## REVISION 1

# 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/cm$^3$. 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 $\omega = 1.567$, $\varepsilon = 1.564$, 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) Å$^3$, Z = 2, *c:a* = 1.330. The seven strongest lines in the X-ray powder-diffraction pattern are as follows: *d* (Å), *I*, (*h k l*): 2.865, 100, ($\bar{1}$ 2 4); 3.287, 96, ($\bar{1}$ 3 1); 4.134, 84, ($\bar{1}$ 2 2); 6.877, 56, (0 0 2); 2.986, 43, (0 3 0); 4.479, 38, (0 2 0); 2.728, 36, (0 2 4). Chemical analysis by electron microprobe gave $SiO_2$ 69.56, $Al_2O_3$ 0.35, $Y_2O_3$ 9.69, $Yb_2O_3$ 0.15, FeO 0.02 CaO 5.75, $Na_2O$ 0.07, $K_2O$ 4.52, BeO(calc) 7.06, $H_2O$(calc) 1.74, sum 98.91 wt.%. The $H_2O$ content was determined by crystal-structure analysis. On the basis of 30 anions with ($H_2O$) + Na = 1 a.p.f.u., the empirical formula is $(Y_{0.89}Yb_{0.01}Ca_{1.06})_{\Sigma 1.96}(H_2O)_{0.98}Na_{0.02}K_{1.00}(Be_{2.93}Al_{0.07})_{\Sigma 3.00}Si_{12.02}O_{30}$. 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 (Mo*K*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-analogue of oftedalite: $ScCa\square_2KBe_3Si_{12}O_{30}$, and the Y-Ca-Be analogue 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 & Sæbø (1965) reported significant Y-REE in milarite from Grorud, Norway. Černý et al. (1991) described Y-rich milarite from the Jaguaraçú pegmatite, Minas Gerais, Brazil, and the Strange Lake peralkaline complex, Labrador-Quebec border, Canada, with up to 7.9 wt.% $Y_2O_3$ and 2.9 wt.% $REE_2O_3$ in the latter. Nysten (1996) reported Y-rich milarite from granitic pegmatites in Sweden with up to 8.89 wt.% $Y_2O_3$. 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: yttropyrochlore-(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-analogue 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, catalogue number M43863.

## OCCURRENCE

The Heftetjem cleavelandite-amazonite pegmatite is situated in a marshy area between Høydalen and Skarsfjell in Tørdal, 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 Heftetjern: (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 x 3 x 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 $\omega = 1.567$, $\varepsilon = 1.564$, 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 wave-numbers. 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 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 & Pichoir (1985) and the chemical composition (mean of ten determinations) is given in Table 1. The empirical formula was calculated on the basis of 30 anions with Be = 3 - Al , and ($H_2O$) was calculated as 0.92 *apfu* (atom per formula unit) as indicated by site-scattering refinement, giving $(Y_{0.89}Yb_{0.01}Ca_{1.06})_{\Sigma 1.96}(\square_{1.00}(H_2O)_{0.92}Na_{0.02})_{\Sigma 2.00}K_{1.00}(Be_{2.93}Al_{0.07})_{\Sigma 3.00}Si_{12.02}O_{30}$, ideally $(YCa)\square_2KBe_3Si_{12}O_{30}$.

## 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 Å for Cu$K\alpha$) 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) $Å^3$.

## 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 (Mo$K\alpha$), multilayer optics and an APEX-II detector. A total of 44,574 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.

## CRYSTAL STRUCTURE

### The tetrahedron framework

The general structure of the milarite-group minerals is a beryllo-aluminosilicate framework (Forbes et al. 1972; Černý et al. 1980) of the form $(4^2 6^4)_4(6^4 9^2)$ (Hawthorne & 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 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 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 ($H_2O$) in the structure (Fig. 2) which provides the balance in scattering at the B site (Table 6).

## Chemical formula

The empirical formula for agakhanovite-(Y) is $(Y_{0.89}Yb_{0.01}Ca_{1.07})_{\Sigma=1.97}(\square_{1.00}(H_2O)_{0.98}Na_{0.02})_{\Sigma=2.00}K_{1.00}(Be_{2.93}Al_{0.07})_{\Sigma=3.00}Si_{12.02}O_{30}$, resulting in a general composition $(Y,Ca)(\square,H_2O,Na)_2\,K(Be,Al)_3Si_{12}O_{30}$ 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-analogue 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.

