

OFTEDALITE, (Sc,Ca,Mn²⁺)₂ K (Be,Al)₃ Si₁₂ O₃₀, A NEW MEMBER OF THE MILARITE GROUP FROM THE HEFTETJERN PEGMATITE, TØRDAL, NORWAY: DESCRIPTION AND CRYSTAL STRUCTURE

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ABSTRACT

Oftedalite, ideally (Sc,Ca,Mn²⁺)₂ K (Be,Al)₃ Si₁₂ O₃₀, is a new mineral species from the Heftetjern granitic pegmatite, north-west of the small parish of Tørdal, southern Norway. It occurs as short prismatic crystals up to 100 µm in diameter, frequently with very thin crystals of Sc-free milarite up to ~10–20 µm across in parallel orientation on the (001) faces, or as a product of replacement with other Sc-bearing minerals. Oftedalite – Sc-rich milarite is greyish white with a colorless streak and vitreous luster; it does not fluoresce under ultraviolet light. It has a poor cleavage parallel to {001}, a Mohs hardness of 6, is brittle with a conchoidal fracture, and has a calculated density of 2.614 g/cm³. It is uniaxial negative, with ε 1.553, ω 1.556 (both ± 0.002), and is nonpleochroic. It is hexagonal, space group *P6/mcc*, *a* 10.097(1), *c* 13.991(2) Å, *V* 1235.3(6) Å³, *Z* = 2. The strongest seven lines in the X-ray powder-diffraction pattern [*d* in Å(*hkl*)] are: 3.229(10)(104, 211), 4.097(7)(112), 5.044(5)(110), 3.504(5)(004), 7.012(4)(002), 1.836(4)(412), 1.751(4)(008, 500), and 2.735(3) (204). A chemical analysis by electron microprobe gave SiO₂ 73.32, Al₂O₃ 0.47, Sc₂O₃ 6.77, Y₂O₃ 0.36, FeO 0.26, MnO 1.32, CaO 4.49, K₂O 4.71, BeO (calc.) 7.41, sum 99.11 wt.%; the Be content was determined as (3 – Al) *apfu*. The resulting empirical formula on the basis of 30 atoms of oxygen is (Sc_{0.96}Ca_{0.79}Mn²⁺_{0.18}Fe²⁺_{0.04})Σ_{2.00} K_{0.98} (Be_{2.91}Al_{0.09})Σ_{3.0} Si_{11.98} O₃₀. The crystal structure of Sc-rich milarite, (Sc_{0.84}Ca_{1.03}Mn²⁺_{0.09}Y_{0.01}Fe²⁺_{0.03})Σ_{2.00} K (Be_{2.86}Al_{0.14})Σ_{3.0} Si₁₂ O₃₀], very close to the ideal composition of oftedalite, was refined to an *R* index of 6.6% based on 430 observed reflections collected on a four-circle diffractometer with MoKα X-radiation and a 1K CCD detector. Oftedalite is isostructural with milarite, ideally ^ACa₂^B□^CK^{T(1)}(Be₂Al)^{T(2)}(Si₁₂O₃₀) (H₂O). The structure consists of a beryllio-aluminosilicate framework of the form (4²6⁴)₄(6⁴9²) in which the *T*(1) site is occupied by Si and forms a [Si₁₂O₃₀] cage, and the *T*(2) site is occupied by (Be + Al) and links the [Si₁₂O₃₀] cages into a framework. The *A*, *B* and *C* sites occur in the interstices of the framework with the following occupancies: *A* (Sc_{0.84}Ca_{1.03}Mn²⁺_{0.09}Y_{0.01}Fe²⁺_{0.03}); *B* □; *C* K_{1.00}; *T*(2) (Be_{2.86}Al_{0.14}).

Keywords: oftedalite, new mineral species, milarite group, Heftetjern granitic pegmatite, Tørdal, Norway, crystal structure, electron-microprobe analysis.

