Supplementary Materials.

Polytypism and oxo-tungsten polyhedra polymerization in novel complex uranyl tungstates

Andrey N. Seliverstov, a,b Evgeny V. Suleimanov, Evgeny V. Chuprunov, Nikolay V. Somov, Elena M. Zhuchkova, Maxim I. Lelet, Konstantin B. Rozov, Wulf Depmeier, Sergey V. Krivovichev e and Evgeny V. Alekseev*,c,f

^aLobachevsky State University of Nizhny Novgorod, Gagarin Av. 23b, 603950 Nizhny Novgorod, Russia. ^bAnorganische Chemie II, Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 1, D-91058 Erlangen, Germany. ^cInstitute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich, D-52428 Jülich, Germany. Fax: +49 2461 61 24 50 E-mail: e.alekseev@fz-juelich.de ^aInstitute für Geowissenschaften, University of Kiel, Ludewig-Meyn-Str. 10, D-24118 Kiel, Germany. ^eDepartment of Crystallography, Saint Petersburg State University, Dekabristov 16, 199155 Sankt

Petersburg, Russia.

f Institute für Kristallographie, RWTH Aachen University, Jägerstraße 17 – 19 D-52066 Aachen, Germany.

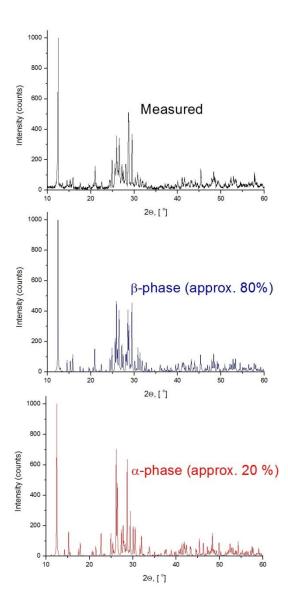


Figure 1 . Theoretical PXRD of 1(red) and 2(blue) and experimental pattern measured from their mixture.

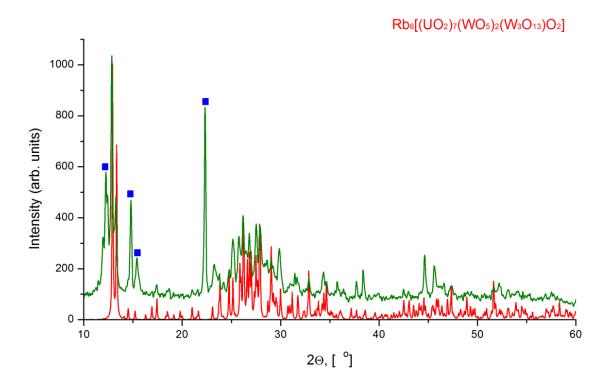


Figure 2. Theoretical (red) and measured (green) patter of 3. The peaks of impurities are shown by blue boxes. The impurities are mostly presented by $R_2U_2O_7$, $Rb_2W_2O_7$ and UO_2WO_4 .

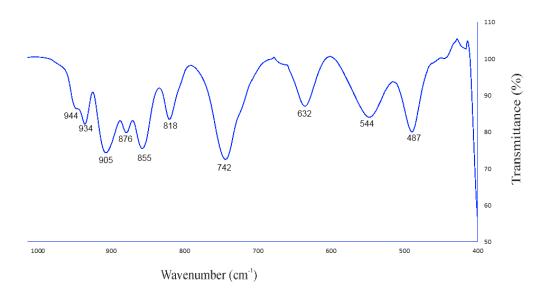


Figure 3. The IR spectra collected from mixture of 1 and 2. The phases are based on identical molecular fragments. The following bands assignment can be given: 944 cm⁻¹ and 934 cm⁻¹ are absorption bands of short tungstyl groups (W=O); 905 cm⁻¹ and 818 cm⁻¹ are v_3 and v_1 modes of UO_2^{2+} group; 876 cm⁻¹, 855 cm⁻¹ and 818 cm⁻¹ are absorption bands of W – O bonds in trigonal bipyramids VO_5 ; the bands at 632 cm⁻¹, 544 cm⁻¹ and 487 cm⁻¹ are vibrations of W – O – U bonds.