American Mineralogist, Volume 96, pages 1455–1460, 2011

Rankamaite from the Urubu pegmatite, Itinga, Minas Gerais, Brazil: Crystal chemistry and Rietveld refinement

Daniel Atencio,[1,*] Reynaldo R. Contreira Filho,[2] Stuart J. Mills,[3] José M.V. Coutinho,[1] Sara B. Honorato,[4] Alejandro P. Ayala,[4] Javier Ellena,[5] and Marcelo B. de Andrade[5]

[1]Departamento de Mineralogia e Geotectônica, Instituto de Geociências, Universidade de São Paulo, Rua do Lago 562, 05508-080 São Paulo, SP, Brazil
[2]Rua Murici 62, Campinas, SP, Brazil
[3]Department of Earth and Ocean Sciences, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada
[4]Departamento de Física, Universidade Federal do Ceará, Caixa Postal 6030, 60455-900 Fortaleza, CE, Brazil
[5]Departamento de Física e Informática, Instituto de Física de São Carlos, Universidade de São Paulo, Caixa Postal 369, 13560-970 São Carlos, SP, Brazil

Abstract

A new occurrence of rankamaite is here described at the Urubu pegmatite, Itinga municipality, Minas Gerais, Brazil. The mineral forms cream-white botryoidal aggregates of acicular to fibrous crystals, intimately associated with simpsonite, thoreaulite, cassiterite, quartz, elbaite, albite, and muscovite. The average of six chemical analyses obtained by electron microprobe is (range in parentheses, wt%): Na_2O 2.08 (1.95–2.13), K_2O 2.61 (2.52–2.74), Al_2O_3 1.96 (1.89–2.00), Fe_2O_3 0.01 (0.00–0.03), TiO_2 0.02 (0.00–0.06), Ta_2O_5 81.04 (79.12–85.18), Nb_2O_5 9.49 (8.58–9.86), total 97.21 (95.95–101.50). The chemical formula derived from this analysis is $(Na_{1.55}K_{1.28})_{\Sigma 2.83}(Ta_{8.45}Nb_{1.64}Al_{0.89}Fe^{3+}_{0.01}Ti_{0.01})_{\Sigma 11.00}[O_{25.02}(OH)_{5.98}]_{\Sigma 31.00}$. Rankamaite is an orthorhombic "tungsten bronze" (OTB), crystallizing in the space group *Cmmm*. Its unit-cell parameters refined from X-ray diffraction powder data are: $a = 17.224(3)$, $b = 17.687(3)$, $c = 3.9361(7)$ Å, $V = 1199.1(3)$ Å^3, $Z = 2$. Rietveld refinement of the powder data was undertaken using the structure of $LaTa_5O_{14}$ as a starting model for the rankamaite structure. The structural formula obtained with the Rietveld analyses is: $(Na_{2.21}K_{1.26})_{\Sigma 3.37}(Ta_{9.12}Nb_{1.30}Al_{0.59})_{\Sigma 11.00}[O_{26.29}(OH)_{4.71}]_{\Sigma 31.00}$. The tantalum atoms are coordinated by six and seven oxygen atoms in the form of distorted TaO_6 octahedra and TaO_7 pentagonal bipyramids, respectively. Every pentagonal bipyramid shares edges with four octahedra, thus forming Ta_5O_{14} units. The potassium atom is in an 11-fold coordination, whereas one sodium atom is in a 10-fold and the other is in a 12-fold coordination. Raman and infrared spectroscopy were used to investigate the room-temperature spectra of rankamaite.

Keywords: Rankamaite, tungsten bronze, tantalate, Urubu pegmatite, Itinga, Minas Gerais, Brazil, Rietveld refinement