SOMMAIRE

L'oftedalite, de composition idéale (Sc,Ca,Mn²⁺)₂ K (Be,Al)₃ Si₁₂ O₃₀, est une nouvelle espèce minérale provenant de la pegmatite granitique de Heftetjern, au nord-ouest de la paroisse de Tørdal, dans le sud de la Norvège. Elle se présente en cristaux prismatiques trappus atteignant un diamètre de 100 µm, en association avec de très minces cristaux de milarite dépourvue de Sc d'environ 10–20 µm de diamètre en orientation parallèle sur les faces (001), ou bien comme produit de remplacement d'autres minéraux porteurs de Sc. La solution solide oftedalite – milarite riche en Sc est blanc grisâtre avec une rayure incolore et un éclat vitreux; elle ne montre aucune fluorescence en lumière ultraviolette. Elle possède un clivage de piètre qualité parallèle à {001} et une dureté de Mohs de 6; elle est cassante avec une fracture conchoïdale, et sa densité calculée est égale à 2.614 g/cm³. Elle est uniaxe négative, avec ε 1.553, ω 1.556 (dans les deux cas ± 0.002), et non pléochroïque. Il s'agit d'un minéral hexagonal, groupe spatial *P6/mcc*, *a* 10.097(1), *c* 13.991(2) Å, *V* 1235.3(6) Å³, *Z* = 2. Les sept raies les plus intenses du spectre de diffraction, méthode des poudres [*d* en Å(*hkl*)] sont: 3.229(10)(104, 211), 4.097(7)(112), 5.044(5)(110), 3.504(5)(004), 7.012(4)(002), 1.836(4)(412), 1.751(4)(008, 500), et 2.735(3) (204). Une analyse chimique avec une microsonde électronique a donné SiO₂ 73.32, Al₂O₃ 0.47, Sc₂O₃ 6.77, Y₂O₃ 0.36, FeO 0.26, MnO 1.32, CaO 4.49, K₂O 4.71, BeO (calc.) 7.41, pour un total de 99.11 % (base pondérale); la teneur en Be a été établie selon la relation (3 – Al) *apfu*. La formule empirique qui en résulte, calculée sur une base de 30 atomes d'oxygène, serait (Sc_{0.96}Ca_{0.79}Mn²⁺_{0.18}Fe²⁺_{0.04})Σ_{2.00} K_{0.98} (Be_{2.91}Al_{0.09})Σ_{3.0} Si_{11.98} O₃₀. La structure cristal-

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line d'un échantillon de milarite scandifère, $(\text{Sc}_{0.84}\text{Ca}_{1.03}\text{Mn}^{2+}_{0.09}\text{Y}_{0.01}\text{Fe}^{2+}_{0.03})_{\Sigma 2.00} \text{K} (\text{Be}_{2.86}\text{Al}_{0.14})_{\Sigma 3.0} \text{Si}_{12}\text{O}_{30}$], voisin de la composition idéale de l'oftedalite, a été affinée jusqu'à un résidu R de 6.6% en utilisant 430 réflexions observées prélevées avec un diffractomètre à quatre cercles, un rayonnement $\text{MoK}\alpha$, et un détecteur à aire 1K de type CCD. L'oftedalite est isostructurale avec la milarite, idéalement $^{\text{A}}\text{Ca}_2 \text{B} \square ^{\text{C}}\text{K} \text{T}(2)(\text{Be}_2\text{Al}) (\text{T}(1)\text{Si}_{12}\text{O}_{30}) (\text{H}_2\text{O})$. La structure comporte une trame béryllo-aluminosilicatée de type $(4^26^4)_4(6^49^2)$ dans laquelle le site $\text{T}(1)$ est rempli par Si et forme une cage $[\text{Si}_{12}\text{O}_{30}]$, et le site $\text{T}(2)$ contient (Be + Al) et assure les liaisons des cages $[\text{Si}_{12}\text{O}_{30}]$ dans une trame. Les sites A, B et C se trouvent dans les interstices de la trame, avec les taux d'occupation suivants: A $(\text{Sc}_{0.84}\text{Ca}_{1.03}\text{Mn}^{2+}_{0.09}\text{Y}_{0.01}\text{Fe}^{2+}_{0.03})$; B \square ; C $\text{K}_{1.00}$; $\text{T}(2)$ $(\text{Be}_{2.86}\text{Al}_{0.14})$.

(Traduit par la Rédaction)

Mots-clés: oftedalite, nouvelle espèce minérale, groupe de la milarite, pegmatite de Heftefjern, Tørdal, Norway, structure cristalline, analyses avec une microsonde électronique.

