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THE CRYSTAL CHEMISTRY OF POTASSIC-FERRISADANAGAITE

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ABSTRACT

The crystal structure of potassic-ferrisadanagaite, $(K_{0.66}Na_{0.32})_{\Sigma 0.98}$ $(Ca_{1.73}Na_{0.23}Mn_{0.04})_{\Sigma 2.00}$ $(Mg_{0.55}Fe^{2+}_{2.16}Mn_{0.25}Fe^{3+}_{1.11}Al_{0.78}Ti_{0.19})_{\Sigma 5.00}$ $(Si_{5.33}Al_{2.67})_{\Sigma 8.00}$ O_{22} $[(OH)_{1.21}F_{0.41}O_{0.38}]_{\Sigma 2.00}$, *a* 9.9309(1), *b* 18.0949(3), *c* 5.3681(1) Å, β 105.19(2)°, *V* 930.9(1) Å^3, *C*2/*m*, *Z* = 2, *D*(calc) = 3.36 g/cm^3, has been refined using the Rietveld method to the following values: $R_p = 3.5$, $R_B = 2.6\%$. Mössbauer spectroscopy was used to characterize the $Fe^{3+}/(Fe^{2+} + Fe^{3+})$ value, and site populations were assigned on the basis of the refined site-scattering values at the *A*-, *B* -, and *C*-group sites, the unit formula calculated from the results of the chemical analysis, and the observed mean bond-lengths. The *T*(1) site is approximately half-occupied by $^{[4]}Al$ (2.15 *apfu*: atoms per formula unit) and the *T*(2) site is significantly occupied by $^{[4]}Al$ (0.66 *apfu* according to the <*T*(2)–O> distance). This distribution is in accord with no $^{T}Al–O–^{T}Al$ linkages in the structure (in accord with the absence of Ca at the *A* site). In the presence of large amounts of ^{T}Al (>> 2 *apfu*), linkage between the octahedron strip and the double-chain of tetrahedra is maintained by incorporation of large cations at the *M*(1), *M*(2) and *M*(3) sites ($Fe^{2+} \rightarrow Mg$, $Fe^{3+} \rightarrow Al$) and maximal kinking of the double-chain of tetrahedra (the latter being facilitated by K ⟶ Na at the *A* site).

Keywords: potassic-ferrisadanagaite, amphibole, crystal structure, Rietveld, Mössbauer spectroscopy, chemical composition.

SOMMAIRE

Nous avons affiné la structure cristalline de la potassic-ferrisadanagaïte, $(K_{0.66}Na_{0.32})_{\Sigma 0.98}$ $(Ca_{1.73}Na_{0.23}Mn_{0.04})_{\Sigma 2.00}$ $(Mg_{0.55}Fe^{2+}_{2.16}Mn_{0.25}Fe^{3+}_{1.11}Al_{0.78}Ti_{0.19})_{\Sigma 5.00}$ $(Si_{5.33}Al_{2.67})_{\Sigma 8.00}$ O_{22} $[(OH)_{1.21}F_{0.41}O_{0.38}]_{\Sigma 2.00}$, *a* 9.9309(1), *b* 18.0949(3), *c* 5.3681(1) Å, β 105.19(2)°, *V* 930.9(1) Å^3, *C*2/*m*, *Z* = 2, *D*(calc) = 3.36 g/cm^3, en utilisant la méthode de Rietveld, ce qui a mené aux résidus suivants: $R_p = 3.5$, $R_B = 2.6\%$. Nous nous sommes servis de la spectroscopie de Mössbauer pour déterminer la valeur du rapport $Fe^{3+}/(Fe^{2+} + Fe^{3+})$. Les occupants des sites ont été assignés à la lumière de valeurs affinées de la dispersion associée aux sites *A*, *B* et *C*, la formule chimique dérivée des résultats de l'analyse chimique, et les longueurs de liaison moyennes observées. Le site *T*(1) est environ à moitié rempli par $^{[4]}Al$ (2.15 atomes par unité formulaire), et $^{[4]}Al$ se trouve aussi en proportion importante au site *T*(2) (0.66 atomes par unité formulaire), d'après la distance <*T*(2)–O>. Cette distribution concorde avec l'absence de liaisons $^{T}Al–O–^{T}Al$ dans la structure (et avec l'absence de Ca au site *A*). En présence d'une telle proportion de ^{T}Al (>> 2 atomes par unité formulaire), l'articulation du ruban d'octaèdres avec la chaîne double de tétraèdres est assurée par l'incorporation de cations à gros rayon aux sites *M*(1), *M*(2) et *M*(3) ($Fe^{2+} \rightarrow Mg$, $Fe^{3+} \rightarrow Al$) et une contraction maximum dans la chaîne double de tétraèdres, facilitée par l'incorporation de K au lieu de Na au site *A*.

