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Ferro-tschermakite from the Ploumanac'h granitic complex, Brittany, France: mineral description

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Abstract: The mineral description is provided for ferro-tschermakite, ideally $^{A}\square^{B}Ca_2{}^{C}(Fe^{2+}_3Al_2)^{T}(Si_6Al_2)O_{22}{}^{W}(OH)_2$. The type specimen has been found in the dump of the Bâtiment et Granit de Ploumanac'h northern granite quarry, La Clarté, Perros-Guirec, Ploumanac'h granitic complex, Brittany, France. The empirical formula derived from electron microprobe analysis and single-crystal structure refinement is: $^{A}(Na_{0.29}K_{0.08})_{\Sigma=0.37}{}^{B}(Ca_{1.69}Fe^{2+}_{0.11}Mn^{2+}_{0.02}Na_{0.18})_{\Sigma=2.00}{}^{C}(Fe^{2+}_{1.84}Mg_{1.54}Al_{1.33}Fe^{3+}_{0.24}V^{3+}_{0.01}Ti_{0.04})_{\Sigma=5.00}{}^{T}(Si_{6.15}Al_{1.85})_{\Sigma=8.00}O_{22}{}^{W}(OH_{1.94}F_{0.06})_{\Sigma=2.00}$. Ferro-tschermakite is biaxial (–), with $\alpha = 1.666(2)$, $\beta = 1.680(2)$, $\gamma = 1.690(2)$ and $2V$ (meas.) = 84(1)°, $2V$ (calc.) = 79.8. The dispersion is medium ($r > v$), and the orientation is: $X \wedge \mathbf{a} = 9.5°$ (in β acute), $Y \| \mathbf{b}$, $Z \wedge \mathbf{c} = 24.3°$ (in β obtuse). The unit-cell parameters are $a = 9.7598(6)$, $b = 18.0220(11)$, $c = 5.3299(3)$ Å, $\beta = 104.826(1)°$, $V = 906.27(9)$ Å^3, $Z = 2$, space group $C2/m$. The strongest ten reflections in the X-ray powder pattern obtained from single-crystal data [d values (in Å), I, (h k l)] are: 8.359, 100, (1 1 0); 2.708, 84, (1 5 1); 3.098, 55, (3 1 0); 2.552, 43, ($\overline{2}$ 0 2); 2.595, 41, (0 6 1); 2.330, 33, ($\overline{3}$ 5 1); 2.159, 27, (2 6 1); 2.936, 27, (2 2 1); 3.338, 27, (1 3 1); 2.012, 24, ($\overline{4}$ 0 2; 3 5 1).

Key words: ferro-tschermakite; amphibole; electron-microprobe analysis; optical properties; powder-diffraction pattern; crystal-structure refinement; Ploumanac'h granitic complex; France.

1. Introduction

After the approval of the new scheme for the classification and nomenclature of the amphibole supergroup (Hawthorne *et al.*, 2012), we have started a systematic investigation to find and characterize all the amphiboles with distinct compositions that have not yet been officially approved by IMA-CNMNC, and for which there is no proper reference in the official IMA list of minerals. We realized that the root-name "tschermakite", with the ideal composition) $^{A}\square^{B}Ca_2{}^{C}(Mg_3Al_2)^{T}(Si_6Al_2)O_{22}{}^{W}(OH)_2$, and its Fe-rich analogues are lacking proper modern characterization. We present in this paper the complete characterization of ferro-tschermakite, which was approved by the IMA-CNMNC vote 2016–116. The holotype ferro-tschermakite is deposited in the mineralogical collections of the Museo di Mineralogia of the Università di Pavia, catalogue number 2016–02.

