Supporting Information

Use of zwitterionic ligands in uranyl hybrid materials: Explorations on the structural features that control water ordering and mobility

Maurice K. Payne, Rebecca C. Laird, Margaret A. Schnell, Samantha R. Mackin, and Tori Z. Forbes*

Department of Chemistry, University of Iowa, Iowa City, IA 52242
**corresponding author: tori-forbes@uiowa.edu*

Additional crystallographic information

Table S1. Select bond distances (Å) and angles (°) for **UIM-5**.

U1-O1'	1.774(2)
U1-O2'	1.775(2)
U1-O1	2.455(3)
U1-O2	2.376(3)
U1-O3	2.347(3)
U1-O4	2.316(3)
U1-O5	2.372(3)
O1'-U1-O2'	179.29(11)

Table S2. Select bond distances (Å) and angles (°) for **UIM-2A**.

U1-O1'	1.7804(19)
U1-O2'	1.7670(19)
U1-O1	2.4903(18)
U1-O2	2.5147(18)
U1-O3	2.3272(18)
U1-O4	2.3277(18)
U1-O5	2.2900(18)
O1'-U1-O2'	179.25(8)

Table S3. Select bond distances (Å) and angles (°) for **UIM-2B**.

U1-O1'	1.775(3)
U1-O2'	1.778(3)
U1-O1	2.327(3)
U1-O2	2.492(3)
U1-O3	2.478(3)
U1-O4	2.273(3)
U1-O5	2.346(3)
O1'-U1-O2'	176.81(12)

Table S4. Select bond distances (Å) and angles (°) for **UIM-2C**.

U1-O1’	1.7820(19)
U1-O2’	1.7736(19)
U1-O1	2.538(2)
U1-O2	2.4754(18)
U1-O3	2.3244(18)
U1-O4	2.294(2)
U1-O5	2.3705(19)
O1’-U1-O2’	176.78(9)

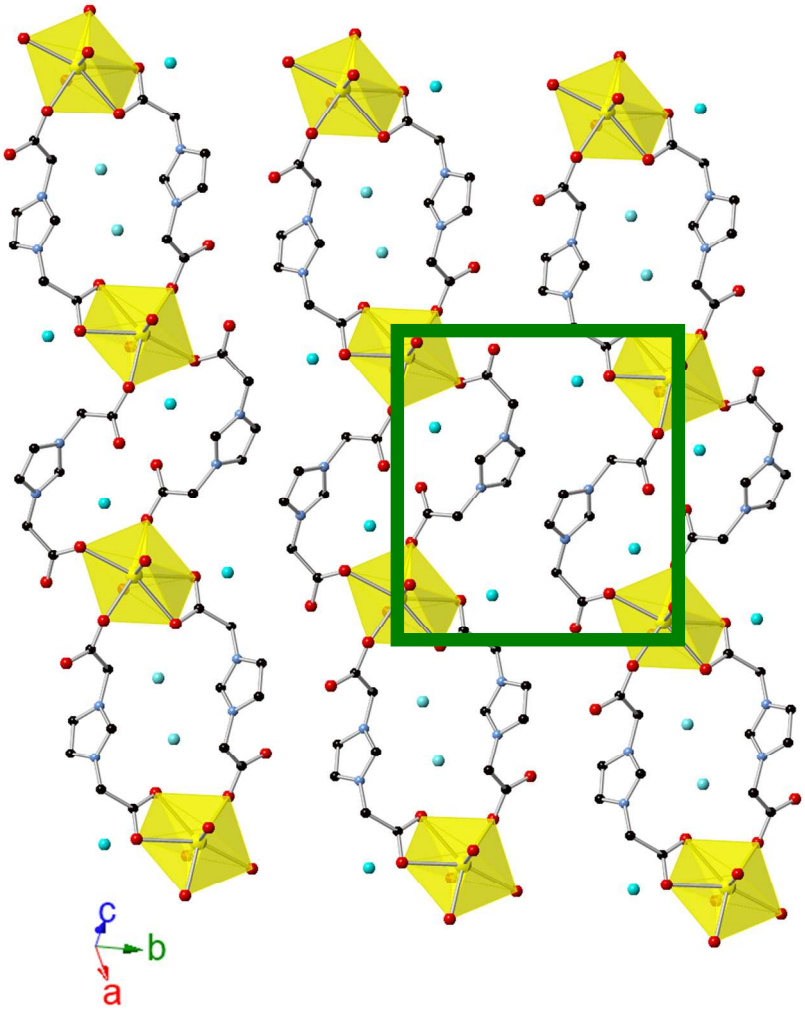

Figure S1. Extended lattice for **UIM-2A** with dominant π-π interaction highlighted with the green square. U represented by yellow polyhedra, whereas the O, C, and N atoms are depicted as red, black and light blue spheres. H atoms and lattice water molecules omitted for clarity.

