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Article in *American Mineralogist* · October 2014

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Agakhanovite-(Y), ideally $(YCa)\square_2KBe_3Si_{12}O_{30}$, a new milarite-group mineral from the Heftetjern pegmatite, Tørdal, Southern Norway: Description and crystal structure

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ABSTRACT

Agakhanovite-(Y), ideally $(YCa)\square_2KBe_3Si_{12}O_{30}$, is a new milarite-group mineral from the Heftetjern pegmatite, Tørdal, southern Norway. Crystals are prismatic along [001], and show the forms {100} and $\{100\}$. Agakhanovite-(Y) is colorless with a white streak and a vitreous luster, and does not fluoresce under ultraviolet light. There is no cleavage or parting, and no twinning was observed. Mohs hardness is 6, and agakhanovite-(Y) is brittle with a conchoidal fracture. The calculated density is 2.672 g/cm³. Optical properties were measured with the Bloss spindle stage for the wavelength 590 nm using a gel filter. Agakhanovite-(Y) is uniaxial (–) with indices of refraction $\omega = 1.567$, $\epsilon = 1.564$, both ± 0.002 ; the calculated birefringence is 0.003 and it is non-pleochroic. Agakhanovite-(Y) is hexagonal, space group *P6/mcc*, $a = 10.3476(2)$, $c = 13.7610(3)$ Å, $V = 1276.02(9)$ Å³, $Z = 2$, $c:a = 1.330$. The seven strongest lines in the X-ray powder-diffraction pattern are as follows: d (Å), I , (hkl): 2.865, 100, ($\bar{1}24$); 3.287, 96, ($\bar{1}31$); 4.134, 84, ($\bar{1}22$); 6.877, 56, (002); 2.986, 43, (030); 4.479, 38, (020); 2.728, 36, (024). Chemical analysis by electron microprobe gave SiO₂ 69.56, Al₂O₃ 0.35, Y₂O₃ 9.69, Yb₂O₃ 0.15, FeO 0.02 CaO 5.75, Na₂O 0.07, K₂O 4.52, BeO(calc) 7.06, H₂O(calc) 1.74, sum 98.91 wt%. The H₂O content was determined by crystal-structure analysis. On the basis of 30 anions, the empirical formula is $(Y_{0.89}Yb_{0.01}Ca_{1.06})_{\Sigma 1.96}(H_2O)_{0.92}Na_{0.02}K_{1.00}(Be_{2.93}Al_{0.07})_{\Sigma 3.00}Si_{12.02}O_{30}$. The crystal structure of agakhanovite-(Y) was refined to an R_1 index of 1.9% based on 660 unique observed reflections collected on a three-circle rotating-anode (MoK α X-radiation) diffractometer equipped with multilayer optics and an APEX-II detector. In the end-member structure of agakhanovite-(Y), the A site is occupied equally by Y and Ca, and the B site is vacant; agakhanovite-(Y) is the Y-analog of oftedalite: $ScCa\square_2KBe_3Si_{12}O_{30}$, and the Y-Ca-Be analog of klöchite, $(Fe^{2+}Fe^{3+})\square_2KZn_3Si_{12}O_{30}$.

Keywords: Agakhanovite-(Y); new mineral species; milarite-group mineral; Heftetjern pegmatite, Tørdal, southern Norway; crystal structure; electron microprobe analysis; optical properties

INTRODUCTION

Oftedal and Sæbø (1965) reported significant Y-REE in milarite from Grorud, Norway. Černý et al. (1991) described Y-rich milarite from the Jaguaraçu pegmatite, Minas Gerais, Brazil, and the Strange Lake peralkaline complex, Labrador-Quebec border, Canada, with up to 7.9 wt% Y₂O₃ and 2.9 wt% REE₂O₃ in the latter. Nysten (1996) reported Y-rich milarite from granitic pegmatites in Sweden with up to 8.89 wt% Y₂O₃. These milarites were all strongly compositionally zoned, preventing characterization and description as a new species. Raade and Kristiansen (2000) and Kristiansen (2009) reported Sc as a major element in one sample of milarite from the granitic pegmatite at Heftetjern, Tørdal, southern Norway. Hawthorne (2002) suggested that this could be a new mineral of the milarite-group, and it was described by Cooper et al. (2006) as the new species oftedalite, ideally $(ScCa)\square_2KBe_3Si_{12}O_{30}$. The Heftetjern pegmatite also contains many minerals with essential Y: ytropyrochlore-(Y), yttrobetafite-(Y), polycrase-(Y), gadolinite-(Y), thalenite-(Y),

