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Fluoro-sodic-ferropedrizite, $NaLi_2(Fe^{2+}_2Al_2Li)Si_8O_{22}F_2$, a new mineral of the amphibole group from the Sutlug River, Tuva Republic, Russia: description and crystal structure

R. OBERTI[1,]*, M. BOIOCCHI[2], N. A. BALL[3] AND F. C. HAWTHORNE[3]

[1] CNR-Istituto di Geoscienze e Georisorse, unità di Pavia, via Ferrata 1, I-27100 Pavia, Italy
[2] Centro Grandi Strumenti, Università di Pavia, via Bassi 21, I-27100 Pavia, Italy
[3] Department of Geological Sciences, University of Manitoba, Winnipeg, Manitoba, R3T 2N2, Canada

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ABSTRACT

Fluoro-sodic-ferropedrizite, ideally $^{A}Na^{B}Li_2{}^{C}(Fe^{2+}_2Al_2Li)^{T}Si_8O_{22}{}^{W}F_2$, is a new mineral of the amphibole group from the Sutlug River, Tuva Republic, Russia. It occurs at the endogenic contact of a Li-pegmatite with country rocks near to a diabase dyke and formed by reaction of the pegmatitic melt with the country rock. Fluoro-sodic-ferropedrizite occurs as prismatic to acicular crystals, ranging in length from 0.1–3 cm and widths of up to 50 μm. Crystals occur in parallel to sub-parallel aggregates up to 5 mm across in a matrix of calcite and plagioclase feldspar. Crystals are pale bluish-grey with a greyish-white streak. Fluoro-sodic-ferropedrizite is brittle, has a Mohs hardness of ~6 and a splintery fracture; it is non-fluorescent with perfect {110} cleavage, no observable parting, and has a calculated density of 3.116 g cm^{-3}. In plane-polarized light, it is pleochroic, X = pale purple-grey, Y = light grey, Z = colourless; $X \wedge a = 71.2°$ (in β acute), $Y \parallel b$, $Z \wedge c = 83.4°$ (in β obtuse). Fluoro-sodic-ferropedrizite is biaxial positive, $\alpha = 1.642(1)$, $\beta = 1.644(1)$, $\gamma = 1.652(1)$; $2V_{(obs)} = 68.0(3)°$, $2V_{(calc)} = 56.4°$.

Fluoro-sodic-ferropedrizite is monoclinic, space group $C2/m$, $a = 9.3720(4)$ Å, $b = 17.6312(8)$ Å, $c = 5.2732(3)$ Å, $\beta = 102.247(4)°$, $V = 851.5(2)$ Å^3, $Z = 2$. The strongest ten X-ray diffraction lines in the powder pattern are (d in Å,(I),(hkl)): 8.146,(10),(110); 2.686,(9),(151); 3.008,(8),(310); 4.430,(7),(021); 2.485,(6),($\bar{2}02$); 3.383,(4),(131); 2.876,(3),($\bar{1}51$, $\bar{3}11$); 2.199,(3),($\bar{3}12$); 4.030,(2),(111) and 3.795,(2),($\bar{1}31$). Analysis by a combination of electron microprobe and crystal-structure refinement gives SiO_2 59.81, Al_2O_3 12.66, TiO_2 0.09, FeO 10.32, MgO 5.56, MnO 0.73, ZnO 0.17, CaO 0.20, Na_2O 2.81, Li_2O 4.80, F 2.43, H_2O_{calc} 1.10, sum = 99.65 wt.%. The formula unit, calculated on the basis of 24(O,OH,F) is $^{A}(Na_{0.68})^{B}(Li_{1.92}Na_{0.05}Ca_{0.03})^{C}(Fe^{2+}_{1.16}Mg_{1.10}Mn^{2+}_{0.08}Zn_{0.02}Al_{1.97}Ti_{0.01}Li_{0.66})$ $^{T}(Si_{7.98}Al_{0.02})O_{22}{}^{W}(F_{1.03}OH_{0.97})$. Crystal-structure refinement shows Li to be completely ordered at the $M(3)$ and $M(4)$ sites. Fluoro-sodic-ferropedrizite, ideally $^{A}Na^{B}Li_2{}^{C}(Fe^{2+}_2Al_2Li)^{T}Si_8O_{22}{}^{W}F_2$, is related to the theoretical end-member 'sodic-pedrizite', $^{A}Na^{B}Li_2{}^{C}(Mg_2Al_2Li)^{T}Si_8O_{22}{}^{W}(OH)_2$, by the substitutions $^{C}Fe^{2+} \rightarrow {}^{C}Mg$ and $^{W}F \rightarrow {}^{W}(OH)$.

