Probing Hydrogen and Halogen-Oxo Interactions in Uranyl Coordination Polymers: A Combined Crystallographic and Computational Study

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I. Additional Figures

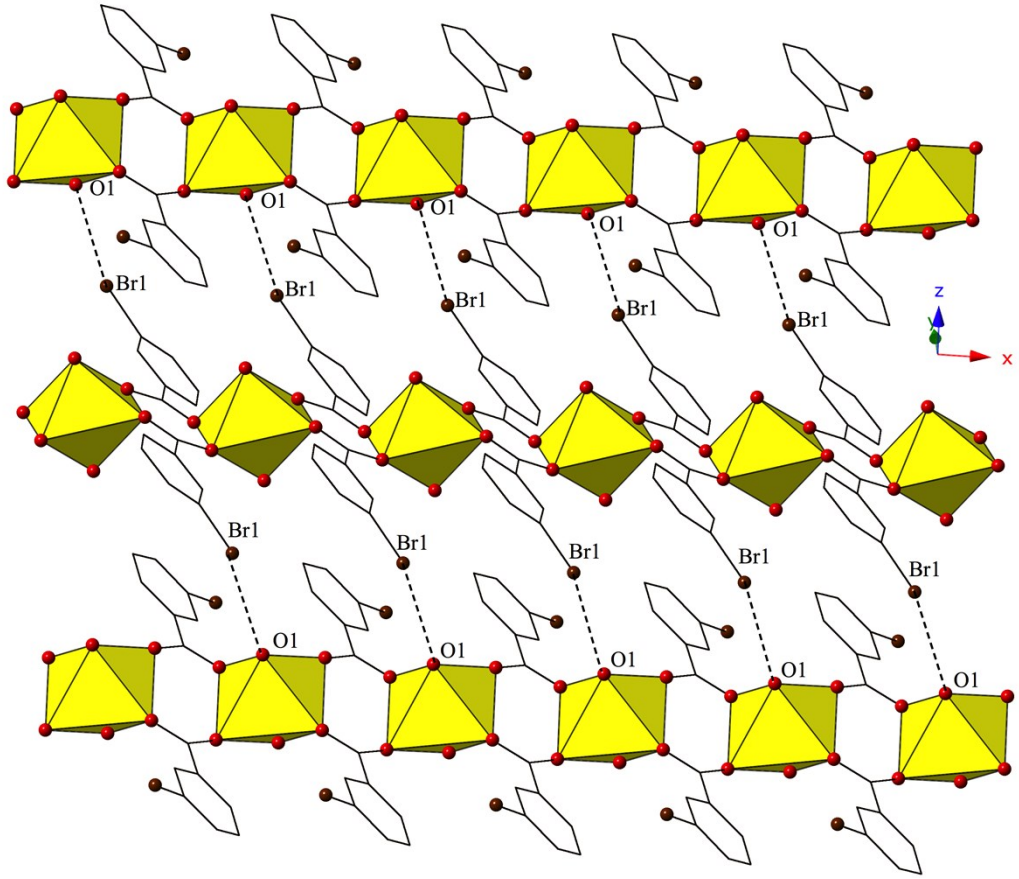

Figure S1 Compound **3** viewed in the (010) plane highlighting Br-O halogen-oxo interactions that assemble chains of **3** into a supramolecular 2D sheet.

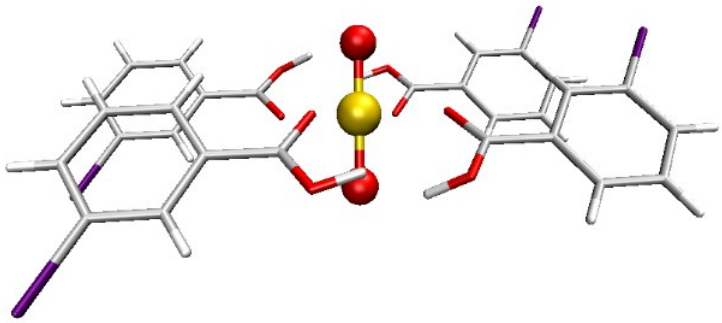

Figure S2 $[UO_2(C_7H_5XO_2)_4]^{2+}$ model, with Hal-oxo interactions removed.