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## FIGURE CAPTIONS

**Figure 1.** Back-scattered-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).

**TABLE 1.** Chemical composition of agakhanovite-(Y)

| Constituent | Wt.% | Range | Stand. Dev. |
|---|---|---|---|
| $SiO_2$ | 69.56 | 68.36-70.45 | 0.58 |
| $Al_2O_3$ | 0.35 | 0.24-0.63 | 0.14 |
| $Y_2O_3$ | 9.69 | 9.43-10.35 | 0.24 |
| $Yb_2O_3$ | 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 |
| $Na_2O$ | 0.07 | 0.03-0.09 | 0.02 |
| $K_2O$ | 4.52 | 4.41-4.57 | 0.04 |
| BeO(calc.) | 7.06 | --- | --- |
| $H_2O$(calc.) | 1.74 | --- | --- |
| Total | 98.91 | | |

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

| $I_{\text{(meas.)}}$ % | $d_{\text{(meas.)}}$ Å | $d_{\text{(calc.)}}$ Å | $h$ | $k$ | $l$ |
|---|---|---|---|---|---|
| 56 | 6.877 | 6.884 | 0 | 0 | 2 |
| 16 | 5.464 | 5.458 | 0 | 1 | 2 |
| 19 | 5.170 | 5.171 | $\bar{1}$ | 2 | 0 |
| 38 | 4.479 | 4.479 | 0 | 2 | 0 |
| 84 | 4.134 | 4.135 | $\bar{1}$ | 2 | 2 |
| 11 | 3.755 | 3.754 | 0 | 2 | 2 |
| 25 | 3.445 | 3.442 | 0 | 0 | 4 |
| 96 | 3.287 | 3.288 | $\bar{1}$ | 3 | 1 |
| 27 | 3.214 | 3.213 | 0 | 1 | 4 |
| 43 | 2.9861 | 2.9857 | 0 | 3 | 0 |
| 100 | 2.8653 | 2.8654 | $\bar{1}$ | 2 | 4 |
| 36 | 2.7283 | 2.7291 | 0 | 2 | 4 |
| | | 2.7244 | $\bar{1}$ | 3 | 3 |
| 15 | 2.5842 | 2.5857 | $\bar{2}$ | 4 | 0 |
| 5 | 2.4832 | 2.4843 | $\bar{1}$ | 4 | 0 |
| 10 B | 2.4280 * | | | | |
| 5 | 2.2513 | 2.2554 | 0 | 3 | 4 |
| 6 | 2.1858 | 2.1847 | $\bar{1}$ | 4 | 3 |
| 8 | 2.0977 | 2.0975 | $\bar{1}$ | 2 | 6 |
| 14 | 2.0159 | 2.0144 | $\bar{1}$ | 4 | 4 |
| 15 | 1.9541 | 1.9546 | $\bar{1}$ | 5 | 0 |
| 21 | 1.8801 | 1.8803 | $\bar{1}$ | 5 | 2 |
| 15 | 1.8450 | 1.8445 | $\bar{1}$ | 4 | 5 |
| 10 | 1.8196 | 1.8193 | 0 | 3 | 6 |
| 10 | 1.7915 | 1.7914 | 0 | 5 | 0 |
| 16 | 1.7181 | 1.7210 | 0 | 0 | 8 |
| | | 1.7163 | $\bar{2}$ | 4 | 6 |
| 16 | 1.6995 | 1.6997 | $\bar{1}$ | 5 | 4 |
| 9 | 1.6793 | 1.6801 | $\bar{2}$ | 6 | 1 |
| 3 | 1.6436 | 1.6438 | $\bar{2}$ | 6 | 2 |
| 6 | 1.6059 | 1.6065 | 0 | 2 | 8 |
| 5 | 1.5909 | 1.5891 | 0 | 5 | 4 |
| | | 1.5882 | $\bar{2}$ | 6 | 3 |
| 3 | 1.5661 | 1.5665 | $\bar{1}$ | 6 | 2 |
| 9 | 1.5406 | 1.5413 | $\bar{3}$ | 6 | 4 |
| 4 | 1.5184 | 1.5182 | $\bar{1}$ | 6 | 3 |
| 9 | 1.4915 | 1.4911 | 0 | 3 | 8 |
| 5 | 1.4590 | 1.4589 | 0 | 6 | 2 |
| 14 | 1.4342 | 1.4343 | $\bar{2}$ | 7 | 0 |

