

## Aluminotaramite, alumino-magnesiotalamite, and fluoro-alumino-magnesiotalamite: Mineral data and crystal chemistry

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### ABSTRACT

Aluminotaramite, ideally  $\text{Na}(\text{CaNa})(\text{Fe}_3^{2+}\text{Al}_2)(\text{Si}_6\text{Al}_2)\text{O}_{22}(\text{OH})_2$ , and alumino-magnesiotalamite, ideally  $\text{Na}(\text{CaNa})(\text{Mg}_3\text{Al}_2)(\text{Si}_6\text{Al}_2)\text{O}_{22}(\text{OH})_2$ , occur in retrogressed eclogites in the Liset kyanite-eclogite pod, near Selje, Vestlandet, Norway. Fluoro-alumino-magnesiotalamite, ideally  $\text{Na}(\text{CaNa})(\text{Mg}_3\text{Al}_2)(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{F}_2$ , occurs in the Jianchang eclogite, Su-Lu coesite-eclogite province, China. These aluminotaramites always replace other higher pressure amphiboles (nyböite and fluoronyböite), and their higher Al content derives from resorbed garnets and lowered pressure during retrogression from the eclogite to the amphibolite facies. This paper reports complete mineral data for the three new holotypes as obtained by EMP analysis, structure refinement, and optical measurements. The three new minerals and mineral names have been approved with votes 2006-023, 2006-024, and 2006-025, respectively, by the IMA Commission on New Minerals, Nomenclature and Classification.

Holotype aluminotaramite has the unit formula:  $^{\text{A}}(\text{Na}_{0.89}\text{K}_{0.01})_{\Sigma 0.90}^{\text{B}}(\text{Fe}_{0.11}^{2+}\text{Na}_{0.82}\text{Ca}_{1.07})_{\Sigma 2.00}^{\text{C}}(\text{Fe}_{1.75}^{2+}\text{Mg}_{1.62}\text{Al}_{1.12}\text{Fe}_{0.42}^{3+}\text{Ti}_{0.07}\text{Zn}_{0.01}\text{Mn}_{0.01})_{\Sigma 5.00}^{\text{T}}(\text{Si}_{6.23}\text{Al}_{1.77})_{\Sigma 8.00}^{\text{O}_{22}}\text{W}(\text{OH}_{1.86}\text{F}_{0.14})_{\Sigma 2.00}$ , and  $a = 9.7489(5)$ ,  $b = 17.9377(7)$ ,  $c = 5.3233(3)$  Å,  $\beta = 104.539(5)^\circ$ ,  $V = 901.1(2)$  Å<sup>3</sup>; the calculated density is 3.29 g/cm<sup>3</sup>.

Holotype alumino-magnesiotalamite has the unit formula:  $^{\text{A}}\text{Na}_{1.07}^{\text{B}}(\text{Fe}_{0.06}^{2+}\text{Na}_{0.73}\text{Ca}_{1.21})_{\Sigma 2.00}^{\text{C}}(\text{Fe}_{1.06}^{2+}\text{Mg}_{2.40}\text{Al}_{1.20}\text{Fe}_{0.31}^{3+}\text{Ti}_{0.03})_{\Sigma 5.00}^{\text{T}}(\text{Si}_{6.09}\text{Al}_{1.91})_{\Sigma 8.00}^{\text{O}_{22}}\text{W}(\text{OH})_{2.00}$ , and  $a = 9.7899(7)$ ,  $b = 17.8991(9)$ ,  $c = 5.3192(5)$  Å,  $\beta = 104.900(7)^\circ$ ,  $V = 900.7(3)$  Å<sup>3</sup>; the calculated density is 3.21 g/cm<sup>3</sup>.

Holotype fluoro-alumino-magnesiotalamite has the unit formula:  $^{\text{A}}\text{Na}_{0.99}^{\text{B}}(\text{Fe}_{0.02}^{2+}\text{Na}_{0.77}\text{Ca}_{1.21})_{\Sigma 2.00}^{\text{C}}(\text{Fe}_{1.11}^{2+}\text{Mg}_{2.12}\text{Al}_{1.04}\text{Fe}_{0.68}^{3+}\text{Ti}_{0.03}\text{Mn}_{0.02})_{\Sigma 5.00}^{\text{T}}(\text{Si}_{6.00}\text{Al}_{2.00})_{\Sigma 8.00}^{\text{O}_{22}}\text{W}(\text{F}_{1.04}\text{OH}_{0.96})_{\Sigma 2.00}$ , and  $a = 9.7414(8)$ ,  $b = 17.9095(13)$ ,  $c = 5.3335(4)$  Å,  $\beta = 104.672(1)^\circ$ ,  $V = 900.2(3)$  Å<sup>3</sup>; the calculated density is 3.26 g/cm<sup>3</sup>.

**Keywords:** Aluminotaramite, alumino-magnesiotalamite, fluoro-alumino-magnesiotalamite

### INTRODUCTION

The need for a formal approval and complete characterization of amphibole end-members whose name is already determined by the current scheme of amphibole classification (Leake et al. 1997, 2004) has been recently discussed by Burke and Leake (2004).

The root name taramite [with composition defined as  $^{\text{A}}\text{Na}^{\text{B}}(\text{CaNa})^{\text{C}}(\text{Fe}_3^{2+}\text{AlFe}^{3+})^{\text{T}}(\text{Si}_6\text{Al}_2)\text{O}_{22}^{\text{W}}(\text{OH})_2$  in Leake et al. 1997] applies to the four ideal end-members having at the C sites the combinations  $\text{Fe}_3^{2+}\text{Fe}_3^{3+}$ ,  $\text{Mg}_3^{2+}\text{Fe}_3^{3+}$ ,  $\text{Fe}_3^{2+}\text{Al}_3^{3+}$ , and  $\text{Mg}_3^{2+}\text{Al}_3^{3+}$ . The original “taramite” came from Walli-Tarama Valley, Mariupol, Ukraine (Morozewicz 1925). Overlap with the same ideal composition in “mboziite” from Mbozi, Mbeya, Tanzania (Brock et al. 1964) was clarified in Leake (1978) where the root name mboziite was abolished in favor of taramite. An important point

is that these original samples had  $^{\text{C}}\text{Fe}^{3+} > ^{\text{C}}\text{Al}$  and came from igneous rocks, i.e., relatively high-temperature ( $T$ ), low-pressure ( $P$ ) environments.