calcian hingganite-(Y), manganoan hellandite-(Y), kainosite-(Y), and kamphaugite-(Y), suggesting the possibility of an Y-analog of oftedalite. Detailed examination of Y-rich parageneses of the Heftetjern pegmatite eventually led in 2011 to the discovery of tractable crystals of high Y content that could be characterized as a new species.

This mineral is named agakhanovite-(Y) after Atali A. Agakhanov (b. 1971), mineralogist at the Fersman Mineralogical Museum, Moscow, Russia, who has worked on a wide variety of pegmatite minerals, and in particular on the minerals of the milarite group. The new mineral and mineral name have been approved by the Commission on New Minerals, Nomenclature and Classification, International Mineralogical Association (IMA 2013-090). The holotype specimen of agakhanovite-(Y) is deposited in the Mineralogy collection of the Royal Ontario Museum, 100 Queens Park, Toronto, Ontario M5S 2C6, Canada, catalog number M43863.

OCCURRENCE

The Heftetjern cleavelandite-amazonite pegmatite is situated in a marshy area between Høydalen and Skarsfjell in Tørdal,

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southern Norway, at an altitude of ~650 m above sea level, at 59°8.6' N 8°45.4' E. The numerous granite pegmatites of the Tørdal area occur within the Nissedal volcano-sedimentary outlier. Both the outlier (1300–1200 Ma) and the older basement (1520–1500 Ma) are intruded by the Tørdal granite (960–850 Ma), which is regarded as the source of the pegmatite swarms (Bergstøl and Juve 1988). The Tørdal area in Telemark is geochemically different from other granite pegmatites in south Norway, being characterized by high levels of Sn, Sc, Y, Be, and Li. Bergstøl and Juve (1988) suggested that some of the Sn and a major part of Sc in the amazonite-cleavelandite pegmatites of the area were leached from the volcanogenic rocks of the Nissedal outlier by the pegmatitic fluids.

Three types of milarite can be distinguished at Hefsetjern: (1) milarite of normal composition (rather common); (2) milarite with roughly 5–7 wt% Sc_2O_3 = oftedalite (Cooper et al. 2006) (extremely rare); (3) milarite with high yttrium content (rare). Moreover, only one sample shows very high Y (~10 wt% Y_2O_3), the holotype described here. Agakhanovite-(Y) occurs in vugs in a granitic pegmatite, indicating that it is a miarolitic-cavity mineral that crystallized from late-stage hydrothermal solutions enriched in Y.

PHYSICAL PROPERTIES

The type specimen is approximately $3 \times 3 \times 1$ cm and consists of microcline, albite, and interstitial quartz crystals, with several hexagonal, colorless crystals of milarite 1–4 mm long with prominent {100} and {001} forms. Agakhanovite-(Y) occurs as aggregates or clusters up to 350 μm wide (Fig. 1) and consisting of colorless transparent crystals, or as tiny solitary hexagonal crystals partly on or between crystals of milarite or embedded in or deposited on the surface of milarite crystals with random orientation. It occurs more rarely as ~20 μm hexagonal crystals perched on the surface of kristiansenite. Individual crystals of agakhanovite-(Y) are up to 20–60 μm long and 10–20 μm thick.

Crystals are prismatic along [001] and show the following forms: {100} and {001}. Agakhanovite-(Y) is colorless with a white streak and a vitreous luster, and does not fluoresce under ultraviolet light. There is no cleavage or parting, and no twinning was observed. Mohs hardness is 6, and agakhanovite-(Y) is brittle with a conchoidal fracture. The calculated density is 2.672 g/cm^3 . Optical properties were measured with a Bloss spindle stage for the wavelength 590 nm using a gel filter. It is uniaxial (–) with indices of refraction $\omega = 1.567$, $\epsilon = 1.564$, both ± 0.002 ; the calculated birefringence is 0.003.