(Traduit par la Rédaction)

Mots-clés: potassic-ferrisadanagaïte, amphibole, structure cristalline, affinement de Rietveld, spectroscopie de Mössbauer, composition chimique.

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INTRODUCTION

The first occurrence of a Si-poor amphibole (Si < 5.5 *apfu*: atoms per formula unit) with Si = 5.27 *apfu* from alkaline rocks at Wolfe, Ontario, Canada, was reported by Appleyard (1975). Sadanagaite, ideal end-member Na Ca_2 ($Fe^{2+}{}_3Al_2$) $(Si_5Al_3)_8$ O_{22} $(OH)_2$ and its Mg-rich analogue, magnesiosadanagaite, were described from two localities in Japan (Shimazaki *et al.* 1984, Sawaki 1989). The same authors reported the occurrence of a new Si-poor amphibole with $Fe^{3+} > {}^{[6]}Al$ but did not submit a proposal to the CNMMN of the IMA. The silica-poor (<5.5 Si *apfu*) calcic amphibole potassic-ferrisadanagaite, ideal end-member K Ca_2 ($Fe^{2+}{}_3Fe^{3+}$) (Si_5Al_3) O_{22} $(OH)_2$, has been found recently in a contact zone of the Ilmen alkaline massif, Ilmen Mountains, southern Urals, Russia (Bazhenov *et al.* 1999; a complete description of the mineral and its geological environment are given in that paper). The behavior of monoclinic amphiboles rich in ${}^{[4]}Al$ has been most recently examined by Oberti *et al.* (1995b) and Hawthorne (1997), who showed that Al–O–Al linkages tend to be avoided except where ${}^{A}Ca$ links to the bridging O atom. Here, we present results of a crystal-structure investigation of potassic-ferrisadanagaite from the Ilmen massif by means of Rietveld refinement from X-ray powder-diffraction data and Mössbauer spectroscopy.

EXPERIMENTAL DETAILS

A separate of potassic-ferrisadanagaite from the Ilmen alkali massif was available for this work. The grain size of the amphibole was too small for conventional single-crystal four-circle diffractometry, thus we used powder-diffraction to characterize its structure.

Mössbauer spectroscopy

A sample of potassic-ferrisadanagaite from the Ilmen massif was gently ground in an agate mortar with acetone and mixed with benzophenone to reduce the possibility of preferred orientation of the crystallites. Mössbauer-absorber thickness for the sample was 5 mg Fe/cm^3. The spectrum was collected at room temperature (293 K) on a conventional transmission Mössbauer spectrometer.

The spectrum of potassic-ferrisadanagaite is typical of spectra for amphiboles, and was fitted to two Voigt doublets corresponding to Fe^{2+} and one Voigt doublet corresponding to Fe^{3+}. Component areas and widths of high- and low-velocity components of each were constrained to be equal, and the Lorentzian linewidth of the Voigt lineshape was fixed at the natural value of 0.195 mm/s. For Fe^{2+} (I) and (II), the center shifts are 1.134(5) and 1.11(10) mm/s (relative to α–Fe), the quadrupole splittings are 2.67(1) and 2.22(22) mm/s, Gaussian standard deviations are 0.107(6) and 0.17(2) mm/s, and the relative areas are 38 and 30%, respectively. For Fe^{3+}, the center shift is 0.38(9) mm/s (relative to α–Fe), the quadrupole splitting is 0.75(18) mm/s, Gaussian standard deviation is 0.164(2) mm/s, and the relative area is 32%.

Powder diffraction

Powder-diffraction data were collected on a focusing STOE–STADIP diffractometer equipped with a curved Ge (111) primary monochromator producing monochromatic Mo$K\alpha_1$ radiation (λ = 0.70926 Å) with a minimum FWHM of 0.08° according to the procedure of Wölfel (1981). The sample, contained in a quartz capillary, was rotated during exposure to minimize preferred orientation. Diffracted intensities were collected in stepwise overlapping mode of a linear position-sensitive detector with about 5° acceptance angle and 0.02° per channel (Wölfel 1983); 2600 data points were collected in the range $2.00 < 2\theta < 54.98°$ (Table 1).