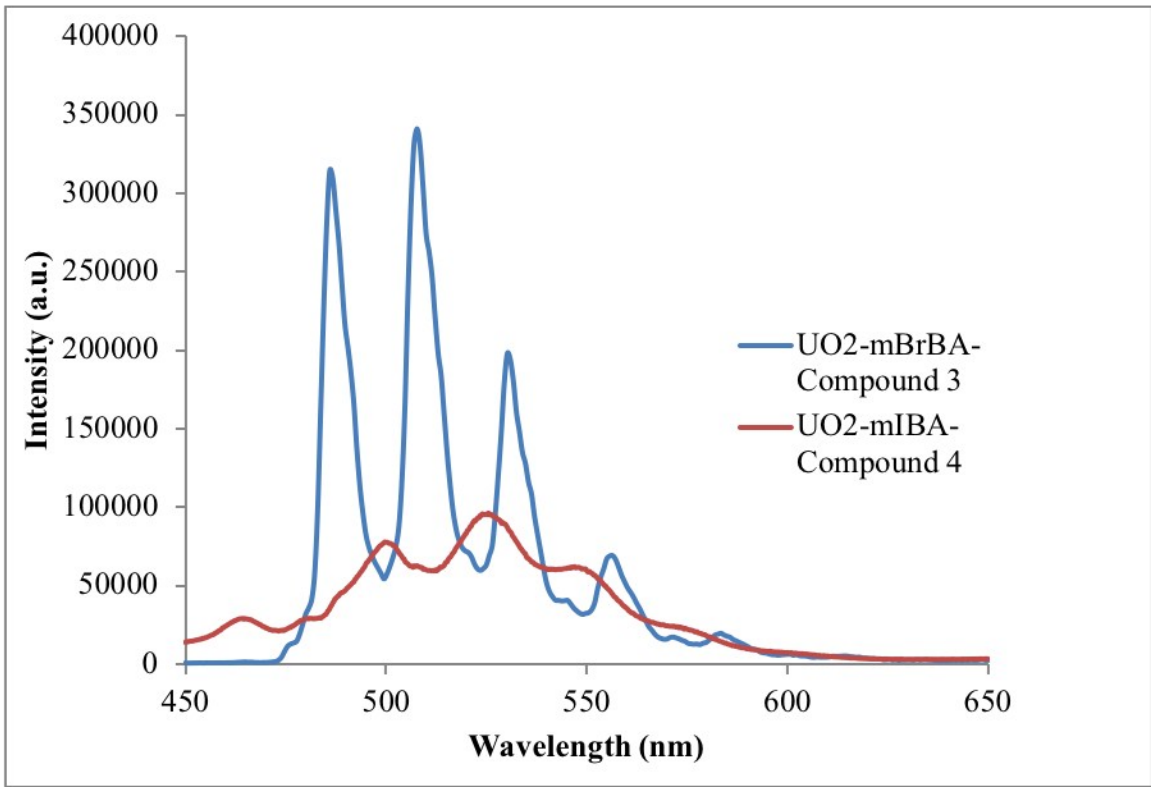

Figure S3 Room temperature, solid-state emission spectra of UO_2-*m*-BrBA compound **3** (blue) and UO_2-*m*-IBA compound **4** (red).

II. Additional DFT Data

Table S1 Comparison of bond lengths in presence and absence of Hal-oxo interactions. All values are in Å.

	Hal=Br				**Hal=I**			
	PBE0		**B3LYP**		**PBE0**		**B3LYP**	
	Hal-oxo	**No Hal-oxo**	**Hal-oxo**	**No Hal-oxo**	**Hal-oxo**	**No Hal-oxo**	**Hal-oxo**	**No Hal-oxo**
U-oxo	1.746	1.746	1.767	1.768	1.748	1.747	1.769	1.770
U-O_{eq}	2.311	2.310	2.315	2.315	2.313	2.310	2.314	2.315

