

## Crystal-structure determination of pinalite

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### ABSTRACT

The crystal structure of pinalite,  $\text{Pb}_3\text{WO}_5\text{Cl}_2$ , is orthorhombic *Amam*, with  $a = 11.073(2)$ ,  $b = 13.067(3)$ ,  $c = 5.617(1)$  Å,  $V = 812.81(3)$  Å<sup>3</sup>, and  $Z = 4$ . It has been refined to an  $R$  index of 0.049 on the basis of 593 unique, observed reflections. There are two crystallographically distinct Pb cations with different coordinations: Pb1 has eightfold-coordination with ligands of 4 Cl atoms, 4 O atoms, and one stereoactive lone-pair, whereas Pb2 has ninefold-coordination with ligands of 4 Cl atoms and 5 O atoms. The W cation has fivefold-coordination with 5 O ligands. The pinalite structure is layered parallel to (100) with Pb-O-Cl layers interleaved with Pb-W-O layers. Pinalite belongs to the bismuth oxychloride group of structures. The Pb-O-Cl layer of pinalite duplicates the basic structure of thorikosite and the Pb-W-O layer of pinalite is able to conform to this fundamental cell through differences in the two Pb coordinations and a unique W coordination. Similarly the structures of nadorite and kettnerite are also shown to replicate the basic bismuth oxychloride structure.