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$Ba(NpO_2)(PO_4)(H_2O)$, its relationship to the uranophane group, and implications for Np incorporation in uranyl minerals

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ABSTRACT

Single crystals of $Ba(NpO_2)(PO_4)(H_2O)$ were obtained using hydrothermal synthesis techniques. The structure was determined using single-crystal X-ray diffraction data collected using Mo$K\alpha$ radiation and an APEX II CCD detector and was refined on the basis of F^2 for all unique data to R_1 = 2.41%. $Ba(NpO_2)(PO_4)(H_2O)$ crystallized in monoclinic space group $P2_1/n$ with a = 6.905(3), b = 7.108(3), c = 13.321(6) Å, β = 105.02°, and V = 631.4 Å^3. The structure contains chains of edge-sharing neptunyl pentagonal bipyramids that link through phosphate tetrahedra to form infinite sheets. This sheet-type is identical to the anion topology of the uranophane group, in particular to that of oursinite, $Co[(UO_2)(SiO_3OH)]_2(H_2O)_6$. Similarities between $Ba(NpO_2)(PO_4)(H_2O)$ and the uranophane group of minerals suggests a charge-balancing mechanism for incorporation of Np^{5+} into uranyl minerals.

Keywords: Neptunium, uranyl mineral, uranophane, nuclear waste, crystal structure, actinide