KEYWORDS: Fluoro-sodic-ferropedrizite, new amphibole, electron microprobe analysis, optical properties, crystal-structure refinement, Sutlug river, Tuva Republic, Russia.

Introduction

ALTHOUGH Li has long been known as a major constituent in amphiboles, it is only in the last 20 y that it has been recognized as a major constituent of the C-group cations (Hawthorne *et al.*, 1993), giving rise to several new amphibole

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* E-mail: oberti@crystal.unipv.it
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species: leakeite, $^{A}\mathrm{Na}^{B}\mathrm{Na}_2{}^{C}(\mathrm{Mg}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$ (Hawthorne *et al.*, 1992); kornite, $^{A}\mathrm{K}^{B}\mathrm{Na}_2{}^{C}(\mathrm{Mg}_2\mathrm{Mn}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$ (Armbruster *et al.*, 1993); fluoro-ferroleakeite, $^{A}\mathrm{Na}^{B}\mathrm{Na}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$ (Hawthorne *et al.*, 1996*a*)**;** potassic-leakeite, $^{A}\mathrm{K}^{B}\mathrm{Na}_2{}^{C}(\mathrm{Mg}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$ (Matsubara *et al.*, 2002); dellaventuraite, $^{A}\mathrm{Na}^{B}\mathrm{Na}_2{}^{C}(\mathrm{MgMn}^{3+}_2\mathrm{LiTi}^{4+})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{O}_2$ (Tait *et al.*, 2005).

Investigation of a series of episyenites from the east sector of the Pedriza massif, Sierra de Guardarrama, Spanish Central System, Spain, led to the discovery of amphiboles with complete solid solution of Na and Li at the *M*(4) site in the amphibole structure (Oberti *et al.*, 2003*a*). The first new species was described by Caballero *et al.* (1998) as clino-sodic-ferri-ferroholmquistite, and many other new species with Fe-rich compositions related to the root-name sodic-pedrizite, $^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Mg}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$ (with Li dominant at the *M*(3) and *M*(4) sites) were described by Oberti *et al.* (2003*b*). However, the then extant amphibole classification scheme (Leake *et al.*, 1997) was unsuited to classify amphiboles with ^{B}Na and ^{B}Li in solid solution at the *M*(4) site (Hawthorne and Oberti, 2006, 2007*b*), and the names originally given to these Li-bearing amphiboles from Pedriza were redefined according to Leake *et al.* (2003) and Burke and Leake (2004), giving rise to ferriottoliniite, $^{A}\square^{B}(\mathrm{NaLi})^{C}(\mathrm{Mg}_3\mathrm{Fe}^{3+}_2)^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$, and ferriwhittakerite, $^{A}\mathrm{Na}^{B}(\mathrm{NaLi})^{C}(\mathrm{Mg}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$. The discovery of these amphiboles, and the observation that the charge arrangement of clinoholmquistite is always associated with high Fe contents, prompted further work on amphiboles from the classic localities where holmquistite and 'clinoholmquistite' were discovered (Ginzburg, 1965). As a result, 'clinoholmquistite' was discredited and the new amphibole fluoro-sodic-pedrizite, $^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Mg}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$, was described (Oberti *et al.*, 2005). Because of the confusion surrounding the names of the pedrizite-group amphiboles, generally given by $^{A}\mathrm{Na}^{B}\mathrm{Li}_2\,C_5\,{}^{T}\mathrm{Si}_8\mathrm{O}_{22}W_2$ (C = Li, Mg, Fe^{2+}, Al, Fe^{3+}; W = (OH), F), we list current names and compositions in Table 1. During this work, another new amphibole was discovered, the 'fluoro-ferro-' equivalent of 'sodic-pedrizite', ideally $^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$; a formal description of the amphibole is given here. The new species and the new name have been approved by the International Mineralogical Association Commission on New Minerals and Classification (2008-070). Holotype material is deposited in the Fersman Mineralogical Museum, Moscow, Russia.

