American Mineralogist, Volume 97, pages 1796–1803, 2012

Crystal structure of pseudojohannite, with a revised formula, $Cu_3(OH)_2[(UO_2)_4O_4(SO_4)_2](H_2O)_{12}$

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Abstract

The crystal structure of pseudojohannite from White Canyon, Utah, was solved by charge-flipping from single-crystal X-ray diffraction data and refined to an $R_{obs} = 0.0347$, based on 2664 observed reflections. Pseudojohannite from White Canyon is triclinic, $P\bar{1}$, with $a = 8.6744(4)$, $b = 8.8692(4)$, $c = 10.0090(5)$ Å, $\alpha = 72.105(4)°$, $\beta = 70.544(4)°$, $\gamma = 76.035(4)°$, and $V = 682.61(5)$ Å^3, with $Z = 1$ and chemical formula $Cu_3(OH)_2[(UO_2)_4O_4(SO_4)_2](H_2O)_{12}$. The crystal structure of pseudojohannite is built up from sheets of zippeite topology that do not contain any OH groups; these sheets are identical to those found in zippeites containing Mg^{2+}, Co^{2+}, and Zn^{2+}. The two Cu^{2+} sites in pseudojohannite are [5]- and [6]-coordinated by H_2O molecules and OH groups. The crystal structure of the pseudojohannite holotype specimen from Jáchymov was refined using Rietveld refinement of high-resolution powder diffraction data. Results indicate that the crystal structures of pseudojohannite from White Canyon and Jáchymov are identical.

Keywords: Pseudojohannite, zippeite group, uranyl sulfate, X-ray diffraction, crystal structure, chemical composition