**TABLE 3.** Miscellaneous information for agakhanovite-(Y)

| | | | |
|---|---|---|---|
| *a* (Å) | 10.3476(2) | Crystal size (μm) | 15 x 15 x 30 |
| *c* | 13.7610(3) | Radiation | Mo*K*α |
| *V* (Å$^3$) | 1276.02(9) | No. of unique reflections | 660 |
| Space Group | *P*6/*mcc* | No. $\lvert F_o \rvert > 5\sigma F$ | 430 |
| *Z* | 2 | *R*(merge) (%) | 2.5 |
| | | $R_1$ (%) | 1.9 |
| | | *wR* (%) | 6.3 |

$R = \Sigma(\lvert F_o\rvert - \lvert F_c\rvert) / \Sigma\lvert F_o\rvert$

$wR = [\Sigma w(\lvert F_o\rvert - \lvert F_c\rvert)^2 / \Sigma F_o^2]^{½}$, $w = 1$

**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 x3 | 2.258(1) | T1-O1 | 1.6153(6) |
| A-O3′ x3 | 2.409(1) | T1-O2 | 1.619(1) |
| <A-O> | 2.334 | T1-O2″ | 1.617(1) |
| | | T1-O3 | 1.595(1) |
| B-O1 x3 | 2.814(3) | <T1-O> | 1.612 |
| B-O3 x3 | 2.764(5) | | |
| <B-O> | 2.789 | T2-O3 x4 | 1.636(1) |
| C-O2 x12 | 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 $H_2O$ | 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*, site occupancies and charge arrangements

| Name | $A_2$ | $B_2$ | C | $T(2)_3$ | $T(1)_{12}$ | $O_{30}$ | Refs. |
|---|---|---|---|---|---|---|---|
| Agakhanovite-(Y) | YCa | $\square_2$ | K | $Be_3$ | $Si_{12}$ | $O_{30}$ | (1) |
| Almarudite | $Mn_2$ | $\square_2$ | K | $Be_2Al$ | $Si_{12}$ | $O_{30}$ | (2) |
| Armenite | $Ca_2$ | $\square_2$ | Ba | $Al_3$ | $(Si_9Al_3)$ | $O_{30}$ | (3) |
| Berezanskite | $Ti_2$ | $\square_2$ | K | $Li_3$ | $Si_{12}$ | $O_{30}$ | (4) |
| Brannockite | $Sn_2$ | $\square_2$ | K | $Li_3$ | $Si_{12}$ | $O_{30}$ | (5) |
| Chayesite | $Mg_2$ | $Na\square$ | K | $Mg_3$ | $Si_{12}$ | $O_{30}$ | (6) |
| Darapiosite | $Mn_2$ | $Na_2$ | K | $LiZn_2$ | $Si_{12}$ | $O_{30}$ | (7) |
| Dusmatovite | $Mn_2$ | $K\square$ | K | $Zn_3$ | $Si_{12}$ | $O_{30}$ | (8) |
| Eifelite | MgNa | $Na_2$ | K | $Mg_3$ | $Si_{12}$ | $O_{30}$ | (9) |
| Friedrichbeckeite | $Mg_2$ | $Na\square$ | K | $Be_3$ | $Si_{12}$ | $O_{30}$ | (10) |
| Klöchite | $Fe^{2+}Fe^{3+}$ | $\square_2$ | K | $Zn_3$ | $Si_{12}$ | $O_{30}$ | (11) |
| Merrihueite | $Fe^{2+}{}_2$ | $Na\square$ | K | $Fe^{2+}{}_3$ | $Si_{12}$ | $O_{30}$ | (12) |
| Milarite | $Ca_2$ | $\square_2$ | K | $Be_2Al$ | $Si_{12}$ | $O_{30}$ | (13) |
| Oftedalite | ScCa | $\square_2$ | K | $Be_3$ | $Si_{12}$ | $O_{30}$ | (14) |
| Osumilite | $Fe^{2+}{}_2$ | $\square_2$ | K | $Al_3$ | $Si_{10}Al_2$ | $O_{30}$ | (15) |
| Osumilite-(Mg) | $Mg_2$ | $\square_2$ | K | $Al_3$ | $Si_{10}Al_2$ | $O_{30}$ | (16) |
| Poudretteite | $Na_2$ | $\square_2$ | K | $B_3$ | $Si_{12}$ | $O_{30}$ | (17) |
| Roedderite | $Mg_2$ | $Na\square$ | K | $Mg_3$ | $Si_{12}$ | $O_{30}$ | (18) |
| Shibkovite | $Ca_2$ | $K\square$ | K | $Zn_3$ | $Si_{12}$ | $O_{30}$ | (19) |
| Sogdianite | $Zr_2$ | $\square_2$ | K | $Li_3$ | $Si_{12}$ | $O_{30}$ | (20) |
| Sugilite | $Fe^{3+}{}_2$ | $Na_2$ | K | $Li_3$ | $Si_{12}$ | $O_{30}$ | (21) |
| Trattnerite | $Fe^{3+}{}_2$ | $\square_2$ | $\square$ | $Mg_3$ | $Si_{12}$ | $O_{30}$ | (22) |
| Yagiite | $Mg_2$ | $\square_2$ | Na | $Al_3$ | $Si_{10}Al_2$ | $O_{30}$ | (23) |

