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Hydrokenomicrolite, $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$, a new microlite-group mineral from Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil

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Abstract

Hydrokenomicrolite, $(\square,H_2O)_2Ta_2(O,OH)_6(H_2O)$ or ideally $\square_2Ta_2[O_4(OH)_2](H_2O)$, is a new microlite-group mineral approved by the CNMNC (IMA 2011-103). It occurs as an accessory mineral in the Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil. Associated minerals are: microcline, albite, quartz, muscovite, spodumene, "lepidolite", cassiterite, tantalite-(Mn), monazite-(Ce), fluorite, "apatite", beryl, "garnet", epidote, magnetite, gahnite, zircon, "tourmaline", bityite, and other microlite-group minerals under study. Hydrokenomicrolite occurs as euhedral octahedral crystals, occasionally modified by rhombododecahedra, untwinned, from 0.2 to 1.5 mm in size. The crystals are pinkish brown and translucent; the streak is white, and the luster is adamantine to resinous. It is non-fluorescent under ultraviolet light. Mohs hardness is 4½–5, tenacity is brittle. Cleavage is not observed; fracture is conchoidal. The calculated density is 6.666 g/cm^3. The mineral is isotropic, n_{calc} = 2.055. The infrared spectrum contains bands of O-H stretching vibrations and H-O-H bending vibrations of H_2O molecules. The chemical composition (n = 3) is [by wavelength-dispersive spectroscopy (WDS), H_2O calculated from crystal-structure analysis, wt%]: CaO 0.12, MnO 0.27, SrO 4.88, BaO 8.63, PbO 0.52, La_2O_3 0.52, Ce_2O_3 0.49, Nd_2O_3 0.55, Bi_2O_3 0.57, UO_2 4.54, TiO_2 0.18, SnO_2 2.60, Nb_2O_5 2.18, Ta_2O_5 66.33, SiO_2 0.46, Cs_2O 0.67, H_2O 4.84, total 98.35. The empirical formula, based on 2 cations at the B site, is $[\square_{0.71}(H_2O)_{0.48}Ba_{0.33}Sr_{0.27}U_{0.10}Mn_{0.02}Nd_{0.02}Ce_{0.02}La_{0.02}Ca_{0.01}\ Bi_{0.01}Pb_{0.01}]_{\Sigma 2.00}$ $(Ta_{1.75}Nb_{0.10}Sn_{0.10}Si_{0.04}Ti_{0.01})_{\Sigma 2.00}[(O_{5.77}(OH)_{0.23}]_{\Sigma 6.00}[(H_2O)_{0.97}Cs_{0.03}]_{\Sigma 1.00}$. The strongest eight X-ray powder-diffraction lines [d in Å(I)(hkl)] are: 6.112(86)(111), 3.191(52)(311), 3.052(100)(222), 2.642(28)(400), 2.035(11)(511)(333), 1.869(29)(440), 1.788(10)(531), and 1.594(24)(622). The crystal structure refinement (R_1 = 0.0363) gave the following data: cubic, $Fd\bar{3}m$, a = 10.454(1) Å, V = 1142.5(2) Å^3, Z = 8. The $Ta(O,OH)_6$ octahedra are linked through all vertices. The refinement results and the approximate empirical bond-valences sums for the positions A (1.0 v.u.) and Y' (0.5 v.u.), compared to valence calculations from electron microprobe analysis (EMPA) and ranges expected for H_2O molecules, confirm the presence of H_2O at the A(16d) site and displaced from the Y(8b) to the Y'(32e) position. The mineral is characterized by H_2O dominance at the Y site, vacancy dominance at the A site, and Ta dominance at the B site.

Keywords: Hydrokenomicrolite, new mineral, Volta Grande pegmatite, Nazareno, Minas Gerais, Brazil, pyrochlore supergroup, microlite group, crystal structure