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A novel arrangement of silicate tetrahedra in the uranyl silicate sheet of oursinite, $(Co_{0.8}Mg_{0.2})[(UO_2)(SiO_3OH)]_2(H_2O)_6$

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ABSTRACT

Oursinite is a rare Co-bearing uranyl silicate of the uranophane group. The structure of oursinite, $(Co_{0.8}Mg_{0.2})[(UO_2)(SiO_3OH)]_2(H_2O)_6$, is orthorhombic, space group *Cmca*, $a = 7.0494(5)$, $b = 17.550(1)$, $c = 12.734(1)$ Å, $V = 1575.4(2)$ Å^3, $Z = 4$. It was solved by direct methods and refined on the basis of F^2 for all unique reflections using least-squares techniques to an agreement index ($R1$) of 2.66%. The structure contains an approximately linear $(UO_2)^{2+}$ uranyl ion that is present as a uranyl pentagonal bipyramid, one symmetrically distinct SiO_3OH acid silicate group, and one $M^{2+}(OH,H_2O)_6$ octahedron (M is dominated by Co). The uranyl pentagonal bipyramids and silicate tetrahedra are linked by the sharing of edges and vertices, giving a sheet based upon the uranophane anion topology. Adjacent sheets are linked by $M^{2+}(OH,H_2O)_6$ octahedra located in the interlayer, and by hydrogen bonds. Each $M^{2+}(OH,H_2O)_6$ octahedron contains two OH groups that are apical ligands of silicate tetrahedra in adjacent uranyl silicate sheets. Although several uranophane-group minerals contain sheets that are based upon the uranophane anion topology, the oursinite sheet involves novel orientations of silicate tetrahedra.

Keywords: Oursinite, uranyl silicate, uranium, crystal structure