*omitting ($H_2O$) in the channels.

References: (1) This study; (2) Mihajlović 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).

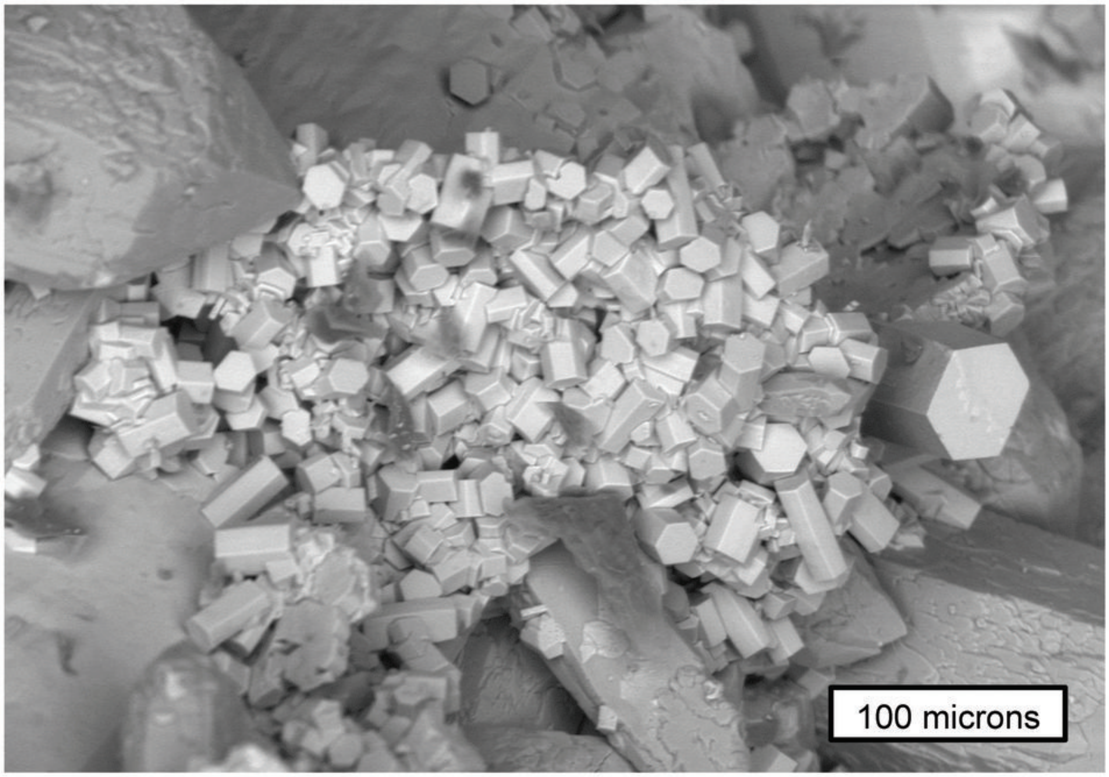

FIGURE 1