2. Occurrence

Ferro-tschermakite was found in a specimen found in the dump of the Bâtiment et Granit de Ploumanac'h northern granite quarry, in the Ploumanac'h granitic complex, at La Clarté, Perros-Guirec, Brittany, France (~48°48′50″ N, ~3°28′50″ W; Fig. S1 in Supplementary Material attached to this article and freely available online on the GSW website of the journal: http://eurjmin.geoscienceworld.org/). The Ploumanac'h granite complex (or Ploumanac'h plutonic complex in Decître *et al.*, 2002), is located on the northern coast of Brittany, at the northern tip of the Trégor, between Trébeurden and Perros-Guirec. On the geological map of France at a scale of 1/1 000 000, the complex occurs at the northern end of the "red granites", which extend from the end of Finistère (Aber-Ildut, Morlaix) in the southwest to the Cotentin peninsula (Flamanville and Barfleur) in the northeast. The Ploumanac'h complex is approximately 12 × 8 km in extent, and is concentrically zoned with an outer aureole (Fig. S2; Barrière, 1977). A reconstruction of geological setting, of magma composition and of the complex crystallization conditions is provided in Decître *et al.* (2002). The Ploumanac'h complex intrudes: (i) the Trébeurden gneisses; (ii) the granite pluton of Perros-Guirec; (iii) the orbicular granite of Milliau Island (Decître *et al.*, 2002). The Perros-Guirec granite (Fig. S3) is a grey-pink granite batholith located east of the Ploumanac'h complex. It is a coarse-grained, porphyroid granite, where the pronounced pink colour is due to the presence of large feldspar crystals. It is

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emplaced in the Icartian basement, dated to the lower Brioverian (615 Ma, the beginning of the Cadomian cycle), and intruded by veins of the pink Ploumanac'h granite (Decître *et al.*, 2002).

3. Appearance and physical properties

The holotype specimen is shown in Fig. 1. It consists of a ~3 cm long aggregate of dark green bladed-to-acicular crystals of ferro-tschermakite associated with white plagioclase and occurs in miarolitic texture in a granite pegmatite. Ferro-tschermakite is dark green, is non-fluorescent, and has a dark green streak and a vitreous lustre.

A spindle stage was used to orientate a crystal to measure refractive indices and 2 V by extinction curves (Bartelmehs *et al.*, 1992). The optical orientation was determined by transferring the crystal from the spindle stage to a single-crystal diffractometer and measuring the relative axial relations by X-ray diffraction. In transmitted plane-polarized light, ferro-tschermakite is pleochroic (X = pale yellow-green, Y = olive green, Z = blue green). It is biaxial (−), $\alpha = 1.666(2)$, $\beta = 1.680(2)$, $\gamma = 1.690(2)$, $2V$ (meas) = 84(1), $2V$ (calc) = 79.8°. The dispersion is medium ($r > v$), and the orientation is: $X \wedge \mathbf{a} = 9.5°$ (in β acute), $Y \| \mathbf{b}$, $Z \wedge \mathbf{c} = 24.3°$ (in β obtuse).

The compatibility index ($1 - (K_p/K_c)$; Mandarino, 1981) is 0.005 (superior) based on the proposed chemical formula.

4. Single-crystal diffraction and powder analysis

Diffraction data for a platy prismatic single crystal 140 × 130 × 50 μm in size were collected in the θ range 2–30° with a Bruker-AXS CCD diffractometer using graphite monochromatized Mo$K\alpha$ X-radiation ($\lambda = 0.7107$ Å). Omega rotation frames (scan width 0.3°, scan time 20 s, sample-to-detector distance 50 mm) were processed with the SAINT software (Bruker, 2003) and intensities were corrected for Lorentz and polarization effects; absorption effects were empirically evaluated by the SADABS software (Krause *et al.*, 2015) and an absorption correction was applied to the data. A total of 6912 collected reflections was reduced to 1377 unique reflections (mean redundancy = 5, $R_{int} = 1.8\%$). Of these, 1249 reflections with $I > 3\sigma I$ were considered as observed during unweighted full-matrix least-squares refinement on F done with a program locally written to handle complex solid-solutions (Cannillo *et al.*, 1983). Scattering curves for fully ionised chemical species were used at sites where chemical substitutions occur; neutral *vs.* ionized scattering curves were used at the T and anion sites [except O(3)]. Full-matrix unweighted least-squares refinement on $I > 3\sigma I$ gave $R_{obs} = 2.5\%$ (1249 reflections) and $R_{all} = 2.7\%$ (1377 reflections). Refined atom coordinates and displacement parameters, and selected bond lengths and angles are given in Tables 1 and 2, respectively. Observed structure factors have been deposited together with the CIF, as part of the supplementary material linked to this article. The refined and analysed crystal of this work has the code 1307 in the amphibole database of the CNR-IGG in Pavia, Italy.

