Poster Presentation

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Uranyl selenates and sulfates: features of structure formation

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Uranium compounds containing tetrahedral oxoanions are of special importance from the environmental and mineralogical points of view. In this work, we examine structural relations and systematics for uranyl compounds with tetrahedrally coordinated Se6+ and S6+ cations. The U6+ atoms is almost always present as approximately linear uranyl-ions [UO2]2+, that are coordinated by four, five or six additional anions in the equatorial plane. For the valence saturation of equatorial anions it is necessary to form additional chemical bonds, hence the uranyl polyhedra are usually polymerize with each other only through the equatorial vertices and edges, that results in prevalence of layered structures among the minerals and synthetic uranyl compounds. Analysis of uranyl selenate structures demonstrates predominance of structural connectivity based upon corner-sharing coordination polyhedra. Crystal structures of uranyl sulfates often based on edge-sharing heteropolyhedral units. In the crystal structures of inorganic uranyl compounds, uranyl selenate and uranyl sulfate complexes are linked via monovalent cations (K+, Na+, etc.) or octahedrally coordinated divalent cations ([Ni(H2O)6]2+, [Zn(H2O)6]2+, [Mg(H2O)6]2+, etc.). In the crystal structures of amine-templated uranyl compounds, structure formation is regulated by hydrogen bonding systems and by arrangement of hydrophobic and hydrophilic parts of molecules with voids and dense fragments of inorganic complexes. The basic structural principle of organic-inorganic uranyl composites templated by electroneutral molecules (such as crown ethers), is the translation of interactions between organic and inorganic components by means of protonated water molecule complexes (e.g., H5O2+ and H3O+). This work was supported by St. Petersburg State University and President of Russian Federation grant for young scientists (no. MK-1737.2014.5). XRD studies have been performed at the X-ray Diffraction Centre of St. Petersburg State University.

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