3)_4(OH)_2$;
9) $Cu_8(Si_4O_{11})_2(OH)_4 \cdot xH_2O$;
10) Composition [%]: CuO – 36.2; MgO – 2.3; CaO – 3.8; MnO – 0.5; SiO_2 – 41.5; H_2O – 14.6; close to $Cu_5Si_6O_{17} \cdot 7H_2O$;
11) Composition [%]: CuO – 43.6; FeO – 0.3; MgO – 1.7; CaO – 1.8; SiO_2 – 40.8; H_2O – 13.8; close to $Cu_9Si_{10}O_{29} \cdot 11H_2O$;
12) $Cu_{2-x}(Al,Fe)_xH_{2-x}(Si_2O_5)(OH)_4 \cdot nH_2O$ (0.46 to 5.87 % Al_2O_3; 0…5.66 % Fe_2O_3);
13) Composition [%]: SiO_2 – 36.79; TiO_2 – 0.23; Al_2O_3 – 29.60; Fe_2O_3 – 2.09; FeO – 17.65; MnO – 0.14; MgO – 2.48; H_2O^+ – 11.03.

Table 4. Data obtained by ^{57}Fe NGR data.

Silicate [a]	T [K]	Site	δ [b] [mm/s]	ΔQ [mm/s]	Γ [c] [mm/s]	A [%]	Refs.
$Mg_{1-x}Fe^{2+}_x(Al_{2-y}Fe^{3+}_y)Si_2O_6(OH,F)_4$							
x = 0.52, y = 0.05	RT	$^{[6]}Fe^{2+}$	1.17(1)	3.20(1)	0.28(1)	91.2	96W1
		$^{[6]}Fe^{3+}$	0.33(1)	0.46(1)	0.31(1)	8.8	
x = 0.70, y = 0.10	RT	$^{[6]}Fe^{2+}$	1.20(1)	3.27(1)	0.33(1)	87.5	96W1
		$^{[6]}Fe^{3+}$	0.39(1)	0.72(1)	0.68(2)	12.5	
Magnesiocarpholite[4]	300	$^{[6]}Fe^{2+}$	1.165(1)	3.204(1)	0.136(1)	96.2	01F1
		$^{[6]}Fe^{3+}$	0.35(2)	0.47(3)	0.16(3)	3.8	
Magnesiocarpholite[5]	300	$^{[6]}Fe^{2+}$	1.168(1)	3.198(1)	0.134(1)	91.3	01F1
		$^{[6]}Fe^{3+}$	0.34(1)	0.50(1)	0.17(1)	8.7	
Ferrocarpholite (natural)	RT	$^{[6]}Fe^{2+}$	1.178	3.198	0.14	96	79S1
		$^{[6]}Fe^{3+}$	0.38	0.55	0.13…0.21	4	

[a] Compositions according to Table 3;
[b] Relative to α-Fe;
[c] Linewidth of NGR line. The $\Gamma/2$ values are given by [79S1, 01F1].

Table 5. Refractive indices.

Silicate [a]	n_α	n_β	n_γ	$2V^o$		Refs.
Carpholite[1]	1.6284	1.6290	1.6386	67		75N1
Carpholite[13]	1.617	1.632	1.639	70		75N1
Ferrocarpholite[2]	1.628	1.644	1.647	49		51D1, 75N1
Balipholite[7]	1.5810	1.5958	1.6008	68…72	optic plane	75W1, 76F1
Shattuckite[8]	1.753(3)	1.782(3)	1.815(3)	88	biaxial positive	64N1, 77E1
Plancheite[9]	1.697	1.718	1.741	88.5		34L1, 77E1
Gilalite[10]	1.560	1.635	1.635	small	biaxial negative	80C1
Apachite[11]	1.610	1.650	1.650	small	biaxial negative	80C1

[a] Compositions according to Table 3.