RAMAN SPECTROSCOPY

The Raman spectrum of agakhanovite-(Y) is shown in Figure 2. The Raman spectrum shows typical Si-O stretches at 1000–1200 cm^{-1} and various “lattice vibrations” at lower wavenumbers. There is an asymmetric envelope from ~3400–3560 cm^{-1} and two small peaks at 3670 and 3730 cm^{-1} that correspond to principal stretching bands of H_2O .

CHEMICAL COMPOSITION

Agakhanovite-(Y) was analyzed with a Cameca SX-100 electron microprobe operating in wavelength-dispersion mode with an accelerating voltage of 15 kV, a specimen current of 20 nA, and a

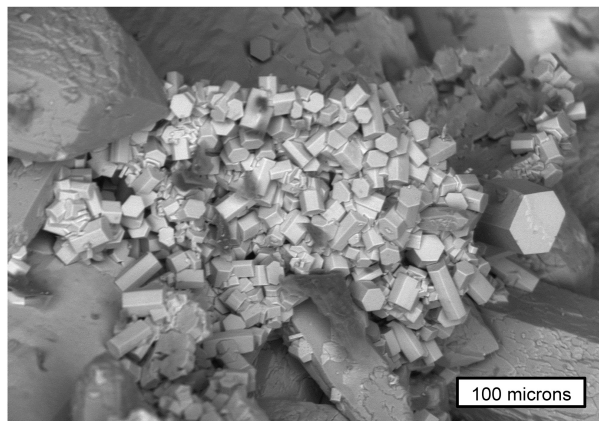


FIGURE 1. Backscattered-electron image of crystals of agakhanovite-(Y) and Y-bearing milarite.

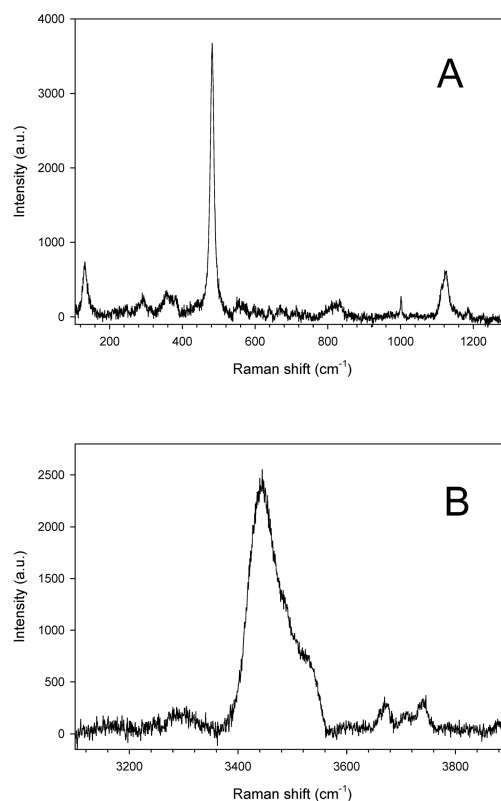


FIGURE 2. The Raman spectrum of agakhanovite-(Y) in the regions 100–1300 cm^{-1} (a) and 3100–3900 cm^{-1} (b).

beam diameter of 5 μm . The following standards were used: quartz – Si; andalusite – Al; YAG – Y; YbPO_4 – Yb; fayalite – Fe; diopside – Ca; albite – Na; orthoclase – K (Mn, Zn, other REE not detected). The data were reduced and corrected by the PAP method of Pouchou and Pichoir (1985) and the chemical composition (mean of 10 determinations) is given in Table 1. The empirical formula was calculated on the basis of 30 anions with

TABLE 1. Chemical composition of agakhanovite-(Y)