INTRODUCTION

When Hawthorne *et al.* (1991) reviewed the crystal chemistry of the milarite group, it comprised 15 species. Over the past fifteen years, six new minerals were added to this array, attesting to the great compositional flexibility of this structure type. In the present paper, we describe yet another member of the milarite group, oftedalite $(\text{Sc,Ca,Mn}^{2+})_2 \text{K} (\text{Be,Al})_3 \text{Si}_{12} \text{O}_{30}$, from the Heftefjern granitic pegmatite in the Tørdal district of southern Norway. In early 1998, when RK announced the occurrence of four scandium minerals in the milarite-bearing Heftefjern pegmatite, PC predicted the possibility of finding a scandium analog of milarite at this locality (as quoted in Kristiansen 2003). In the very first samples collected in 1998, RK recognized a milarite-like mineral in one sample, physically distinct from the previously known milarite. He sent a crystal to Franz Bernhard (Graz) who estimated ~5 to ~7 wt.% Sc_2O_3 in its composition. The material was later forwarded to the Mineralogy–Crystallography group at the University of Manitoba, where the data for the new-mineral-species proposal were collected. A second sample of oftedalite – Sc-rich-milarite was found by RK in 2001 as a product of replacement involving four Sc-silicate minerals (Raade & Bernhard 2003, Raade *et al.* 2004).

The new mineral is named in honor of the late Ivar Oftedal (1894–1976), former Professor of Mineralogy at the Institute of Geology, University of Oslo, who contributed extensively to the geochemistry of Sc, and who wrote the first papers on the mineralogy of the Tørdal pegmatites. The species and name of oftedalite were approved by the Commission on New Minerals and Mineral Names, International Mineralogical Association (IMA 2003–045a). A small chip of oftedalite – Sc-rich-milarite, numbered H04/98 in RK's collection, is deposited in the mineralogy collection of the Canadian Museum of Nature, Ottawa. A small fragment of oftedalite – Sc-rich-milarite is also stored at the Steiermärkisches Landesmuseum, Graz, Austria.

OCCURRENCE

The type locality of oftedalite, the Heftefjern pegmatite, is located at 8°45' E, 59°11' N, about 4.3

km NW of the small parish of Tørdal in Telemark County, southern Norway. The pegmatite is a member of an extensive group of pegmatites related to the postorogenic Tørdal granite. This granite was dated at 960 to 880 Ma (Bergstøl & Juve 1988), and the Skarsfjell pegmatite, closely related to the nearby Heftefjern pegmatite, gave 950 to 880 Ma by Rb–Sr on lepidolite and microcline (Neumann 1960, Bergstøl & Juve 1988). The granite is hosted in part by a basement gneiss (1520 to 1500 Ma) and in part by the Rjukan metasedimentary–metavolcanic group of the Telemark Supracrustal Suite, deposited 1300 to 1200 Ma ago (Dons 1960) and metamorphosed to the low-pressure epidote–amphibolite to amphibolite facies at about 1060 Ma (Mitchell 1967, Oftedal 1980, Bergstøl & Juve 1988). The pegmatite population, generally confined to the Rjukan group, is mostly barren, but the more evolved pegmatites contain a (Li, Be, Sc, Y>Ce, Sn, Ti, Nb, Ta)-bearing assemblage of accessory minerals (Bergstøl & Juve 1988, Juve & Bergstøl 1990, 1995, Kristiansen 2003, Raade & Kristiansen 2002, Raade & Bernhard 2003, Raade *et al.* 2004). The granite-cum-pegmatite suite was characterized as a member of the mixed NYF–LCT family, generated by contamination of an A-type NYF magma by LCT components assimilated from the host supracrustal rocks (Černý 1991).

The Heftefjern pegmatite comprises a dike ~300 m long and 5 to 40 m thick in outcrop, and the outcrop of Sc-bearing minerals is less than 10 m long, 3–4 m wide, and less than 2 m deep. The pegmatite is poorly zoned; it consists dominantly of amazonitic K-feldspar, microcline, albite–oligoclase, albite (variety “cleavelandite”), quartz (in part smoky) and a variety of dark to white micas, from minor biotite to zinnwalditic phases enriched in Rb, Cs, Zn and Sc (Juve & Bergstøl 1990). As in most pegmatites of the Tørdal district, a thin fine- to coarse-grained border-zone is followed by a zone of graphic intergrowth of feldspars and quartz, a core-margin zone of coarse blocky texture with abundant albite, and a quartz core. Accessory minerals are concentrated mainly in the margin of the core. Primary accessory phases include beryl, bazzite, spessartine, gadolinite-(Y), cerian scandian epidote, tourmaline, scandian helvite, phenakite, cassiterite, scandian ixiolite, zircon, monazite-(Ce), Sc-bearing minerals of