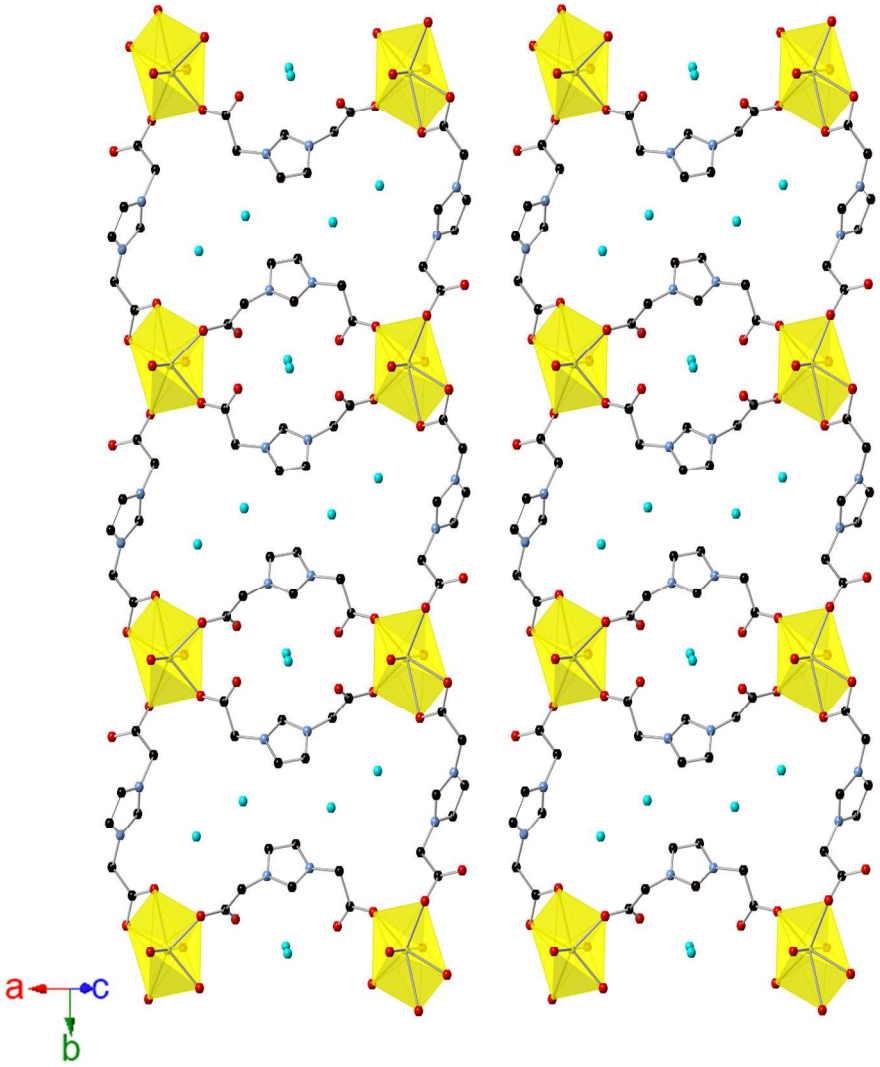

Figure S2. Extended lattice for **UIM-2B**. U represented by yellow polyhedra, whereas the O, C, and N atoms are depicted as red, black and light blue spheres. H atoms and lattice water molecules omitted for clarity.

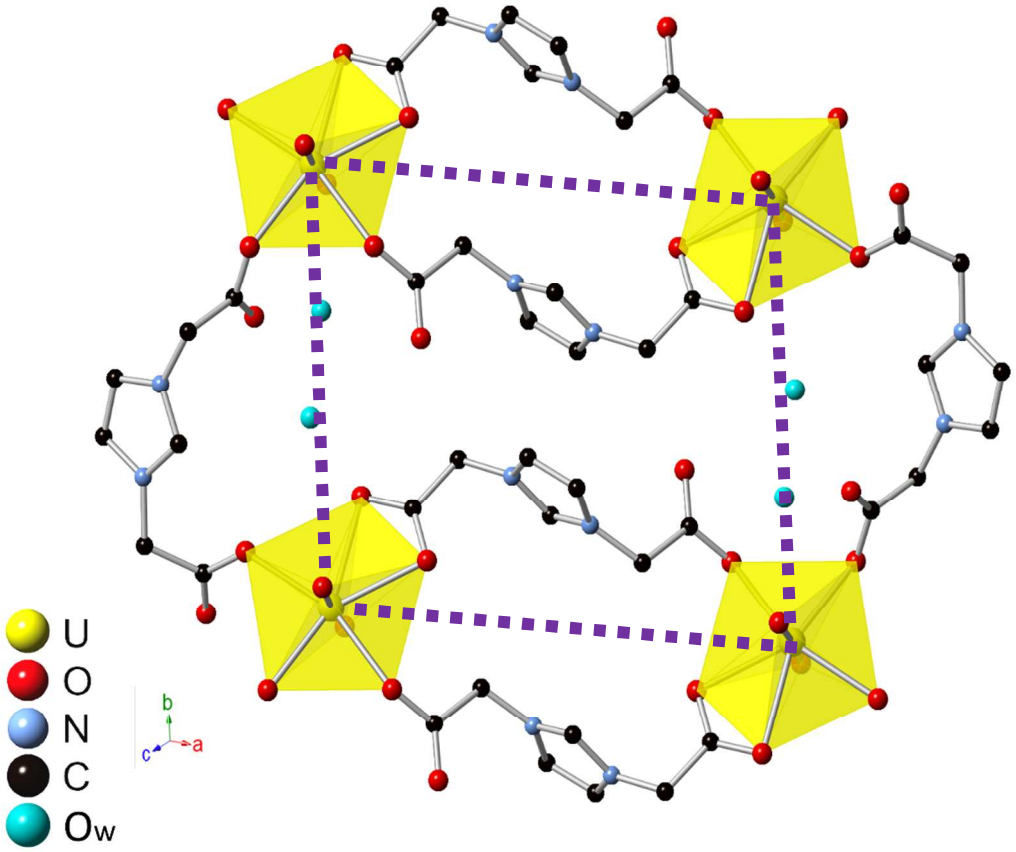

Figure S3. Extended lattice for **UIM-2C** depicting the variations in ligand binding modes. The dashed parallelogram highlights the differences in the crystal packing that leads to structural variations within the UIM-2 polymorphs. U represented by yellow polyhedra, whereas the O, C, and N atoms are depicted as red, black and light blue spheres. H atoms and lattice water molecules omitted for clarity.

