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Revision of the crystal structure and chemical formula of weeksite, $K_2(UO_2)_2(Si_5O_{13})\cdot 4H_2O$

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Abstract

The previously published structure determination of weeksite from the Anderson mine, Arizona, U.S.A., suggested that it is orthorhombic, *Cmmb*, with $a = 14.209(2)$, $b = 14.248(2)$, $c = 35.869(4)$ Å, and $V = 7262(2)$ Å^3, and an ideal chemical formula $(K,Ba)_{1-2}(UO_2)_2(Si_5O_{13})\cdot H_2O$. Using single-crystal X-ray diffraction, electron microprobe analysis, and thermal analysis, we reexamined weeksite from the same locality. Our results demonstrate that weeksite is monoclinic, with the space group *C*2/*m* and unit-cell parameters $a = 14.1957(4)$, $b = 14.2291(5)$, $c = 9.6305(3)$ Å, $\beta = 111.578(3)°$, $V = 1808.96(10)$ Å^3, and an ideal formula $K_2(UO_2)_2(Si_5O_{13})\cdot 4H_2O$. The previously reported orthorhombic unit cell is shown to result from twinning of the monoclinic cell. The structure refinement yielded $R_1 = 2.84\%$ for 1632 observed reflections [$I_{obs} > 3\sigma(I)$] and 5.42% for all 2379 reflections. The total H_2O content derived from the structure refinement agrees well with that from the thermal analysis. Although the general topology of our structure resembles that reported previously, all Si sites in our structure are fully occupied, in contrast to the previous structure determination, which includes four partially occupied SiO_4 tetrahedra. From our structure data on weeksite, it appears evident that the orthorhombic cell of the newly discovered weeksite-type mineral coutinhoite, $Th_xB_{1-2x}(UO_2)_2Si_5O_{13}\cdot 3H_2O$, needs to be reevaluated.

Keywords: Weeksite, uranyl silicate, crystal structure, X-ray diffraction, open framework