

Birchite, a new mineral from Broken Hill, New South Wales, Australia: Description and structure refinement

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ABSTRACT

The new mineral species birchite, idealized formula $\text{Cd}_2\text{Cu}_2(\text{PO}_4)_2(\text{SO}_4)\cdot 5\text{H}_2\text{O}$, occurs on specimens from the Block 14 Opencut, Broken Hill, New South Wales, Australia, as sprays and aggregates of crystals to 0.75 mm across on a host rock composed of quartz, garnet, galena, chalcopyrite, and fluorapatite. It is a late-stage supergene mineral formed as part of a suite of secondary phosphate minerals under low-temperature conditions. Associated secondary minerals are covellite, cerussite, anglesite, plumbogummite-hinsdalite, pyromorphite, libethenite, and sampleite. Individual crystals are bladed to prismatic and acicular in habit, with a maximum length of 0.3 mm and width of 0.05 mm. The crystals are elongated along [001] and sometimes also flattened on (100). The crystal forms are major {100} and {010}, and minor {101} and {001}. Birchite is orthorhombic, space group *Pnma*, with unit-cell parameters refined from powder X-ray diffraction data, $a = 10.489(6)$, $b = 20.901(7)$, $c = 6.155(5)$ Å, $V = 1349.6(3)$ Å³, and $Z = 4$. The eight strongest lines in the diffraction pattern are [$d(\text{Å})/I(hkl)$]: 10.451(100)(020); 5.146(28)(111); 4.223(38)(131); 3.484(39)(060); 2.902(70)(260); 2.719(33)(132); 2.652(32)(042); 1.919(80)(432). Birchite is translucent (masses) to transparent (crystals); pale blue with a vitreous luster. Optically, birchite is biaxial positive, with $n_\alpha = 1.624(4)$, $n_\beta = 1.636(5)$, $n_\gamma = 1.669(4)$, and $2V_{\text{calc}} = +63^\circ$. The optical orientation is $\mathbf{X} = \mathbf{b}$, $\mathbf{Y} = \mathbf{a}$, $\mathbf{Z} = \mathbf{c}$; the optical axis plane lies within the {100} plane. Birchite shows very faint pleochroism, $\mathbf{X} =$ pale bluish, $\mathbf{Z} =$ pale greenish, absorption $\mathbf{Z} \geq \mathbf{X}$. Birchite is brittle, has a conchoidal fracture and is nonfluorescent. Hardness (Mohs) is 3.5–4; the measured density is 3.61(4) g/cm³, and the calculated density is 3.647 g/cm³ (from the empirical formula). Average electron microprobe analysis (wt%): CdO 36.79, CuO 21.22, CaO 0.17, MnO 0.17, ZnO 1.07, P₂O₅ 20.21, SO₃ 9.70, H₂O (from crystal-structure analysis) 12.37, total 101.70. The empirical formula, calculated on the basis of 17 O atoms and with H₂O calculated to give 5H₂O is $(\text{Cu}_{1.94}\text{Zn}_{0.10})_{\Sigma 2.04}(\text{Cd}_{2.09}\text{Ca}_{0.02}\text{Mn}_{0.02})_{\Sigma 2.13}\text{P}_{2.07}\text{S}_{0.88}\text{O}_{12}\cdot 5\text{H}_2\text{O}$. The crystal structure has been refined to an *R* index of 4.3% for 846 observed reflections measured with MoK α X-radiation. Alternating [CdO₄(H₂O)₂] octahedra and [CuO₃(H₂O)₂] square-pyramids share edges to form chains that extend along the *a* axis, which are linked by (PO₄) tetrahedra to form [CdCu(PO₄)(H₂O)₂O] sheets in the (010) plane. Two such sheets are linked via (PO₄) tetrahedra vertices to form a layer in the (010) plane. Two layers, which are related by mirror symmetry, are linked via (SO₄) tetrahedra vertices to form a heteropolyhedral framework structure. Interstitial channels within the framework extend along both the *a* and *c* axes and are occupied by a H₂O group. The mineral is named for William D. Birch, Senior Curator of Geosciences at Museum Victoria, Australia.

Keywords: Birchite, new mineral species, crystal structure, cadmium oxysalt, phosphate, sulfate, Broken Hill, New South Wales