

From 2D Layers to 3D Frameworks: Expanding the Structural Diversity of Uranyl Compounds by Cation-Cation Interactions

Bin Xiao^{†,‡}, Hartmut Schlenz[†], Jakob Dellen[†], Dirk Bosbach[†], Evgeny V. Suleimanov[§], and Evgeny V. Alekseev^{†,‡,*}

[†]Institute of Energy and Climate Research (IEK-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

[‡]Institut für Kristallographie, RWTH Aachen University, 52066 Aachen, Germany

[§]Department of Chemistry, Lobachevsky State University of Nizhny Novgorod, 603950, Nizhny Novgorod, Russia

*contact E-Mail: e.alekseev@fz-juelich.de

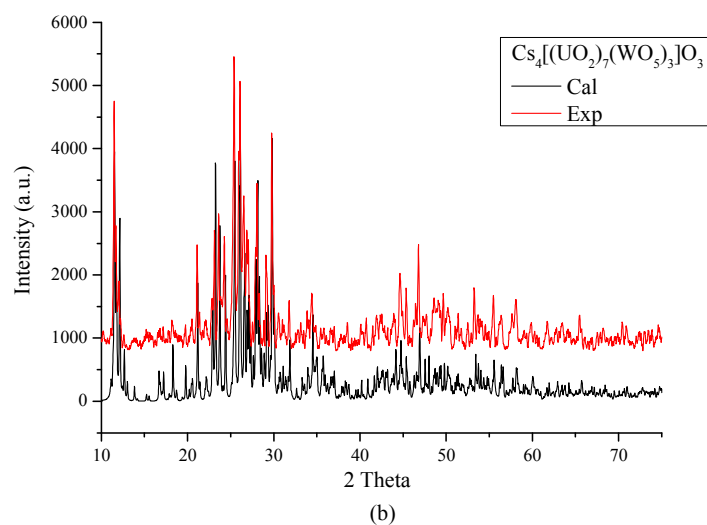
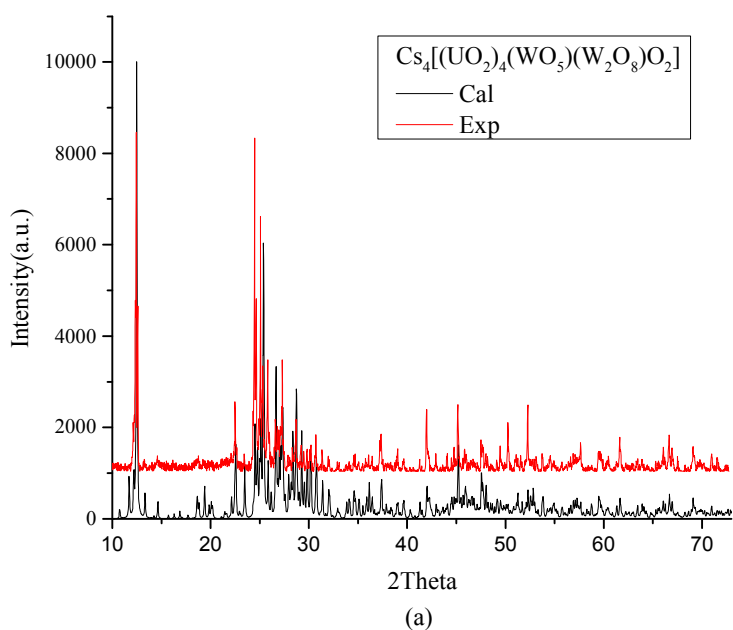


Figure SI1. Comparison between experimental and theoretical powder X-ray for (a) $\text{Cs}_4[(\text{UO}_2)_4(\text{WO}_5)(\text{W}_2\text{O}_8)\text{O}_2]$ (CsUW-1) and (b) $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$ (CsUW-2), respectively.

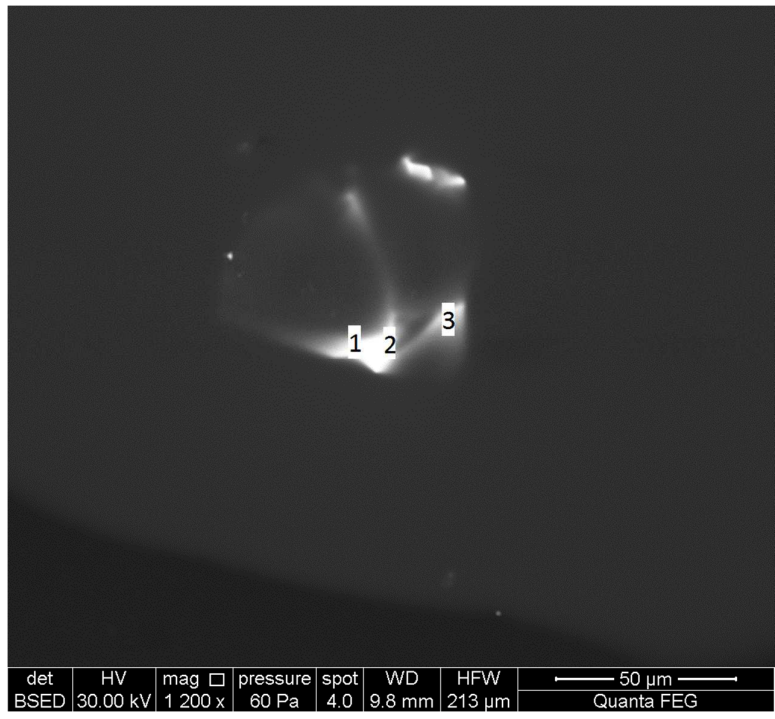


Figure SI2 (a). SEM spectra of Cs₄[(UO₂)₄(WO₅)(W₂O₈)O₂].