Rietveld refinement of the potassic-ferrisadanagaite structure using the atom coordinates of a subsilicic hastingsite (Hawthorne & Grundy 1977) as a starting model was done with the Wyriet 3.3 program (Schneider 1989). The Pearson VII reflection-profile function was used with reflection profiles considered over a range of six full-width-at-half-maximum (FWHM) and graphical modeling of background. Asymmetry was refined for reflections with 2θ less than 30°. Occupancies of the *A* and *M* sites were refined.

RESULTS

Mössbauer spectroscopy

The Fe^{2+} absorption in the spectrum of potassic-ferrisadanagaite consists of strongly overlapped doublets (Fig. 1), and the parameters cannot be determined unambiguously. They are typical for Fe^{2+} occupying one or more of the *M*(1), *M*(2) and *M*(3) sites in the amphibole structure, but specific site-populations for Fe^{2+} cannot be determined owing to excessive line-overlap.

TABLE 1. CRYSTALLOGRAPHIC DATA FOR POTASSIC-FERRISADANAGAITE

a (Å)	9.9309(1)	Bragg reflections	1160
b	18.0949(3)	Refined parameters	74
c	5.3681(1)	R_p (%)	3.49
β (°)	105.19(2)	R_{wp} (%)	4.84
V ($Å^3$)	930.9(1)	R_{exp} (%)	2.14
Z	2	R_B (%)	2.56
Space group	*C*2/*m*	R_F (%)	2.58
D_{calc} (g/cm^3)	3.36	*s**	2.26
2θ (°)-range	2.00–54.98	*DWD***	0.52
Asymmetry, 2θ (°)	< 30	σ_x***	2.099

* $s = R_{wp} / R_{exp}$, R_{exp}: expected value of R_{wp}
***DWD*: Durbin-Watson *d* statistic (Hill & Flack 1987)
***σ_x: multiplier for the E.S.D.'s (Bérar & Lelann 1991)

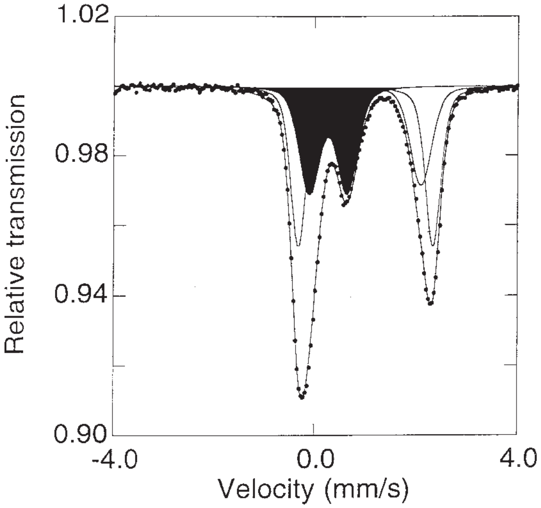

FIG. 1. Room-temperature Mössbauer spectrum of potassic-ferrisadanagaite, showing two Fe^{2+} doublets (unshaded) and one Fe^{3+} doublet (shaded black).

There is no detectable evidence for Fe^{2+} at the *M*(4) site. The Fe^{3+} absorption was fitted to a single quadrupole doublet. An $Fe^{3+}/\Sigma Fe$ ratio of 32% was determined from the refined area-ratios.

Rietveld refinement

Final refinement converged to $R_{wp} = 0.048$, $s = R_{wp} / R_{exp}$ (goodness of fit) of 2.26, Durbin–Watson *d*-statistic (Hill & Flack 1987) DWD of 0.52; all estimated standard deviations have been multiplied by $\sigma_x = 2.099$ to correct for serial correlation (Bérar & Lelann 1991). Atom coordinates and isotropic-displacement factors are given in Table 2, selected interatomic distances are listed In Table 3, and the refined site-scattering values (Hawthorne *et al.* 1995) are given in Table 4. The refined powder pattern is shown in Figure 2.

