



Article

Ferri-fluoro-katophorite from Bear Lake diggings, Bancroft area, Ontario, Canada: a new species of amphibole, ideally $\text{Na}(\text{NaCa})(\text{Mg}_4\text{Fe}^{3+})(\text{Si}_7\text{Al})\text{O}_{22}\text{F}_2$

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Abstract

Ferri-fluoro-katophorite is the second species characterised involving the rootname katophorite in the sodium–calcium subgroup of the amphibole supergroup. The mineral and its name were approved by the International Mineralogical Association Commission on New Minerals, Nomenclature and Classification, IMA2015-096. It was found in the Bear Lake diggings, Bancroft area, Ontario, Canada, where coarse euhedral crystals of amphibole, phlogopite, sanidine solid-solution (now coarsely exsolved to microcline perthite), titanite, augite, zircon and fluorapatite crystallised from a low-viscosity silicocarbonatitic magma of crustal origin. Greenish grey prismatic crystals of ferri-fluoro-katophorite generally protrude from the walls into a body of coarsely crystalline calcite, but they also occur away from the walls, completely enclosed by calcite. The empirical formula derived from electron microprobe analysis and single-crystal structure refinement is: $^A(\text{Na}_{0.55}\text{K}_{0.32})_{\Sigma 0.87}^B(\text{Na}_{0.79}\text{Ca}_{1.18}\text{Mn}_{0.03}^{2+})_{\Sigma 2.00}^C(\text{Mg}_{3.29}\text{Mn}_{0.02}^{2+}\text{Fe}_{1.19}\text{Fe}_{0.31}^{3+}\text{Al}_{0.09}\text{Ti}_{0.08}^{4+}\text{Li}_{0.02})_{\Sigma 5.00}^T(\text{Si}_{7.39}\text{Al}_{0.61})_{\Sigma 8.00}\text{O}_{22}^W[\text{F}_{1.23}(\text{OH})_{0.77}]_{\Sigma 2.00}$. Ferri-fluoro-katophorite is biaxial (–), with $\alpha = 1.640(2)$, $\beta = 1.652(2)$, $\gamma = 1.658(2)$, $2V_{\text{meas.}} = 68.9(2)^\circ$ and $2V_{\text{calc.}} = 70.1^\circ$. The unit-cell parameters are $a = 9.887(3)$, $b = 18.023(9)$, $c = 5.292(2)$ Å, $\beta = 104.66(3)^\circ$, $V = 912.3(6)$ Å³, $Z = 2$ and space group $C2/m$. The strongest ten lines in the powder X-ray pattern [d values (in Å) $I(hkl)$] are: 2.708, 100, (151); 2.388, 74, (131); 3.139, 72, (310); 8.449, 69, (110); 2.540, 65, ($\bar{2}02$); 2.591, 53, (061); 2.739, 47, ($\bar{3}31$); 2.165, 45, (261); 3.279, 44, ($\bar{2}40$); 2.341, 43, ($\bar{3}51$).

Keywords: ferri-fluoro-katophorite, new amphibole species, electron-microprobe analysis, optical properties, powder-diffraction pattern, crystal-structure refinement, Bear Lake diggings, Ontario, Canada

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Introduction

We present the complete characterisation of ferri-fluoro-katophorite, ideally $\text{Na}(\text{NaCa})(\text{Mg}_4\text{Fe}^{3+})(\text{Si}_7\text{Al})\text{O}_{22}\text{F}_2$, a new species of amphibole of the sodium–calcium subgroup of the amphibole supergroup. The mineral and its name were approved by the International Mineralogical Association (IMA) Commission on New Minerals, Nomenclature and Classification (CNMNC), vote 2015-096. Hawthorne *et al.* (2006) characterised a series of amphiboles from the Bear Lake diggings, Bancroft area, Ontario, Canada (44°53'N, 78°19'W). Two of them (BL10 and BL11) were classified as 'potassian-fluor-magnesian-katophorite'. According to the nomenclature rules now in force, root names are assigned to $^C(\text{MgAl})$ compositions (Hawthorne *et al.*, 2012), and hence BL10 and BL11 must now be named ferri-fluoro-katophorite. A systematic work characterising all the missing (or named; Burke and Leake, 2004) amphibole species is in progress after the publication of that report, and sample

BL11 was used to complete the mineral description for ferri-fluoro-katophorite.

