Phosphohedyphane, Ca₂Pb₃(PO₄)₃Cl, the phosphate analog of hedyphane: Description and crystal structure

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ABSTRACT

Phosphohedyphane, Ca₂Pb₃(PO₄)₃Cl, space group $P6_3/m$, a = 9.857(1), c = 7.130(2) Å, V = 599.9(2)Å³, Z = 2, is a new mineral from the Capitana mine, Copiapó, Atacama Province, Chile and has been identified from numerous other deposits world-wide. At the Capitana mine, it occurs as transparent, colorless, tapering hexagonal prisms, as individuals up to about 0.5 mm in length and 0.1 mm in diameter, which are commonly doubly terminated. Crystals often occur in subparallel intergrowths and irregular clusters. Phosphohedyphane forms as a secondary mineral in the oxidized zone of the Capitana mine, a Cu-Pb-Ag deposit, where it closely associated with quartz, duftite, and bayldonite. Crystals exhibit core-to-rim chemical zonation and electron analyses of cores/rims yielded CaO 9.24/7.76, PbO 67.60/69.35, P₂O₅ 18.40/17.00, As₂O₅ 2.73/3.68, Cl 3.32/3.22, -O = Cl -0.75/-0.73, total 100.54/100.28 wt%. The name phosphohedyphane is for the relationship of the mineral to hedyphane. The mineral has an apatite structure with ordering of Ca and Pb in the two non-equivalent large cation sites, as in hedyphane. The structure refinement indicates that the Ca2(6h) site is completely occupied by Pb and the Ca1(4f) site is occupied by 92% Ca and 8% Pb. The tetrahedral site refines to 91% P and 9% As. The refinement indicates the 0.0.0 position to be fully occupied by Cl. The ordering of Ca and Pb in phosphohedyphane has important implications with respect to the chlorapatite-pyromorphite solid solution series. An analysis of compositions of natural members of the pyromorphite-mimetite-turneaureite-chlorapatite system suggests the existence of complete solid solution among pyromorphite, mimetite, hedyphane, and phosphohedyphane. No stable solid solutions appear to exist between the joins phosphohedyphane-hedyphane and chlorapatite-turneaureite in natural systems.

Keywords: Phosphohedyphane, new mineral, crystal structure, chemical analysis, solid solution, pyromorphite, apatite group