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Revision of the crystal structure and chemical formula of haiweeite, $Ca(UO_2)_2(Si_5O_{12})(OH)_2 \cdot 6H_2O$

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Abstract

The previously published crystal structure study suggested that haiweeite is orthorhombic, *Cmcm*, with $a = 7.125(1)$, $b = 17.937(2)$, $c = 18.342(2)$ Å, and $V = 2344.3(7)$ Å^3, and an ideal chemical formula $Ca[(UO_2)_2Si_5O_{12}(OH)_2]\cdot 3H_2O$, with $Z = 4$. Using single-crystal X-ray diffraction and electron microprobe analysis we re-examined haiweeite from the Teofilo Otoni, Minas Gerais, Brazil. Our diffraction experiment provided weak reflections responsible for doubling of the *b* cell parameter (for the current space-group settings), leading finally to the choice of a different space group. Haiweeite is thus orthorhombic, the space group *Pbcn*, with the unit-cell parameters $a = 18.3000(5)$, $b = 14.2331(3)$, $c = 17.9192(5)$ Å, $V = 4667.3(2)$ Å^3, and an ideal formula $Ca[(UO_2)_2(SiO_3OH)_2(Si_3O_6)]\cdot 6H_2O$ (6.25 H_2O inferred from the thermal analysis; 7.50 H_2O from the structure model), with $Z = 8$. The structure refinement yielded $R_1 = 0.0512$ for 2498 observed reflections [$I_{obs} > 3\sigma(I)$] and $wR_2 = 0.1286$ for all 6117 unique reflections. Structure solution confirmed by subsequent refinement provided a structure model with full occupancies for U, Si, and Ca atoms, contrasting to previous average structure model. Although the general topology of our structure resembles that reported previously, all Si and O sites in our structure are fully occupied, in contrast to the previous structure determination.

Keywords: Haiweeite, uranyl silicate, sheets of polyhedra, crystal structure, X-ray diffraction