Electron-microprobe analyses (EMP), secondary ion mass spectrometry (SIMS) and structure refinement (SREF) for this sample were reported by Hawthorne *et al.* (2006). In the present work, the analytical data have been optimised according to current knowledge of amphibole crystal-chemistry. The holotype material of ferri-fluoro-katophorite is deposited in the mineral collection of the Department of Natural History, Royal Ontario Museum, Canada, catalogue number M57071.

Occurrence and optical properties

The Bear Lake diggings are located 8.4 km west of Tory Hill, Monmouth Township, in the Bancroft District of southeastern Ontario, Canada. They are underlain by rocks of the Glamorgan complex, consisting mostly of quartzofeldspathic gneiss, amphibolite and marble (Armstrong and Gittins, 1968).

The complex equilibrated at amphibolite grade during the Elzevirian compressive pulse of the Grenvillian collisional orogeny, at ~1280–1300 Ma (McLelland *et al.* 2010). The supra-crustal rocks, buried to 25 km or so, record a temperature of 725–750°C (Anovitz and Essene, 1990; Streepey *et al.*, 1997). Towards the end of the Grenville event, at the Late Ottawa stage, the

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gravitational collapse of the overthickened crust led to the rise of the asthenosphere and of mantle-derived fluids, which induced the local melting of marble units. The resulting calcite dykes were emplaced between 1070 and 1040 Ma ago, at a stage of regional extension. They are steep and subparallel, and extend approximately east–west. They are typically 1 to 2 metres across, and pinch out at irregular intervals in an *en échelon* fashion (Vertolli *et al.*, 1998). The carbonatitic melt aggressively dissolved adjacent gneissic rocks, and in this way became a crustally derived silicocarbonatitic melt.

Coarse euhedral crystals of amphibole (samples BL10 and BL11), phlogopite, sanidine solid-solution (now coarsely exsolved to microcline perthite), titanite, augite, zircon and fluorapatite crystallised from this low-viscosity magma. These crystals (up to 8 cm long along *c*) generally protrude from the walls into the body of coarsely crystalline calcite, but they also are found away from the walls, completely enclosed by calcite, suggestive of rapid freezing of the silicocarbonatitic magma. The temperature of crystallisation of the assemblage was above the crest of the alkali feldspar solvus (i.e. above 625°C).

The refined and analysed crystal used in this work was taken from rock specimen BL11. It has a composition close to the end-member, and has the code 762 in the amphibole database of the CNR-IGG Pavia.

In the type specimen, ferri-fluoro-katophorite occurs as greenish grey prismatic to lamellar crystals with perfect {110} cleavage. The streak is grey and the tenacity is brittle.

A spindle stage was used to orient a crystal for measurement of refractive indices and 2V 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-polarised light ($\lambda = 590 \text{ cm}^{-1}$), ferri-fluoro-katophorite is pleochroic: *X* = very light grey, *Y* = medium grey, *Z* = light grey, non fluorescent, and has a vitreous lustre. It is biaxial (–), $\alpha = 1.640(2)$, $\beta = 1.652(2)$, $\gamma = 1.658(2)$, $2V_{\text{meas.}} = 68.9(5)$ and $2V_{\text{calc.}} = 70.1^\circ$. The orientation is: $X \wedge a = 45.4^\circ$ (in β obtuse), $Y \parallel b$, $Z \wedge c = 30.7^\circ$ (in β acute).