Aluminotaramitic amphiboles with  $^{\text{C}}\text{Fe}^{3+} < ^{\text{C}}\text{Al}$ , initially with  $\text{Mg} > \text{Fe}^{2+}$  and later also with  $\text{Mg} < \text{Fe}^{2+}$ , were discovered in the Liset kyanite-eclogite pod, near Selje, Vestlandet, Norway (Ungaretti et al. 1981, 1985; Kechid and Smith 1982; Kechid 1984; Oberti et al. 1989). This locality occurs within the Norwegian “coesite-eclogite province” (Smith 1988, 1992) as Liset shows evidence of “deduced coesite” (Smith 1984). Of particular interest is a continuous trend in chemical composition from nyböite through alumino-magnesiotalamite toward sadanagaite that fits with decreasing  $^{[6]}\text{Al}/(^{[6]}\text{Al} + ^{[4]}\text{Al})$  (Smith 1988), which correlates with decreasing  $P/T$  ratio. Subsequently, nyböite and alumino-magnesiotalamite were found by Smith et al. (1990) in a sample from the Jianchang eclogite. This sample came from the “Su-Lu coesite-eclogite province,” China (first defined by Yang and Smith 1989; see also Yang 1991 and Yang et al. 1998).

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A similar trend from nyböite through alumino-magnesiotalamite toward sadanagaite occurs at Jianchang (Smith 1992; Yang 1997; G. Godard, unpub. data). At both localities, nyböite is clearly the highest *P* amphibole, and Smith (1995) suggested that it may have coexisted with coesite. Subsequently aluminotalamite was found on Île Dumet, Brittany (France), where the depressurization retrogression trend starts from glaucophane, as the pressure there was not as high as the coesite-eclogite subfacies (Lasnier and Smith 1989; Smith et al. 1999). Information on alumino-taramite compositions with various Mg/Fe<sup>2+</sup> ratios from Norway, China and France will be presented by Smith, Yang, and Godard (in preparation). Here we focus on the mineral data and the crystal chemistry of the three specific crystals whose names have recently been recognized by the IMA.

The names defining two out of these three amphiboles already exist in the official IMA "Amphibole Nomenclature," but no type specimen had ever been submitted and thus aluminotalamite and alumino-magnesiotalamite are unfortunately to be considered "named amphibole" according to Burke and Leake (2004). This work presents complete mineral characterizations for the two above-mentioned species and fluoro-alumino-magnesiotalamite. Formal approval has been given by IMA-CNMNC for 2006-023 (aluminotalamite), 2006-024 (alumino-magnesiotalamite), and 2006-025 (fluoro-alumino-magnesiotalamite). The correspondence between the new mineral names and the codes of the holotype specimens used in this work are given in Table 1.

## MINERAL DATA

### Occurrence and paragenesis

Aluminotalamite occurs in the Liset kyanite-eclogite pod, near Selje, Møre og Romsdal County, Vestlandet, Norway (Ungaretti et al. 1981, 1985; Kechid and Smith 1982; Kechid 1984; Oberti et al. 1989), the type locality for lisetite (Smith et al. 1986). The rock sample in which the holotype was found is a retrogressed eclogite (sample K22). Associated minerals are nyböite, clinopyroxene, garnet, rutile, paragonite, plagioclase, quartz, zoisite, and apatite. Aluminotalamite replaced the amphibole (nyböite) formed previously under high-*P* eclogite-facies conditions when uplift and retrogression toward amphibolite-facies conditions occurred. Resorbed garnet provided the extra Al, Fe<sup>2+</sup>, and Ca needed to form aluminotalamite from nyböite. A key point is that aluminotalamite coexists with retrogressive plagioclase, whereas nyböite does not.

Alumino-magnesiotalamite occurs in the Liset kyanite-eclogite pod, near Selje, Møre og Romsdal County, Vestlandet, Norway. The rock sample where the holotype has been found is a retrogressed eclogite (sample Q99), and the paragenesis is the same as that of aluminotalamite.

Fluoro-alumino-magnesiotalamite occurs in the Jianchang eclogite, Su-Lu coesite-eclogite province, China (Smith et al. 1990). The rock-sample number is DJ102. Associated min-

erals are fluoronyböite (Oberti et al. 2003), clinopyroxene (~Jd<sub>70</sub>Ae<sub>20</sub>Di<sub>10</sub>), garnet (~Alm<sub>60</sub>Prp<sub>21</sub>Grs<sub>17</sub>Sps<sub>02</sub>), rutile, apatite, paragonite, plagioclase, and quartz. Fluoro-alumino-magnesiotalamite replaced the amphibole formed under high-*P* eclogite-facies conditions (fluoronyböite) when uplift and retrogression toward amphibolite-facies conditions occurred. As noted previously, the extra Al and Ca came from partially resorbed garnet.

### Appearance and physical properties

All the taramites of this work occur as submillimeter grains, are brittle, have vitreous luster and are not fluorescent. The density could not be measured because of the small grain size.

**Aluminotalamite.** Color: bluish green. Cleavage: {110}, rather poor. Density (calc.) = 3.29 g/cm<sup>3</sup>.

**Alumino-magnesiotalamite.** Color: greenish gray. Cleavage: {110}, good. Morphology: prismatic. Density (calc.) = 3.21 g/cm<sup>3</sup>.