Occurrence

The sample containing holotype fluoro-sodic-ferropedrizite (code 64715) was obtained from the Fersman Mineralogical Museum, Russian Academy of Sciences, Moscow, Russia, in order to study all the samples closely related to 67493, the holotype sample of 'clinoholmquistite' (Ginzburg, 1965). The sample was listed as coming from the Sutlug River, Tuva Republic, Russia. It occurs at the endogenic contact of a Li pegmatite with country rocks near to a diabase dyke and formed by reaction of the pegmatitic melt with the country rock. Crystals are prismatic to acicular and range in length from 0.1–3.0 cm with widths of up to 50 µm. They occur in

TABLE 1. Monoclinic $^{M(4)}$Li-bearing amphiboles of the pedrizite type: $^{A}\mathrm{Na}^{B}\mathrm{Li}_2C_5{}^{T}\mathrm{Si}_8\mathrm{O}_{22}W_2$.

Name	End-member formula	Ref.
Sodic-pedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Mg}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$	(1)
Fluoro-sodic-pedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Mg}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$	(2)
Sodic-ferripedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Mg}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$	(3)
Sodic-ferri-ferropedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$	(4)
Fluoro-sodic-ferropedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$	(5)
Sodic-ferropedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Al}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}(\mathrm{OH})_2$	(1)
Fluoro-sodic-ferro-ferripedrizite	$^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Fe}^{3+}_2\mathrm{Li})^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$	(1)

References: (1) Not yet formally described as a species; (2) Oberti *et al.* (2005); (3) Caballero *et al.* (2002); (4) Oberti *et al.* (2003*a*); (5) this work.

parallel to sub-parallel aggregates up to 5 mm across in a matrix of calcite and feldspar.

Physical and optical properties

Fluoro-sodic-ferropedrizite is pale bluish-grey with a vitreous lustre. It has a greyish-white streak and shows no fluorescence under long-wave or short-wave ultraviolet light. Grains are prismatic to acicular [001] and are bounded by {110} cleavage faces with the prism direction terminated by irregular fractures. Fluoro-sodic-ferropedrizite has a Mohs hardness of ~6 and is brittle with a splintery fracture; it has the characteristic perfect {110} cleavage of monoclinic amphiboles, intersecting at ~56º. The calculated density is 3.116 g cm^{-3}.

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 light, fluoro-sodic-ferropedrizite is pleochroic with X = pale purple-grey, Y = light grey, Z = colourless, $X \wedge a = 71.2^\circ$ (in β acute), $Y \parallel b$, $Z \wedge c = 83.4^\circ$ (in β obtuse). It is biaxial positive with indices of refraction $\alpha = 1.642(1)$, $\beta = 1.644(1)$, $\gamma = 1.652(1)$ measured with gel-filtered Na light ($\lambda = 589.9$ nm); $2V_{obs} = 68.0(3)^\circ$, $2V_{calc} = 56.4^\circ$.

Chemical composition

Fluoro-sodic-ferropedrizite was analysed primarily by electron microprobe using a Cameca SX100 operating in the wavelength-dispersive mode with an accelerating voltage of 15 kV, probe current of 10 nA, final beam diameter of 5 μm, peak-count time of 20 s and background-count time of 10 s. The following standards, (X-ray lines and analysing crystals) were used: synthetic fluorophlogopite (F-*K*α on LTAP); jadeite (Na-*K*α on TAP); periclase (Mg-*K*α on LTAP); corundum (Al-*K*α on TAP); wollastonite (Si-*K*α on TAP and Ca-*K*α on LPET); rutile (Ti-*K*α on LPET); Mn metal (Mn-*K*α on LLiF); magnetite (Fe-*K*α on LLiF); Zn metal (Zn-*K*α on LLiF). Data reduction was performed using the φ(ρZ) procedure of Pouchou and Pichoir (1985). Lithium was derived by Structure REFinement (SREF) (see section on crystal-structure refinement). The average of 10 analyses on a single grain is given in Table 2.

Refinement of the crystal structure shows both Fe and Mn to be in the divalent state. The end-member formula is $^{A}\mathrm{Na}^{B}\mathrm{Li}_2{}^{C}(\mathrm{Fe}^{2+}_2\mathrm{Al}_2\mathrm{Li})\,^{T}\mathrm{Si}_8\mathrm{O}_{22}{}^{W}\mathrm{F}_2$, which corresponds to Na_2O 3.76, Li_2O 5.44, FeO 17.44, Al_2O_3 12.37, SiO_2 58.33, F 4.61, less O≡F 1.94, total = 100.00 wt.%. The compatibility index ($1 - K_P/K_C$) is 0.0018 (superior).