TABLE 2. ATOM COORDINATES AND ISOTROPIC-DISPLACEMENT FACTORS FOR POTASSIC-FERRISADANAGAITE

Site	*x*	*y*	*z*	B_{iso} (Å^2)
T(1)	0.2813(2)	0.087(1)	0.3117(1)	0.8(2)
T(2)	0.2897(3)	0.174(1)	0.8144(1)	0.7(1)
M(1)	0	0.091(1)	1/2	0.1(2)
M(2)	0	0.180(1)	0	0.2(1)
M(3)	0	0	0	0.2(1)
M(4)	0	0.283(1)	1/2	0.1(1)
A	0	1/2	0	5.5(6)
O(1)	0.1035(3)	0.093(1)	0.2108(1)	0.2(2)
O(2)	0.1184(4)	0.176(1)	0.7380(2)	0.7(3)
O(3)	0.1034(3)	0	0.7038(2)	0.9(2)
O(4)	0.3708(3)	0.250(1)	0.7939(1)	0.1(2)
O(5)	0.3500(4)	0.140(1)	0.1161(2)	1.1(1)
O(6)	0.3414(3)	0.118(1)	0.6109(1)	0.4(2)
O(7)	0.3404(3)	0	0.2940(1)	0.6(4)

TABLE 3. SELECTED INTERATOMIC DISTANCES (Å) IN POTASSIC-FERRISADANAGAITE

T(1)–O(1)		1.709(3)	*M*(2)–O(1)		2.05(1)
T(1)–O(5)		1.69(1)	*M*(2)–O(2)		2.057(3)
T(1)–O(6)		1.657(8)	*M*(2)–O(4)		1.93(1)
T(1)–O(7)		1.69(1)	<*M*(2)–O>		2.01
<*T*(1)–O>		1.69			
			M(3)–O(1)	×4	2.13(1)
T(2)–O(2)		1.642(2)	*M*(3)–O(3)	×2	2.106(2)
T(2)–O(4)		1.61(1)	<*M*(3)–O>		2.12
T(2)–O(5)		1.688(9)			
T(2)–O(6)		1.66(1)	*M*(4)–O(2)	×2	2.44(2)
<*T*(2)–O>		1.65	*M*(4)–O(4)	×2	2.356(6)
			M(4)–O(5)	×2	2.60(1)
M(1)–O(1)	×2	2.074(2)	*M*(4)–O(6)	×2	2.55(1)
M(1)–O(2)	×2	2.14(1)	<*M*(4)–O>		2.49
M(1)–O(3)	×2	2.09(1)			
<*M*(1)–O>		2.10	*A*–O(5)	×4	3.08(1)
			A–O(6)	×4	3.11(1)
O(5)–O(6)–O(5)		162.7(1)	*A*–O(7)	×2	2.512(2)
			<*A*–O>		2.98

Chemical composition

The chemical composition, taken from Bazhenov *et al.* (1999), is shown in Table 5, with the FeO and Fe_2O_3 contents modified to reflect the $Fe^{3+} / (Fe^{2+} + Fe^{3+})$ ratio determined here by Mössbauer spectroscopy. The unit formula was calculated on the basis of 24(O,OH,F) under two assumptions: (1) OH + F = 2 *apfu*; (2) OH + F = 2 – 2Ti *apfu*; the latter calculation assumes that Ti enters the *M*(1) site *via* the substitution ${}^{M(1)}Ti^{4+} + 2\,{}^{O(3)}O^{2-} \rightarrow {}^{M(1)}(Mg + Fe^{2+}) + 2\,{}^{O(3)}OH$ (Oberti *et al.* 1992, Hawthorne *et al.* 1998). Inspection of the *M*(1)–O bond lengths in most amphiboles with low Ti and OH + F ≪ 2 *apfu* (*e.g.*, Appendix B4 of Hawthorne 1983) shows that *M*(1)–O(3) ≥ <*M*(1)–O>. However, in dehydroxylated amphiboles with OH + F < 2 *apfu* and significant Ti^{4+} and Fe^{3+} at *M*(1) [and *M*(3)], *M*(1)–O(3) << <*M*(1)–O>. Inspection of Table 3 shows that *M*(1)–O(3) (2.09 Å) is less than <*M*(1)–O> (2.10 Å), indicating that potassic-ferrisadanagaite is dehydroxylated and has Ti^{4+}

TABLE 4. REFINED SITE-SCATTERING VALUES AND ASSIGNED SITE-POPULATIONS FOR POTASSIC-FERRISADANAGAITE

Site	Site scattering	Normalized site scattering*	Site populations (*apfu*)	
M(1)	43.1	44.1	1.30 Fe^{2+} + 0.19 Ti^{4+} + 0.51 Mg	44.1
M(2)	41.6	42.6	0.78 Al + 1.11 Fe^{3+} + 0.11 Fe^{2+}	41.9
M(3)	23.9	24.5	0.70 Fe^{2+} + 0.21 Mn^{2+} + 0.09 Mg	24.5
M(4)	35	35.8	0.04 Mn^{2+} + 1.73 Ca + 0.23 Na	38.1
A	16	16.4	0.32 Na + 0.66 K	16.1

* Normalized to the total number of electrons of the *A*-, *B*- and *C*-group cations in unit formula (2), Table 5.

