American Mineralogist, Volume 89, pages 1561–1565, 2004

LETTER

Porous titanosilicate nanorods in the structure of yuksporite, $(Sr,Ba)_2K_4(Ca,Na)_{14}(\square,Mn,Fe)\{(Ti,Nb)_4(O,OH)_4[Si_6O_{17}]_2[Si_2O_7]_3\}(H_2O,OH)_n$, resolved using synchrotron radiation

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ABSTRACT

The crystal structure of yuksporite, $(Sr,Ba)_2K_4(Ca,Na)_{14}(\square,Mn,Fe)\{(Ti,Nb)_4(O,OH)_4[Si_6O_{17}]_2[Si_2O_7]_3\}(H_2O,OH)_n$, where $n \sim 3$ [monoclinic, $P2_1/m$, $a = 7.126(3)$, $b = 24.913(6)$, $c = 17.075(7)$ Å, $\beta = 101.89(3)°$, $V = 2966.4(17)$ Å^3] has been solved using X-ray synchrotron radiation data collected from a needle-like crystal with dimensions of $6 \times 6 \times 50$ μm^3 at the Swiss-Norwegian beamline BM01 of the European Synchrotron Research Facility (ESRF, Grenoble, France). The structure was refined to $R_1 = 0.101$ on the basis of 2359 unique observed reflections with $|F_o| \geq 4\sigma_F$. The structure of yuksporite is based upon titanosilicate nanorods elongated along **a** and with an elliptical cross-section of ca. 16×19 Å $= 1.6 \times 1.9$ nm. Silicate tetrahedra form double xonotlite-like chains $^1_\infty[Si_6O_{17}]$ oriented parallel to (001). Two $^1_\infty[Si_6O_{17}]$ chains are linked into a rod via TiO_6 octahedra and Si_2O_7 double tetrahedra. The $\{(Ti,Nb)_4(O,OH)_4[Si_6O_{17}]_2[Si_2O_7]_3\}$ nanorods are porous. The internal pores are defined by eight-membered rings (8MR) with open diameters of 3.2 Å. The interior of the titanosilicate nanorods is occupied by Sr, Ba, K, and Na cations and H_2O molecules. The nanorods are separated by walls of Ca coordination polyhedra that are parallel to (010) and link the rods into a three-dimensional structure.