III. Powder X-ray Diffraction Data

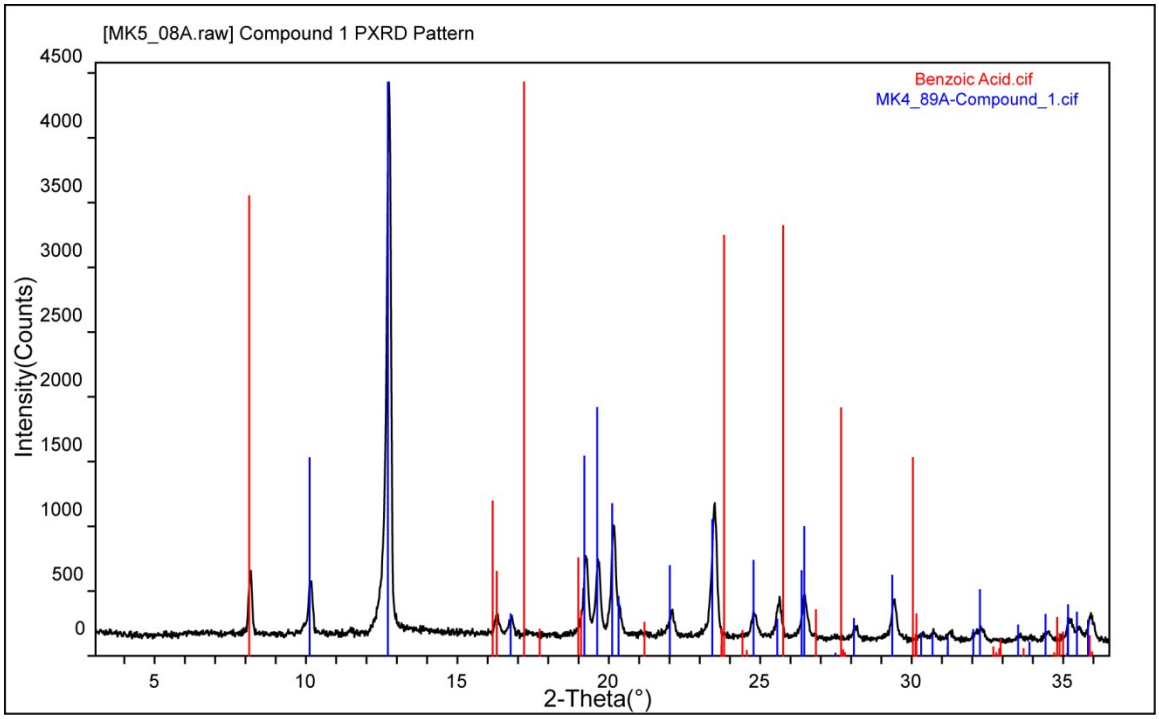

Figure S4 The observed PXRD pattern of compound **1** with calculated pattern overlaid in red. We acknowledge an impurity in the bulk product, which has been identified as benzoic acid (calculated CIF overlaid in blue).

