Ronneburgite, K₂MnV₄O₁₂, a new mineral from Ronneburg, Thuringia, Germany: Description and crystal structure

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ABSTRACT

Ronneburgite is a new chain vanadate mineral from Ronneburg, Thuringia, Germany. It occurs as reddish-brown crystals of equant, flattened, or short prismatic habit, up to 0.5 mm in length. The crystals have an adamantine luster and are translucent. Ronneburgite is biaxial negative with refractive indices $n_{\alpha} = 1.925(5)$, $n_{\beta} = 1.960(10)$, $n_{\gamma} = 1.988(4)$, and $2V_x = 82^{\circ}$. Electron microprobe analysis ($K_2O = 16.93$, MnO = 12.44, MgO = 0.62, $V_2O_5 = 68.54$; total = 98.53 wt%) gives the empirical formula $K_{1.91}Mn_{0.93}Mg_{0.08}V_{4.00}O_{11.96}$, which simplifies to $K_2MnV_4O_{12}$. Ronneburgite is monoclinic, space group $P2_1/n$, with a = 8.183(3), b = 9.247(3), c = 8.651(2) Å, and $\beta = 109.74(2)^{\circ}$. The measured density is 2.84 g/cm³; the calculated density for Z = 2 is 2.85 g/cm³. Single-crystal X-ray structure determination ($R_1 = 0.046$ for 1846 reflections) shows that ronneburgite contains infinite vierer-single metavanadate chains $[(VO_3)_n]^{n-}$ of corner-sharing VO_4 tetrahedra along [101]. Although the empirical formula and calculated bond valences indicate that V is 5+ and Mn is 2+, the crystal color, a "poor" structural compatibility index, and Mn-O distances between those expected for Mn²⁺-O and Mn³⁺-O indicate that some Mn³⁺ and V^{4+} ions are present. K⁺ ions and octahedral Mnⁿ⁺ ions bridge between the metavanadate chains by coordinating to their oxygen atoms.