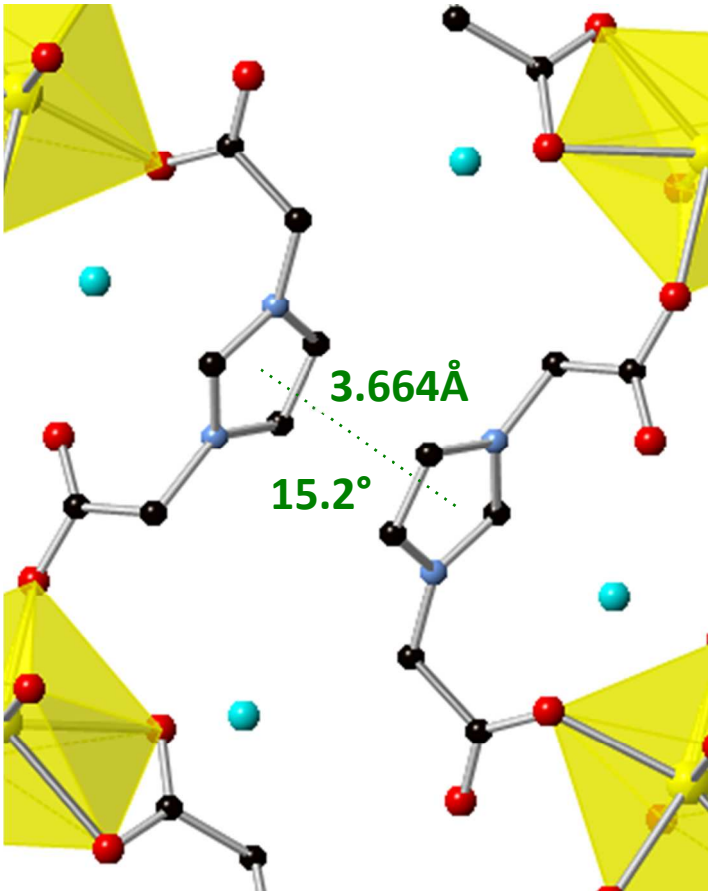

Figure S4. Representative π-π interactions for **UIM-2A** with centroid to centroid distances and interplanar angles for this interaction highlighted in green.

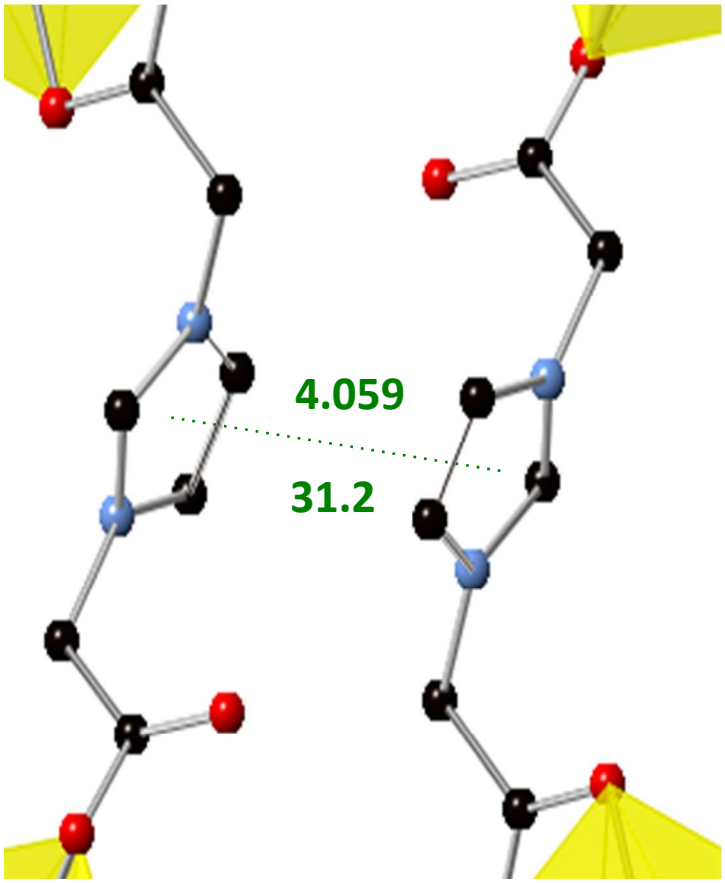

Figure S5. Representative π-π interactions for **UIM-2B** with centroid to centroid distances and interplanar angles for this interaction highlighted in green.