**Fluoro-alumino-magnesiotalamite.** The mineral occurs as very small grains (<100 μm). Color: bluish green. Cleavage: {110}, rather poor. Density (calc.) = 3.26 g/cm<sup>3</sup>.

### Optical properties

**Aluminotalamite.** Biaxial (-), n<sub>α</sub> = 1.663(1), n<sub>β</sub> = 1.675(2), n<sub>γ</sub> = 1.684(1) (589 nm). 2*V*<sub>x</sub> (meas.) = 71(1)°, 2*V*<sub>x</sub> (calc.) = 81°. Dispersion: *r* << *v*, extreme. Extremely inclined monoclinic dispersion. The optic axis with the smaller angle to the **c** axis is much more dispersed than the other axis. Orientation: *Y* = **b**. O.A. plane = (010). *Z* ^ **c** = 11(1)°. Pleochroism: *X* = colorless, *Y* = dark purple, *Z* = greenish blue.

**Alumino-magnesiotalamite.** Biaxial (-), n<sub>α</sub> = 1.654(1), n<sub>β</sub> = 1.666(2), n<sub>γ</sub> = 1.671(1) (589 nm). 2*V*<sub>x</sub> (meas.) = 74(1)°, 2*V*<sub>x</sub> (calc.) = 65°. Dispersion: *r* << *v* extreme. Extremely inclined monoclinic dispersion. The optic axis with the smaller angle to the **c** axis is much more dispersed than the other axis. Orientation: *Y* = **b**. O.A. plane = (010). *Z* ^ **c** = 15(1)°. Pleochroism: *X* = colorless, *Y* = dark purple, *Z* = blue.

**Fluoro-alumino-magnesiotalamite.** Biaxial (-), n<sub>α</sub> = 1.627(2), n<sub>β</sub> = 1.635(2), n<sub>γ</sub> = 1.641(2) (589 nm). 2*V*<sub>x</sub> (meas.) = 66(1)°, 2*V*<sub>x</sub> (calc.) = 81°. Dispersion: *r* << *v*, extreme. Extremely inclined monoclinic dispersion. The optic axis with the smaller angle to the **c** axis is much more dispersed than the other axis. Orientation: *Y* = **b**. O.A. plane = (010). *Z* ^ **c** = 19(2)°. Pleochroism: *X* = colorless, *Y* = light purple, *Z* = blue.

### EMP ANALYSIS

Chemical analyses of the refined crystals were done with a CAMECA SX-50 electron microprobe (WDS mode, 15 kV, 15 nA, 5 μm beam diameter). The following standards were used for *K*α X-ray lines: Si and Ca = wollastonite (TAP); Ti = rutile (LIF); Al = corundum (TAP), Fe = magnetite (LiF); Mn = Mn metal (LiF); Zn = Zn metal (LIF), Mg = periclase (TAP); Na = jadeite (TAP); K = orthoclase (PET); F = fluorophlogopite syn. (TAP); Cl = sylvite (PET). H<sub>2</sub>O was calculated from the unit formula to obtain 2 (OH + F) in the absence of dehydrogenation, as suggested by the crystal-chemical study. The total Fe content was first estimated as FeO; the ferrous and ferric populations were estimated later, imposing electro-

TABLE 1. Sample codes and classification

End-member name	Ideal formula	Sample code	SEQ*
aluminotalamite	Na(CaNa)(Fe <sup>3+</sup> Al <sub>2</sub> )(Si <sub>6</sub> Al <sub>2</sub> )O <sub>22</sub> (OH) <sub>2</sub>	K22-2	1131
alumino-magnesiotalamite	Na(CaNa)(Mg <sub>2</sub> Al <sub>2</sub> )(Si <sub>6</sub> Al <sub>2</sub> )O <sub>22</sub> (OH) <sub>2</sub>	Q99-3	421
fluoro-alumino-magnesiotalamite	Na(CaNa)(Mg <sub>2</sub> Al <sub>2</sub> )(Si <sub>6</sub> Al <sub>2</sub> )O <sub>22</sub> F <sub>2</sub>	DJ102-23	1066

\* SEQ is the sequence code in the CNR-IGG-PV amphibole database.

neutrality and crystal-chemical constraints obtained from the structure refinement. The results are reported in Table 2.

**Aluminotaramite:** The empirical formula, based on 24 (O,OH,F) pfu is  ${}^A\text{Na}_{0.89}\text{K}_{0.01}\text{Fe}_{0.11}^{2+}\text{Na}_{0.82}\text{Ca}_{1.07}\text{Mg}_{1.62}\text{Al}_{1.12}\text{Fe}_{0.42}^{3+}\text{Ti}_{0.07}\text{Zn}_{0.01}\text{Mn}_{0.01}\text{Si}_{6.23}\text{Al}_{1.77}\text{O}_{22}\text{W}(\text{OH}_{1.86}\text{F}_{0.14})_{22.00}$ . The end-member formula is  ${}^A\text{Na}^B(\text{Ca Na})^C(\text{Fe}_2^3\text{Al}_2)^T(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{W}(\text{OH})_2$ , which requires  $\text{Na}_2\text{O}$  6.77,  $\text{CaO}$  6.12,  $\text{FeO}$  23.53,  $\text{Al}_2\text{O}_3$  22.26,  $\text{SiO}_2$  39.35,  $\text{H}_2\text{O}$  1.97, Total 100.00 wt%.

**Alumino-magnesirotaramite:** The empirical formula, based on 24 (O,OH) pfu is  ${}^A\text{Na}_{1.07}\text{Fe}_{0.06}^{2+}\text{Na}_{0.73}\text{Ca}_{1.21}\text{Mg}_{2.40}\text{Al}_{1.20}\text{Fe}_{0.31}^{3+}\text{Ti}_{0.03}\text{Si}_{6.09}\text{Al}_{1.91}\text{O}_{22}\text{W}(\text{OH})_{2.00}$ . The end-member formula is  ${}^A\text{Na}^B(\text{Ca Na})^C(\text{Mg}_3\text{Al}_2)^T(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{W}(\text{OH})_2$ , which requires  $\text{Na}_2\text{O}$  7.55,  $\text{MgO}$  14.72,  $\text{CaO}$  6.83,  $\text{Al}_2\text{O}_3$  24.83,  $\text{SiO}_2$  43.89,  $\text{H}_2\text{O}$  2.19, Total 100.00 wt%.