Single-crystal and powder diffraction analysis

Diffraction data for a prismatic single-crystal fragment $220 \mu\text{m} \times 220 \mu\text{m} \times 300 \mu\text{m}$ in size were collected in the θ range 2–30° using a Philips PW1100 diffractometer with graphite-monochromatised MoK α X-radiation ($\lambda = 0.7107 \text{ \AA}$). The scan width and the scan speed used were 2.40° and $0.06^\circ\text{sec}^{-1}$, respectively. Two monoclinic equivalents (*hkl* and *h-kl*) were collected. Intensities were corrected for Lorentz and polarisation effects and for absorption (ψ -scan method; North *et al.*, 1968) and then merged, giving 1384 unique reflections ($R_{\text{int}} = 2.1\%$). The 1059 reflections with $I_o > 3\sigma(I)$ were considered as observed during unweighted full-matrix least-squares refinement on *F*. Scattering curves for fully ionised chemical species were used at sites where chemical substitutions occur; neutral *vs.* ionised scattering curves were used at the *T* and anion sites [except O(3)] (cf. Oberti *et al.* (1992) for more details on the procedure). A residual corresponding to the H atom was found in the difference-Fourier map and inserted in the model with a fixed occupancy equal to 0.80 atoms per formula unit (apfu) and a fixed B_{eq} atom-displacement parameter equal to 1.0 \AA^2 . Full-matrix least-squares refinement on $I > 3\sigma(I)$ converged to $R_{\text{obs}} = 1.7\%$ and $R_{\text{all}} = 3.1\%$. Details concerning data collection and structure refinement are provided in

Table 1. Miscellaneous information on data collection and structure refinement of ferri-fluoro-katophorite.

Crystal data	
Ideal formula	Na(NaCa)(Mg ₄ Fe ³⁺)(Si ₇ Al)O ₂₂ F ₂
Crystal dimensions (mm)	0.30 × 0.22 × 0.22
Crystal system, space group	Monoclinic, <i>C2/m</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	9.887(3), 18.023(9), 5.292(2)
β (°)	104.66(3)
<i>V</i> (Å ³)	912.3(6)
<i>Z</i>	2
Calculated density (g cm ⁻³)	3.19
μ (mm ⁻¹)	2.56
Data collection	
Crystal description	prism
Instrument	PHILIPS PW1100, punctual detector
Radiation type, wavelength (Å)	MoK α , $\lambda = 0.7107$
θ range (°)	2–30
Absorption correction	ψ scan
T_{min} , T_{max}	0.73, 0.81
No. of measured, independent and observed [$I > 3\sigma(I)$] reflections	2762, 1384, 1059
R_{int}	0.021
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.705
Data completeness (%)	100
Indices range of <i>h</i> , <i>k</i> , <i>l</i>	–13 ≤ <i>h</i> ≤ 13; –24 ≤ <i>k</i> ≤ 24; 0 ≤ <i>l</i> ≤ 7
Refinement	
Refinement method	Full matrix, unweighted least squares on <i>F</i>
No. of reflections, parameters, restraints	1059, 126, 0
R_1 [$I > 2\sigma(I)$], R_1 (all)	0.017, 0.031
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e ⁻ Å ⁻³)	0.84, –0.60

Table 1. Refined atom coordinates and displacement parameters, and selected bond lengths and angles are given in Tables 2 and 3, respectively. Observed structure factors have been deposited together with the cif as Supplementary material (see below).

The *a:b:c* ratio calculated from the unit cell parameters is 0.549:1:0.294

Powder X-ray diffraction data (CuK α , $\lambda = 1.54178 \text{ \AA}$) were obtained using the *XPREP* utility of *SAINTE* (Bruker, 2003), which generates a 2D powder diffractogram (Debye-Scherrer technique) starting from the F^2 collected on the single crystal and taking into account solely the information concerning the unit-cell dimensions and the Laue symmetry. No Lorentz and polarisation corrections were applied. Data are given in Table 4.