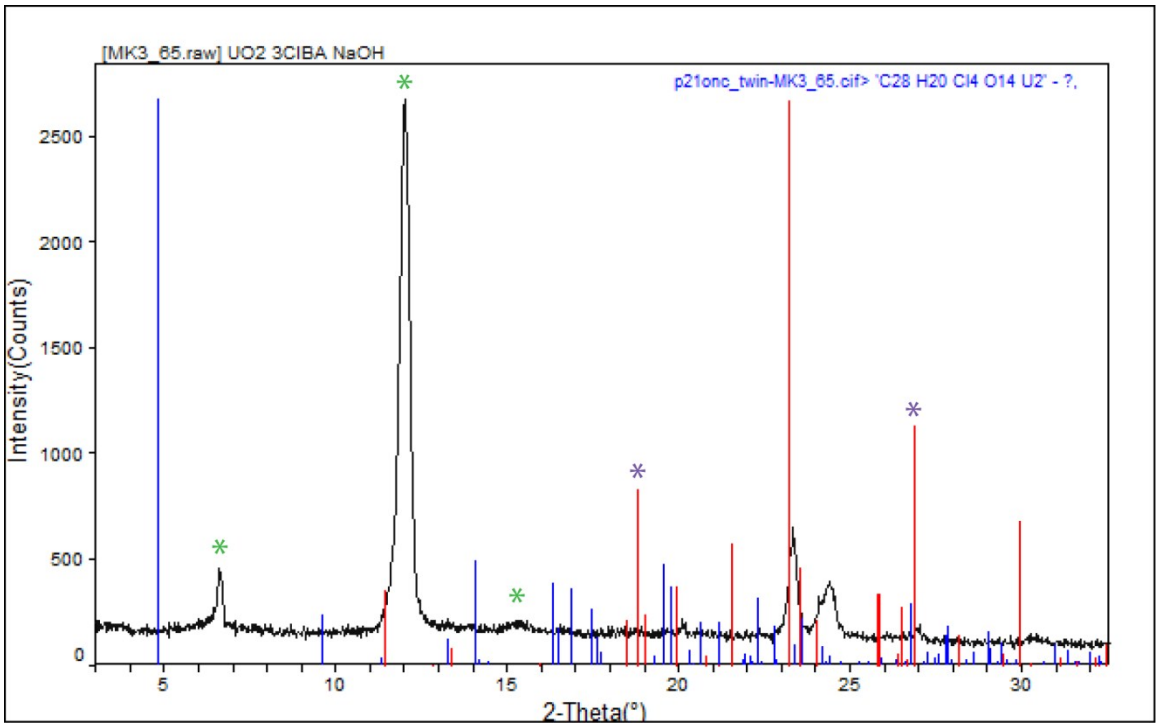

Figure S5 The observed PXRD pattern of compound **2** with calculated pattern overlaid in blue. We acknowledge that the calculated CIF is a poor match with the bulk product, yet single crystals of **2** were the only crystalline product we were able to isolate over multiple trials. Some of the additional peaks in the pattern of **2** have been identified as *m*-chlorobenzoic acid (calculated CIF overlaid in red) and these are indicated with purple asterisks. Impurities that could not be identified at 6 and 15 degrees 2-theta are noted with green asterisks.

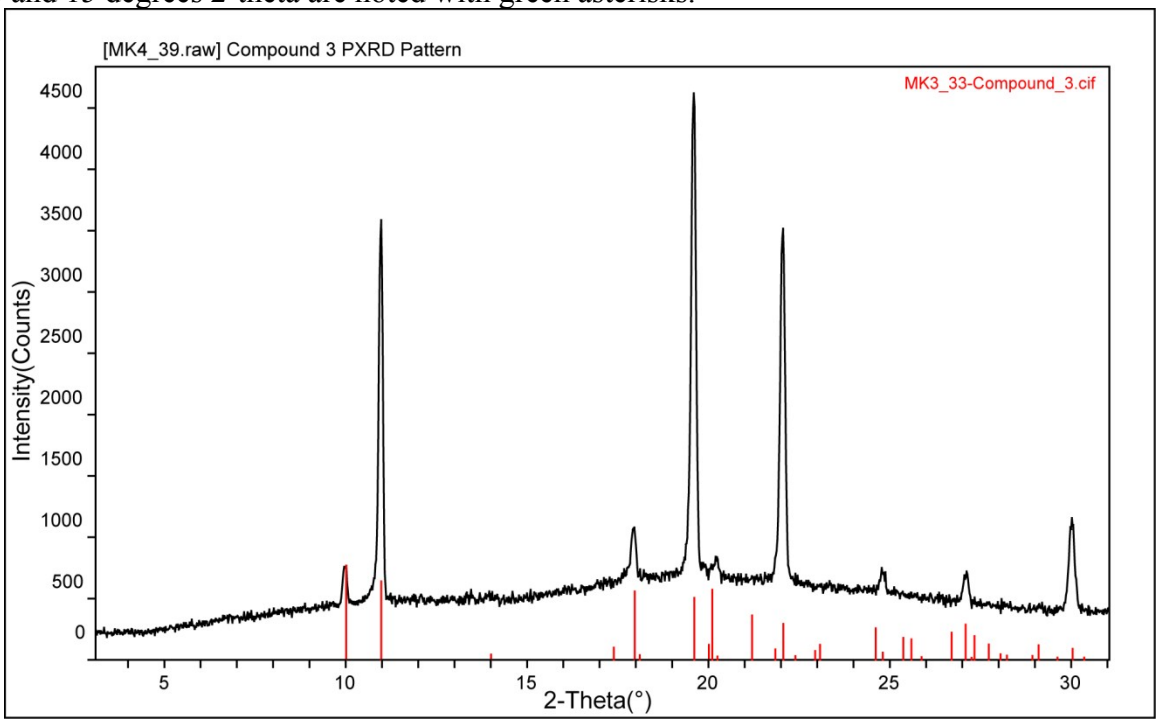

Figure S6 The observed PXRD pattern of compound **3** with calculated pattern overlaid in red.