**Fluoro-alumino-magnesirotaramite:** The empirical formula, based on 24 (O,OH,F) pfu is  ${}^A\text{Na}_{0.99}\text{Fe}_{0.02}^{2+}\text{Na}_{0.77}\text{Ca}_{1.21}\text{Mg}_{2.11}\text{Mn}_{0.02}\text{Si}_{6.00}\text{Al}_{2.00}\text{O}_{22}\text{W}(\text{F}_{1.04}\text{OH}_{0.96})_{22.00}$ . The end-member formula is  ${}^A\text{Na}^B(\text{Ca Na})^C(\text{Mg}_3\text{Al}_2)^T(\text{Si}_6\text{Al}_2)\text{O}_{22}\text{W}\text{F}_2$ , which requires  $\text{Na}_2\text{O}$  7.51,  $\text{MgO}$  14.65,  $\text{CaO}$  6.79,  $\text{Al}_2\text{O}_3$  24.71,  $\text{SiO}_2$  43.68,  $\text{F}$  4.60,  $-\text{O} = \text{F} - 1.94$ , Total 100.00 wt%.

## CRYSTALLOGRAPHY

Single-crystal X-ray studies for the two samples from Liset were done with a Philips PW1100 4-circle diffractometer ( $\lambda = \text{MoK}\alpha$ ). The unit-cell parameters were calculated from least-squares refinement of the  $d^*$  values obtained for 60 rows of the reciprocal lattice by measuring the center of gravity of each reflection and of its antireflection in the range:  $-70 < 2\theta < 70^\circ$ . Two monoclinic equivalents were collected; corrections for absorption and  $L_p$  were applied. Due to the small size of the crystal, data collection for fluoro-alumino-magnesirotaramite was done in the  $2\theta$  range  $4-60^\circ$  with a Bruker AXS diffractometer equipped with an area detector; the resulting mean redundancy was 5.11.

For all samples, the reflections with  $I_o > 3\sigma(I_o)$  were considered as observed during unweighted full-matrix least-squares refinement on  $F$ . Scattering curves for fully ionized chemical species were used at sites where chemical substitutions occur; neutral vs. ionized scattering curves were used at the T and anion sites (except O3). More details on the refinement procedure are given in Oberti et al. (1992). Selected crystal data are given in Table 3, atom coordinates, refined site-scattering values and anisotropic-displacement parameters in Table 4, and selected geometrical parameters in Table 5.

The X-ray powder-diffraction data were simulated (for  $\lambda = \text{CuK}\alpha$ ) combining the structure factors from single-crystal diffraction study at the proper  $2\theta$  values, taking multiplicities and  $L_p$  factors into account (XPREP software, Bruker-Axis Inc.). The results are given in Table 6.

**TABLE 2.** Chemical analysis and unit formulae calculated based on 24 (O,OH,F) and 2 (OH,F) for the three refined taramite crystals of this work

	K22-2	Q99-3	DJ102-23		K22-2	Q99-3	DJ102-23
SiO <sub>2</sub>	41.87	42.00	40.73	Si	6.23	6.09	6.00
TiO <sub>2</sub>	0.69	0.31	0.24	Al	1.77	1.91	2.00
Al <sub>2</sub> O <sub>3</sub>	16.43	18.20	17.5	ΣT	8.00	8.00	8.00
Cr <sub>2</sub> O <sub>3</sub>	0.00	na	0.01	Al	1.12	1.20	1.04
Fe <sub>2</sub> O <sub>3</sub>	3.68	2.84	6.12	Mg	1.62	2.40	2.12
FeO	14.92	9.24	9.20	Ti	0.07	0.03	0.03
MnO	0.05	na	0.14	Fe <sup>2+</sup>	1.75	1.06	1.11
MgO	7.36	11.10	9.66	Fe <sup>3+</sup>	0.42	0.31	0.68
ZnO	0.06	na	0.02	Mn <sup>2+</sup>	0.01	na	0.02
CaO	6.74	7.78	7.66	Zn	0.01	na	0.00
Na <sub>2</sub> O	5.93	6.42	6.15	ΣC	5.00	5.00	5.00
K <sub>2</sub> O	0.07	na	0.01	Ca	1.07	1.21	1.21
(H <sub>2</sub> O) <sub>cal</sub>	1.87	2.07	0.98	Na	0.82	0.73	0.77
F	0.28	na	2.22	Fe <sup>2+</sup>	0.11	0.06	0.02
Cl	0.01	na	0.01	Σ B	2.00	2.00	2.00
O = F,Cl	0.12	0.00	0.94	Na	0.89	1.07	0.99
				K	0.01	na	0.00
				ΣA	0.90	1.07	0.99
				F	0.14	na	1.04
				OH	1.86	2.00	0.96
				ΣW	2.00	2.00	2.00
ss values calculated from unit formulae				refined ss values			
ss C	92.51	80.68	86.66	ss C	92.35	82.93	88.95
ss B	33.28	33.79	33.19	ss B	33.58	33.78	33.36
ss A	9.98	11.77	10.89	ss A	10.12	11.00	10.93
Total	135.77	126.24	130.74	Total	136.05	127.71	133.24
ss W	16.14	16.00	17.04	ss W	16.25	16.00	17.35

Note: ss = site scattering; na = not analyzed.