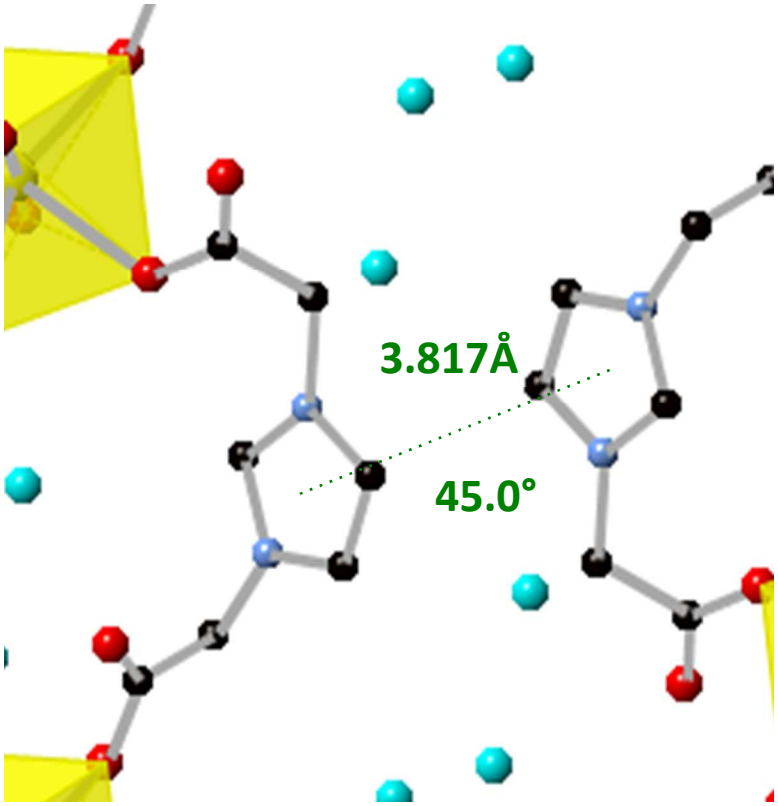

Figure S6. Representative π-π interactions for **UIM-2C** with centroid to centroid distances and interplanar angles for this interaction highlighted in green.