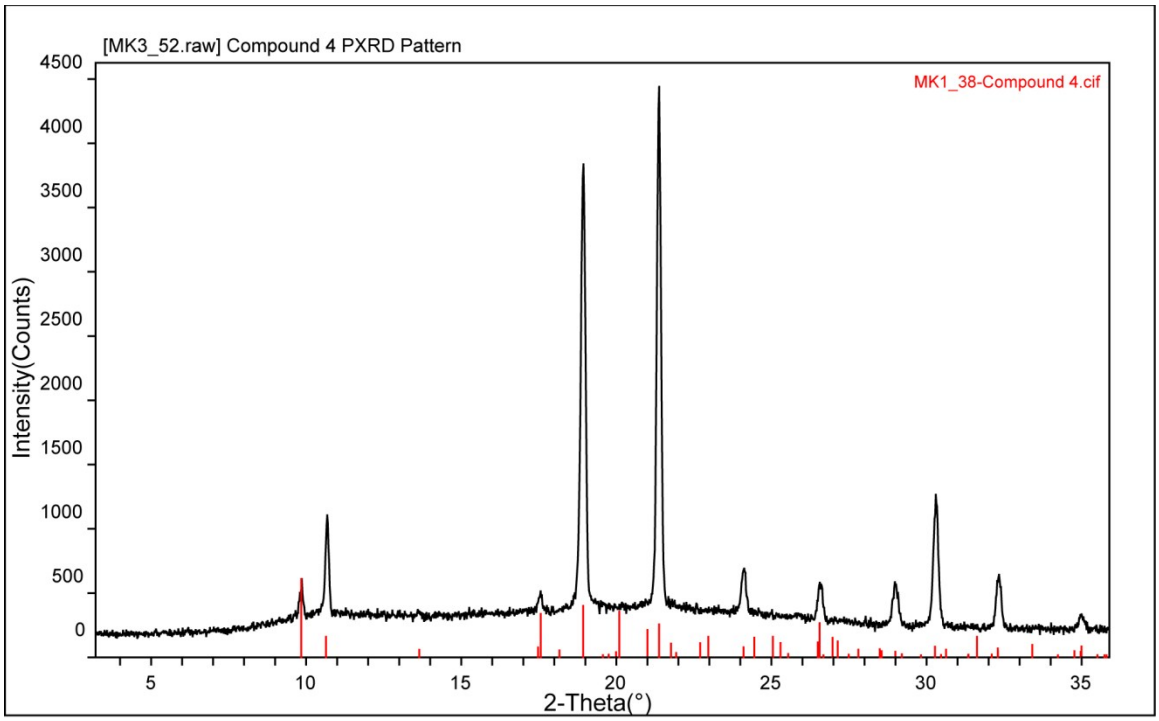

Figure S7 The observed PXRD pattern of compound **4** with calculated pattern overlaid in red.

IV. Thermal Ellipsoid Plots

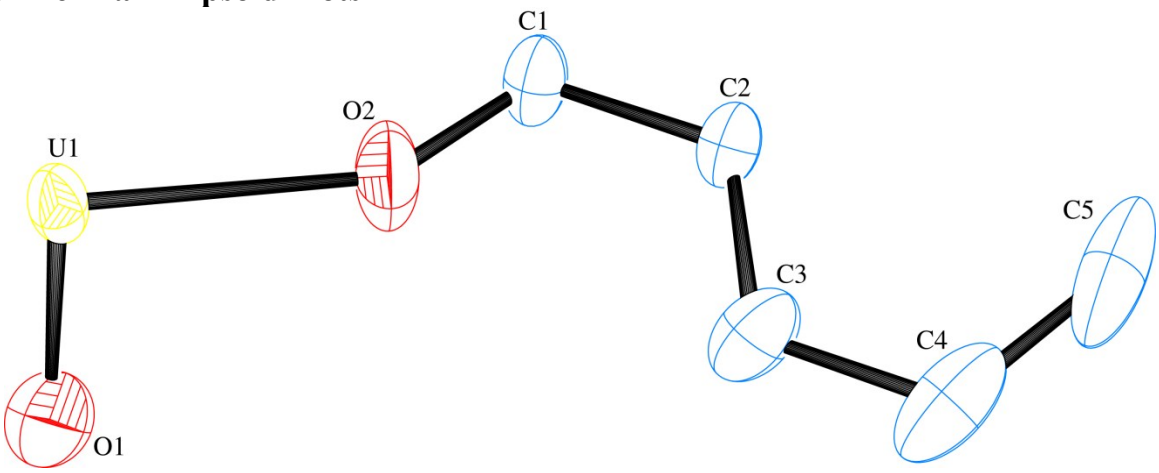

Figure S8 ORTEP illustration of compound **1**. Ellipsoids are shown at 50% probability level.