## Compatibility

$1 - (K_p/K_C) = -0.005$  (superior) for aluminotaramite,  $-0.107$  (superior) for alumino-magnesirotaramite, and  $0.029$  (excellent) for fluoro-alumino-magnesirotaramite.

## Type material

Holotype materials (the analyzed crystals and crystal concentrates from the same rock sample) are deposited at the Museo di Mineralogia, Dipartimento di Scienze della Terra, Università degli Studi di Pavia, under the codes 2006-01 (aluminotaramite), 2006-02, (alumino-magnesirotaramite), and 2006-03 (fluoro-alumino-magnesirotaramite).

## CRYSTAL CHEMISTRY

According to the current rules for amphibole classifications (Leake et al. 1997, 2004), all the studied crystals refer to the root name taramite, with <sup>Ti</sup>Al close to 2 apfu, the A site almost filled by Na, and the B site close to (CaNa). This rootname has the code (1122) in the ABCD system of Smith (1988), compared to nyböite that is (1221); these are among the most substituted clin amphiboles compared to tremolite (0000), which is considered as the origin of amphibole multivariate space. Petrological analysis shows that the taramites formed according to the first step of the plagioclase exchange,  ${}^B\text{Na}^+ + {}^T\text{Si}^{4+} \rightarrow {}^B\text{Ca}^{2+} + {}^T\text{Al}^{3+}$ , involving the transition from nyböite,  $\text{NaNa}_2(\text{Mg}_3\text{Al}_2)(\text{Si}_7\text{Al})\text{O}_{22}(\text{OH})_2$ , to alumino-magnesirotaramite,  $\text{Na}(\text{CaNa})(\text{Mg}_3\text{Al}_2)(\text{Si}_6\text{Al}_2)\text{O}_{22}(\text{OH})_2$ . Continuation of this exchange, which involves the transition from alumino-magnesirotaramite toward alumino-magnesirotaramite,  $\text{NaCa}_2(\text{Mg}_3\text{Al}_2)(\text{Si}_5\text{Al}_3)\text{O}_{22}(\text{OH})_2$ , is also observed at both localities (Liset: Smith 1988; Oberti et al. 1989; Jianchang: Smith et al. 1990). Decreasing  ${}^{6}\text{Al}/({}^{6}\text{Al} + {}^{4}\text{Al})$  due to this exchange is related to decreasing  $P$ - $T$  ratio due to a definite substantial decrease in  $P$  (from over 2 GPa down to about 1 GPa: Smith 1988, 1992, 1995) and an uncertain but smaller variation in  $T$  (with  $T$  ranging around 800 °C).

The three taramite samples of this work allow discussion of the structural changes occurring as a function of C- and W-site populations, and of those occurring when early high- $P$  amphiboles are replaced by low  ${}^{6}\text{Al}/({}^{6}\text{Al} + {}^{4}\text{Al})$  species during evolution to medium- $P$  amphibolite-facies conditions. Table 7 reports the final site populations, with comparisons between the refined and calculated site-scattering values and between the refined mean bond lengths and those calculated from structure modeling.

In all three samples, M2 is the smallest among the octahedra,

**TABLE 3.** Selected crystal data for the three taramites of this work

	K22-2	Q99-3	DJ102-23
$a$ (Å)	9.7489(5)	9.7899(7)	9.7414(8)
$b$ (Å)	17.9377(7)	17.8991(9)	17.9095(13)
$c$ (Å)	5.3233(3)	5.3192(5)	5.3335(4)
$\beta$ (°)	104.539(5)	104.900(7)	104.672(1)
$V$ (Å <sup>3</sup> )	901.1(2)	900.7(3)	900.2(3)
$2\theta$ range (°)	4-60	4-60	4-60
no. all	1370	1376	1395
no. obs (>3 $\sigma$ )	1201	1146	1111
Space group	$C2/m$	$C2/m$	$C2/m$
$R_{\text{sym}}$ (%)	1.1	1.0	4.6
$R_{\text{obs}}$ (%)	1.5	1.3	2.3
$R_{\text{int}}$ (%)	1.9	2.1	3.2
$a:b:c$	0.5435:1:0.2968	0.5469:1:0.2972	0.5439:1:0.2978

**TABLE 4.** Refined site-scattering values (ss, epfu), atom coordinates and atomic-displacement parameters ( $B_{\text{eq}}$ , Å<sup>2</sup>;  $\beta_{ii}$  × 10<sup>4</sup>) for the three taramites of this work