Constituent	wt%	Range	St. dev.
SiO ₂	69.56	68.36–70.45	0.58
Al ₂ O ₃	0.35	0.24–0.63	0.14
Y ₂ O ₃	9.69	9.43–10.35	0.24
Yb ₂ O ₃	0.15	0.06–0.30	0.07
FeO	0.02	0.00–0.04	0.01
CaO	5.75	5.66–5.95	0.08
Na ₂ O	0.07	0.03–0.09	0.02
K ₂ O	4.52	4.41–4.57	0.04
BeO(calc)	7.06	–	–
H ₂ O(calc)	1.74	–	–
Total	98.91		

Be = 3 – Al, and (H₂O) was calculated as 0.92 apfu (atom per formula unit) as indicated by site-scattering refinement, giving (Y_{0.89}Yb_{0.01}Ca_{1.06})_{Σ1.96}[□_{1.06}(H₂O)_{0.92}Na_{0.02}]_{Σ2.00}K_{1.00}(Be_{2.93}Al_{0.07})_{Σ3.00}Si_{12.02}O₃₀, ideally (YCa)□₂KBe₃Si₁₂O₃₀.

X-RAY POWDER DIFFRACTION

X-ray powder-diffraction data were obtained using a Gandolfi attachment mounted on a Bruker D8 rotating-anode Discover SuperSpeed micro-powder diffractometer with a multi-wire 2D detector. Data (in angstroms for CuKα) are listed in Table 2. Unit-cell parameters refined from the powder data are as follows: $a = 10.342(1)$, $c = 13.768(3)$ Å, $V = 1275.5(4)$ Å³.

CRYSTAL-STRUCTURE SOLUTION AND REFINEMENT

A crystal was attached to a tapered glass fiber and mounted on a Bruker D8 three-circle diffractometer equipped with a rotating-anode generator (MoKα), multilayer optics and an APEX-II detector. A total of 44574 intensities was collected to 60° 2θ using 2 s per 0.2° frames with a crystal-to-detector distance of 5 cm. Empirical absorption corrections (SADABS; Sheldrick 2008) were applied and equivalent reflections were corrected for Lorentz, polarization, and background effects, averaged and reduced to structure factors. The unit-cell dimensions were obtained by least-squares refinement of the positions of 9975 reflections with $I > 10\sigma I$ and are given in Table 3, together with other information pertaining to data collection and structure refinement.

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. The structure was refined in the space group $P6/mcc$ by full-matrix least-squares with anisotropic-displacement parameters on all atoms to convergence at a final R_1 index of 1.90%. Refined atom coordinates and anisotropic-displacement parameters are listed in Table 4, selected interatomic distances are given in Table 5, and refined site-scattering values (Hawthorne et al. 1995) and assigned site-populations are given in Table 6. (A CIF¹ is available.)

CRYSTAL STRUCTURE

The tetrahedron framework

The general structure of the milarite-group minerals is a beryllio-aluminosilicate framework (Forbes et al. 1972; Černý et al. 1980) of the form (4²6⁴)₄(6⁴9²) (Hawthorne and Smith 1986; Hawthorne et al. 1991) with several of the interstitial sites occupied by a wide variety of cations. The T1 site is occupied solely by Si, as indicated by the empirical formula

TABLE 2. Powder-diffraction data for agakhanovite-(Y)

I_{meas} (%)	d_{meas} (Å)	d_{calc} (Å)	hkl
56	6.877	6.884	002
16	5.464	5.458	012
19	5.170	5.171	120
38	4.479	4.479	020
84	4.134	4.135	122
11	3.755	3.754	022
25	3.445	3.442	004
96	3.287	3.288	131
27	3.214	3.213	014
43	2.9861	2.9857	030
100	2.8653	2.8654	124
36	2.7283	2.7291	024
		2.7244	133
15	2.5842	2.5857	240
5	2.4832	2.4843	140
10 B	2.4280 ^a		
5	2.2513	2.2554	034
6	2.1858	2.1847	143
8	2.0977	2.0975	126
14	2.0159	2.0144	144
15	1.9541	1.9546	150
21	1.8801	1.8803	152
15	1.8450	1.8445	145
10	1.8196	1.8193	036
10	1.7915	1.7914	050
16	1.7181	1.7210	008
		1.7163	246
16	1.6995	1.6997	154
9	1.6793	1.6801	261
3	1.6436	1.6438	262
6	1.6059	1.6065	028
5	1.5909	1.5891	054
		1.5882	263
3	1.5661	1.5665	162
9	1.5406	1.5413	364
4	1.5184	1.5182	163
9	1.4915	1.4911	038
5	1.4590	1.4589	062
14	1.4342	1.4343	270

^a Broad, not used in the refinement.