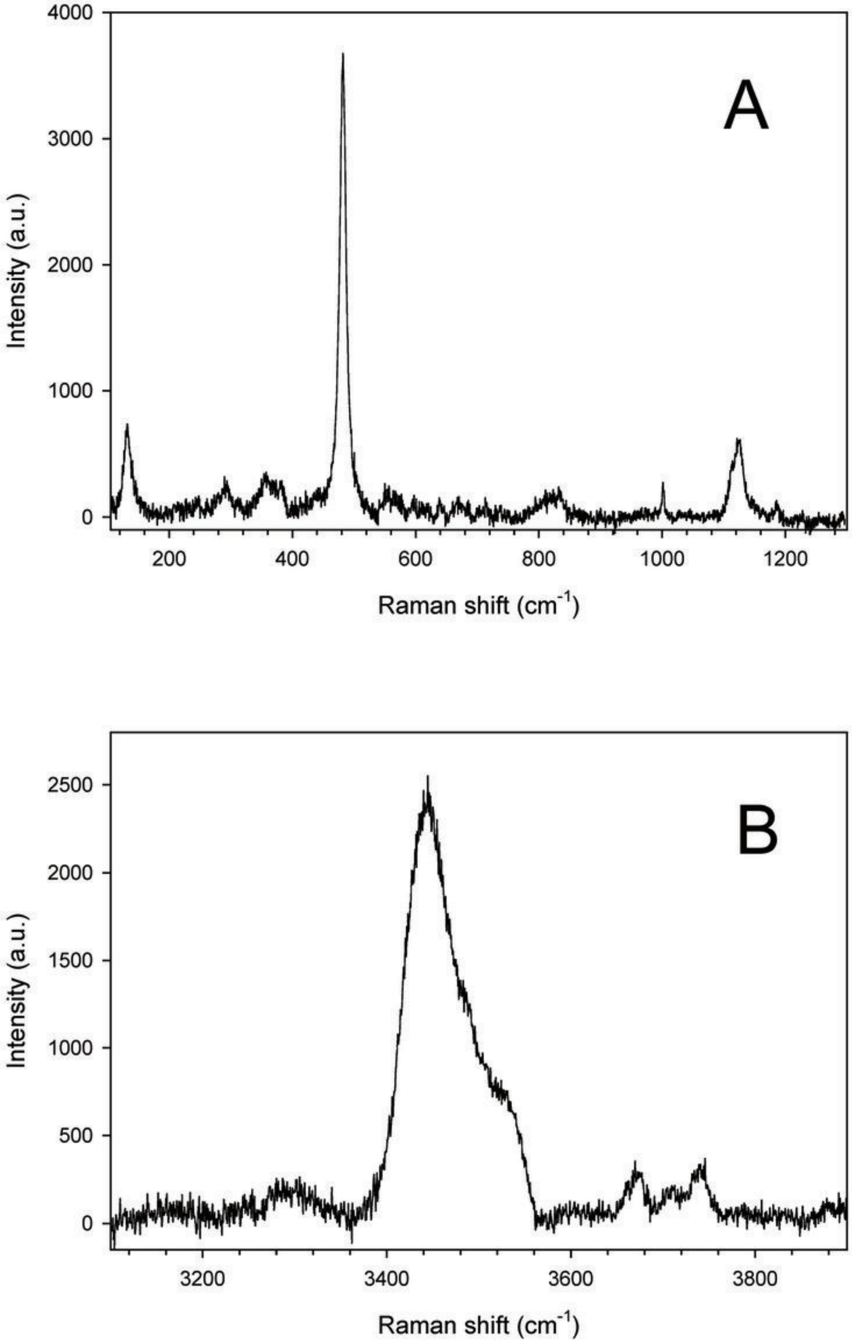
A
Intensity (a.u.)
4000
3000
2000
1000
0
200
400
600
800
1000
1200
Raman shift (cm-1)
B
Intensity (a.u.)
2500
2000
1500
1000
500
0
3200
3400
3600
3800
Raman shift (cm-1)

FIGURE 2