Atom	ss	x/a	y/b	z/c	$B_{\text{eq}}$	$\beta_{11}$	$\beta_{22}$	$\beta_{33}$	$\beta_{12}$	$\beta_{13}$	$\beta_{23}$
<b>K22-2: aluminotaramite</b>											
O1		0.1049(1)	0.0931(1)	0.2096(2)	0.77(2)	19	7	67	-2	12	-3
O2		0.1199(1)	0.1750(1)	0.7443(2)	0.72(2)	14	6	79	0	6	2
O3	16.25(5)	0.1104(2)	0	0.7068(3)	0.89(3)	18	8	93	-	5	-
O4		0.3700(1)	0.2518(1)	0.7950(2)	0.89(2)	29	5	98	-2	19	2
O5		0.3540(1)	0.1387(1)	0.1049(2)	0.97(2)	19	9	88	-1	4	14
O6		0.3422(1)	0.1187(1)	0.6045(2)	0.99(2)	19	9	100	1	9	-11
O7		0.3368(2)	0	0.2788(3)	1.19(4)	25	10	137	-	18	-
T1		0.2812(1)	0.0870(1)	0.3001(1)	0.45(1)	11	4	46	-1	5	-1
T2		0.2928(1)	0.1737(1)	0.8141(1)	0.49(1)	12	4	50	-1	7	0
M1	36.73(8)	0	0.0904(1)	½	0.60(1)	18	6	45	-	12	-
M2	33.65(9)	0	0.1791(1)	0	0.54(1)	14	4	60	-	9	-
M3	21.97(3)	0	0	0	0.53(1)	18	3	48	-	7	-
M4	31.85(10)	0	0.2799(1)	½	0.83(1)	26	6	86	-	29	-
M4'	1.73(5)	0	0.2569(5)	½	0.4(1)						
A	1.72(3)	0	½	0	2.9(4)	61	29	330	-	99	-
Am	3.43(8)	0.0500(10)	½	0.1065(16)	3.3(2)	92	37	199	-	64	-
A2	4.97(8)	0	0.4711(3)	0	2.3(1)	55	14	374	-	101	-
H	1.9(1)	0.188(4)	0	0.767(6)	1.8(7)						
<b>Q99-3: alumino-magnesirotaramite</b>											
O1		0.1047(1)	0.0920(1)	0.2116(3)	0.73(2)	18	7	63	-1	9	-2
O2		0.1196(1)	0.1743(1)	0.7427(2)	0.68(2)	14	6	68	1	4	0
O3		0.1096(1)	0	0.7094(2)	0.71(3)	15	6	73	0	4	0
O4		0.3687(1)	0.2520(1)	0.7944(2)	0.73(2)	26	4	74	-2	20	1
O5		0.3535(1)	0.1399(1)	0.1090(2)	0.87(2)	19	8	74	-1	1	11
O6		0.3425(1)	0.1178(1)	0.6094(2)	0.88(2)	18	8	96	0	11	-11
O7		0.3381(1)	0	0.2764(3)	1.09(3)	24	10	115	-	17	-
T1		0.2809(1)	0.0869(1)	0.3021(1)	0.44(1)	11	4	43	-1	3	-1
T2		0.2921(1)	0.1740(1)	0.8158(1)	0.43(1)	12	3	42	-1	5	0
M1	30.56(8)	0	0.0901(1)	½	0.55(1)	18	5	41	-	9	-
M2	34.12(8)	0	0.1782(1)	0	0.54(1)	14	4	55	-	7	-
M3	18.25(4)	0	0	0	0.50(1)	17	3	43	-	5	-
M4	33.78(11)	0	0.2806(1)	½	0.77(1)	24	6	79	-	22	-
A	1.99(3)	0	1/2	0	3.2(2)	67	34	314	-	89	-
Am	2.40(7)	0.0401(9)	1/2	0.0980(15)	2.5(2)	61	31	142	-	48	-
A2	6.61(7)	0	0.4703(2)	0	2.3(1)	56	14	325	-	80	-
H	1.40(50)	0.1978(33)	0	0.7640(61)	0.8(4)						
<b>DJ102-23: fluoro-alumino-magnesirotaramite</b>											
O1		0.1046(1)	0.0917(1)	0.2098(3)	0.79(3)	21	7	70	-2	15	-4
O2		0.1194(2)	0.1743(1)	0.7444(3)	0.72(3)	15	6	73	1	5	0
O3	17.35(9)	0.1096(2)	0	0.7079(4)	1.08(5)	28	8	108	-	10	-
O4		0.3687(2)	0.2529(1)	0.7956(3)	0.76(3)	26	5	84	-2	23	-1
O5		0.3550(2)	0.1395(1)	0.1064(3)	0.94(3)	20	10	81	-3	7	10
O6		0.3430(2)	0.1193(1)	0.6052(3)	0.98(4)	20	9	103	0	14	-9
O7		0.3400(2)	0	0.2809(5)	1.18(6)	25	11	125	-	22	-
T1		0.2822(1)	0.0870(1)	0.3010(1)	0.53(1)	14	5	46	-1	5	-1
T2		0.2930(1)	0.1740(1)	0.8156(1)	0.52(1)	15	4	45	-1	6	0
M1	33.80(12)	0	0.0908(1)	½	0.71(2)	25	6	52	-	12	-
M2	36.07(11)	0	0.1783(1)	0	0.61(2)	17	5	62	-	11	-
M3	19.08(4)	0	0	0	0.64(2)	22	4	55	-	7	-
M4	33.36(16)	0	0.2804(1)	½	0.92(2)	31	7	90	-	28	-
A	0.90(4)	0	1/2	0	2.5(8)	70	19	273	-	73	-
Am	6.18(10)	0.0489(6)	1/2	0.1032(11)	2.3(1)	45	31	160	-	48	-
A2	3.85(10)	0	0.4729(5)	0	2.6(2)	72	14	388	-	104	-
H	0.95(15)	0.205(9)	0	0.767(16)	1.0(8)						

and hosts all high-charged cations (always <2 apfu) plus minor amounts of divalent cations (with  $M_2Mg \gg M_2Fe^{2+}$ ). The larger divalent cations ( $Fe^{2+}$  and  $Mn^{2+}$ ) are preferentially incorporated at the largest M3 octahedron.

Interestingly, the octahedra in taramites maintain the structural features previously observed in other F-free high-*P* amphiboles (nyböite and glaucophane; Oberti et al. 2003), i.e., structural relaxation at the M3 site as a result of small trivalent cations occupying the two adjacent M2 sites and the need to maintain linkage with the double-chain of tetrahedra. The relaxation is even more evident in fluoro-alumino-magnesirotaramite

for which, as observed in fluoronyböite (Oberti et al. 2003), both the M1 and especially the M3 octahedra are far larger than expected on the basis of the site population and of the F content at the O3 site. The M1 and M3 sites are the only octahedra bonded to O3, and the observed relaxation confirms that the  $F_1(OH)_{-1}$  exchange does not produce the decrease in the mean bond lengths (0.013 Å per F apfu; Oberti et al. 1993) expected in these medium-*P* amphiboles.