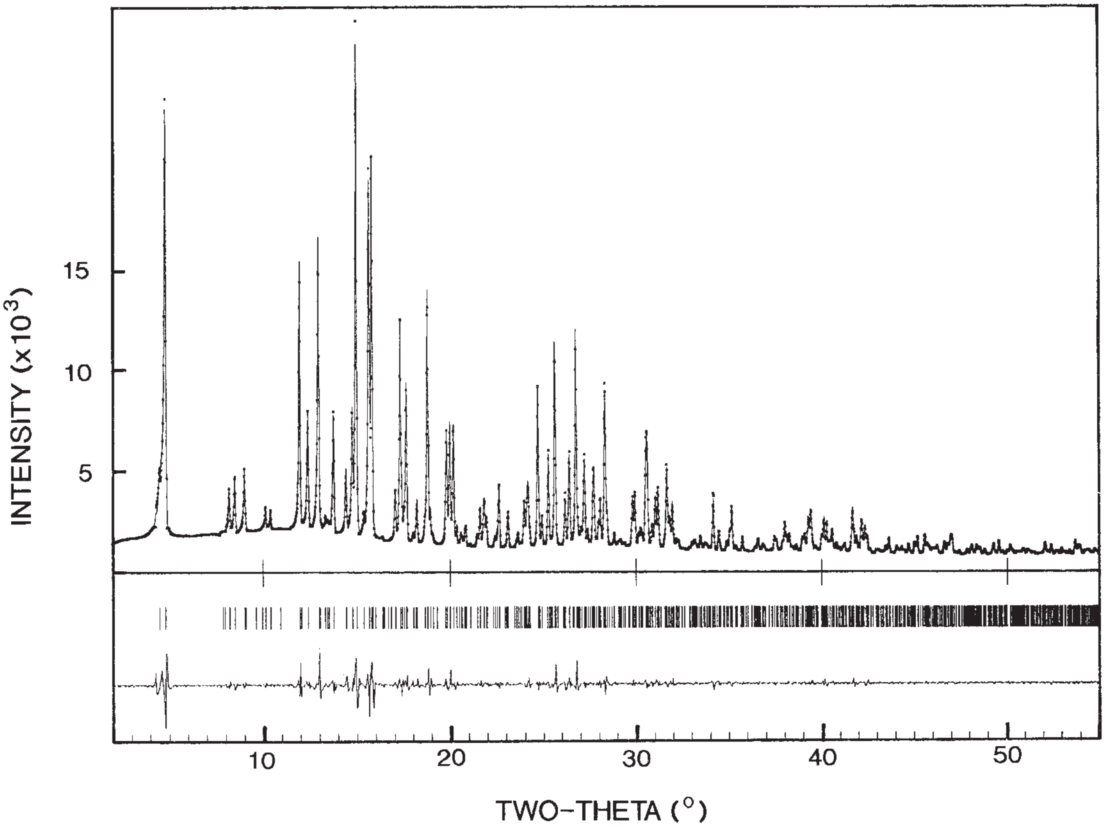

FIG. 2. The refined powder pattern for potassic-ferrisadanagaite; the observed pattern is shown by small circles, the calculated pattern is the continuous line through the small circles, the vertical lines below the pattern show the positions of all the *h k l* lines, and at the bottom is the difference pattern (observed minus calculated).

at the *M*(1) site. Thus unit formula (2) of Table 5 is to be preferred over unit formula (1).

DISCUSSION

Assignment of site populations

The total scattering from the *C*-, *B*- and *A*-group sites is 159.6 *epfu* (electrons per formula unit), and the corresponding number of electrons calculated from unit formulae (1) and (2) (Table 5) are 163.6 and 165.4 *epfu*, respectively; thus the Rietveld results are slightly underestimating the scattering of the cations. However, we can overcome this problem by renormalizing the refined site-scattering values to the number of *epfu* calculated from the electron-microprobe analysis. The site populations were assigned using unit-formula (2) of Table 4.