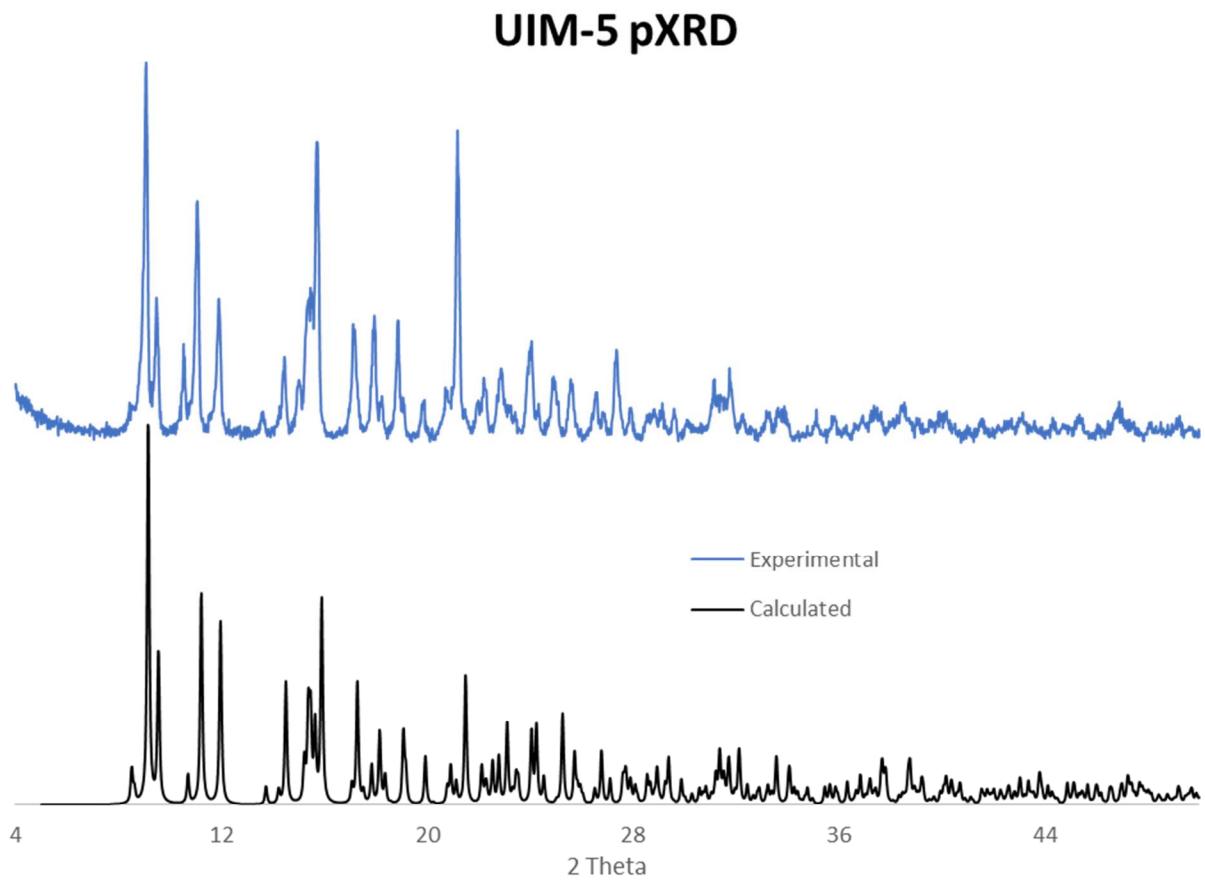

Figure S7. Experimental and calculated pXRD pattern of **UIM-5.**

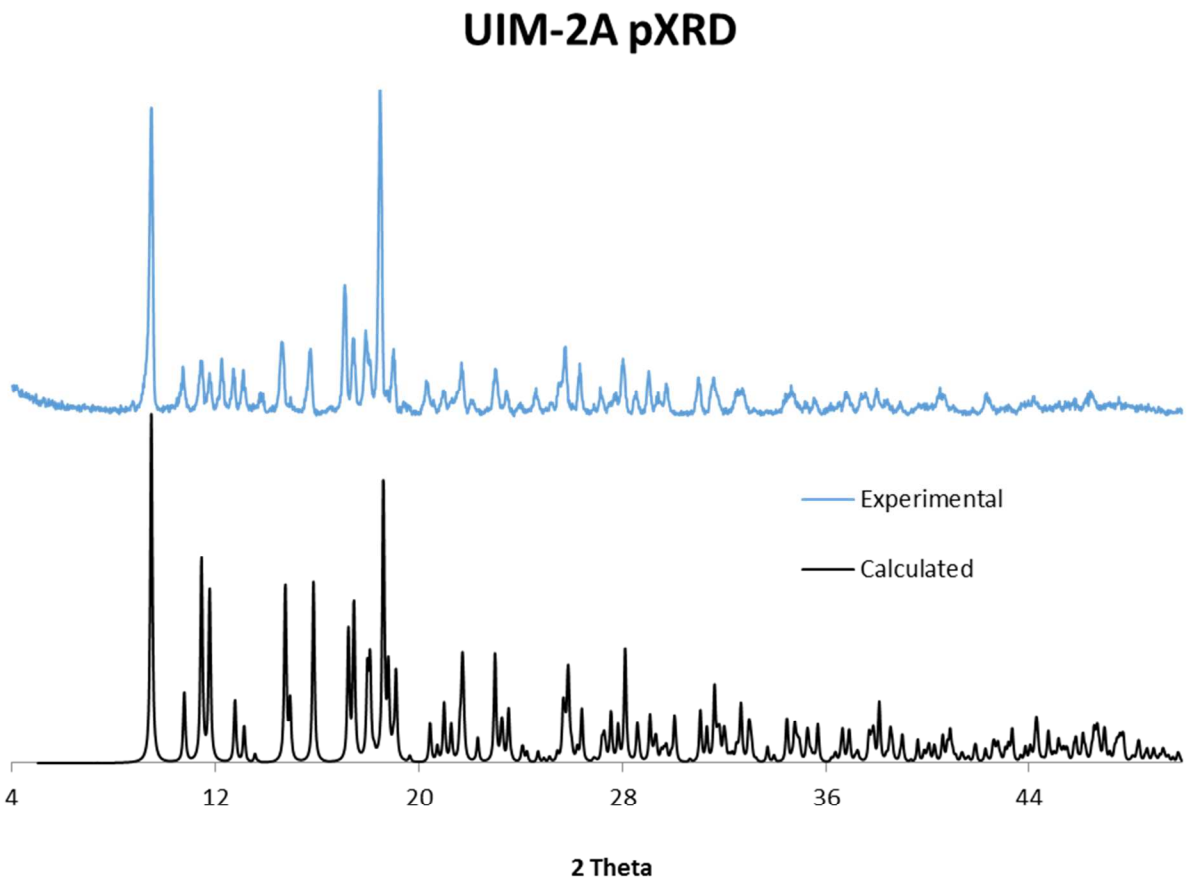

Figure S8. Experimental and calculated pXRD pattern of **UIM-2A.**

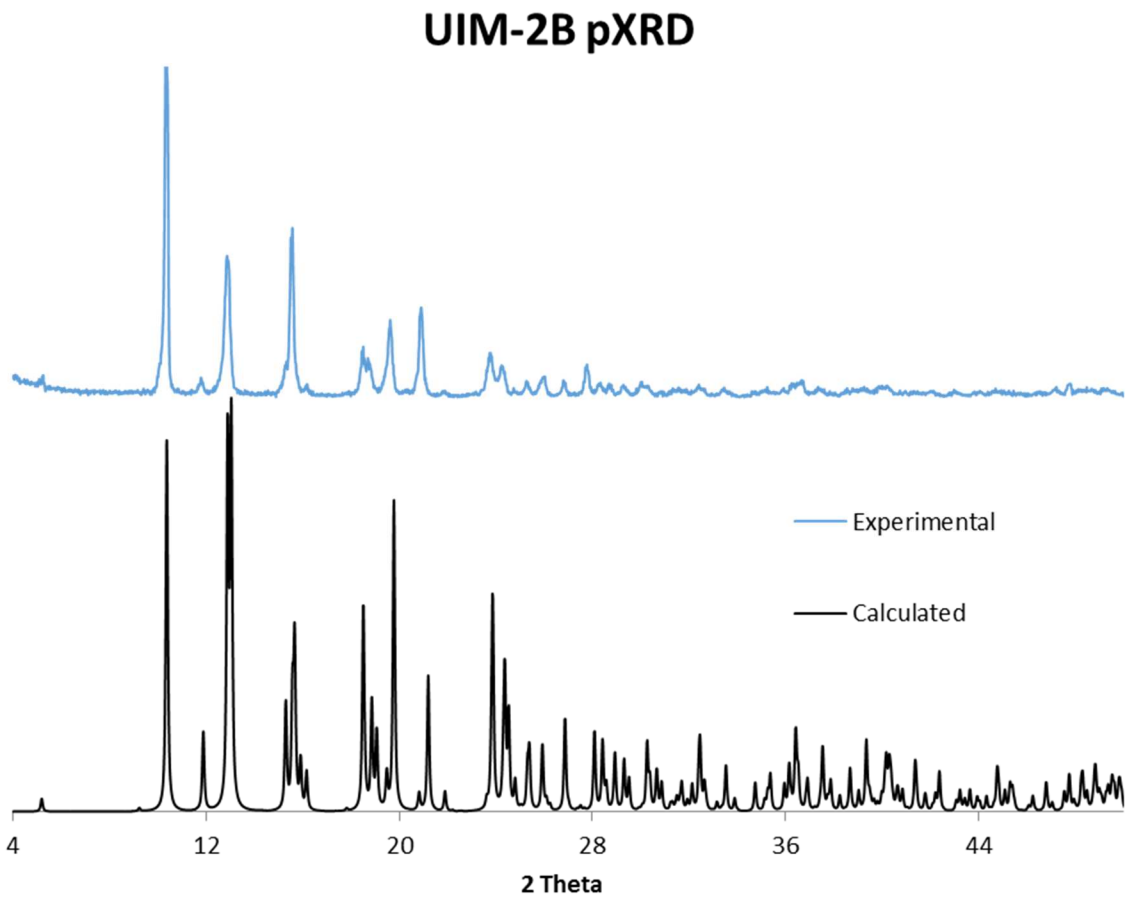

Figure S9. Experimental and calculated pXRD pattern of **UIM-2B.**

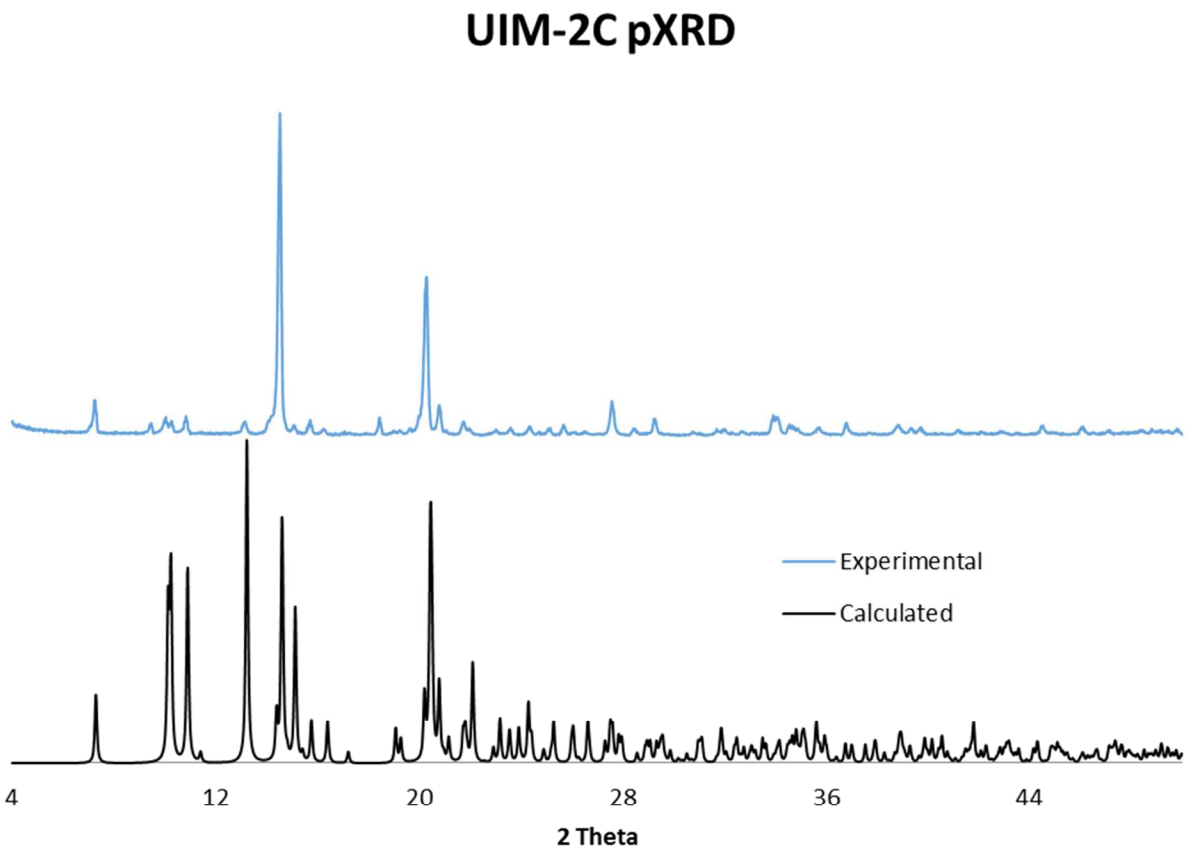

Figure S10. Experimental and calculated pXRD pattern of **UIM-2C.**