TABLE 3. Miscellaneous information for agakhanovite-(Y)

a (Å)	10.3476(2)	Crystal size (μm)	15 × 15 × 30
c	13.7610(3)	Radiation	MoKα
V (Å ³)	1276.02(9)	No. of unique reflections	660
Space Group	$P6/mcc$	No. $ F_o^* > 5\sigma F$	430
Z	2	$R(\text{merge})$ (%)	2.5
		R_1 (%)	1.9
		wR (%)	6.3

Notes: $R = \sum(|F_o^*| - |F_c^*|) / \sum |F_o^*|$, $wR = [\sum w(|F_o^*| - |F_c^*|)^2 / \sum F_o^*]^2$, $w = 1$.

given above and by the observed <T1-O> distance of 1.612 Å (Table 5). Hawthorne et al. (1991) developed a relation between <T2-O> and Be/(Be + Al) in the milarite structures; the observed <T2-O> distance of 1.636 Å (Table 5) and the assigned T2 site-population of 2.93 Be + 0.07 Al (Table 6) are in exact accord with this relation.

The interstitial sites

The refined site-scattering value at the A site is in close accord with the site populations assigned from the unit formula derived from the electron-microprobe analysis (Table 6). The observed <A-O> distance of 2.334 Å (Table 5) and the site

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TABLE 4. Atom coordinates and displacement parameters for agakhanovite-(Y)

	x	y	z	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}	U_{eq}
A	1/3	2/3	0.2363(1)	0.0071(2)	0.0071(2)	0.0139(11)	0	0	0.0036(1)	0.0094(4)
B	1/3	2/3	0.0545(6)	0.044(3)	0.044(3)	0.031(4)	0	0	0.022(2)	0.039(3)
C	0	0	1/4	0.0187(5)	0.0187(5)	0.0220(6)	0	0	0.0093(2)	0.0198(4)
T1	0.08107(4)	0.33803(4)	0.11267(3)	0.0082(2)	0.0106(2)	0.0073(2)	-0.0013(1)	-0.0002(1)	0.0048(2)	0.0086(1)
T2	0	1/2	1/4	0.009(2)	0.0092(13)	0.0088(15)	0	0	0.0045(8)	0.0091(10)
O1	0.0938(2)	0.3867(2)	0	0.0308(10)	0.0211(8)	0.0076(7)	0	0	0.0130(7)	0.0199(4)
O2	0.1955(1)	0.2774(1)	0.1334(1)	0.0173(6)	0.0247(6)	0.0193(6)	-0.0049(5)	-0.0031(5)	0.0158(5)	0.0181(3)
O3	0.1155(1)	0.4748(1)	0.18233(7)	0.0123(5)	0.0132(5)	0.0111(5)	-0.0031(4)	0.0001(4)	0.0075(4)	0.0117(2)

TABLE 5. Selected interatomic distances (Å) in agakhanovite-(Y)

A-O3 ×3	2.258(1)	T1-O1	1.6153(6)
A-O3' ×3	2.409(1)	T1-O2	1.619(1)
<A-O>	2.334	T1-O2 ^a	1.617(1)
		T1-O3	1.595(1)
B-O1 ×3	2.814(3)	<T1-O>	1.612
B-O3 ×3	2.764(5)		
<B-O>	2.789	T2-O3 ×4	1.636(1)
C-O2 ×12	3.016(1)		

TABLE 6. Refined and calculated^a site-scattering values (epfu) and assigned site-populations (apfu) in agakhanovite-(Y)