The T sites: As Al ($Z = 13$) and Si ($Z = 14$) have very close scattering factors for X-rays, Al and Si can only be assigned to the *T*(1) and *T*(2) sites on the basis of the <*T*(1)–O> and <*T*(2)–O> bond-lengths. Equations for this procedure are given by Hawthorne (1983) and Oberti *et al.* (1995a). There is a check on the accuracy of the sum of the $^{[4]}$Al site-populations, as this value is derived also by calculating the unit formula from the chemical composition of amphibole. Table 6 lists the predicted site-populations, together with the predicted and observed $^{[4]}$Al values for potassic-ferrisadanagaite and amphibole (58) of Hawthorne [1983; $(Na_{0.83}K_{0.30})$ $(Ca_{1.74}Na_{0.12}Fe_{0.14})$ $(Mg_{1.17}Fe^{2+}_{2.17}Mn_{0.04}Al_{0.58}Fe^{3+}_{0.79}Ti_{0.39})$ $(Si_{5.27}Al_{2.73})$ O_{22} $(OH)_2$]. The latter amphibole was initially described as subsilicic hastingsite by Hawthorne & Grundy (1977), then as subsilicic titanian magnesian hastingsite by Hawthorne (1983); according to the current amphibole-nomenclature scheme (Leake *et al.* 1997), it is a potassian ferrian sadanagaite. Note that the scheme indicated by Hawthorne (1997) is obeyed approximately: there is a limit of ~2 *apfu* on the site populations of Al at *T*(1) in order to avoid ^{T}Al–O–^{T}Al linkages in the absence of Ca at the *A* site.

The M(1,2,3) sites: The total scattering from these sites is 108.6 *epfu* (electrons per formula unit:

TABLE 5. CHEMICAL COMPOSITION (wt.%)* AND FORMULA UNIT (*apfu*) FOR POTASSIC-FERRISADANAGAITE

			(1)**	(2)**
SiO_2	33.24	Si	5.3	5.33
Al_2O_2	18.25	$^{[4]}Al$	2.7	2.67
TiO_2	1.58	ΣT	8	8
$^{†}Fe_2O_3$	9.25			
$^{†}FeO$	16.13	$^{[6]}Al$	0.7	0.78
MnO	1.83	Ti	0.2	0.19
MgO	2.31	Fe^{3+}	1.1	1.11
CaO	10.04	Fe^{2+}	2.2	2.16
Na_2O	1.78	Mn	0.3	0.25
K_2O	3.2	Mg	0.6	0.55
H_2O	1.3	ΣC	5	5.04
F	0.8			
O≡F	−0.47	ΣC–5	–	0
Total	99.24	Ca	1.7	1.73
		Na	0.3	0.23
		ΣB	2	2
		Na	0.3	0.32
		K	0.7	0.66
		ΣA	0.9	0.98
		OH	1.6	1.21
		F	0.4	0.41
		O	–	0.38

* Taken from Bazhenov *et al.* (1999)
** (1) OH + F = 2 *apfu*, H_2O = 1.50 wt.%; (2) OH + F = 2 – 2 Ti *apfu*, H_2O = 1.13 wt.%
† from Mössbauer spectroscopy

TABLE 6. ASSIGNED SITE-POPULATIONS FOR $^{[4]}Al$ IN POTASSIC-FERRISADANAGAITE (KSAD) AND AMPHIBOLE (58)

	KSAD		-58	
	H(1983)*	O(1995a)**	H(1983)	O(1995a)
$^{T(1)}Al$	2.15	2.26	1.96	2.07
$^{T(2)}Al$	0.66	0.53	0.74	0.64
^{T}Al	2.81	2.79	2.7	2.71
$^{T}Al^{EMP}$	2.67	2.67	2.73	2.73

* equations from Hawthorne (1983)
** $^{T(2)}Al = \langle T(2)–O\rangle – \langle T(2)–O\rangle_c / 0.02836$, modified after Oberti *et al.* (1995b)

Hawthorne *et al.* 1995); the corresponding number of electrons calculated from the unit formula (Table 5) is 111.2. This is reasonable agreement (Δ = 2.4%) for Rietveld data, and the difference between the two values is also in accord with the fact that the isotropic-displacement factors for the *M*(1), *M*(2) and *M*(3) sites are anomalously low when compared to analogous single-crystal values. Presuming that the relative scattering at the *M*(1), *M*(2) and *M*(3) sites is more accurately determined than the actual values, we have renormalized the refined site-scattering values (Table 4) such that their sum is concordant with unit formula (2) of Table 5.