The differences between the refined and calculated mean octahedral distances are even larger in fluoro-alumino-magnesirotaramite ( $\Delta M1 + 0.015$  Å,  $\Delta M3 + 0.013$  Å) than in fluoronyböite



TABLE 6.— Continued

<i>l</i>	2θ	<i>d</i>	<i>hkl</i>	<i>l</i>	2θ	<i>d</i>	<i>hkl</i>	<i>l</i>	2θ	<i>d</i>	<i>hkl</i>	<i>l</i>	2θ	<i>d</i>	<i>hkl</i>
<b>DJ102-23: fluoro-alumino-magnesirotaramite</b>															
13.9	9.88	8.954	0 2 0	15.6	32.20	2.780	3 3 0	1.5	42.98	2.104	4 4 1	7.8	50.98	1.791	0 10 0
<b>82.2</b>	<b>10.61</b>	<b>8.340</b>	<b>1 1 0</b>	<b>100.0</b>	<b>33.18</b>	<b>2.700</b>	<b>1 5 1</b>	18.6	44.08	2.054	2 0 2				1 9 1
1.4	17.19	5.159	0 0 1	5.0	33.99	2.637	1 1 2	<b>28.2</b>	<b>45.13</b>	<b>2.009</b>	<b>4 0 2</b>	1.1	51.82	1.764	1 1 3
1.5	17.60	5.040	1 3 0	<b>53.6</b>	<b>34.72</b>	<b>2.583</b>	<b>0 6 1</b>				<b>3 5 1</b>				3 7 1
16.7	18.08	4.907	1 1 1				<b>0 0 2</b>	5.6	45.73	1.984	3 7 0	5.5	52.63	1.739	5 1 2
2.7	18.83	4.712	2 0 0	<b>63.6</b>	<b>35.17</b>	<b>2.551</b>	<b>2 0 2</b>	3.1	46.33	1.960	1 5 2	1.3	53.28	1.719	0 0 3
21.6	19.83	4.476	0 4 0	1.3	36.61	2.455	2 2 2				3 7 1	6.3	53.94	1.700	5 5 1
			0 2 1	1.0	36.92	2.435	1 3 2				2 8 1				1 3 3
0.4	21.31	4.170	2 2 0	2.4	37.50	2.398	3 1 1	2.5	46.64	1.947	1 9 0	9.1	54.30	1.689	0 10 1
3.1	22.20	4.005	1 1 1				2 6 1	2.7	46.95	1.935	3 5 2				0 2 3
7.6	22.93	3.879	1 3 1	6.9	38.11	2.361	3 5 0	2.2	47.39	1.918	4 2 1	7.1	54.51	1.683	2 8 2
0.5	24.25	3.670	2 2 1	<b>39.4</b>	<b>38.79</b>	<b>2.321</b>	<b>3 5 1</b>	5.4	48.59	1.874	5 1 0	3.3	55.10	1.667	3 9 1
<b>47.1</b>	<b>26.33</b>	<b>3.384</b>	<b>1 3 1</b>	20.7	39.11	2.303	4 2 1	6.8	48.88	1.863	2 4 2	24.3	56.06	1.640	4 6 1
27.0	27.48	3.246	2 4 0	25.5	39.49	2.282	1 7 1				4 6 1	7.2	56.72	1.623	4 8 0
<b>67.4</b>	<b>28.86</b>	<b>3.094</b>	<b>3 1 0</b>				3 1 2	9.3	49.14	1.854	1 9 1	12.8	57.44	1.604	1 11 0
4.0	29.74	3.004	3 1 1	2.7	40.15	2.246	3 3 1	6.2	49.33	1.847	1 7 2	23.7	58.04	1.589	1 5 3
3.9	29.94	2.985	0 6 0	7.7	40.70	2.217	2 4 2	4.2	49.66	1.836	4 4 2	5.8	58.79	1.571	6 0 0
<b>32.9</b>	<b>30.43</b>	<b>2.937</b>	<b>2 2 1</b>	<b>35.2</b>	<b>41.96</b>	<b>2.153</b>	<b>2 6 1</b>					7.6	59.46	1.555	4 0 2

TABLE 7. Site populations and agreement parameters for aluminotaramite (K22-2, first line), alumino-magnesirotaramite (Q99-3, second line), and fluoro-alumino-magnesirotaramite (DJ102-23, third line)

Site	Site population (apfu)	ss (epfu)		mbl (Å)	
		refined	calculated	refined	calculated
T1	1.77 Al + 2.23 Si			1.672	1.671
	1.91 Al + 2.09 Si			1.677	1.676
	2.00 Al + 2.00 Si			1.678	1.677
M1	1.07 Mg + 0.93 Fe <sup>2+</sup>	36.73	37.02	2.100	2.098
	1.57 Mg + 0.43 Fe <sup>2+</sup>	30.56	30.02	2.091	2.088
	1.35 Mg + 0.65 Fe <sup>2+</sup>	33.80	33.10	2.095	2.080
M2	0.27 Mg + 1.12 Al + 0.11 Fe <sup>2+</sup> + 0.42 Fe <sup>3+</sup> + 0.07 Ti + 0.01 Zn	33.65	33.42	1.980	1.982
	0.25 Mg + 1.20 Al + 0.21 Fe <sup>2+</sup> + 0.31 Fe <sup>3+</sup> + 0.03 Ti	34.12	32.78	1.988	1.984
	0.22 Mg + 1.04 Al + 0.03 Fe <sup>2+</sup> + 0.68 Fe <sup>3+</sup> + 0.03 Ti	36.07	35.28	1.980	1.981
M3	0.28 Mg + 0.71 Fe <sup>2+</sup> + 0.01 Mn	21.97	22.07	2.117	2.111
	0.58 Mg + 0.42 Fe <sup>2+</sup>	18.25	17.88	2.103	2.098
	0.55 Mg + 0.43 Fe <sup>2+</sup> + 0.02 Mn	19.08	18.28	2.100	2.087
M4 + M4'	1.07 Ca + 0.82 Na + 0.11 Fe <sup>2+</sup>	33.58	33.28		
	1.21 Ca + 0.73 Na + 0.06 Fe <sup>2+</sup>	33.78	33.79		
	1.21 Ca + 0.77 Na + 0.02 Fe <sup>2+</sup>	33.36	33.19		
A + Am + A2	0.89 Na + 0.01 K	10.12	9.98		
	1.07 Na	11.00	11.77		
	0.99 Na	10.93	10.89		
O3	1.86 O + 0.14 F	16.25	16.14		
	2.00 O	16.00	16.00		
	0.96 O + 1.04 F	17.35	17.04		

Note: ss = site scattering, mbl = mean bond length.