X-ray crystallography

The powder-diffraction pattern was recorded from a small fragment on a Gandolfi camera with Fe-filtered Cu-*K*α X-radiation. Cell dimensions were refined from the corrected *d* values; the indexed powder pattern and refined cell dimensions are given in Table 3. Peak intensities reported in Table 3 are those estimated by eye from the darkening on the film. The possible space groups are *C*2/*m*, *C*2 and *Cm*; crystal-structure refinement confirmed the space group *C*2/*m*.

TABLE 2. Chemical composition (wt.%) and unit formula (a.p.f.u.) for fluoro-sodic-ferropedrizite.

SiO_2	59.81	Si	7.98
TiO_2	0.09	$^{[4]}Al$	0.02
Al_2O_3	12.66	Sum *T*	8.00
FeO	10.32		
MnO	0.73	$^{[6]}Al$	1.97
ZnO	0.17	Ti^{4+}	0.01
MgO	5.56	Fe^{2+}	1.16
CaO	0.20	Mn	0.08
Na_2O	2.81	Zn	0.02
Li_2O*	4.80	Mg	1.10
H_2O**	1.10	Li	0.66
F	2.43	Sum *C*	5.00
sub total	100.68		
less O≡F	1.02	Ca	0.03
Total	99.66	Na	0.05
		Li	1.92
		Sum *B*	2.00
		Na	0.68
		Sum *A*	0.68
		F	1.03
		OH	0.97
		Sum *W*	2.00

* calculated from SREF results
** calculated based on (OH+F) = 2 a.p.f.u.

TABLE 3. X-ray powder-diffraction data for fluoro-sodic-ferropedrizite.

I_{obs}	I_{SREF}	d_{obs} (Å)	d_{calc} (Å)	*hkl*	I_{obs}	I_{SREF}	d_{obs} (Å)	d_{calc} (Å)	*hkl*
10	91	8.146	8.129	110	1	8	2.431	2.428	170
1	6	4.773	4.786	$\bar{1}11$	2	18	2.246	2.247	$\bar{1}71$
1	6	4.573	4.580	200		23	"	2.245	$\bar{3}51$
*7	28	4.430	4.458	021	3	22	2.199	2.200	$\bar{3}12$
60	"	4.407		040	1	13	2.152	2.152	171
2	16	4.030	4.032	111	2	28	2.138	2.138	261
2	23	3.795	3.796	$\bar{1}31$	*2	12	2.070	2.074	$\bar{3}32$
2	24	3.530	3.533	$\bar{2}21$		13	"	2.071	202
4	42	3.383	3.385	131	1	10	1.993	1.992	351
1	13	3.172	3.176	240	*1	4	1.900	1.905	$\bar{3}71$
8	82	3.008	3.009	310		8		1.901	421
2	14	2.935	2.938	221	*1	5	1.873	1.877	$\bar{3}52$
* 3	25	2.876	2.876	$\bar{1}51$		9		1.874	242
	18	"	2.874	$\bar{3}11$	1	10	1.823	1.823	$\bar{1}91$
2	24	2.704	2.710	330		6		1.822	510
9	100	2.686	2.685	151	2	11	1.769	1.771	191
1	11	2.611	2.610	$\bar{3}31$	<1	10	1.664	1.663	$\bar{5}12$
1	13	2.583	2.584	002	<1	6	1.649	1.649	$\bar{2}82$
1	21	2.554	2.554	061	2	28	1.624	1.623	461
6	54	2.485	2.487	$\bar{2}02$	<1	9	1.588	1.588	480
					2	26	1.577	1.576	$\bar{1}53$

114.6 mm Debye-Scherrer powder camera with Gandolfi attachment using Ni-filtered Cu radiation (λ Cu-*K*α = 1.54178 Å). Intensities estimated visually. Not corrected for shrinkage, and no internal standard was used.
* lines omitted for unit-cell refinement. Indexed on a = 9.373(3) Å, b = 17.629(6) Å, c = 5.287(2) Å, β = 102.21(3)º, V = 853.8(4) Å^3. I_{SREF} = relative intensities calculated from the structure refinement.