Table SI2 (a). EDS results for Cs₄[(UO₂)₄(WO₅)(W₂O₈)O₂] (U is set to 1).

Point	Cs	U	W
1	1.1	1.0	0.77
2	1.2	1.0	0.87
3	0.9	1.0	0.72
Mean	1.1	1.0	0.79

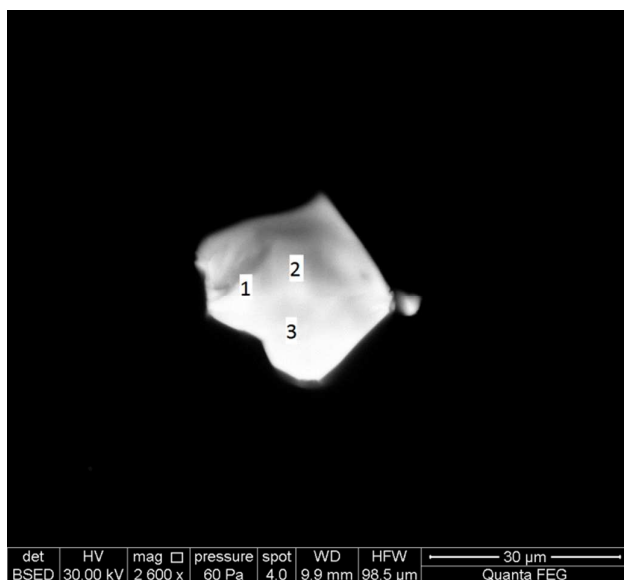


Figure SI2 (b). SEM spectra of $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$.

Table SI2 (b). EDS results for $\text{Cs}_4[(\text{UO}_2)_7(\text{WO}_5)_3\text{O}_3]$ (U is set to 1).

Point	Cs	U	W
1	0.55	1.0	0.45
2	0.65	1.0	0.57
3	0.52	1.0	0.32
Mean	0.57	1.0	0.45

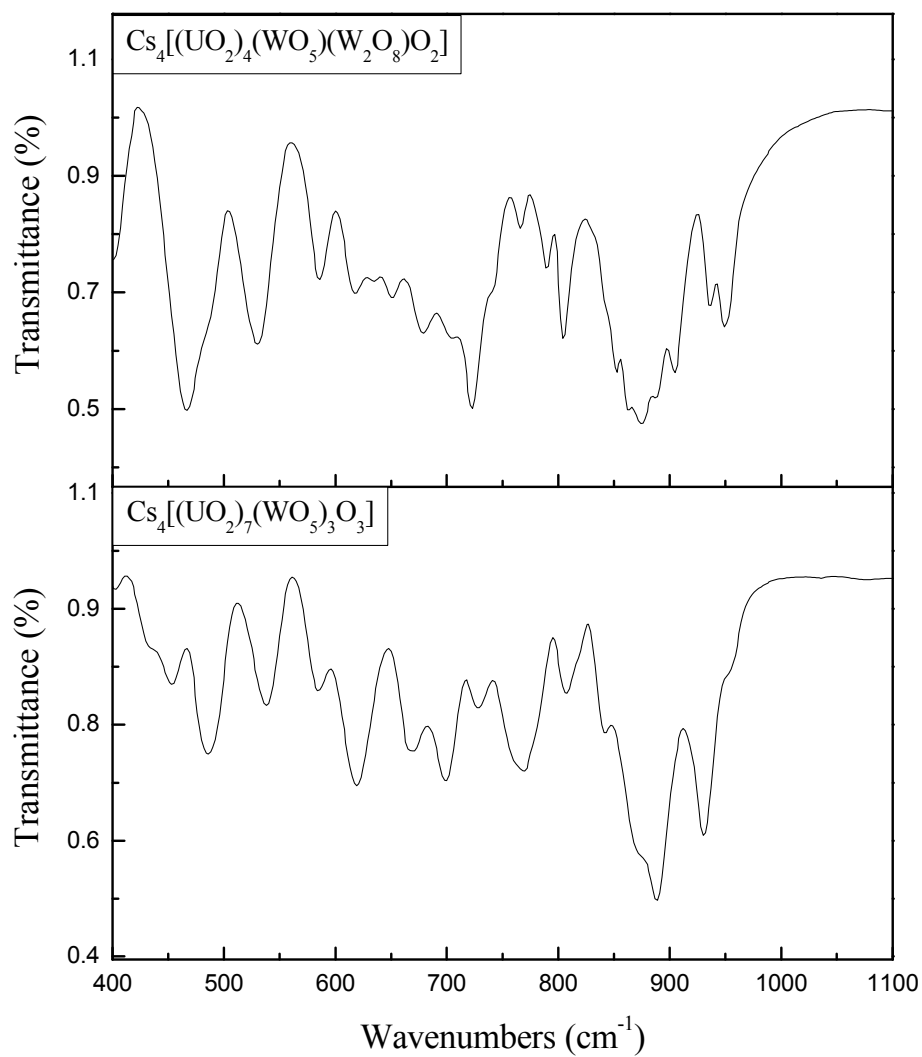


Figure SI3. IR spectra for Cs₄[(UO₂)₄(WO₅)(W₂O₈)O₂] (**CsUW-1**) and Cs₄[(UO₂)₇(WO₅)₃O₃] (**CsUW-2**), respectively