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SYNTHESIS AND CRYSTAL STRUCTURE OF A NEW POTASSIUM URANYL SELENATE $K_{2.5}[(UO_2)_2(SeO_4)_3(H_2O)](NO_3)_{0.5}(H_2O)_4$

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The problem of safe disposal of industrial wastes, in particular, radioactive wastes, is important for the modern technological civilization. Of special interest are the studies of secondary uranium phases, which formation is possible under conditions of geological repository of radioactive waste and spent nuclear fuel. Detailed studies and the modeling experiments under laboratory conditions demonstrated that, during oxidation of spent nuclear fuel, the whole spectrum of secondary uranyl minerals and compounds is formed. Uranium compounds containing Se are of special importance, because ^{79}Se isotope is chemically and radiologically toxic fission product with the half life of 1.1×10^6 years.

Under oxidizing conditions, U^{6+} cations are almost invariably present as approximately linear uranyl-ions $[O=U=O]^{2+}$, coordinated in their equatorial planes by four, five or six additional anions. Valence requirements of the apical O atoms in the bipyramids are almost completely satisfied, and the uranyl polyhedra usually polymerize by sharing equatorial vertices and edges with adjacent polyhedra. The high anisotropy of bond distribution results in prevalence of layered structures among the minerals and synthetic uranyl compounds. Uranyl selenates, containing potassium atoms are of great interest due to special way of alkali atoms arrangement in between the U-Se structural units (Gurzhiy et. al., 2011, 2012). Here we report on the synthesis and structural study of a new potassium uranyl selenate.

Single crystals of $K_{2.5}[(UO_2)_2(SeO_4)_3(H_2O)](NO_3)_{0.5}(H_2O)_4$ (**I**) were prepared by evaporation from 2 ml aqueous solution of uranyl nitrate, potassium carbonate and selenic acid. Yellow – green transparent crystals was mounted in an Bruker Smart Apex II diffractometer equipped with an CCD – type planar de8tector. The unit cell parameters were determined by the least squares method. Compound (**I**) has a monoclinic symmetry, space group $C2/c$, a = 20.290(4) Å, b = 10.380(2) Å, c = 21.436(4) Å, β = 103.446(3)^o, V = 4391.0(13) Å^3. The crystal structure was solved by direct methods from X-ray diffraction data and refined by the least-squares method to R_1 = 0.027 (wR_2 = 0.066) for 6405 reflections with $|F_o| \geq 4\sigma_F$.

The structure of **I** is based on the $[(UO_2)_2(SeO_4)_3(H_2O)]^{2-}$ layers formed via corner sharing uranyl pentagonal bypiramides and selenate tetrahedral and parallel to (-101) plane. The negative charge of the layered complex is compensated by potassium atoms arranged in the interlayer space. The topology of the layeres in the structure of **I** is novel for the uranyl selenates.

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