Crystal-structure refinement and crystal chemistry

A single crystal was selected for data collection and SREF based on optical and diffraction properties. Unit-cell dimensions were calculated by least-squares refinement of the d values obtained from 50 rows of the reciprocal lattice by measuring the centroid of gravity of each reflection and of the corresponding antireflection in the range $-60º < 2\theta < 60º$. Two monoclinic equivalents were collected in the 2θ range 4–60º, and corrections were applied for absorption and Lp. Reflections with $I_o > 3\ \sigma(I)$ were considered as observed during an unweighted full-matrix least-squares refinement on F done using a program specifically written at CNR-IGG-PV to deal with complex solid-solutions. Scattering curves for fully ionized scattering 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)]. Crystal data are summarized in Table 4. Table 5 reports the atomic coordinates and the components of the anisotropic-displacement parameters, and Table 6 reports selected interatomic distances and parameters related to the conformation of the double-chain of tetrahedra. A table listing the observed and calculated structure factors has been deposited with the Principal Editor of *Mineralogical Magazine* and is available from www.minersoc.org/pages/e_journals/dep_mat_mm.html.

Site populations and Li quantification were derived from the results of EMP analysis and structure refinement. Previous experience has shown that, based on our knowledge of the crystal chemistry of Li in amphiboles, it is possible to measure the amount and distribution of Li directly by SREF. The refined bond lengths of the tetrahedra indicate that they are occupied solely by Si; the bond-length and site-scattering refined at the $M(1)$ site indicate that all Mg occurs at this site; comparison of the refined and calculated bond distances at the three M octahedra indicates that Fe and Mn are in the divalent state. Based on these constraints and on the results of the EMP analysis, the Li_2O content was

TABLE 4. Miscellaneous information for fluoro-sodic-ferropedrizite.

a (Å)	9.3720(4)	Crystal size (μm)	200 × 200 × 330
b (Å)	17.6312(8)	Radiation/monochromater	Mo-$K\alpha$/Graphite
c (Å)	5.2732(3)	Total no. of reflections	1300
β (º)	102.247(4)	No. unique reflections	984
V (Å^3)	851.5(2)	R_{merge} %	1.80
Sp. Gr.	$C2/m$	R_{obs} %	1.72
Z	2	R_{all} %	3.06
D_{calc} (g cm^{-3})	3.116	Goodness of Fit	0.982
		Largest diff. peak/hole (e Å^{-3})	0.38/−0.31

calculated, and the corresponding value of Li in a.p.f.u. is in agreement with the refined site-scattering values at the $M(3)$ and $M(4)$ sites. The final site populations (Table 7) are also in accord with the crystal-chemical constraint derived for ^{C}Li amphiboles, i.e., ^{A}Na $\geqslant$ ^{C}Li (Oberti *et al.*, 2003*b*). Fluoro-sodic-ferropedrizite has ^{A}Na ordered at the $A(m)$ site, in agreement with the results for all other fluoro-amphiboles (Hawthorne *et al.*, 1996*b*; Hawthorne and Oberti, 2007*a*). The $A-A(m)$ distance is exceptionally long in this sample (0.905(5) Å *vs.* 0.850(8) in fluoro-sodic pedrizite); a large displacement of Na from the central A position is common in ^{C}Li-rich and in ^{B,C}Li-rich compositions, and has been explained by bond-valence requirements (Oberti *et al.* 2003*a*). The presence of more than one F a.p.f.u. at the O(3) site reduces the steric hindrance with the proton, and increases the Na-F interaction, so that the $A(m)-$O(3) distance is particularly short in this composition (2.859(5) Å *vs.* 2.908(8) in fluoro-sodic pedrizite) and O(3) can be considered in the coordination sphere of $^{A(m)}$Na.

Discussion

End-member fluoro-sodic-ferropedrizite has the formula $^{A}\text{Na}^{B}\text{Li}_2{}^{C}(\text{Fe}^{2+}_2\text{Al}_2\text{Li})^{T}\text{Si}_8\text{O}_{22}{}^{W}\text{F}_2$. This may be derived from the still-uncharacterized end-member 'sodic-pedrizite', $^{A}\text{Na}^{B}\text{Li}_2{}^{C}(\text{Mg}_2\text{Al}_2\text{Li})^{T}\text{Si}_8\text{O}_{22}{}^{W}(\text{OH})_2$, by the homovalent

TABLE 5. Atomic coordinates, refined site-scattering values (ss, e.p.f.u.), atomic-displacement parameters (B$_{\text{eq}}$, Å^2; $\beta_{ii} \times 10^4$) for fluoro-sodic-ferropedrizite.

