Čejkaite, the triclinic polymorph of Na₄(UO₂)(CO₃)₃—a new mineral from Jáchymov, Czech Republic

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ABSTRACT

Čejkaite, a new mineral from Jáchymov, NW Bohemia, Czech Republic, forms a thin earthy efflorescence over a calcite vein associated with disintegrated uraninite. The color is pale yellow to beige, the streak is light yellow, and the luster is vitreous. The broad secondary mineral association includes and ersonite and schröckingerite. Chemical analysis (by ICP-MS and TG) gave (in wt%): $Na_2O = 21.39$, MgO = 0.15, FeO = 0.53, UO₃ = 53.93, and CO₂ = 24.00 (calculated by difference). The simplified chemical formula is $Na_4UO_2(CO_3)_3$. The mineral is triclinic, space group P1 or P1, a = 9.291(2), b = 9.292(2), c = 12.895(2) Å, $\alpha = 90.73(2), \beta = 90.82(2), \gamma = 120.00(1)^{\circ}, V = 963.7(4)$ Å³, Z = 4, $D_{\text{meas}} = 3.67(1)$ g/cm³, and $D_{\text{calc}} = 3.766(5)$ g/cm³. The strongest seven lines in the X-ray powder-diffraction pattern [d in Å(I)(hkl)] are: 8.022(92)(110, 010, 100), 5.080(57)(102, 012), 5.024(60)(112, 112), 4.967(68)(012, 102), 4.639(100)(120, 210, 110), 3.221(63)(004), 2.681(60) $(\overline{330}, \overline{114}, 030, 300)$. Optical data could not be measured due to the extremely small grain size, but the calculated mean refractive index is 1.5825. Crystal size varies from 0.2 to 0.6 µm and shows an indistinct hexagonal outline. Thermal decomposition of synthetic čejkaite proceeds in three main steps. DTA endotherm at 430 °C corresponds to the decomposition of the uranyl tricarbonate groups. IR spectrum of čejkaite confirms the presence of crystallographically nonequivalent $(CO_3)^{2-}$ groups and the absence of water. The average U-O bond length in $(UO_2)^{2+}$, calculated from $v_3 = 848$ cm⁻¹, is $R_{\rm UO} \sim 1.81$ Å. A model based on the crystal structure of trigonal Na₄(UO₂)(CO₃)₃ was adopted and applied to solve the čejkaite crystal structure by the Rietveld method (7238 unique reflections, $R_{\rm p}$ = 0.076, $R_{wp} = 0.104$). Uranium is eight-coordinated, and forms a [UO₂O₆] skeleton with almost linear O-U-O that is roughly perpendicular to an irregular cycle formed by six O atoms that, in turn, belong to three more-or-less regular and planar CO₃ groups. Atoms Na1, Na1a, and Na2 are octahedrally coordinated, whereas Na3 is pentagonally coordinated. The mineral name honors Jiří Čejka for his notable contributions to the crystal chemistry of U minerals.