Chemical analysis

Chemical analysis (10 points) on the crystal used for structure refinement was done using a Cameca SX-100 electron microprobe (wavelength-dispersive spectroscopy mode, 15 kV, 20 nA, count time 20 s and 5 μm beam diameter). The Li content was measured by SIMS analysis (Ottolini *et al.*, 1993). The standards used were: Si and Ca: diopside (TAP); Ti: titanite (LPET); Al: andalusite (TAP); 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); and Cl: tugtupite (LPET). Both Cl and Ni were below the detection limits. The Fe³⁺/Fe_{tot} ratio was calculated based on SREF results for the *A*-site occupancy (and hence for the total number of cations), and the amount of H₂O used in the calculation is that needed to obtain F + OH + Cl = 2 apfu (atoms per formula unit). The oxide wt.% and the calculated unit-formula are

Table 2. Atom coordinates, refined site-scattering (ss, epfu) values and atom-displacement parameters (B_{eq} , \AA^2 ; β_{ij} $\times 10^4$) for ferri-fluoro-katophorite crystal 762.

Site	ss*	x/a	y/b	z/c	B_{eq}	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)		0.11015(13)	0.08652(7)	0.2169(2)	0.64(3)	17	6	49	-2	9	-1
O(2)		0.11940(12)	0.17056(7)	0.7284(2)	0.69(3)	14	7	62	-1	5	-2
O(3)	17.44(8)	0.1054(2)	0	0.7123(3)	0.86(4)	23	7	77	-	9	-
O(4)		0.36355(14)	0.24902(7)	0.7943(2)	0.89(3)	29	6	89	-4	20	-3
O(5)		0.34776(14)	0.13327(7)	0.0970(3)	0.99(3)	18	12	77	1	9	13
O(6)		0.34358(13)	0.11806(7)	0.5943(3)	0.85(3)	19	8	78	0	12	-8
O(7)		0.3385(2)	0	0.2925(4)	1.03(4)	24	5	137	-	8	-
T(1)		0.27989(5)	0.08494(2)	0.29849(9)	0.454(9)	12	4	42	-1	4	-1
T(2)		0.28869(5)	0.17153(2)	0.80563(9)	0.472(9)	12	4	43	-1	7	0
M(1)	29.18(11)	0	0.08891(4)	1/2	0.60(2)	19	5	46	-	11	-
M(2)	38.53(11)	0	0.17925(3)	0	0.569(13)	14	5	57	-	11	-
M(3)	14.56(4)	0	0	0	0.53(2)	18	4	42	-	5	-
M(4)	33.31(14)	0	0.27788(4)	1/2	1.02(2)	32	7	114	-	38	-
A	3.66(2)	0	1/2	0	1.81(11)	39	20	179	-	62	-
A(m)	7.49(8)	0.0419(4)	1/2	0.0927(7)	2.42(8)	57	25	221	-	61	-
A(2)	1.06(9)	0	0.469(2)	0	2.73(5)						
H	0.8**	0.188(6)	0	0.768(10)	1.0						

*ss – site scattering in electrons per formula unit (epfu).
 **Kept fixed to the value obtained from the analysis.

Table 3. Selected interatomic distances (\AA), angles ($^\circ$), tetrahedral and octahedral angle variances (TAV, OAV, $^\circ\text{\AA}^2$) and quadratic elongations (TQE, OQE) according to Robinson *et al.* (1971) for ferri-fluoro-katophorite crystal 762.

