Pauloabibite, trigonal NaNbO$_3$, isostructural with ilmenite, from the Jacupiranga carbonatite, Cajati, São Paulo, Brazil

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Abstract

Pauloabibite (IMA 2012-090), trigonal NaNbO$_3$, occurs in the Jacupiranga carbonatite, in Cajati County, São Paulo State, Brazil, associated with dolomite, calcite, magnetite, phlogopite, pyrite, pyrrhotite, ancylite-(Ce), tochilinite, fluorapatite, "pyrochlore", vigezzite, 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/cm^3. The mineral is uniaxial; n(mean)$_{calc}$ is 2.078. Chemical composition ($n = 17$, WDS, wt%) is: Na$_2$O 16.36, MgO 0.04, CaO 1.36, MnO 0.82, FeO 0.11, SrO 0.02, BaO 0.16, SiO$_2$ 0.03, TiO$_2$ 0.86, Nb$_2$O$_5$ 78.66, Ta$_2$O$_5$ 0.34, total 98.76. The empirical formula is (Na$_{0.88}$Ca$_{0.04}$Mn$^{2+}_{0.02}$)$_{\Sigma0.94}$(Nb$_{0.98}$Ti$_{0.02}$)$_{\Sigma1.00}$O$_3$. X-ray powder-diffraction lines (calculated pattern) [d in Å(I)(hkl)] are: 5.2066(100)(003), 4.4257(82)(101), 3.9730(45)(012), 2.9809(54)(104), 2.3718(88)(2$\bar{1}$3), 1.9865(28)(024), 1.8620(53)(2$\bar{1}$6), and 1.5383(30)(300). It is trigonal, space group: $R\bar{3}$, $a = 5.3287(5)$, $c = 15.6197(17)$ Å, $V = 384.10(7)$ Å^3, $Z = 6$. The crystal structure was solved ($R_1 = 0.0285$, $wR_2 = 0.0636$ 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