American Mineralogist, Volume 99, pages 2084–2088, 2014

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 *P*6/*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*, (*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 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, 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 (Mo$K\alpha$ 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