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# Uranotungstite, the only natural uranyl tungstate: Crystal structure revealed from 3D electron diffraction

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## Abstract

Uranotungstite is an uranyl-tungstate mineral that was until recently only partially characterized with a formula originally given as $(Fe^{2+},Ba,Pb)(UO_2)_2(WO_4)(OH)_4 \cdot 12H_2O$ and an unknown crystal structure. This mineral has been reinvestigated by electron microprobe analysis coupled with three-dimensional electron diffraction. According to the electron microprobe data, the holotype material from the Menzenschwand uranium deposit (Black Forest, Germany) has the empirical formula $(Ba_{0.35}Pb_{0.27})_{\Sigma 0.62}[(U^{6+}O_2)_2(W^{6+}_{0.98}Fe^{3+}_{0.26}\square_{0.75})O_{4.7}(OH)_{2.5}(H_2O)_{1.75}](H_2O)_{1.67}$ (average of 8 points calculated on the basis of 2U apfu; $H_2O$ content derived from the structure). According to the precession-assisted 3D ED data, holotype uranotungstite from Menzenschwand is monoclinic, $P2_1/m$, with $a = 6.318(5)$ Å, $b = 7.388(9)$ Å, $c = 13.71(4)$ Å, $\beta = 99.04(13)°$, and $V = 632(2)$ Å$^3$ ($Z = 2$). The structure refinement of the 3D ED data using the dynamical approach ($R_{obs} = 0.0846$ for 3287 independent observed reflections) provided a structure model composed of heteropolyhedral sheets. A β-$U_3O_8$-type sheet of idealized composition $[(UO_2)_2W^{6+}Fe^{3+}_{0.25}\square_{0.75}O_{4.75}(OH)_{1.5}(H_2O)_{1.75}]^{0.25-}$ is composed of $UO_7$ polyhedra linked by $(W,Fe)O_5$ polyhedra in which the W:Fe ratio is variable as well as the bulk occupancy of this site; the W site may also host a minor proportion of Cu, Mg, or V. In uranotungstite, the interlayer spaces between adjacent U-W-O sheets host water on one side and, on the other side, a partially occupied cation site mostly occupied by Ba and, to a lesser extent, Pb, as well as a partially occupied $H_2O$ site. This work is the first structural description of a natural uranyl-tungstate mineral and confirms the great structural and chemical flexibility of β-$U_3O_8$ type of sheets.

**Keywords:** Uranotungstite, uranyl tungstate, crystal structure, crystal chemistry, Menzenschwand, 3D electron diffraction