the pyrochlore group, yttrantalite and yttrian fluorite. A late mineral assemblage encountered mainly in vugs and fractures comprises bertrandite, bavenite, cesian bazzite, stannian titanite, rynersonite, yttrian milarite, kainosite-(Y), hellandite-(Y), calcian hingganite-(Y), stilpnomelane, thortveitite, cascandite, kristiansenite and scandiobabingtonite.

Oftedalite – Sc-rich-milarite was found in two samples: one containing green tourmaline, yttrian milarite, bazzite and an unidentified micaceous mineral, the other containing thortveitite, bazzite, kristiansenite and bertrandite. The specimen of Sc-rich milarite described here comes from the first assemblage; additional compositional data are available from the second specimen, as mentioned below (sample H03/01b of Raade *et al.* 2004).

PHYSICAL PROPERTIES

Oftedalite – Sc-rich-milarite occurs as short six-sided prismatic crystals up to 100 μm in diameter, with prominent $\{100\}$ and $\{001\}$ forms. Very thin crystals of Sc-free milarite, ~ 10 to 20 μm across, grow locally in parallel orientation on the $\{001\}$ faces of oftedalite. Crystals are greyish white with a colorless streak and vitreous luster, and do not fluoresce under ultraviolet light. They have poor cleavage parallel to $\{001\}$, a Mohs hardness of 6, and are brittle with a conchoidal fracture; no parting or twinning was observed. Crystals of oftedalite – Sc-rich milarite are generally very inhomogeneous, showing solid solution toward milarite, and are unsuitable for the determination of density; the calculated density is 2.614 g/cm^3 . Optical properties in transmitted light were measured on a Bloss spindle stage in monochromated Na light ($\lambda = 590 \text{ nm}$) on the single crystal used for the crystal-structure study and electron-microprobe analysis, and the program EXCALBR II (Bartelmehs *et al.* 1992) was used to determine optic orientation. Oftedalite – Sc-rich-mila-

rite is uniaxial negative with ε 1.553, ω 1.556 (both ± 0.002), and is nonpleochroic.

CHEMICAL COMPOSITION

Crystals were analyzed with a Cameca SX-50 electron microprobe operating in the wavelength-dispersion mode with an accelerating voltage of 20 kV, a specimen current of 15 nA, and a beam diameter of 5 μm . The following standards were used: quartz (Si), andalusite (Al), synthetic NaScSi₂O₆ (Sc), YAG (Y), fayalite (Fe), spessartine (Mn), diopside (Ca), and sanidine (K). The data were reduced and corrected by the PAP method of Pouchou & Pichoir (1984, 1985). Table 1 gives the chemical composition (mean of ten determinations) and formula unit based on 30 anions *pfu* (per formula unit) and $\text{Be} = 3 - \text{Al } apfu$ (as determined by site-scattering refinement during the crystal-structure refinement). Crystals of oftedalite – Sc-rich-milarite are inhomogeneous, and we were not able to find single grains of oftedalite or even grains the average composition of which corresponded to that of oftedalite. Composition (1) (Table 1) pertains to a small zone of oftedalite in a composite crystal; composition (2) is the average composition (on 10 points) of the crystal of Sc-rich milarite used to refine the crystal structure.

X-RAY POWDER DIFFRACTION

The single crystal used for the structure study, the electron-microprobe work and optics was mounted on a Debye-Scherrer powder camera with a Gandolfi attachment and the powder-diffraction pattern was recorded with Ni-filtered CuK α X-radiation ($\lambda = 1.5406 \text{ \AA}$). Table 2 shows the X-ray powder-diffraction data for Sc-rich milarite. The unit-cell dimensions were refined from 21 reflections representing *d*-values between 7.012 and 1.188 \AA which could be indexed unambiguously on the basis of intensities from the single-crystal diffraction work. These values (Table 2) are close to the values determined on the same crystal of Sc-rich milarite by single-crystal diffraction (Table 3).