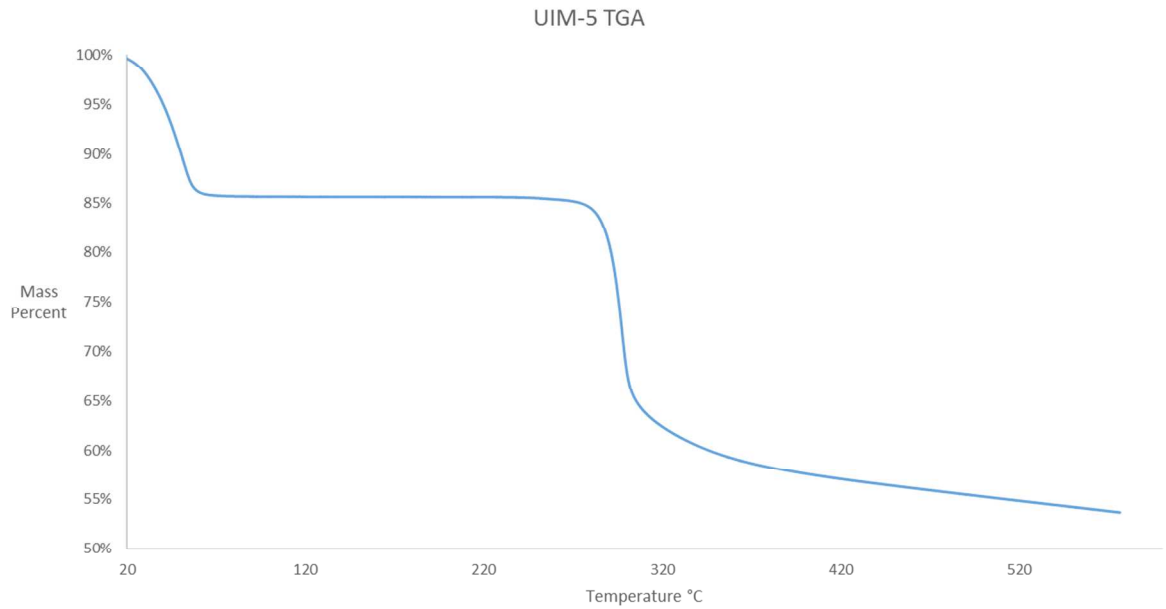

Figure S11. Thermogravimetric analysis of **UIM-5.**

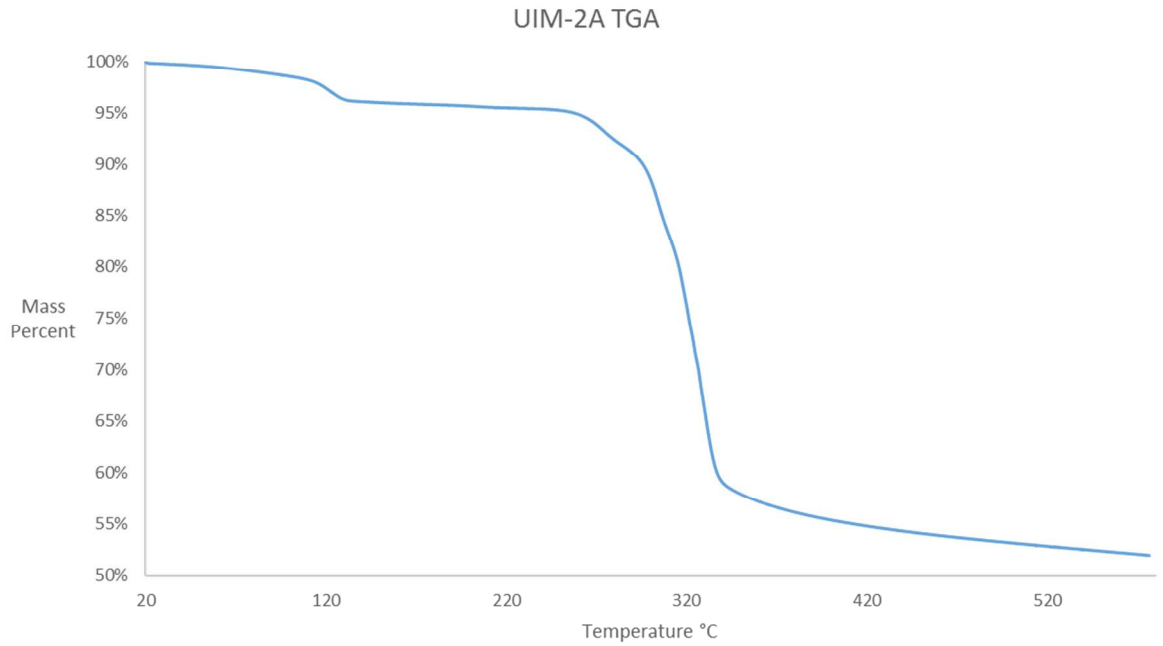

Figure S12. Thermogravimetric analysis of **UIM-2A.**

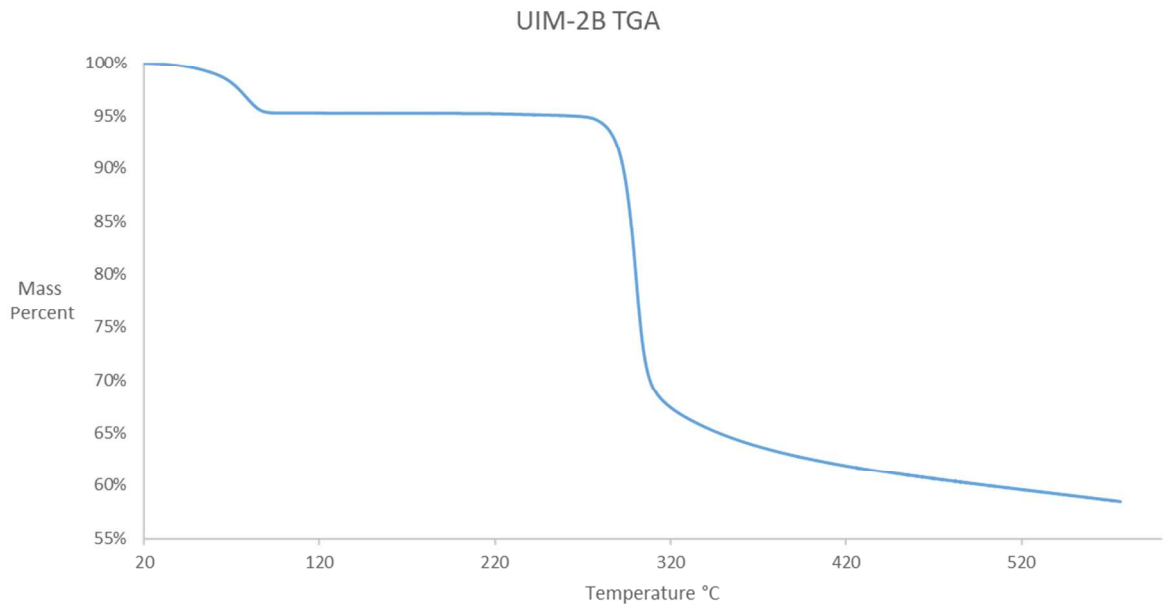

Figure S13. Thermogravimetric analysis of **UIM-2B.**

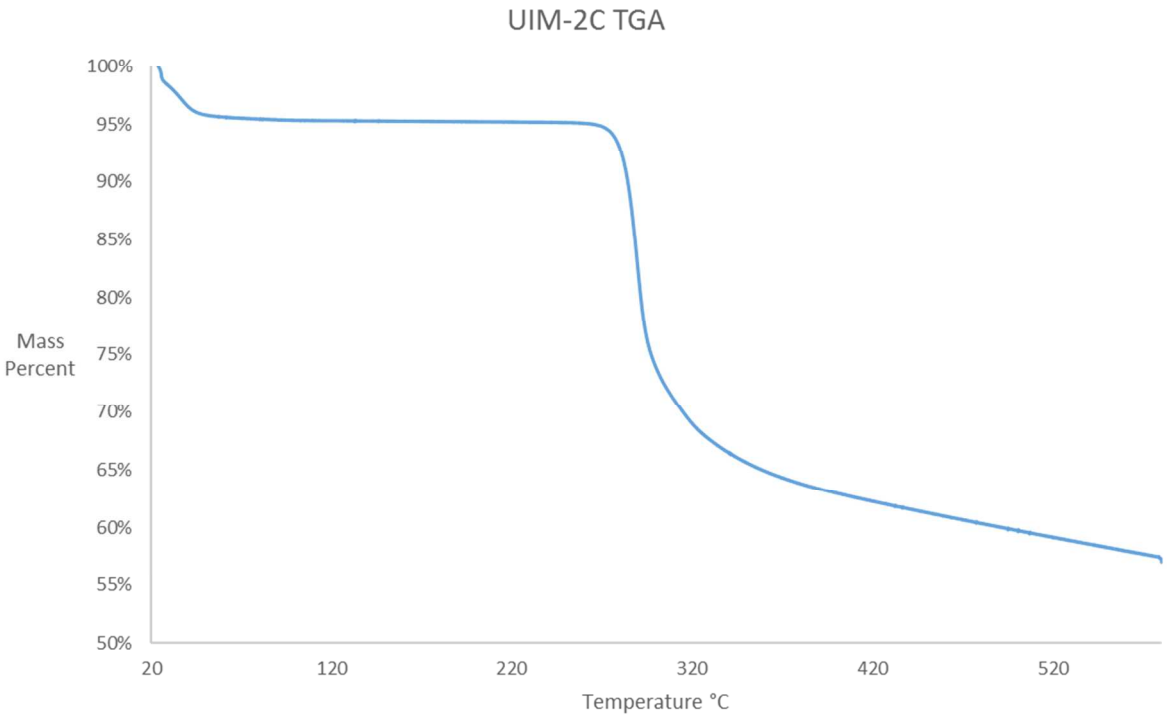

Figure S14. Thermogravimetric analysis of **UIM-2C.**

Table S5. CHN Analysis for UIM series.