Atom	ss (e.p.f.u.)	x/a	y/b	z/c	B$_{\text{eq}}$	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
O(1)		0.1088(1)	0.0943(1)	0.1986(2)	0.50(2)	12	4	55	0	6	0
O(2)		0.1198(1)	0.1750(1)	0.7416(2)	0.56(2)	13	6	52	0	6	1
O(3)	16.96(4)	0.1173(2)	0	0.6948(3)	0.93(4)	26	7	101	–	7	–
O(4)		0.3773(1)	0.2532(1)	0.7914(2)	0.68(2)	20	4	77	−4	6	0
O(5)		0.3579(1)	0.1290(1)	0.0648(2)	0.77(2)	16	9	64	0	9	13
O(6)		0.3462(1)	0.1234(1)	0.5626(2)	0.85(2)	16	10	65	2	2	−12
O(7)		0.3367(2)	0	0.2875(3)	0.81(4)	20	3	131	–	15	–
$T(1)$		0.2844(1)	0.0879(1)	0.2787(1)	0.35(1)	10	3	35	0	4	0
$T(2)$		0.2974(1)	0.1738(1)	0.7919(1)	0.37(1)	10	3	34	−1	4	−1
$M(1)$	35.29(5)	0	0.0894(1)	½	0.54(1)	18	5	49	–	11	–
$M(2)$	27.50(6)	0	0.1794(1)	0	0.42(1)	11	3	43	–	5	–
$M(3)$	10.41(2)	0	0	0	0.33(1)	14	2	28	–	0	–
$M(4)$	6.92(6)	0	0.2571(3)	½	1.59(1)	40	20	95	–	24	–
A	0.67(3)	0	½	0	3.28(3)	192	9	346	–	219	–
$A(m)$	7.03(7)	0.0715(5)	½	0.1452(9)	2.37(2)	102	15	233	–	114	–
H	1.0(1)	0.195(7)	0	0.730(11)	0.48(8)						

TABLE 6. Selected interatomic distances (Å) and angles (º) in fluoro-sodic-ferropedrizite.

T(1)–O(1)	1.614(1)	*T*(2)–O(2)	1.629(1)
T(1)–O(5)	1.613(1)	*T*(2)–O(4)	1.589(1)
T(1)–O(6)	1.612(2)	*T*(2)–O(5)	1.634(1)
T(1)–O(7)	1.624(1)	*T*(2)–O(6)	1.641(1)
<*T*(1)–O>	1.616	<*T*(2)–O>	1.623
M(1)–O(1) ×2	2.064(1)	*M*(2)–O(1) ×2	1.984(1)
M(1)–O(2) ×2	2.134(1)	*M*(2)–O(2) ×2	1.942(1)
M(1)–O(3) ×2	2.065(1)	*M*(2)–O(4) ×2	1.846(1)
<*M*(1)–O>	2.088	<*M*(2)–O>	1.924
M(3)–O(1) ×4	2.109(1)	*M*(4)–O(2) ×2	2.092(3)
M(3)–O(3) ×2	2.133(2)	*M*(4)–O(4) ×2	2.113(1)
<*M*(3)–O>	2.117	*M*(4)–O(5) ×2	3.126(3)
		M(4)–O(6) ×2	2.612(4)
A–O(5) ×4	2.693(1)	<$^{[6]}$*M*(4)–O>	2.272
A–O(6) ×4	3.274(1)	<$^{[8]}$*M*(4)–O>	2.486
A–O(7) ×2	2.372(2)		
<*A*–O>	2.861	*A*(*m*)–O(5) ×2	3.000(3)
		A(*m*)–O(5) ×2	2.673(2)
O(3)–H	0.717(2)	*A*(*m*)–O(6) ×2	2.683(3)
		A(*m*)–O(7)	2.471(4)
T(1)–O(5)–*T*(2)	135.5(1)	*A*(*m*)–O(7)	2.932(5)
T(1)–O(6)–*T*(2)	142.4(1)	*A*(*m*)–O(7)	2.604(4)
T(1)–O(7)–*T*(1)	145.4(2)	*A*(*m*)–O(3)	2.859(5)
O(5)–O(6)–O(5)	173.7(2)	<$^{[9]}$*A*(*m*)–O>	2.746
O(6)–O(7)–O(6)	113.2(2)	<$^{[10]}$*A*(*m*)–O>	2.758

substitutions $^{C}\mathrm{Fe}^{2+} \rightarrow {}^{C}\mathrm{Mg}$ and $^{W}\mathrm{F} \rightarrow {}^{W}(\mathrm{OH})$. It is worth noting that only the fluoro-species have been found (so far) for $^{C}[(\mathrm{Mg,Fe})^{2+}\mathrm{Al}^{3+}]$ compositions, whereas $^{C}[(\mathrm{Mg,Fe})^{2+}\mathrm{Fe}^{3+}]$ compositions are always poor in F (Table 1). This feature may be geochemically controlled, but also suggests a cooperative dimensional control among the three *M* octahedra. The fluoro-sodic-ferropedrizite

