

PŮVODNÍ PRÁCE/ORIGINAL PAPER

Ojedinělý výskyt bayleyitu, $Mg_2[(UO_2)(CO_3)_3] \cdot 18H_2O$, z Jáchymova

Unique occurrence of bayleyite, $Mg_2[(UO_2)(CO_3)_3] \cdot 18H_2O$, from Jáchymov

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Abstract

A rare supergene uranyl carbonate mineral, bayleyite, was found on a single specimen originated from the 3rd level of the Barbora shaft, the Jáchymov ore district, Czech Republic. Bayleyite occurs there as a yellow, very small, imperfect crystals of glassy lustre forming crystalline aggregates up to 3 mm on a small fragment of the rock. Liebigite, schröckingerite, rabbittite and natrozippeite were found in the mineral association. According to single-crystal X-ray data bayleyite is monoclinic, space group $P2_1/a$, with $a = 26.535(1)$, $b = 15.244(2)$, $c = 6.497(3)$ Å, $\beta = 92.942(10)$, and $V = 2624.5(13)$ Å³. Crystal structure was refined to $R_1 = 2.68\%$ on the basis of 5008 unique observed reflections [$I_{obs} > 3\sigma(I)$] collected on a Oxford Diffraction Gemini diffractometer with a Atlas CCD detector and MoKα radiation. Chemical analyses of bayleyite yielded the average composition MgO 12.68, FeO 0.06, Al₂O₃ 0.05, SiO₂ 0.45, UO₃ 51.97, CO₂_{calc.} 21.27, H₂O_{calc.} 29.46, total 115.94 wt. % corresponding to the empirical formula $(Mg_{1.73}Al_{0.01}Fe_{0.01})_{\Sigma 1.75}(UO_2)_{1.00}[(CO_3)_{2.66}(SiO_4)_{0.04}] \cdot 18H_2O$ calculated on the basis of U = 1 apfu (CO₃ content derived from the charge-balance). Raman spectrum of bayleyite is dominated by the symmetric stretching vibration of UO₂²⁺ ion, and stretching and bending modes of planar CO₃ groups. Inferred uranyl bond-lengths and possible hydrogen bond lengths obtained from the Raman frequencies of corresponding vibrations, based on the empirical relations, are consistent with values from the refined structure.

Key words: bayleyite, uranyl carbonate, crystal structure, electron microprobe data, Raman spectroscopy, Jáchymov

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