Fig. 1. The holotype specimen of ferro-tschermakite, from the Ploumanac'h granitic complex (scale in cm).

The a:b:c ratio calculated from the unit cell parameters is 0.542:1:0.296.

X-ray powder-diffraction data (Cu$K\alpha$, $\lambda = 1.54178$ Å) were obtained using the XPREP utility of SAINT (Bruker, 2003), which generates a 2D powder diffractogram (Debye–Scherrer technique) starting from the F_{obs} collected on the single crystal and taking into account solely the information concerning the unit-cell dimensions and the Laue symmetry. No Lorentz and polarization corrections were applied. Data are given in Table 3.

5. Chemical analysis and unit-formula

Chemical analysis (10 points) of the crystal used for structure refinement was done with a Cameca SX-100 electron microprobe (WDS mode, 15 kV, 20 nA, counting time 20 s, 5 μm beam diameter). The standards used are as follows: Si and Ca, diopside (TAP); Ti, titanite (LPET); Al, andalusite (TAP); Cr, chromite (LPET); V, VP_2O_7 (LLiF); Fe, fayalite (LLiF); Mn, spessartine (LLiF); Mg, forsterite (LTAP); Zn, gahnite (LLiF); Ni, pentlandite (LLiF); Na, albite (TAP); K, orthoclase (LPET); F, fluoro-riebeckite (TAP); Cl, tugtupite (LPET). The amount of H_2O used in the calculation is that required to give F + OH + Cl = 2 anions and 15.37 cations per formula unit, in accord with amphibole stoichiometry and the results of the structure refinement (which constrains the total number of cations and excludes the presence of the oxo-component). These assumptions fix the Fe^{3+}/Fe_{tot} ratio. The oxide wt% and the calculated unit-formula are reported in Table 4. The proposed empirical formula (based on 24 anions pfu and 15.37 cations pfu, a value compatible with the results of the structure refinement) is $^{A}(Na_{0.29}K_{0.08})_{\Sigma=0.37}{}^{B}(\mathbf{Ca_{1.69}}Fe^{2+}_{0.11}Mn^{2+}_{0.02}Na_{0.18})_{\Sigma=2.00}$

Table 1. Atom coordinates, refined site-scattering values (ss, epfu), atom-displacement parameters (B_{eq}, Å^2; $\beta_{ij} \times 10^4$) for ferro-tschermakite crystal 1307.

