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Fluorphosphohedyphane, $Ca_2Pb_3(PO_4)_3F$, the first apatite supergroup mineral with essential Pb and F

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Abstract

The new mineral fluorphosphohedyphane, $Ca_2Pb_3(PO_4)_3F$, the F-analog of phosphohedyphane, is hexagonal with space group $P6_3/m$ and cell parameters $a = 9.6402(12)$, $c = 7.0121(8)$ Å, $V = 564.4(1)$ Å^3, and $Z = 2$. It occurs in the oxidation zone of a small Pb-Cu-Zn-Ag deposit, the Blue Bell claims, about 11 km west of Baker, San Bernardino County, California. It forms as sub-parallel intergrowths and irregular clusters of transparent, colorless, highly lustrous, hexagonal prisms with pyramidal terminations. It is found in cracks and narrow veins in a highly siliceous hornfels in association with cerussite, chrysocolla, fluorite, fluorapatite, goethite, gypsum, mimetite, opal, phosphohedyphane, plumbogummite, plumbophyllite, plumbotsumite, pyromorphite, quartz, and wulfenite. The streak of the new mineral is white, the luster is subadamantine, and the Mohs hardness is about 4. The mineral is brittle with subconcoidal fracture and no cleavage. The calculated density is 5.445 g/cm^3 based upon the empirical formula. Optical properties (589 nm): uniaxial (–), $\omega = 1.836(5)$, $\varepsilon = 1.824(5)$, nonpleochroic. SEM-EDS analyses yielded the averages and ranges in wt%: O 21.28 (20.31–22.14), F 1.59 (1.38–1.91), P 10.33 (9.81–10.83), Ca 9.66 (8.97–10.67), Pb 60.08 (57.67–61.21), total 102.95 (102.02–103.88), providing the empirical formula (based on P = 3): $Ca_{2.00}(Pb_{2.61}Ca_{0.17})_{\Sigma 2.78}P_3O_{11.91}F_{0.75}$. Infrared spectroscopy showed no evidence of OH or carbonate. The strongest powder X-ray diffraction lines are [d(hkl)I]: 8.38(100)22, 3.974(111)28, 3.506(002)25, 2.877(121,211)100, 1.878(213,123)26. Fluorphosphohedyphane has the apatite structure ($R_1 = 1.75\%$ for 444 reflections with $F_o > 4\sigma F$) with ordering of Ca and Pb in two cation sites, as in hedyphane and phosphohedyphane. The Pb^{2+} cation exhibits a stereoactive $6s^2$ lone-electron-pair. The X anion site at (0, 0, ½) is fully occupied by F forming six bonds of 2.867 Å to Pb atoms, in contrast to the six Pb-Cl bonds of 3.068 Å in phosphohedyphane.

Keywords: Fluorphosphohedyphane, new mineral, crystal structure, apatite supergroup, hedyphane group, Pb^{2+} $6s^2$ lone-electron-pair, Blue Bell claims, California