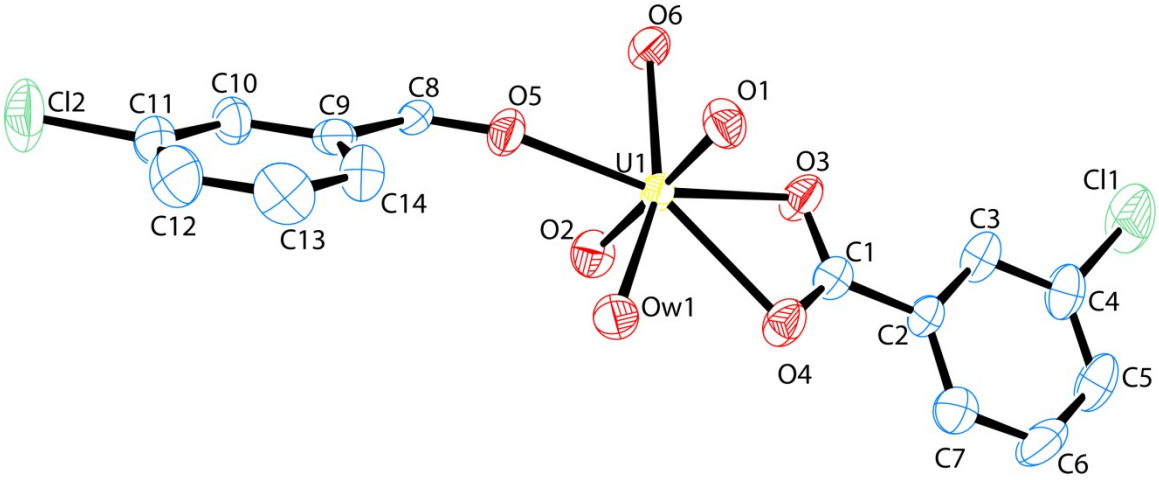

Figure S9 ORTEP illustration of compound **2**. Ellipsoids are shown at 50% probability level.

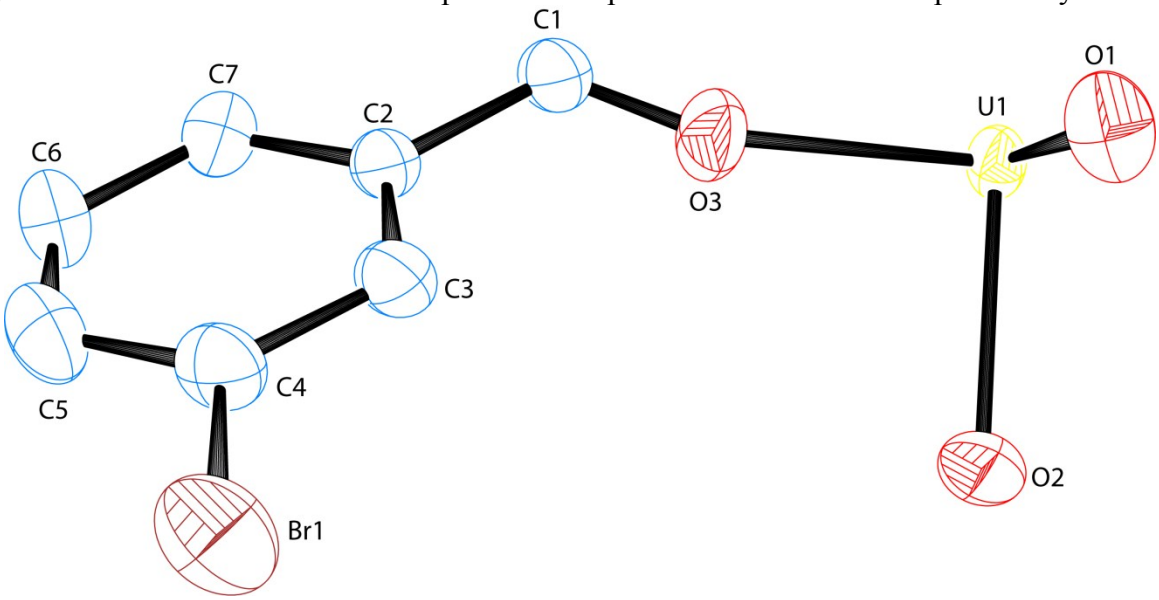

Figure S10 ORTEP illustration of compound **3**. Ellipsoids are shown at 50% probability level.