CRYSTAL-STRUCTURE REFINEMENT

Numerous grains were examined, but in no case could we isolate a grain of pure oftedalite; all grains were found to be heterogeneous mixtures of oftedalite and Sc-rich milarite, with the latter composition predominating. A single-crystal of average composition close to that of oftedalite (Table 1) was attached to a glass fiber and mounted on a Bruker P4 diffractometer equipped with a 1K CCD detector and a MoK α X-ray tube. A total of 13,903 reflections was measured (11,319 in the Ewald sphere) out to 60° 2 θ with a frame time of 60 s and a frame width of 0.2°. Of the 639 unique reflections, 430 reflections were considered as observed [$|F_o| \geq 5\sigma F$]. The data were corrected for absorption,

TABLE 1. CHEMICAL COMPOSITION (wt.%) AND FORMULA (*apfu*) FOR (1) OFTEDALITE AND (2) SC-RICH MILARITE

	(1)	(2)		(1)	(2)
SiO ₂	73.32	73.44	Si	11.98	12.00
Al ₂ O ₃	0.47	0.75			
Sc ₂ O ₃	6.77	5.90	Al	0.09	0.14
Y ₂ O ₃	0.36	0.15	Be	<u>2.91</u>	<u>2.86</u>
FeO	0.26	0.22	Σ	3.00	3.00
MnO	1.32	0.63			
CaO	4.49	5.88	K	0.98	1.00
K ₂ O	4.71	4.78			
BeO*	<u>7.41</u>	<u>7.27</u>	Sc	0.96	0.84
Sum	99.11	99.02	Ca	0.79	1.03
			Mn ²⁺	0.18	0.09
			Y	0.03	0.01
			Fe ²⁺	<u>0.04</u>	<u>0.03</u>
			Σ	2.00	2.00

* calculated as $\text{Be} = 3 - \text{Al } apfu$.

Lorentz, polarization and background effects, averaged and reduced to structure factors. After data collection, the crystal used for X-ray diffraction was attached to the surface of a Perspex disc, polished, carbon-coated and analyzed with a Cameca SX-50 electron microprobe as described above.

All calculations were done with the SHELXTL PC (Plus) system of programs; *R* indices are of the form given in Table 3 and are expressed as percentages. Systematic absences in the single-crystal X-ray-diffraction data are consistent with the space group *P6/mcc*, the space group for (most of) the milarite-group minerals. The starting coordinates were those of milarite (Černý *et al.* 1980), and the following scattering factors were used: *A* = Sc (variable occupancy), the *B* site was

observed to be vacant, *C* = K (fixed), *T*(2) = Be (variable occupancy). Refinement rapidly converged to an *R* index of 6.6%. Refined coordinates and anisotropic-displacement factors are listed in Table 4, selected interatomic distances are given in Table 5, and site-scattering values and assigned site-populations are given in Table 6. Observed and calculated structure-factors may be obtained from The Depository of Unpublished Data, CISTI, National Research Council, Ottawa, Ontario K1A 0S2, Canada.

CRYSTAL STRUCTURE

The tetrahedron framework

As discussed by Hawthorne & Smith (1986) and Hawthorne *et al.* (1991), the general structure of the milarite-group minerals is a beryllio-aluminosilicate framework of the form $(4^26^4)_4(6^49^2)$, with several of the interstitial sites occupied by a wide variety of cations. The observed $\langle T(1)-O \rangle$ distance, 1.605 Å (Table 5), indicates that the *T*(1) site is occupied solely by Si, as indicated by the empirical formula (Table 1). The observed $\langle T(2)-O \rangle$ distance, 1.638 Å (Table 5), and the site population for *T*(2) given in Table 6 are in exact accord with the relation between $\langle T(2)-O \rangle$ and Be / (Be + Al) given by Hawthorne *et al.* (1991).

The interstitial sites

Site-scattering refinement indicated that only the *A* and *C* sites are occupied and the *B* and *D* sites are vacant in the crystal examined. The refined site-scattering value at the *A* site is in almost exact accord with the site populations assigned from the unit formula derived from the electron-microprobe analysis (Table 6). The observed $\langle A-O \rangle$ distance, 2.232 Å (Table 5), and the site population for *A* given in Table 6 are in close accord with the relation between $\langle A-O \rangle$ and the aggregate radius of the cations occupying the *A* site given by Hawthorne *et al.* (1991). The $\langle C-O \rangle$ distance, 3.047 Å (Table 5), is reasonably close to the grand $\langle C-O \rangle$ distance, 3.017 Å, observed in milarite structures (Hawthorne *et al.* 1991).

