Pauloabibite, trigonal NaNbO₃, isostructural with ilmenite, from the Jacupiranga
carbonatite, Cajati, São Paulo, Brazil

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ABSTRACT

Pauloabibite (IMA 2012-090), trigonal NaNbO₃, occurs in the Jacupiranga carbonatite, in Cajati County, São Paulo State, Brazil, associated with dolomite, calcite, magnetite, phlogopite, pyrite, pyrrhotite, ancybite-(Ce), tochilinite, fluorapatite, “pyrochlore”, viggzezite, and strontianite. Pauloabibite occurs as encrustations of platy crystals, up to 2 mm in size, partially intergrown with an unidentified Ca-Nb-oxide, embedded in dolomite crystals, which in this zone of the mine can reach centimeter sizes. Cleavage is perfect on {001}. Pauloabibite is transparent and displays a sub-adamantine luster; it is pinkish brown and the streak is white. The calculated density is 4.246 g/cm³. The mineral is uniaxial; n(mean)_c is 2.078. Chemical composition (n = 17, WDS, wt%) is: Na₂O 16.36, MgO 0.04, CaO 1.36, MnO 0.82, FeO 0.11, SrO 0.16, BaO 0.02, TiO₂ 0.33, Nb₂O₅ 78.66, Ta₂O₅ 0.34, total 98.76. The empirical formula is (Na₀.₈₂Ca₀.₀₄Mn₀.₃₂Fe₀.₀₁Sr₀.₀₂Ba₀.₀₂Ti₀.₀₁O₁₆.₃₆MgO 0.0₄CaO 0.0₂MnO 0.8₂FeO 0.1₁SrO 0.0₂BaO 0.0₂TiO₂ 0.0₃Nb₂O₅ 78.₆₆Ta₂O₅ 0.₃₄, total 100). X-ray powder-diffraction lines (calculated pattern) [d in Å, hkl] are: 5.2666(100) (003), 4.4257(82) (101), 3.9730(45) (012), 2.9809(54) (104), 2.3718(88) (2T3), 1.9865(28) (024), 1.8620(53) (2T6), and 1.5383(30) (300). It is trigonal, space group: R₃c, a = 5.3287(5), c = 15.6197(17) Å, V = 384.10(7) Å³, Z = 6. The crystal structure was solved (R₁ = 0.0285, wR₂ = 0.0636 for 309 observed reflections). Pauloabibite is isostructural with ilmenite and is polymorphic with isolueshite (cubic) and lueshite (orthorhombic). The name is in honor of Paulo Abib Andery (1922–1976).

Keywords: Pauloabibite, new mineral, carbonatite, ilmenite structure, crystal structure, chemical composition, Jacupiranga mine, Cajati, Brazil

INTRODUCTION

Pauloabibite (IMA 2012-090), trigonal NaNbO₃, is polymorphic with isolueshite (cubic) and lueshite (orthorhombic) (Table 1). Natroniobite, a poorly described mineral (Bulakh et al. 1960), may be a monoclinic polymorph of NaNbO₃, or a mineral with formula NaNb₃O₈(OH), related to fersmite (Chakhmouradian et al. 1997; Chakhmouradian and Mitchell 1998) and plumbonacrite (Chakhmouradian and Mitchell 1998) investigated a museum specimen labeled “natroniobite” (not the type specimen) and concluded that it is a “complex aggregate of lueshite and its replacement products, set in a matrix of dolomite and fluorapatite.” Monoclinic synthetic compounds with formula NaNbO₃ are known (e.g., Solovev et al. 1961; Johnston et al. 2010), but the X-ray diffraction pattern of natroniobite does not match those of these other compounds.

Pauloabibite is trigonal, isostructural with ilmenite and other R₃c oxides that display a crystal structure formed by the hexagonal close packing of oxygen atoms, with two-thirds of the octahedral interstices occupied by two unique sites of di- and tetravalent or uni- and pentavalent cations. In corundum and other R₃c oxides, two-thirds of the octahedral interstices are occupied by trivalent cations in one unique site. Data for these minerals are included in Table 2.

The synthetic analog of pauloabibite has been studied by several research groups. It was reported by Kinomura et al. (1984) and Kumata et al. (1990) from a two-step synthesis method, involving the preparation of Na₃NbO₃·13H₂O followed by hydrothermal reaction with NaOH in a silver-lined vessel at 250 °C. It was also prepared directly in one step under mild hydrothermal conditions by lowering pH and using close-to-stoichiometric amounts of reagents at 240 °C (Modeshia et al. 2009; Johnston et al. 2011). The equivalent to lueshite (space group Pbnm) was not yet synthesized, but phase transitions in natural lueshite were observed in the sequence: Cmcm at 575 °C, P4/nmm at 625 °C, and Pn5m, equivalent to isolueshite, at

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