Adolfpateraite, K(UO₂)(SO₄)(OH)(H₂O), a new uranyl sulphate mineral from Jáchymov, Czech Republic

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ABSTRACT

Adolfpateraite, monoclinic $K(UO_2)(SO_4)(OH)(H_2O)$, is a new supergene mineral from the Svornost mine, Jáchymov ore district, Czech Republic. It forms sulfur yellow to greenish yellow crystalline aggregates, up to 2 mm in diameter. Crystals are transparent to translucent with a vitreous luster, without observable cleavage. The streak is pale yellow. The Mohs hardness is ~2. The mineral shows a green fluorescence in long-wave ultraviolet radiation. Adolf pateraite is pleochroic, with $\alpha =$ colorless and $\gamma =$ yellow (β could not been examined). It is biaxial, with $\alpha = 1.597(2)$, $\gamma = 1.659(2)$ (β could not been measured), birefringence 0.062. The empirical chemical formula (mean of 4 electron microprobe point analyses) was calculated based on 8 O apfu and is $K_{0.94}(UO_2)_{1.00}(SO_4)_{1.02}(OH)_{0.90}(H_2O)_{1.00}$ (water content calculated). The simplified formula is K(UO₂)(SO₄)(OH)(H₂O), requiring K₂O 10.70, UO₃ 64.97, SO₃ 18.19, H₂O 6.14, total 100.00 wt%. Adolfpateraite is monoclinic, space group $P_{2_1/c}$, a = 8.0462(1), b = 7.9256(1), c = 11.3206(2) Å, β = $107.726(2)^\circ$, V = 687.65(2)Å³, Z = 4, and $D_{calc} = 4.24$ g/cm³. The five strongest reflections in the X-ray powder diffraction pattern are $[d_{obs}$ in Å (I) (*hkl*)]: 7.658 (76) (100), 5.386 (100) (002), 5.218 (85) ($\overline{102}$), 3.718 (46) (021), 3.700 (37) (202). The crystal structure has been refined from single-crystal X-ray diffraction data to $R_1 = 0.0166$ with GOF = 1.30, based on 1915 observed reflections $[I_{obs} > 3\sigma(I)]$. The crystal structure consists of chains of uranyl polyhedra extended along [010], with OH⁻ located on the shared vertex between the bipyramids. The sulfate tetrahedra decorate the outer side of the chain with bridging bidentate linkages between the uranyl pentagonal bipyramids. H₂O groups are located on the edges of the chains on the non-linking vertex of each uranyl pentagonal bipyramid. K⁺ atoms are located between the chains providing additional linkage of these together with H-bonds. The fundamental vibrational modes of uranyl ion, sulfate tetrahedra, and H₂O groups were tentatively assigned in the infrared and Raman spectra. The new mineral is named to honor Adolf Patera (1819–1894), Czech chemist, mineralogist, and metallurgist.

Keywords: Adolfpateraite, uranyl sulfate, crystal structure, chemical composition, Jáchymov