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

LUIZ A.D. MENEZES FILHO¹†, DANIEL ATENCIO²*, MARCELO B. ANDRADE³, ROBERT T. DOWNS⁴, MÁRIO L.S.C. CHAVES¹, ANTONIO W. ROMANO¹, RICARDO SCHOLZ⁵ and ABA I.C. PERSIANO⁶

¹Instituto de Geociências, Universidade Federal de Minas Gerais, Avenida Antônio Carlos, 6627, 31270-901, Belo Horizonte, Minas Gerais, Brazil
²Instituto de Geociências, Universidade de São Paulo, Avenida Doutor Lineu Prestes, 3246, 05508-090, São Paulo, São Paulo, Brazil
³Instituto de Física of São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970, São Carlos, São Paulo, Brazil
⁴Department of Geosciences, University of Arizona, Tucson, Arizona 85721-0077, U.S.A.
⁵Departamento de Geologia da Escola de Minas da Universidade Federal de Ouro Preto, Campus Morro do Cruzeiro, Ouro Preto, 35400-000, Minas Gerais, Brazil
⁶Departamento de Física do Instituto de Ciências Exatas da Universidade Federal de Minas Gerais, Avenida Antônio Carlos, 6627, 31279-901, Belo Horizonte, Minas Gerais, Brazil

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, anhydrite, to chlorite, fluorapatite, “pyrochlore”,巍等zity, and strontianite. Pauloabibite occurs as incrustations 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) 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 0.02, BaO 0.16, SiO₂ 0.03, TiO₂ 0.86, Nb₂O₅ 78.66, Ta₂O₅ 0.34, total 98.76. The empirical formula is (Na₈.0₂Ca₀.04Mn₁₀.45₀.5₂Mg₁.0₁₄₀.0₁₂₁.0₁₁₄.0₁₂O₃. The x-ray powder-diffraction lines (calculated pattern) [001] (hkl) are: 5.2066(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: R₃̅₃, a = 5.3287(5), c = 15.6197(17), A, 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 ilmenolite (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 ilmenolite (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 Na₀.₀₈Ca₀.₀₆Mn₁₄.₀₂₂₄₀.₀₁₂₁.₀₁₁₄.₀₁₂O₃. The x-ray powder-diffraction lines (calculated pattern) [001] (hkl) are: 5.2066(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: R₃̅₃, a = 5.3287(5), c = 15.6197(17), A, 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 ilmenolite (cubic) and lueshite (orthorhombic). The name is in honor of Paulo Abib Andery (1922–1976).

Pauloabibite (IMA 2012-090), trigonal NaNbO₃, is polymorphic with ilmenolite (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 Na₀.₀₈Ca₀.₀₆Mn₁₄.₀₂₂₄₀.₀₁₂₁.₀₁₁₄.₀₁₂O₃. The x-ray powder-diffraction lines (calculated pattern) [001] (hkl) are: 5.2066(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: R₃̅₃, a = 5.3287(5), c = 15.6197(17), A, 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 ilmenolite (cubic) and lueshite (orthorhombic). The name is in honor of Paulo Abib Andery (1922–1976).

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 Na₀.₀₈Ca₀.₀₆Mn₁₄.₀₂₂₄₀.₀₁₂₁.₀₁₁₄.₀₁₂O₃ 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 Pn3m, equivalent to ilmenolite, at

* E-mail: datencio@usp.br
† Deceased 9 July 2014.