Site	Ss	*x*	*y*	*z*	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)		0.1041(2)	0.09409(8)	0.2089(3)	1.01(3)	27	8	100	−2	18	−2
O(2)		0.1193(2)	0.17647(8)	0.7443(3)	0.96(3)	24	7	103	0	9	2
O(3)	16.30(10)	0.1114(2)	0	0.7098(4)	1.10(5)	28	8	118	–	14	–
O(4)		0.3722(2)	0.25142(8)	0.7958(3)	1.15(3)	39	6	124	−3	23	3
O(5)		0.3525(2)	0.14032(8)	0.1103(3)	1.13(3)	29	9	104	−1	11	9
O(6)		0.3413(2)	0.12069(9)	0.6025(3)	1.20(3)	31	10	117	1	14	−7
O(7)		0.3312(3)	0	0.2850(5)	1.56(5)	42	10	173	–	15	–
T(1)		0.28060(6)	0.08693(3)	0.30164(11)	0.72(2)	22	5	71	−1	9	−1
T(2)		0.29292(6)	0.17407(3)	0.81664(11)	0.74(2)	22	5	75	−1	12	0
M(1)	38.67(11)	0	0.09024(3)	½	0.79(2)	28	5	71	–	14	–
M(2)	30.73(10)	0	0.17824(4)	0	0.78(2)	24	5	82	–	12	–
M(3)	22.42(4)	0	0	0	0.80(2)	29	5	76	–	14	–
M(4)	38.0(2)	0	0.28043(4)	½	1.06(2)	33	8	105	–	27	–
M(4′)	1.51(7)	0	0.2578(12)	½	1.0						
A	1.49(6)	0	½	0	2.0						
A(*m*)	1.32(9)	0.033(3)	½	0.085(7)	2.0						
A(2)	1.72(9)	0	0.4675(13)	0	2.0						
H	1.8(2)	0.183(8)	0	0.765(13)	1.0						

Table 2. Selected interatomic distances (Å), angles (°), bond angle variances (°^{2}) and quadratic elongations (AV and QE; Robinson *et al.*, 1971) in ferro-tschermakite crystal 1307.

T(1)–O(1)	1.671(2)	*T*(2)–O(2)	1.639(2)	*M*(4)–O(2) × 2	2.405(2)
T(1)–O(5)	1.681(2)	*T*(2)–O(4)	1.612(2)	*M*(4)–O(4) × 2	2.319(2)
T(1)–O(6)	1.675(2)	*T*(2)–O(5)	1.641(2)	*M*(4)–O(5) × 2	2.626(2)
T(1)–O(7)	1.6519(9)	*T*(2)–O(6)	1.651(2)	*M*(4)–O(6) × 2	2.511(2)
<*T*(1)–O>	1.670	<*T*(2)–O>	1.636	<*M*(4)–O>	2.465
TAV	3.60	TAV	18.23		
TQE	1.0009	TQE	1.0047		
M(1)–O(1) × 2	2.0621(14)	*M*(2)–O(1) × 2	1.998(2)	*M*(3)–O(1) × 4	2.137(2)
M(1)–O(2) × 2	2.166(2)	*M*(2)–O(2) × 2	2.0066(14)	*M*(3)–O(3) × 2	2.106(2)
M(1)–O(3) × 2	2.111(2)	*M*(2)–O(4) × 2	1.911(2)	<*M*(3)–O>	2.127
<*M*(1)–O>	2.113	<*M*(2)–O>	1.972	OAV	114.31
OAV	65.50	OAV	19.58	OQE	1.0363
OQE	1.0207	OQE	1.0064		
A–O(5) × 4	3.041(2)	*A*(2)–O(5) × 2	2.57(2)	*A*(*m*)–O(5) × 2	3.10(2)
A–O(6) × 4	3.153(2)	*A*(2)–O(6) × 2	2.780(14)	*A*(*m*)–O(5) × 2	3.06(2)
A–O(7) × 2	2.510(3)	*A*(2)–O(7) × 2	2.578(6)	*A*(*m*)–O(6) × 2	2.82(2)
<*A*–O>	2.979	<*A*(2)–O>	2.64	*A*(*m*)–O(7)	2.46(3)
				A(*m*)–O(7)	3.28(3)
M(4′)–O(2) × 2	2.10(2)			*A*(*m*)–O(7)	2.65(2)
M(4′)–O(4) × 2	2.253(2)			<*A*(*m*)–O>	2.93
M(4′)–O(5) × 2	2.869(14)	*T*(1)–O(5)–*T*(2)	133.62(10)		
M(4′)–O(6) × 2	2.82(2)	*T*(1)–O(6)–*T*(2)	141.21(10)	O(5)–O(6)–O(5)	164.22(9)
<*M*(4′)–O>	2.51	*T*(1)–O(7)–*T*(1)	143.0(2)	O(6)–O(7)–O(6)	104.96(11)

