

Uramphite, $(\text{NH}_4)(\text{UO}_2)(\text{PO}_4)\cdot 3\text{H}_2\text{O}$, from the second world occurrence, Beshtau uranium deposit, Northern Caucasus, Russia: Crystal-structure refinement, infrared spectroscopy, and relation to uramarsite

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ABSTRACT

Uramphite, $(\text{NH}_4)(\text{UO}_2)(\text{PO}_4)\cdot 3\text{H}_2\text{O}$, was found at Beshtau uranium deposit, Northern Caucasus, Russia, as the second world occurrence besides its type locality, Tura-Kavak uranium-coal deposit in Kyrgyzstan. In Beshtau, it occurs as yellow tabular crystals up to 0.3 mm grouped in crusts on a matrix composed of albite, microcline, quartz, and chamosite in association with liebigite, meta-autunite, and plumbogummite. The empirical formula calculated on the basis of 6 O apfu and 3 H₂O is $[(\text{NH}_4)_{0.91}\text{K}_{0.08}]_{\Sigma 0.99}\text{P}_{0.99}\text{U}_{1.01}^{6+}\text{O}_6\cdot 3\text{H}_2\text{O}$. According to single-crystal X-ray diffraction, uramphite is tetragonal, $P4/nmm$, with $a = 6.9971(3)$, $c = 8.9787(9)$ Å, $V = 439.59(6)$ Å³, and $Z = 2$. The crystal structure was refined to $R_1 = 3.28\%$ for 255 unique observed reflections with $|F_o| \geq 4\sigma_F$. A model for the distribution of H₂O and NH₄⁺ molecules in the interlayer space based on the electron density distribution data is proposed. The mineral belongs to the meta-autunite group. The IR spectrum shows the splitting of the band of H-N-H bending vibrations into four components, which is explained here by the resonance splitting of a group of NH₄⁺ cations occurring around the fourfold axis at close distances from each other. Uramphite is related to uramarsite, $(\text{NH}_4)(\text{UO}_2)(\text{AsO}_4)\cdot 3\text{H}_2\text{O}$. The two minerals have similar crystal structures and IR spectra. However, they are not isostructural. Uramarsite is triclinic, contains a significant amount of P in arsenate sites, and significantly differs from uramphite by the arrangement of H₂O and NH₄⁺ molecules in the interlayer space (planar and well organized in uramphite vs. disordered in uramarsite).

Keywords: Uramphite, crystal structure, infrared spectroscopy, chemistry, Beshtau uranium deposit, uramarsite