TABLE 7. Site populations, site scattering and mean bond-lengths for fluoro-sodic-ferropedrizite.

Site	Site population (a.p.f.u.)	Site scattering (e.p.f.u.)		Mean bond length (Å)	
		refined	calculated	refined	calculated*
T(1)	0.02 Al + 3.98 Si			1.616	1.619
T(2)	4 Si			1.623	1.628
M(1)	1.11 Mg + 0.87 Fe^{2+} + 0.02 Zn	35.29	36.54	2.088	2.086
M(2)	1.97 Al + 0.02 Fe^{2+} + 0.01 Ti	27.50	26.35	1.924	1.927
M(3)	0.66 Li + 0.26 Fe^{2+} + 0.08 Mn	10.41	10.74	2.117	2.111
Σ*C* sites		73.20	73.63		
B sites	1.91 Li + 0.05 Na + 0.03 Ca	6.92	6.91		
A sites	0.68 Na	7.70	7.45		
W site	1.03 F + 0.97 OH	16.96	17.03		

* based on the models obtained from the IGG-PV amphibole database (Oberti *et al.*, 2007).

described here – ${}^{A}(\mathrm{Na}_{0.68})^{B}(\mathrm{Li}_{1.92}\mathrm{Na}_{0.05}\mathrm{Ca}_{0.03})$ ${}^{C}(\mathrm{Fe}^{2+}_{1.16}\mathrm{Mg}_{1.10}\mathrm{Mn}^{2+}_{0.08}\mathrm{Zn}_{0.02}\mathrm{Al}_{1.97}\mathrm{Ti}_{0.01}\mathrm{Li}_{0.66})$ ${}^{T}(\mathrm{Si}_{7.98}\mathrm{Al}_{0.02})\mathrm{O}_{22}{}^{W}(\mathrm{F}_{1.03}\mathrm{OH}_{0.97})$ – differs only in the Mg/Fe^{2+} ratio from the otherwise compositionally identical fluoro-sodic-pedrizite reported by Oberti *et al*. (2005) – ${}^{A}(\mathrm{Na}_{0.64}\mathrm{K}_{0.01})^{B}(\mathrm{Li}_{1.93}\mathrm{Na}_{0.03}\mathrm{Ca}_{0.04})^{C}(\mathrm{Fe}^{2+}_{0.53}\mathrm{Mg}_{1.81}\mathrm{Mn}^{2+}_{0.02}\mathrm{Zn}_{0.01}\mathrm{Al}_{1.98}\mathrm{Li}_{0.64})^{T}(\mathrm{Si}_{7.96}\mathrm{Al}_{0.04})\mathrm{O}_{22}{}^{W}(\mathrm{F}_{1.10}\mathrm{OH}_{0.90})$. Comparison of the structural parameters for both these amphiboles shows that in the fluoro-sodic-ferropedrizite described here:

(1) the sizes of both tetrahedra, the *M*(2) octahedron and the *M*(4) polyhedron are smaller (0.002, 0.004 and 0.011 Å respectively);

(2) the *A* site is almost unaffected;

(3) the sizes of the *M*(1) and *M*(3) octahedra are larger, in accord with the higher content of ${}^{C}\mathrm{Fe}^{2+}$ (which is ordered at these two sites);

(4) in each structure, the stretching of the double chain of tetrahedra along the *c* axis [as measured by the O(5)–O(6)–O(5) angle] is identical, whereas the stretching along the *b* axis [as measured by O(6)–O(7)–O(6)] is larger by 10º (113.2 *vs*. 112.8º).

These features confirm the strong relation between the size of the *C* cations (in particular, the amount of Fe^{2+}) and the length of the *b* edge observed in amphiboles (Colville *et al*., 1966; Hawthorne, 1983).

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