T(1)–O(1)		1.6238(14)	T(2)–O(2)		1.6193(14)	M(4)–O(2)	×2	2.423(2)
T(1)–O(5)		1.6454(14)	T(2)–O(4)		1.589(2)	M(4)–O(4)	×2	2.354(2)
T(1)–O(6)		1.645(2)	T(2)–O(5)		1.655(2)	M(4)–O(5)	×2	2.784(2)
T(1)–O(7)		1.6399(11)	T(2)–O(6)		1.6676(14)	M(4)–O(6)	×2	2.559(2)
<T1–O>		1.638	<T2–O>		1.633	<M(4)–O>		2.530
TAV		6.55	TAV		19.90			
TQE		1.0015	TQE		1.0048			
M(1)–O(1)	×2	2.0635(14)	M(2)–O(1)	×2	2.159(2)	M(3)–O(1)	×4	2.074(2)
M(1)–O(2)	×2	2.0730(14)	M(2)–O(2)	×2	2.0842(14)	M(3)–O(3)	×2	2.052(2)
M(1)–O(3)	×2	2.0794(14)	M(2)–O(4)	×2	1.983(2)	<M(3)–O>		2.067
<M(1)–O>		2.072	<M(2)–O>		2.076	OAV		52.95
OAV		41.95	OAV		34.44	OQE		1.0165
OQE		1.0127	OQE		1.0112			
A–O(5)	×4	2.948(2)	A(m)–O(5)	×2	3.079(4)	A(2)–O(5)	×2	2.51(3)
A–O(6)	×4	3.138(2)	A(m)–O(5)	×2	2.919(3)	A(2)–O(6)	×2	2.79(2)
A–O(7)	×2	2.490(2)	A(m)–O(6)	×2	2.757(4)	A(2)–O(7)	×2	2.551(8)
<A–O>		2.932	A(m)–O(7)		2.498(6)	<A(2)–O>		2.619
			A(m)–O(7)		3.168(6)			
O(3)–H		0.79(7)	A(m)–O(7)		2.603(6)	M(1)–M(2)		3.1067(12)
			<A(m)–O>		2.864	T(1)–O(5)–T(2)		135.95(8)
						T(1)–O(6)–T(2)		137.47(8)
O(5)–O(6)–O(5)		168.05(10)	O(6)–O(7)–O(6)		106.64(10)	T(1)–O(7)–T(1)		137.99(9)

Table 4. Powder X-ray diffraction data for ferri-fluoro-katophorite crystal 762.

l_{calc}	d_{calc}	hkl	l_{calc}	d_{calc}	hkl	l_{calc}	d_{calc}	hkl	l_{calc}	d_{calc}	hkl
13.90	9.011	0 2 0	46.85	2.739	$\bar{3} 3 1$	35.06	2.022	3 5 1	7.08	1.802	0 10 0
69.33	8.449	1 1 0	100.00	2.708	1 5 1			4 0 2			1 9 1
20.31	4.890	$\bar{1} 1 1$	52.55	2.591	0 6 1	7.55	2.003	3 7 0	6.47	1.752	5 1 2
23.54	4.506	0 4 0	65.39	2.540	2 0 2	8.54	1.960	1 9 0	19.60	1.687	$\bar{1} 3 3$
5.70	4.000	1 1 1	8.85	2.388	3 5 0	6.87	1.938	3 5 2			2 8 2
9.58	3.879	$\bar{1} 3 1$	43.21	2.341	$\bar{3} 5 1$			4 2 1	12.05	1.678	3 9 1
74.23	3.388	1 3 1	24.29	2.296	$\bar{1} 7 1$	8.16	1.902	5 1 0			0 2 3
44.28	3.279	2 4 0	28.88	2.282	$\bar{3} 1 2$	7.17	1.881	4 6 1	30.37	1.655	4 6 1
71.54	3.139	3 1 0	10.53	2.213	$\bar{2} 4 2$	11.92	1.864	2 4 2	11.17	1.640	4 8 0
6.00	3.034	$\bar{3} 1 1$	44.60	2.165	2 6 1			$\bar{1} 9 1$	15.00	1.615	1 11 0
37.73	2.950	2 2 1	15.17	2.149	$\bar{3} 3 2$	7.25	1.845	$\bar{1} 7 2$	7.90	1.594	6 0 0
23.23	2.816	3 3 0			2 0 2			4 4 2	27.49	1.581	$\bar{1} 5 3$
									10.55	1.561	4 0 2

Note: the strongest eight reflections are in bold. Only peaks with $l_{rel} \geq 5$ are reported.

Table 5. Chemical composition (average of 10 points) and unit formula* for ferri-fluoro-katophorite (762), and a comparison between observed and calculated site-scattering values.