CHEMICAL FORMULA

The general composition for oftedalite is $(Sc,Ca,Mn^{2+})_2 K (Be,Al)_3 Si_{12} O_{30}$. The definition of oftedalite requires that Sc be dominant at the *A* site; note that this is the case for composition (1) but not for composition (2) (Table 1) despite the fact that they contain similar amounts of Sc. Consider the composition $(ScCa) K Be_3 Si_{12} O_{30}$; there are two ways in which Sc can exceed Ca and yet maintain electroneutrality; (1) substitution of a lower-valence cation at another cation site (*e.g.*, Al for Si); (2) replacement of Ca by a third (divalent) cation at the *A* site. Examination of composition (1) indicates

TABLE 2. X-RAY POWDER-DIFFRACTION DATA FOR SC-RICH MILARITE

l_{calc}	d_{exp} , Å	d_{calc} , Å	hkl	l_{calc}	d_{exp} , Å	d_{calc} , Å	hkl
* 4	7.012	7.004	0 0 2	4	1.836b	1.842	4 1 2
* 1	5.477	5.468	1 0 2	"	"	1.834	3 1 5
* 5	5.044	5.052	1 1 0	* 4	1.751	1.751	0 0 8
* 2	4.367	4.375	2 0 0	"	"	1.750	5 0 0
* 7	4.097	4.097	1 1 2	* 3	1.715	1.715	2 2 6
* 2	3.711	3.711	2 0 2	* 3	1.677	1.677	4 1 4
* 5	3.504	3.502	0 0 4	1	1.643	1.642	4 2 1
10	3.229	3.251	1 0 4	1	1.624	1.626	2 0 8
"	"	3.219	2 1 1	* 2	1.518	1.518	3 3 4
1	2.923	2.917	3 0 0	2	1.503	1.501	3 0 8
* 6	2.880	2.878	1 1 4	* 2	1.439	1.439	2 2 8
* 3	2.735	2.734	2 0 4	2	1.427	1.428	6 0 2
* 1	2.697	2.699	2 1 3	"	"	1.424	4 2 5
* 2	2.526	2.526	2 2 0	3	1.402b	1.408	2 1 9
* 2	2.425	2.427	3 1 0	"	"	1.401	5 2 0
2	2.386	2.391	3 1 1	"	"	1.394	5 2 1
"	"	2.376	2 2 2	3	1.348	1.350	1 1 10
* 2	2.152	2.153	3 1 3	"	"	1.346	6 0 4
1	2.109	2.119	1 1 6	* 2	1.310	1.310	3 1 9
3	1.995	1.995	3 1 4	2	1.203	1.201	5 2 6
"	"	1.987	3 2 1	* 2	1.188	1.188	2 1 11
* 2	1.911	1.910	4 1 0	"	"	1.188	4 4 4
2	1.895	1.892	4 1 1				

114.6 mm Debye-Scherrer powder camera with Gandolfi attachment, Cu radiation and Ni filter, (λ CuK α = 1.5406 Å); intensities estimated visually, b = broad line. Not corrected for shrinkage and no internal standard.

*: lines used for unit-cell refinement: a 10.104(2), c 14.008(3) Å, V 1238.6(4) Å³.

TABLE 3. MISCELLANEOUS INFORMATION: SC-RICH MILARITE

<i>a</i> (Å)	10.097(1)	crystal size (μm)	60 x 60 x 100
<i>c</i>	13.991(2)	radiation	MoK α
<i>V</i> (Å ³)	1235.3(6)	No. of unique reflections	639
Space Group	<i>P6/mcc</i>	No. <i>F_h</i> > 5σ <i>F</i>	430
<i>Z</i>	2	<i>R</i> (merge) (%)	4.0
		<i>R_w</i> (%)	6.6
		<i>wR</i> (%)	7.1

$R = \sum (F_o - F_c) / \sum F_c$
 $wR = [\sum w(F_o - F_c)^2 / \sum wF_c^2]^{1/2}$, $w = 1$