$^{C}(\mathbf{Fe^{2+}_{1.84}}Mg_{1.54}Al_{1.33}\mathbf{Fe^{3+}_{0.24}}V^{3+}_{0.01}Ti_{0.04})_{\Sigma=5.00}{}^{T}(\mathbf{Si_{6.15}}Al_{1.85})_{\Sigma=8.00}O_{22}{}^{W}(\mathbf{OH_{1.94}}F_{0.06})_{\Sigma=2.00}$ (where the dominant cations/anions in the homovalent groups are in bold). The end-member formula is $^{A}\square\,{}^{B}Ca_2\,{}^{C}(Fe^{2+}_3Al_2)\,{}^{T}(Si_6Al_2)\,O_{22}\,{}^{W}(OH)_2$, which requires SiO_2 39.61, Al_2O_3 22.41, FeO 23.68, CaO 12.32, H_2O 1.98, total 100.00 wt%.

Based on the empirical formula, the calculated density of the ferro-tschermakite sample of this work is 3.260 g/cm^3.

6. The crystal-chemistry of ferro-tschermakite

The site populations were obtained by distributing the ions of the unit formula (Table 4) under the constraints of the refined site-scattering values (Hawthorne *et al.*, 1995) and mean bond-lengths for the C cations (Table 2). The results are reported in Table 5. The agreement between the refined and calculated site-scattering values for the B and C cations is very close. In particular, the calculated

Table 3. Powder X-ray diffraction data for ferro-tschermakite crystal 1307.

I_{rel}	d(calc)	h	k	l	I_{rel}	d(calc)	h	k	l	I_{rel}	d(calc)	h	k	l	I_{rel}	d(calc)	h	k	l
16.3	9.010	0	2	0	**27.0**	**2.936**	**2**	**2**	**1**	5.8	2.221	$\overline{2}$	4	2	5.0	1.699	0	10	1
100.0	**8.359**	**1**	**1**	**0**	7.9	2.786	3	3	0	5.6	2.179	1	7	1			$\overline{1}$	3	3
8.2	5.067	$\overline{1}$	3	0	**83.6**	**2.708**	**1**	**5**	**1**	**27.2**	**2.159**	**2**	**6**	**1**	8.7	1.688	$\overline{2}$	8	2
15.5	4.912	$\overline{1}$	1	1	**41.4**	**2.595**	**0**	**6**	**1**	13.8	2.051	$\overline{2}$	0	2			0	2	3
14.8	4.505	0	4	0	**43.3**	**2.552**	**$\overline{2}$**	**0**	**2**	**23.5**	**2.012**	$\overline{4}$	0	2	20.0	1.643	4	6	1
10.9	3.890	$\overline{1}$	3	1	6.4	2.369	$\overline{3}$	5	0			**3**	**5**	**1**	5.4	1.629	4	8	0
26.8	**3.388**	**1**	**3**	**1**	**32.8**	**2.330**	**$\overline{3}$**	**5**	**1**	6.3	1.993	$\overline{3}$	7	0	12.3	1.614	$\overline{1}$	11	0
21.4	3.258	2	4	0	15.9	2.309	$\overline{4}$	2	1	11.3	1.865	$\overline{1}$	9	1	18.1	1.590	$\overline{1}$	5	3
55.4	**3.098**	**3**	**1**	**0**	19.2	2.284	$\overline{3}$	1	3	8.1	1.801	0	1	0	5.7	1.553	4	0	2

Note: The strongest ten reflections are in bold. Only peaks with $I_{rel} \geq 5$ are reported.

Table 4. Chemical composition (10 points), unit formula (based on 24 anions and 15.37 cations) and a comparison between observed and calculated group site-scattering for ferro-tschermakite crystal 1307. * Calculated on a 2 (OH,F) apfu basis.