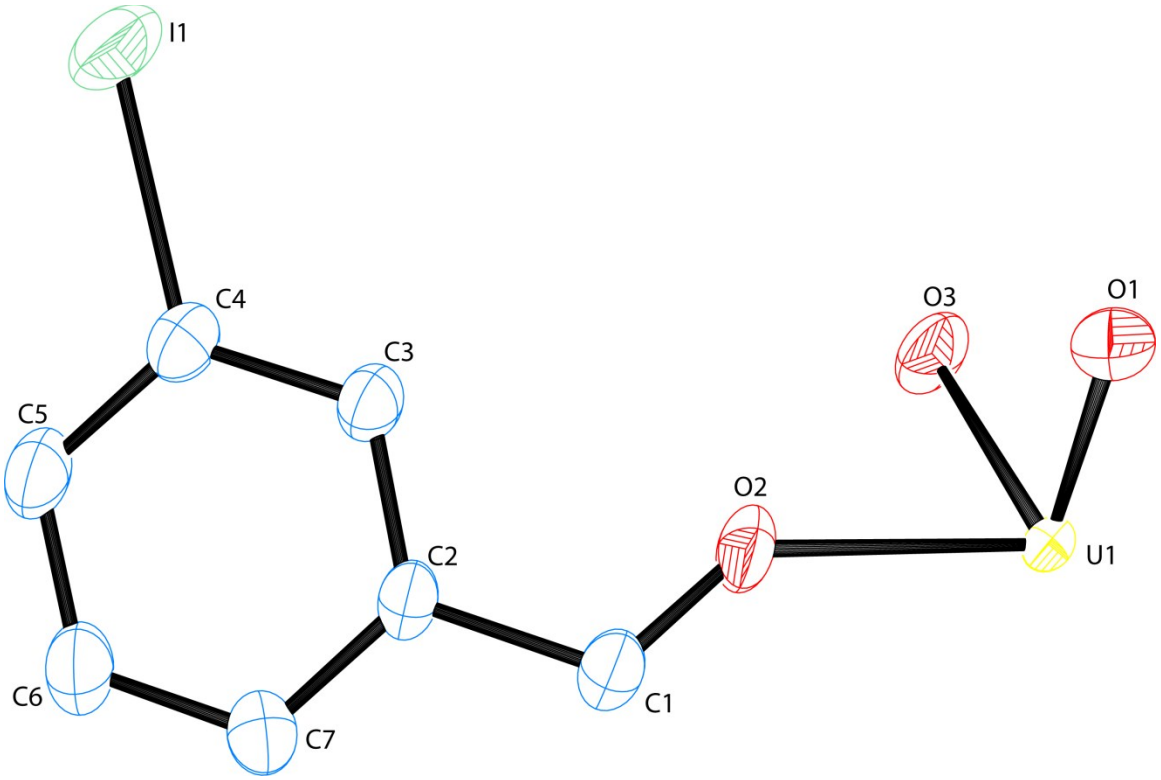

Figure S11 ORTEP illustration of compound **4**. Ellipsoids are shown at 50% probability level.

V. Tables of Bond Distances

Table S2 U-O Axial Bond Lengths in UO_2^{2+} compounds (**1-4)**

Compound	d_{U1-O1} [Å]	d_{U1-O2} [Å]
1	1.748(4)	
2	1.762(3)	1.761(3)
3	1.743(3)	
4	1.764(3)	

Table S3 U-O Equatorial Bond Lengths in UO_2^{2+} compounds (**1-4**)

Compound	d_{U1-O2} [Å]	d_{U1-O3} [Å]	d_{U1-O4} [Å]	d_{U1-O5} [Å]	d_{U1-O6} [Å]	d_{U1-OW1} [Å]
1	2.297(3)					
2		2.391(3)	2.446(3)	2.328(3)	2.328(3)	2.477(3)
3	2.286(3)	2.312(3)				
4	2.316(3)	2.288(3)				