Oxide	Wt.% (esd)		Apfu		Apfu
SiO ₂	50.46(38)	Na ⁺	0.55	Al ³⁺	0.09
TiO ₂	0.74(5)	K ⁺	0.32	Fe ³⁺	0.31
Al ₂ O ₃	4.02(12)	Sum A	0.87	Ti ⁴⁺	0.08
Fe ₂ O ₃	2.84			Mg ²⁺	3.29
FeO	9.68	Na ⁺	0.79	Mn ²⁺	0.02
[FeO] _{tot}	[12.24(41)]	Ca ²⁺	1.18	Fe ²⁺	1.19
MnO	0.40(5)	Mn ²⁺	0.03	Zn ²⁺	–
MgO	15.06(39)	Sum B	2.00	Li ⁺	0.02
ZnO	0.03(2)			Sum C	5.00
Li ₂ O	0.04	Si ⁴⁺	7.39		
CaO	5.53(40)	Al ³⁺	0.61	(OH) ⁻	0.77
Na ₂ O	4.70(6)	Sum T	8.00	F ⁻	1.23
K ₂ O	1.69(2)			Sum W	2.00
H ₂ O*	0.79				
F	2.66(29)				
O = F	-1.12	C	82.27		
Total	99.52	B	33.31		
		A	12.20		
		Σ cations	127.78		
		W	17.45		

*calculated based on 15.87 cations and 24 (O, OH, F, Cl) with (OH + F + Cl) = 2 apfu. esd – estimated standard deviation.

Table 6. Site populations* for ferri-fluoro-katophorite, crystal 762.

Site	Site population (apfu)	Site scattering (epfu)		Mean bond length (Å)	
		Refined	Calculated	Refined	Calculated
T(1)	3.39 Si ⁴⁺ + 0.61 Al ³⁺			1.638	1.637
T(2)	4.00 Si ⁴⁺				
M(1)	1.63 Mg ²⁺ + 0.37 Fe ²⁺	29.18	29.18	2.072	2.071
M(2)	0.87 Mg ²⁺ + 0.63 Fe ²⁺ + 0.02 Mn ²⁺ + 0.31 Fe ³⁺ +0.09 Al ³⁺ + 0.08 Ti ⁴⁺	38.53	38.31	2.076	2.075
M(3)	0.79 Mg ²⁺ + 0.19 Fe ²⁺ + 0.02 Li ⁺	14.56	14.48	2.067	2.072
ΣC cations		82.27	81.97		
B cations	0.79 Na ⁺ + 1.18 Ca ²⁺ + 0.03 Mn ²⁺	33.31	33.04		
A cations	0.55 Na ⁺ + 0.32 K ⁺	12.20	12.13		
W anions	1.23 F ⁻ + 0.77 (OH) ⁻	17.45	17.23		

*Hawthorne *et al.* (1995).

reported in Table 5. The proposed empirical formula for crystal 762 is: ^A(Na_{0.55}K_{0.32})_{Σ0.87}^B(Ca_{1.18}Na_{0.79}Mn_{0.03})_{Σ2.00}^C(Mg_{3.29}Fe_{1.19}Fe_{0.31}Al_{0.09}Ti_{0.08}Mn_{0.02}Li_{0.02})_{Σ5.00}^T(Si_{7.39}Al_{0.61})_{Σ8.00}O₂₂^W[F_{1.23}(OH)_{0.77}]_{Σ2.00} (where the dominant cations or anions in the relevant homovalent series are in bold). The simplified end-member formula is ^ANa^B(NaCa)^C(Mg₄Fe³⁺)^T(Si₇Al)_{0.22}^WF₂, which requires SiO₂: 49.33, Al₂O₃: 5.98, Fe₂O₃: 9.36, MgO: 18.90, Na₂O: 7.27, F: 4.46, F=O: -1.88, total = 100.00 wt.%.

Based on this empirical formula, the calculated density of ferri-fluoro-katophorite BL11 is 3.19 g/cm³. The compatibility index (1 - (K_P/K_C); Mandarino, 1981) is -0.007 (superior).

Comments on the crystal-chemistry of ferri-fluoro-katophorite

Site populations were derived from the unit formula and the results of the structure refinement and are given in Table 6.