TABLE 4. ATOM COORDINATES AND DISPLACEMENT PARAMETERS FOR Sc-RICH MILARITE

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
Sc	1/3	2/3	1/4	0.0070(11)	0.0070(11)	0.0131(18)	0	0	0.0035(5)	0.0090(9)
C	0	0	1/4	0.0175(18)	0.0175(18)	0.026(4)	0	0	0.0087(9)	0.0204(18)
T(1)	0.0884(2)	0.3466(2)	0.10937(14)	0.0058(9)	0.0057(8)	0.0110(8)	-0.0024(8)	-0.0011(8)	0.0027(7)	0.0076(7)
T(2)	0	1/2	1/4	0.010(8)	0.009(6)	0.008(8)	0	0	0.005(4)	0.009(6)
O(1)	0.1044(10)	0.4005(9)	0	0.021(4)	0.017(4)	0.005(3)	0	0	0.011(4)	0.014(3)
O(2)	0.2030(7)	0.2818(8)	0.1300(4)	0.023(3)	0.028(3)	0.028(3)	-0.002(3)	-0.003(3)	0.023(3)	0.022(3)
O(3)	0.1216(7)	0.4817(6)	0.1816(4)	0.023(3)	0.013(3)	0.015(2)	-0.004(2)	-0.001(2)	0.012(2)	0.016(2)

TABLE 5. SELECTED INTERATOMIC DISTANCES (Å) IN Sc-RICH MILARITE

A-O(3)	x6	2.232(5)	T(1)-O(1)	1.805(3)
			T(1)-O(2)	1.814(9)
C-O(2)	x12	3.047(3)	T(1)-O(2)a	1.609(7)
			T(1)-O(3)	1.593(6)
T(2)-O(3)	x4	1.638(7)	<T(1)-O>	1.605

a: x-y, x, z

TABLE 6. REFINED AND CALCULATED SITE-SCATTERING VALUES (apfu) AND ASSIGNED SITE-POPULATIONS (apfu) IN Sc-RICH MILARITE

Site	Refined site-scattering	Site populations from unit formula	Calculated site-scattering
A	41.8(7)	0.84 Sc + 1.03 Ca + 0.01 Y + 0.09 Mn ²⁺ + 0.03 Fe ²⁺	41.7
C	19	1.0 K	19
T(2)	13.0(9)	2.86 Be + 0.14 Al	13.3

that mechanism (2) is operative in oftedalite: Sc is the dominant cation at the A site [composition (1), Table 1] but does not exceed 1 apfu. In composition (1), Sc is dominant because Ca is partly replaced by Mn²⁺ and Fe²⁺, whereas Sc shows only minor replacement by Y; the amounts of divalent and trivalent cations at the A site are still 1.0 and 1.0 apfu, respectively. The composition field for oftedalite is shown in Figure 1, assuming that Sc cannot exceed 1.00 apfu.

The current members of the milarite group are listed in Table 7, where the minerals have been ordered into subgroups according to the formal charge at the T(2) site, and the end-member formulae according to the criteria of Hawthorne (2002) are listed. Armenite has been included here even though it is orthorhombic, as it is pseudo-hexagonal and has an orthorhombic superstructure. In the end-member compositions listed in Table 7, note that the C site, with a rank of 1, is the only site that is not occupied by two species in the collection of end-members given. It is this peculiarity of the milarite structure that is a major factor in the chemical flexibility of this structure type, and suggests

