Bederite, a new pegmatite phosphate mineral from Nevados de Palermo, Argentina: Description and crystal structure

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ABSTRACT

Bederite, ideally \Box Ca₂Mn²⁺Fe³⁺Mn²⁺(PO₄)₆(H₂O)₂, orthorhombic, a = 12.559(2), b = 12.834(1), c= 11.714(2) Å, V = 1887.8(4) Å³, Z = 4, space group *Pcab*, is a new mineral from the El Peñón pegmatite, Nevados de Palermo, Salta Province, República Argentina. The mineral occurs as rare ellipsoidal nodules (~5 cm in diameter) enclosed in potassium feldspar or quartz at the core-margin zone of a beryl-type rare-element pegmatite. Associated minerals are quartz, potassium feldspar, muscovite, beryl, columbite, possibly heterosite, and powdery coatings of Mn- and Fe-oxides; in the dumps of the pegmatite, there are numerous other phosphates including altered triphylite-lithiophyllite, arrojadite, eosphorite, laueite, brazilianite, and fairfieldite. Bederite is very dark brown to black with a dark olive-green streak and a vitreous luster. It is brittle with an irregular fracture and a good cleavage parallel to {100}, Mohs hardness is 5, and the observed and calculated densities are 3.48(1) and 3.50 g/cm³, respectively. In transmitted plane-polarized light, bederite is pleochroic X = Y =olive green, Z = brown with X = Y > Z and X = a, Y = c, Z = b. In cross-polarized light, it is biaxial negative with strong dispersion, v > r, 2V(obs) = 54° and 2V(calc) = 60°. Refractive indices are as follows: $\alpha = 1.729(3)$, $\beta = 1.738(3)$, $\gamma = 1.741(3)$. Chemical analysis by electron microprobe plus the Penfield method and thermogravimetry gave P₂O₅ 41.76, Al₂O₃ 0.82, Fe₂O₃ 12.00, FeO 2.25, MnO 20.59, MgO 3.45, ZnO 0.40, CaO 10.91, SrO 0.43, Na₂O 0.63, H₂O 3.52, sum 96.76 wt% where the Fe₂O₃ and FeO contents were derived from the refined crystal structure. The five strongest lines in the X-ray powder diffraction pattern are as follows: d (Å), I, (h k l): 2.768, 100, (4 0 2); 2.927, 78, (0 0 4); 3.006, 67, (1 4 1); 2.814, 35, (0 4 2); 2.110, 33, (1 6 0). The crystal structure of bederite was refined to an R index of 2.8% based on 2530 observed ($>5\sigma$ F) reflections measured with MoK α X-radiation. Bederite is isostructral with wicksite, grischunite, and an unnamed wicksite-like phase; it is related to wicksite by the substitutions ${}^{Na}\square + {}^{M2}Fe^{3+} \rightarrow {}^{Na}Na + {}^{M2}Mg$, ${}^{M1}Mn^{2+} \rightarrow {}^{M1}Fe^{2+}$ and ${}^{M3}Mn^{2+} \rightarrow {}^{M3}Fe^{2+}$.