Oxide	wt%(esd)	Range	Oxide	wt%(esd)	Range	apfu		apfu	
SiO_2	41.32(21)	40.61–42.55	H_2O*	1.96		Si	6.15	Ca	1.69
TiO_2	0.37(2)	0.35–0.39	F	0.12(15)	0.00–0.24	Al	1.85	Na	0.29
Al_2O_3	18.13(13)	17.72–18.41	Cl	–		Sum T	8.00	Fe^{2+}	0.11
Fe_2O_3	2.09		O=F	−0.05				Mn^{2+}	0.02
Cr_2O_3	0.02(24)	0.00–0.03	Total	99.47		Ti^{4+}	0.04	Sum B	2.00
V_2O_3	0.05(4)	0.01–0.08				Al^{3+}	1.33		
FeO	15.66					Fe^{3+}	0.24	Na	0.29
$[FeO]_{tot}$	[17.55(27)]	17.18–17.82				V^{3+}	0.01	K	0.08
MgO	6.94(7)	6.73–7.15				Cr^{3+}	–	Sum A	0.37
MnO	0.20(5)	0.15–0.22	Group site-scattering (epfu)			Mg	1.54		
NiO	0.01(2)	0.00–0.03		obs (SREF)	calc (EMP)	Mn^{2+}	–	OH^-	1.94
ZnO	0.02(6)	0.00–0.04	C	91.82	90.96	Fe^{2+}	1.84	F^-	0.06
CaO	10.58(32)	18.48–10.64	B	39.47	39.15	Ni	–	Sum W	2.00
Na_2O	1.61(32)	1.30–1.74	A	4.53	4.71	Zn	–		
K_2O	0.45(2)	0.42–0.46	Total	135.81	134.82	Sum C	5.00		

Table 5. Site populations for ferro-tschermakite crystal 1307. There is close agreement (see text for more detail) between the refined values of site-scattering (ss, electrons per formula unit) and mean bond-lengths (mbl, Å) and those calculated based on the proposed site populations.

Site	Site population (apfu)	ss (epfu)		mbl (Å)	
		Refined	Calculated	Refined	Calculated
T(1)	2.15 Si + 1.85 Al			1.670	1.673
T(2)	4.00 Si			1.636	
M(1)	1.04 Fe^{2+} + 0.96 Mg	38.67	38.56	2.113	2.102
M(2)	0.34 Mg + 0.04 Fe^{2+} + 1.33 Al + 0.24 Fe^{3+} + 0.01V^{3+} + 0.04 Ti^{4+}	30.73	29.76	1.972	1.971
M(3)	0.76 Fe^{2+} + 0.24 Mg	22.42	22.64	2.127	2.113
Σ C cations		91.82	90.96		
B cations	1.69 Ca + 0.11 Fe^{2+} + 0.02 Mn^{2+} + 0.18 Na	39.47	39.15		
A cations	0.29 Na + 0.08 K	4.53	4.71		
W anions	1.94 OH + 0.06 F				

<M(2)–O> distance – which is a linear function of the averaged ionic radius of the constituents and is thus sensitive to the Fe^{3+}/Fe^{2+} ratio (Hawthorne & Oberti, 2007; Oberti *et al.*, 2007) – is in excellent agreement with the refined value, which confirms the assumption done during the formula recalculation. In contrast, the calculated <M(1)–O> and <M(3)–O> distances are significantly shorter than the measured values, a feature which is coherent with a unusual distortion of the relevant octahedra (Table 2). However, this difference excludes the presence of trivalent cations at the M(1) and M(3) sites, and hence any deprotonation, so that the assumption of 24 (O,OH,F) atoms per formula unit (apfu) in the calculation of the formula unit is further supported.

