

## **Wyartite: Crystallographic evidence for the first pentavalent-uranium mineral**

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### **ABSTRACT**

Determination of the structure of wyartite provides the first evidence for a pentavalent-U mineral. The structure of wyartite,  $\text{CaU}^{5+}(\text{UO}_2)_2(\text{CO}_3)\text{O}_4(\text{OH})(\text{H}_2\text{O})_7$ ,  $Z = 4$ , orthorhombic,  $a = 11.2706(8)$ ,  $b = 7.1055(5)$ ,  $c = 20.807(1)$  Å,  $V = 1666.3(3)$  Å<sup>3</sup>, space group  $P2_12_12_1$ , was solved by direct methods and refined to an agreement index ( $R$ ) of 4.9% for 2309 unique reflections collected using  $\text{MoK}\alpha$  X-radiation and a CCD-based detector. The structure contains three unique U positions; two contain  $\text{U}^{6+}$  and involve uranyl ions with typical pentagonal-bipyramidal coordination. Seven anions coordinate the other U position, but there is no uranyl ion present. The polyhedral geometry, the bond-valence sum incident at this U site, and electroneutrality requirements, all indicate that this site contains  $\text{U}^{5+}$ . The  $\text{U}\phi_7$  ( $\phi$ : O, OH,  $\text{H}_2\text{O}$ ) polyhedra share edges and corners to form a unique sheet in which a  $\text{CO}_3$  group shares an edge with the  $\text{U}^{5+}\phi_7$  polyhedron. The structure contains one Ca site coordinated by seven anions. The Ca atom and its associated  $\text{H}_2\text{O}$  groups occupy interlayer sites, along with two  $\text{H}_2\text{O}$  groups that are held in the structure by H bonds only. The  $\text{Ca}\phi_7$  polyhedron is linked to one adjacent sheet by sharing an edge with the  $\text{CO}_3$  group and an O atom with a  $\text{U}^{6+}\phi_7$  polyhedron. Structural units are linked together through hydrogen bonds only.