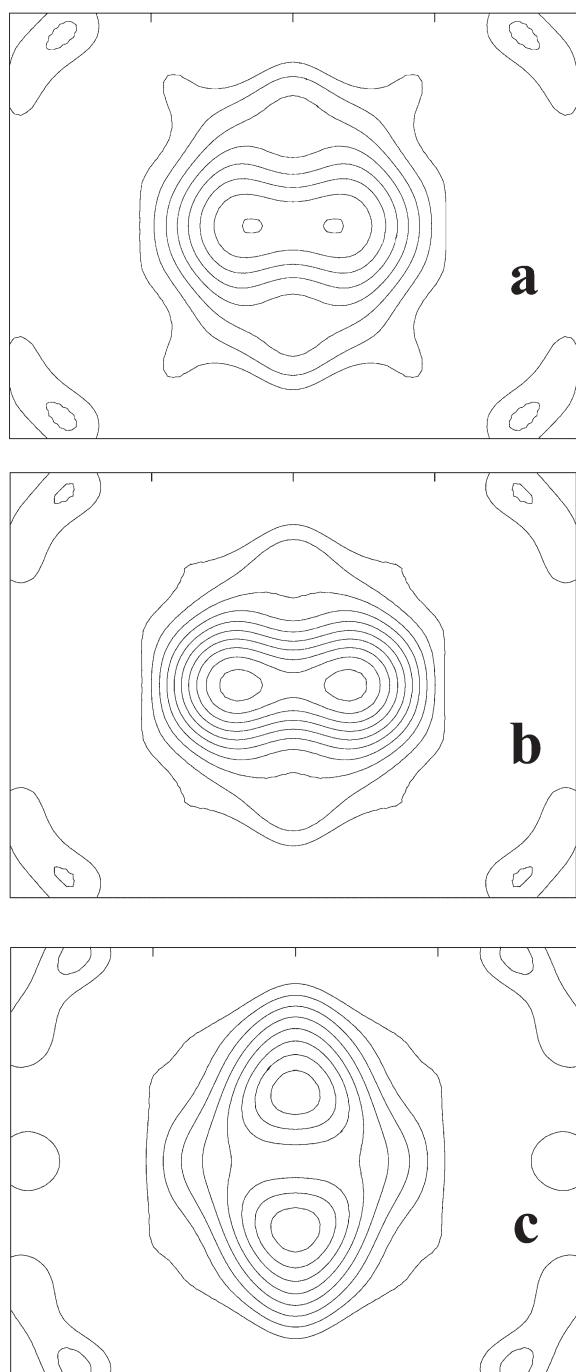
(ΔM1 + 0.005 Å, ΔM3 + 0.011 Å). This feature further supports the previous statements, as the steric requirement imposed by the matching with the double chain of tetrahedra is even stronger, because additional <sup>27</sup>Al apfu in fluoro-alumino-magnesirotaramite increases both the <T1-O> distance and the kinking of the double chain of tetrahedra.

In nyböite with ideally 2 <sup>c</sup>Al and 1 <sup>T1</sup>Al apfu, further bond strength on O1 is provided by the M1 cation, which has a M1-O1 distance of 2.059 Å, much shorter than in glaucophane (2.070 Å) with ideally 2 <sup>c</sup>Al and 0 <sup>T1</sup>Al apfu. In alumino-magnesirotaramite, with ideally 2 <sup>c</sup>Al and 2 <sup>T1</sup>Al apfu, the M1-O distance is even shorter (2.053 Å) to provide more bond strength at O1. The same observation holds for the M2-O1 distance, which is 2.026 Å in alumino-magnesirotaramite (2 <sup>T1</sup>Al apfu), 2.040 Å in nyböite (1 <sup>T1</sup>Al apfu) and 2.041 Å in glaucophane (0 <sup>T1</sup>Al apfu).

Also, the increasing <sup>T1</sup>Al content from glaucophane through

nyböite to alumino-magnesirotaramite allows relaxation of the T-T separation to values more compatible with the ionic radii (3.004, 3.023, and 3.046 Å, respectively), and thus improves the stability of the taramite structure under high-*T* conditions.

Finally, analysis of the electron density at the A site shows the expected behavior for Na ordering (Hawthorne et al. 1996; Oberti et al. 2003). In aluminotaramite and alumino-magnesirotaramite, Na is partitioned between the A2 and the Am sites (according to the preferred local arrangements <sup>M4</sup>Ca-<sup>O3</sup>OH-<sup>A2</sup>Na and <sup>M4</sup>Na-<sup>O3</sup>OH-<sup>Am</sup>Na), whereas in fluoro-alumino-magnesirotaramite Na is almost completely hosted at the Am site, because the presence of F improves the preference for the Am site also in the local arrangements involving <sup>M4</sup>Ca. Inspection of the final *F<sub>o</sub>* maps (Fig. 1) illustrates the different distribution of the electron density at the A site in the studied taramite crystals.



**FIGURE 1.**  $F_0$  maps calculated on sections parallel to  $(-201)$  and centered at  $0, \frac{1}{2}, 0$  for (a) aluminotaramite, (b) alumino-magnesiotalaramite, and (c) fluoro-alumino-magnesiotalaramite showing the electron density around the A-group sites. The  $b$  axis is horizontal and contours are drawn with step of  $1 e\text{\AA}^{-1}$  starting from 1.

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