Table 6. A comparison of the optical and crystallographic properties available for "tschermakite" (no longer such after Hawthorne *et al.*, 2012), ferro-tschermakite (this work) and "ferri-tschermakite".

	"Tschermakite"[1]	Ferro-tschermakite [2]	"Ferri-tschernakite"[3]
Colour	Green	Dark green	Pale green
Optical class		Biaxial (–)	Biaxial (–)
Pleochroism		*X* = pale yellow-green, *Y* = olive green, Z = blue-green	*X* = pale yellowish green, *Y* = Z = pale brownish green
Orientation	Z ^ **c** = 20°*	Y ‖ **b** Z ^ **c** = 24.3° (in β acute)	
α	1.657*	1.666	1.652
β		1.680	1.664
γ		1.690	1.675
$2V_{meas}$ (°)	80°*	84°	58°
Space group	*C*2/*m*	*C*2/*m*	
a (Å)	9.8059(5)	9.7598(6)	
b (Å)	17.9721(8)	18.022(1)	
c (Å)	5.3012(2)	5.3299(3)	
β (°)	105.063(1)	104.826(1)	
V (Å^3)	902.15	906.27	
<*T*(1)–O> (Å)	1.661	1.670	
<*T*(2)–O> (Å)	1.637	1.636	
<*M*(1)–O> (Å)	2.088	2.113	
<*M*(2)–O> (Å)	2.018	1.972	
<*M*(3)–O> (Å)	2.080	2.127	
<*M*(4)–O> (Å)	2.476	2.465	
T(1)–O(5)–*T*(2)	133.6	133.6	
T(1)–O(6)–*T*(2)	138.8	141.2	
T(1)–O(7)–*T*(1)	138.4	143.0	
Reference	Abdu & Hawthorne (2009)	This work	Ogura (1958)

[1] $^{A(}K_{0.05}Na_{0.38})_{\Sigma=0.43}{}^{B}(Ca_{1.80}Fe^{2+}_{0.15}Na_{0.05})_{\Sigma=2.00}(Mg_{3.65}Fe^{2+}_{0.18}Mn^{2+}_{0.03}Al_{0.81}Cr_{0.19}Fe^{3+}_{0.09}Ti_{0.05})_{\Sigma=5.00}{}^{T}(Si_{6.43}Al_{1.57})_{\Sigma=8.00}O_{22}{}^{W}(OH_{1.95}F_{0.04}Cl_{0.01})_{\Sigma=2.00}$.

[2] $^{A}(Na_{0.29}K_{0.08})_{\Sigma=0.37}{}^{B}(Ca_{1.69}Fe^{2+}_{0.11}Mn^{2+}_{0.02}Na_{0.18})_{\Sigma=2.00}{}^{C}(Fe^{2+}_{1.84}Mg_{1.54}Al_{1.33}Fe^{3+}_{0.24}V^{3+}_{0.01}Ti_{0.04})_{\Sigma=5.00}{}^{T}(Si_{6.15}Al_{1.85})_{\Sigma=8.00}O_{22}{}^{W}(OH_{1.94}F_{0.06})_{\Sigma=2.00}$.

[3] $^{A}(K_{0.15}Na_{0.31})_{\Sigma=0.46}{}^{B}(Ca_{1.48}Fe^{2+}_{0.26}Mn^{2+}_{0.07}Na_{0.19})_{\Sigma=2.00}(Mg_{2.16}Fe^{2+}_{1.44}Al_{0.61}Fe^{3+}_{0.67}Ti_{0.13})_{\Sigma=5.01}{}^{T}(Si_{6.17}Al_{1.81}P_{0.02})_{\Sigma=8.00}O_{22}{}^{W}OH_{2.00}$.

* Extrapolated by Winchell (1945) for end-member tschermakite $^{A}\square{}^{B}Ca_2{}^{C}(Mg_3Al_2){}^{T}(Si_6Al_2)O_{22}{}^{W}(OH)_2$.

