American Mineralogist, Volume 88, pages 962–966, 2003

A new uranyl carbonate sheet in the crystal structure of fontanite, $Ca[(UO_2)_3(CO_3)_2O_2](H_2O)_6$

KARRIE-ANN HUGHES AND PETER C. BURNS*

Department of Civil Engineering and Geological Sciences, University of Notre Dame, 156 Fitzpatrick Hall, Notre Dame, Indiana 46556, U.S.A.

ABSTRACT

The structure of fontanite, $Ca[(UO_2)_3(CO_3)_2O_2](H_2O)_6$, is monoclinic, space group $P2_1/n$, a = 6.968(3), b = 17.276(7), c = 15.377(6) Å, β = 90.064(6)°, V = 1851(1) Å^3, Z = 4. The structure 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 9.9%. The structure contains two symmetrically distinct uranyl pentagonal bipyramids, one uranyl hexagonal bipyramid, and two CO_3 triangles. The uranyl polyhedra form chains by sharing equatorial edges, and CO_3 groups occur on either side of the chains, where they share equatorial edges of the uranyl hexagonal bipyramids. The CO_3 groups share their third ligand with a uranyl pentagonal bipyramid of an adjacent chain, resulting in uranyl carbonate sheets of composition $[(UO_2)_3(CO_3)_2O_2]^{2-}$. The single symmetrically unique Ca^{2+} cation is located between the sheets, and is coordinated by two O atoms of uranyl ions of adjacent sheets, and six H_2O groups. The uranyl carbonate sheet in fontanite is novel, but is based upon the phosphuranylite anion topology that is the basis of uranyl phosphate, uranyl selenite, and uranyl sulfate sheets in a variety of minerals.