Compound	C theory %	C found %	H theory %	H found %	N theory %	N found %
UIM-5	22.59	22.53 ± 0.14	3.52	3.39 ± 0.044	7.53	7.52 ± 0.045
UIM-2A	25.01	24.75 ± 0.24	2.70	2.52 ± 0.042	8.33	7.17 ± 0.31
UIM-2B	25.01	25.33 ± 0.028	2.70	2.40 ± 0.061	8.33	8.19 ± 0.42
UIM-2C	25.01	25.79 ± 0.075	2.70	2.13 ± 0.071	8.33	8.52 ± 0.023
UIM-0	26.43	24.67 ± 0.061	2.22	2.68 ± 0.017	8.81	8.40 ± 0.28

Table S6. Comparing vibrational spectroscopies to uranyl bond length. [a]

	Raman		**Experimental Uranyl Bonds**			**Infrared**	
Compound	ν_1 (sym)	Calc U-O distance (Å)	U1-O1'	U1-O2'	Average	ν_3 (asym)	Calc U-O distance (Å)
UIM-5	835	1.776	1.774	1.775	1.775	906	1.780
UIM-2A	834	1.777	1.7804	1.767	1.774	908	1.779
UIM-2B	834	1.777	1.775	1.778	1.777	912	1.776
UIM-2C	830	1.781	1.782	1.7736	1.778	910	1.777
UIM-0	832	1.779	1.771	1.786	1.779	906	1.780

a. Bartlett, J.R., Cooney, R.P., *J. Mol. Struct.,* **1989,** 193, 295