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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, $CaU^{5+}(UO_2)_2(CO_3)O_4(OH)(H_2O)_7$, $Z = 4$, orthorhombic, $a = 11.2706(8)$, $b = 7.1055(5)$, $c = 20.807(1)$ Å, $V = 1666.3(3)$ Å^3, 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 Mo$K\alpha$ X-radiation and a CCD-based detector. The structure contains three unique U positions; two contain 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 U^{5+}. The $U\phi_7$ (ϕ: O, OH, H_2O) polyhedra share edges and corners to form a unique sheet in which a CO_3 group shares an edge with the $U^{5+}\phi_7$ polyhedron. The structure contains one Ca site coordinated by seven anions. The Ca atom and its associated H_2O groups occupy interlayer sites, along with two H_2O groups that are held in the structure by H bonds only. The $Ca\phi_7$ polyhedron is linked to one adjacent sheet by sharing an edge with the CO_3 group and an O atom with a $U^{6+}\phi_7$ polyhedron. Structural units are linked together through hydrogen bonds only.