The presence of the *A*(*m*) and *M*(4′) subsites confirm, respectively, the presence of $^{A(m)}$K and of a significant amount of small B cations.

7. Relation to other species

Ferro-tschermakite is a newly characterized member of the calcium amphibole group with the end-member formula $^{A}\square{}^{B}Ca_2{}^{C}(Fe^{2+}_3Al_2){}^{T}(Si_6Al_2)O_{22}{}^{W}(OH)_2$ (Hawthorne *et al.*, 2012). It forms a series with tschermakite, $^{A}\square{}^{B}Ca_2{}^{C}(Mg_3Al_2){}^{T}(Si_6Al_2)O_{22}{}^{W}(OH)_2$, the only composition related to the rootname "tschermakite" so far recognized as a valid mineral species by IMA-CNMNC (Winchell, 1945; Abdu & Hawthorne, 2009). However, the composition reported by Abdu & Hawthorne (2009) should no longer be called tschermakite according to the classification rules in force, because the amount of trivalent C cations (which was not an issue in the previous classification schemes of Leake, 1978, and Leake *et al.*, 1997) is much lower than 1.50 apfu, and that amphibole now falls in the compositional field of magnesio-hornblende (although with a significant pargasite component). A comparison of the results of the structure refinement for "tschermakite" and ferro-tschermakite reported in Table 6 is coherent with the reported unit formulae. In particular, crystal 1307 has: (i) a lower amount of A cations (as inferred from the refined site-scattering values at the *A* sites); (ii) a higher amount of ^{T}Al, ordered at the *T*(1) site (as inferred from the longer <*T*(1)–O> distance); (iii) a higher amount of trivalent C cations ordered at the *M*(2) site (as inferred from the shorter <*M*(2)–O> distance); (iv) a higher Fe^{2+} content (from the higher refined site-scattering values at the *M*(1) and *M*(3) sites and the longer <*M*(1)–O> and <*M*(3)–O> distances). As a consequence of (ii) and (iii), the double chain of tetrahedra in ferro-tschermakite is more stretched along both the *b* and *c* directions (as inferred from the *T*–O–*T* angles).

Given the absence of proper mineral description in the literature, tschermakite $\square Ca_2(Mg_3Al_2)(Si_6Al_2)O_{22}(OH)_2$, ferri-tschermakite $\square Ca_2(Mg_3Fe^{3+}_2)(Si_6Al_2)O_{22}(OH)_2$ and ferro-ferri-tschermakite, $\square Ca_2(Fe^{2+}_3Fe^{3+}_2)(Si_6Al_2)O_{22}(OH)_2$, have to be considered as named amphiboles (Burke & Leake, 2004) and potential new minerals.

Of the 25 analysis reported by Deer *et al.* (1997) with reference to the tschermakite–ferro-tschermakite series (Table 12, pp. 248–249), only nine fit the stoichiometric requirement for C cations fixed by Hawthorne *et al.* (2012). Of those, five can be referred to as ferro-tschermakite: #15 from a garnet–staurolite amphibolite at Ovala (Gabon; Demange, 1976), #17 from a metacarbonate rock at Waits River (Vermont; Léger & Ferry, 1991), #19 from a hornblende schist at Lake Kutemajärvi (Finland; Seitsaari, 1951), #22 from an amphibolite at Permiö (Finland; Seitsaari, 1952), and #24a from an almandine–biotite–chlorite gneiss at Joyceville (Massachusetts; Doolan *et al.*, 1978), which is closest to the end-member composition. Hawthorne & Grundy (1973) report a ferro-tschermakite from the Frood Mine, Sudbury, Canada, that is close to the composition reported here. Only analysis #14 in Deer *et al.* (1997), which refer to a sample from a gneissose quartz-diorite at Furudono, Gosaisyo-Takanuki district (Japan; Ogura, 1958), where $Fe^{3+} = 0.669$ and $Al = 0.612$ apfu, conforms to the ferri-dominant species.

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