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A new uranyl phosphate chain in the structure of parsonsite

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ABSTRACT

The structure of parsonsite, $Pb_2[(UO_2)(PO_4)_2]$, $Z = 2$, triclinic, space group $P\bar{1}$, $a = 6.842(4)$, $b = 10.383(6)$, $c = 6.670(4)$ Å, $\alpha = 101.26(7)°$, $\beta = 98.17(7)°$, $\gamma = 86.38(7)°$, $V = 459.8(7)$ Å^3, has been solved by direct methods and refined to $R = 6.0$ and a goodness-of-fit (S) of 0.92 using 1187 unique observed reflections ($|F| \geq 4\sigma_F$) collected with Mo$K\alpha$ X-rays and a CCD-based detector. The single unique U^{6+} cation is present as a $(UO_2)^{2+}$ uranyl ion (Ur) and is coordinated by five additional atoms of O arranged at the equatorial corners of a pentagonal bipyramid capped by the O_{Ur} atoms. Uranyl polyhedra share an edge-forming dimers, which are cross-linked by edge- and vertex-sharing with two distinct phosphate tetrahedra, resulting in a new uranyl phosphate chain. Two symmetrically distinct Pb^{2+} cations are coordinated by nine and six oxygen atoms, and link adjacent uranyl phosphate chains. Parsonsite is the first uranyl phosphate mineral structure that is based upon chains of polymerized polyhedra of higher bond-valence; others contain sheets that are either based upon the autunite or phosphuranylite anion-topologies.