Site	Refined site-scattering	Assigned site populations	Calculated site-scattering
A	59.6(2)	0.91 Y + 0.01 Yb + 1.08 Ca	57.8
B	9.4(2)	0.02 Na + 0.92 H ₂ O	9.4
C	19	1.0 K	19
T2	12.6(2)	2.93 Be + 0.07 Al	12.6

^a Corresponding to the assigned site-populations.**TABLE 7.** Current minerals of the milarite group: compositions^a, site occupancies, and charge arrangements

Name	A ₂	B ₂	C	T(2) ₃	T(1) ₁₂	O ₃₀	Refs.
Agakhanovite-(Y)	YCa	□ ₂	K	Be ₃	Si ₁₂	O ₃₀	(1)
Almarudite	Mn ₂	□ ₂	K	Be ₂ Al	Si ₁₂	O ₃₀	(2)
Armenite	Ca ₂	□ ₂	Ba	Al ₃	(Si ₉ Al ₃)	O ₃₀	(3)
Berezanskite	Ti ₂	□ ₂	K	Li ₃	Si ₁₂	O ₃₀	(4)
Brannockite	Sn ₂	□ ₂	K	Li ₃	Si ₁₂	O ₃₀	(5)
Chayesite	Mg ₂	Na□	K	Mg ₃	Si ₁₂	O ₃₀	(6)
Darapiosite	Mn ₂	Na ₂	K	LiZn ₂	Si ₁₂	O ₃₀	(7)
Dusmatovite	Mn ₂	K□	K	Zn ₃	Si ₁₂	O ₃₀	(8)
Eifelite	MgNa	Na ₂	K	Mg ₃	Si ₁₂	O ₃₀	(9)
Friedrichbeckite	Mg ₂	Na□	K	Be ₃	Si ₁₂	O ₃₀	(10)
Klöchite	Fe ²⁺ Fe ³⁺	□ ₂	K	Zn ₃	Si ₁₂	O ₃₀	(11)
Merrhueite	Fe ₂ ³⁺	Na□	K	Fe ₂ ³⁺	Si ₁₂	O ₃₀	(12)
Milarite	Ca ₂	□ ₂	K	Be ₂ Al	Si ₁₂	O ₃₀	(13)
Oftedalite	ScCa	□ ₂	K	Be ₃	Si ₁₂	O ₃₀	(14)
Osumilite	Fe ₂ ³⁺	□ ₂	K	Al ₃	Si ₁₀ Al ₂	O ₃₀	(15)
Osumilite-(Mg)	Mg ₂	□ ₂	K	Al ₃	Si ₁₀ Al ₂	O ₃₀	(16)
Poudretteite	Na ₂	□ ₂	K	B ₃	Si ₁₂	O ₃₀	(17)
Roedderite	Mg ₂	Na□	K	Mg ₃	Si ₁₂	O ₃₀	(18)
Shibkovite	Ca ₂	K□	K	Zn ₃	Si ₁₂	O ₃₀	(19)
Sogdianite	Zr ₂	□ ₂	K	Li ₃	Si ₁₂	O ₃₀	(20)
Sugilite	Fe ₂ ³⁺	Na ₂	K	Li ₃	Si ₁₂	O ₃₀	(21)
Trattnerite	Fe ₂ ³⁺	□ ₂	□	Mg ₃	Si ₁₂	O ₃₀	(22)
Yagiite	Mg ₂	□ ₂	Na	Al ₃	Si ₁₀ Al ₂	O ₃₀	(23)

Notes: References: (1) This study; (2) Mihajlovic et al. (2004); (3) Neumann (1941); (4) Pautov and Agakhanov (1997); (5) White et al. (1973), Armbruster and Oberhänsli (1988b); (6) Velde et al. (1989); (7) Semenov et al. (1975), Ferraris et al. (1999); (8) Pautov et al. (1996), Sokolova and Pautov (1995); (9) Abraham et al. (1983); (10) Lengauer et al. (2009); (11) Bojar et al. (2011); (12) Dodd et al. (1965); (13) Hawthorne et al. (1991); (14) Cooper et al. (2006); (15) Miyashiro (1956), Armbruster and Oberhänsli (1988a); (16) Chukanov et al. (2012), Balassone et al. (2008); (17) Grice et al. (1987); (18) Fuchs et al. (1966), Hentschel et al. (1980), Armbruster (1989); (19) Pautov et al. (1998), Sokolova et al. (1999); (20) Dusmatov et al. (1968), Cooper et al. (1999), Sokolova et al. (2000); (21) Murakami et al. (1976), Kato et al. (1976); (22) Postl et al. (2004); (23) Bunch and Fuchs (1969).