TABLE 7. SITE POPULATIONS IN END-MEMBER COMPOSITIONS OF MINERALS OF THE MILARITE GROUP

	A ₆	B ₂	C	T(1) ₁₂	T(2) ₁	Ref.
Berezanskite	Ti ⁴⁺ ₆	□ ₂	K	Si ₁₂	Li ₁	(1)
Brannockite	Sn ⁴⁺ ₆	□ ₂	K	Si ₁₂	Li ₁	(2)
Darapioisite	Mn ²⁺ Zr	Na ₂	K	Si ₁₂	Li ₁	(3)
Sogdianite	Zr ₂	□ ₂	K	Si ₁₂	Li ₁	(4)
Sugilite	Fe ³⁺ ₆	Na ₂	K	Si ₁₂	Li ₁	(2)
Dusmatovite	Mn ²⁺ ₆	□Na	K	Si ₁₂	Zn ₁	(5)
Eifelite	MgNa	Na ₂	K	Si ₁₂	Mg ₁	(6)
Morzhueite (syn)	Mg ₆	□K	K	Si ₁₂	Mg ₁	(7)
Synthetic	Mn ²⁺ ₆	□K	K	Si ₁₂	Mn ²⁺ ₁	(8)
Oftedalite	ScCa	□ ₂	K	Si ₁₂	Be ₁	(9)
Roedderite	Mg ₆	□Na	K	Si ₁₂	Mg ₁	(10)
Shibkovite	Ca ₂	□K	K	Si ₁₂	Zn ₁	(11)
Tratnerite	Fe ₂	□ ₂	□	Si ₁₂	Mg ₁	(12)
Chayesite	Mg ₆	Li ₂	K	Si ₁₂	Mg ₁ Fe ²⁺	(13)
Synthetic	Mn ²⁺ ₆	□ ₂	K	Si ₁₂	Zn ₁ Fe ²⁺	(14)
Milarite	Ca ₆	□ ₂	K	Si ₁₂	Be ₁ Al	(15)
Almarudite	Mn ²⁺ ₆	□ ₂	K	Si ₁₂	(Be, Al)	(16)
Armenite	Ca ₆	□ ₂	Ba	Si ₁₂ Al	Al ₁	(17)
Osumilite	Fe ²⁺ ₆	□ ₂	K	Si ₁₂ Al	Al ₁	(18)
Osumilite-(Mg)	Mg ₆	□ ₂	K	Si ₁₂ Al	Al ₁	(18)
Poudretteite	Na ₆	□ ₂	K	Si ₁₂	B ₁	(19)
Yagiite	Mg ₆	□ ₂	Na	Si ₁₂ Al	Al ₁	(20)
Ba Mg ₅ Al ₂ Si ₁₀ O ₂₃	Mg ₆	□ ₂	Ba	Si ₁₂ Al	Al ₁	(21)
Sr Mg ₅ Al ₂ Si ₁₀ O ₂₃	Mg ₆	□ ₂	Sr	Si ₁₂ Al	Al ₁	(21)
Mg ₅ Al ₂ Si ₁₁ O ₂₃	Mg ₆	□ ₂	□	Si ₁₂ Al	Al ₁	(21)

References: (1) Pautov & Agakhanov (1997), (2) Armbruster & Oberhänsli (1988b), (3) Ferraris *et al.* (1999), (4) Sokolova *et al.* (2000), (5) Sokolova & Pautov (1995), (6) Abraham *et al.* (1983), (7) Dodd *et al.* (1965), Khan *et al.* (1971), (8) Sandomirskii *et al.* (1977), (9) this study, (10) Armbruster (1989), (11) Sokolova *et al.* (1999), (12) Post *et al.* (2004), (13) Velde *et al.* (1989), (14) Pushcharovskii *et al.* (1972), (15) Černý *et al.* (1980), Hawthorne *et al.* (1991), (16) Mihajlovic *et al.* (2004), (17) Armbruster & Czank (1992), Armbruster (1999), (18) Armbruster & Oberhänsli (1988a), (19) Grice *et al.* (1987), (20) Bunch & Fuchs (1969), (21) Winter *et al.* (1995).

that many milarite-group minerals remain to be found in the appropriate parageneses (Boggs 1994).

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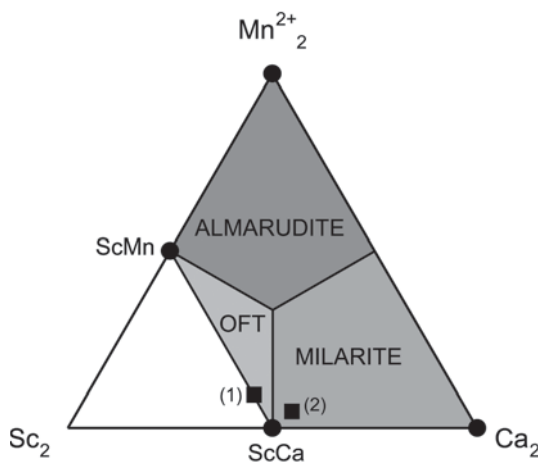


FIG. 1. The compositional field of oftedalite (OFT) as a function of the occupancy of the A site in the milarite-type structure.

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