The *M*(1) and *M*(3) sites are presumed to be occupied by Mg, Fe^{2+}, Fe^{3+} and Ti^{4+}. The Ti^{4+} is assigned to the *M*(1) site (Oberti *et al.* 1992, Hawthorne *et al.* 1998) as it participates in the substitution discussed above. This leaves Mg and Fe* (= Fe^{2+} + Mn^{2+}), which can be assigned directly from the renormalized site-scattering values; we also assign Mn^{2+} completely to the *M*(3) site because of the long <*M*(3)–O> bond-length, but emphasize that this assignment is somewhat speculative. This leaves the remaining *C*-group cations from the formula unit (Table 5) to be assigned to the *M*(2) site; the resultant number of electrons at the *M*(2) site is in close agreement (41.9 *versus* 42.6 *epfu*, Table 4) with the refined site-scattering value. The short *M*(1)–O(3) distance (Table 3) also suggests the presence of some Fe^{3+} at the *M*(1) site, but the observed <*M*(1)–O> distance, 2.103 Å (Table 3), indicates that the amount must be quite small.

Articulation of the octahedron strip and the double-chain of tetrahedra

Hawthorne & Grundy (1973, 1977) and Robinson *et al.* (1973) proposed that the amount of kinking of an amphibole double-chain is a function of the $^{[4]}Al$ content of the structure. Hawthorne (1979, 1983) introduced a simple model for examining dimensional aspects of linkage between the octahedron strip and the double-chain of tetrahedra in the *C*2/*m* amphibole structure. Obviously, the details of the linkage between the octahedron strip and the chain of tetrahedra are dependent on the lateral dimensions of the octahedron strip (which is controlled primarily by the mean size of the *C*-group cations) and the double-chain of tetrahedra (which is controlled primarily by the amount of $^{[4]}Al$ occupancy of the *T* sites). As the repeat distance of the double-chain of tetrahedra increases, linkage may be maintained by increasing the size of the *C*-group cations and by kinking of the double chain [which may be measured by the O(5)–O(6)–O(5) angle]. In this regard, it is notable that both potassic-ferrisadanagaite and amphibole (58), which have the most aluminous double-chains, also are Fe-rich (and K-rich). Hawthorne (1983) showed that the relative sizes of the octahedron strip and the chain of tetrahedra, as measured by the ratio 3<*M*–O> / 4<*T*–O>, is positively correlated with the O(5)–O(6)–O(5) angle of the double chain (represented as sin[O(5)–O(6)–O(5)]/2). This relation is shown in Figure 3, with potassic-ferrisadanagaite and amphibole (58) identified specifically. The latter two amphiboles plot at the bottom end of the trend, in accord with their high $^{[4]}Al$ values, and show the importance of articulation requirements in affecting details of both stereochemistry and chemical composition.

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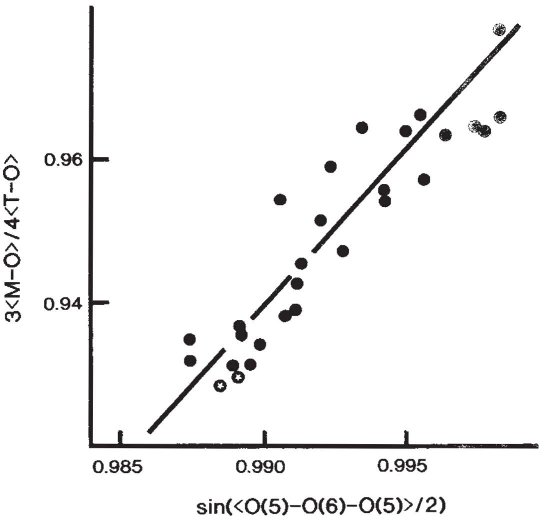

FIG. 3. Variation in relative size of the octahedron strip and the chain of tetrahedra in *C*2/*m* calcic amphiboles [3<*M*–O> / 4<*T*–O>] as a function of the kinking angle [O(5)–O(6)–O(5)] of the double chain of tetrahedra; circles: data of Hawthorne (1983); starred circles: data for potassic-ferrisadanagaite and amphibole (58); after Hawthorne (1983).

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