Table 7. Comparison of the optical and crystallographic properties for the two known amphiboles related to the root name katophorite.

	Ferri-fluoro-katophorite BL 11	Katophorite AMNH H32734
	This work	Oberti <i>et al.</i> (2015)
Colour	Greenish grey	Pale blue
Optical class	Biaxial (-)	Biaxial (-)
Pleochroism	α = very light grey, β = medium grey, γ = light grey	α = pale blue, β = light-blue-green, γ = colourless
Orientation	X ∧ a = 45.4° (β obtuse), Y // b, Z ∧ c = 30.7° (β acute)	X ∧ a = 30.6° (β obtuse), Y // b, Z ∧ c = 15.8° (β acute)
Absorption	Y > Z > X	Y > X > Z
α	1.640(2)	1.638(2)
β	1.652(2)	1.642(2)
γ	1.658(2)	1.644(2)
2V _{obs}	68.9(5)°	73(1)°
a (Å)	9.887(3)	9.8573(8)
b (Å)	18.023(9)	17.9617(15)
c (Å)	5.292(2)	5.2833(4)
β (°)	104.66(3)	104.707(2)
V (Å ³)	912.3(6)	904.8(1)
<T(1)-O> (Å)	1.638	1.643
<T(2)-O> (Å)	1.633	1.634
<M(1)-O> (Å)	2.072	2.067
<M(2)-O> (Å)	2.076	2.058
<M(3)-O> (Å)	2.067	2.083
<M(4)-O> (Å)	2.530	2.520

There is excellent agreement between the refined site-scattering values (ss, electrons per formula unit) and the corresponding mean bond lengths (mbl, Å) and those calculated based on the assigned site-populations

The results show that Ti⁴⁺ is ordered at the M(2) site, together with all the other high-charge cations, which is in accord with the absence of an oxo component (O²⁻) at the O(3) site; this result validates the constraint (OH,F,Cl) = 2 apfu used to calculate the unit formula. As already discussed in Hawthorne *et al.* (2006), and explained on the basis of 'local' bond-valence requirements, the A cations are strongly ordered at the A(m) subsite, where the interactions with F are stronger (Oberti *et al.*, 2007).

Relation with other species and a review of related compositions

The sample designated 'ferri-katophorite' by Pushcharovski *et al.* (2003) has the formula ^A(Na_{0.87}K_{0.13})^B(Na_{1.18}Ca_{0.82})^C[^{M(1)}(Mg_{1.41}Fe_{0.42}Ti_{0.17})^{M(2)}(Fe_{1.31}Mg_{0.69})^{M(3)}(Mg_{0.60}Fe_{0.38}Mn_{0.02})]^T[^{T(1)}(Si_{3.16}Al_{0.84})^{T(2)}Si₄]_{0.22}^W(O_{1.05}OH_{0.66}F_{0.29}), which according to current nomenclature (Hawthorne *et al.*, 2012) is a member of the oxo-amphiboles group, and should, in principle, deserve a new rootname. However, this mineral has never been officially approved by IMA-CNMNC, and the proposed formula has major crystal-chemical problems because the sum of the highly charged cations at the M(1) site does not compensate for the oxo component.

Therefore, the only published composition corresponding to katophorite is the recently approved katophorite from Myanmar (IMA 2013-140; Oberti *et al.*, 2015), which has the unit formula ^A(Na_{0.85}K_{0.04})_{Σ0.89}^B(Ca_{1.22}Na_{0.78})_{Σ2.00}^C(Mg_{3.76}Al_{0.43}Fe_{0.30}Ca_{0.27}Fe_{0.18}Li_{0.05}Ti_{0.01})_{Σ5.00}^T(Si_{7.21}Al_{0.79})_{Σ8.00}O₂₂^W[(OH)_{1.67}O_{0.30}F_{0.03}]_{Σ2.00}.

A comparison is provided in Table 7 between the optical and crystallographic properties of these two known species related to the rootname katophorite.

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