^a Omitting (H₂O) in the channels.

population for A given in Table 6 are in reasonable accord with the relation between <A-O> and the aggregate radius of the cations occupying the A site given by Hawthorne et al. (1991).

The <C-O> distance of 3.016 Å (Table 5) is almost exactly equal to the grand <C-O> distance of 3.017 Å reported by Hawthorne et al. (1991) for milarite structures. The B site has a refined site-scattering value of 9.4(2) epfu and the Na content of the crystal is 0.02 apfu. The Raman spectrum indicates the presence of major (H₂O) in the structure (Fig. 2) that provides the balance in scattering at the B site (Table 6).

Chemical formula

The empirical formula for agakhanovite-(Y) is $(Y_{0.89}Yb_{0.01}Ca_{1.07})_{\Sigma=1.97}[\square_{1.06}(H_2O)_{0.92}Na_{0.02}]_{\Sigma=2.00}K_{1.00}(Be_{2.93}Al_{0.07})_{\Sigma=3.00}Si_{12.02}O_{30}$, resulting in a general composition $(Y,Ca)(\square_2H_2O,Na)_2K(Be,Al)_3Si_{12}O_{30}$ and an end-member composition $(YCa)\square_2KBe_3Si_{12}O_{30}$. Note that the occurrence of two heterovalent cations at a single site in the structure is in accord with the criteria for an end-member (Hawthorne 2002).

Agakhanovite-(Y) is the Y-analog of oftedalite (ScCa) $\square_2KBe_3Si_{12}O_{30}$, related by the substitution $Y = Sc$. It also has the same charge arrangement as klöchite, $(Fe^{2+}Fe^{3+})\square_2KZn_3Si_{12}O_{30}$ (Bojar et al. 2011), to which it is related by the substitution $Y + Ca + Be_3 = Fe^{3+} + Fe^{2+} + Zn_3$. The current members of the milarite group are listed in Table 7. Note that armenite is only pseudo-hexagonal and has an orthorhombic superstructure. In the end-member compositions listed in Table 7, the C site (with a rank of 1) is the only site that is not occupied by two species in the set of end-members given here. It is this peculiarity of the milarite structure that is a major factor in the chemical flexibility of this structure type.

IMPLICATIONS

There are currently 24 milarite-group minerals known from a wide variety of parageneses, and it is certain that others will be found in the future. The discovery of agakhanovite-(Y) draws attention to the following significant question: Why are some structural arrangements very compliant in terms of the ions that they can contain as dominant chemical species, giving rise to relatively large numbers of isostructural mineral species, whereas other structural arrangements are chemically restrictive and are adopted by only one or two mineral species? The issue of what affects the relative chemical stabilities of specific bond topologies is one that challenges our understanding of structure stability and deserves serious consideration in the future.

ACKNOWLEDGMENTS

We thank Mark Cooper for his help with this work; Harald Folvik, Natural History Museum, University of Oslo, for the SEM photo of agakhanovite-(Y); and Franz Bernhard, Technical University of Graz, for an early indication of high Y content in milarite. Support was provided by a Canada Research Chair in Crystallography and Mineralogy, and by Discovery, Equipment and Major Installation grants of the Natural Sciences and Engineering Research Council of Canada, and by Innovation grants from the Canada Foundation for Innovation to F.C.H.

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MANUSCRIPT RECEIVED JANUARY 8, 2014

MANUSCRIPT ACCEPTED APRIL 21, 2014

MANUSCRIPT HANDLED BY G. DIEGO GATTA