Supporting information

Uranyl Carboxyphosphonates derived from Hydrothermal in situ Ligand Reaction: Syntheses, Structures and Computational Investigations

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Table S1. Selected bond lengths (Å) and angles (°) for uranyl carboxyphosphonates **DPTP-U1**, **DPTP-U2** and **DPTP** ligand.

DPTP-U1		**DPTP-U2**		**DPTP**	
U(1)-O(1)	1.757(5)	U(1)-O(1)	1.780(11)	P(1)-O(1)	1.5444(18)
U(1)-O(2)	1.767(5)	U(1)-O(2)	1.781(12)	P(1)-O(2)	1.4875(16)
U(1)-O(6)	2.264(5)	U(1)-O(6)	2.246(11)	P(1)-O(3)	1.5255(16)
U(1)-O(5)#1	2.302(5)	U(1)-O(8)	2.364(11)	P(1)-C(1)	1.815(2)
U(1)-O(9)#2	2.359(5)	U(1)-O(12)#1	2.365(10)	C(4)-O(4)	1.315(3)
U(1)-O(10)#1	2.436(6)	U(1)-O(11)#2	2.466(10)	C(4)-O(5)	1.184(3)
U(1)-O(1W)	2.506(6)	U(1)-O(12)#2	2.597(11)	C(1)-C(2)	1.396(3)
U(2)-O(3)	1.761(5)	U(2)-O(3)	1.754(12)	C(1)-C(3)	1.398(3)
U(2)-O(3)#3	1.761(5)	U(2)-O(4)	1.761(11)	C(2)-C(3)#1	1.390(3)
U(2)-O(4)#3	2.307(5)	U(2)-O(5)	2.292(10)	C(3)-C(2)#1	1.390(3)
U(2)-O(4)	2.307(5)	U(2)-O(7)#3	2.305(10)	C(3)-C(4)	1.513(3)
U(2)-O(8)#2	2.335(5)	U(2)-O(10)#4	2.326(11)		
U(2)-O(8)#4	2.336(5)	U(2)-O(14)#4	2.499(11)	O(2)-P(1)-O(3)	113.57(10)
		U(2)-O(1W)	2.505(12)	O(2)-P(1)-O(1)	112.63(10)
P(1)-O(6)	1.508(6)	P(1)-O(5)	1.509(11)	O(3)-P(1)-O(1)	107.93(10)
P(1)-O(5)	1.516(5)	P(1)-O(6)	1.525(11)	O(2)-P(1)-C(1)	108.95(10)
P(1)-O(4)	1.523(5)	P(1)-O(7)	1.527(10)	O(3)-P(1)-C(1)	106.17(9)
P(1)-C(1)	1.832(7)	P(1)-C(1)	1.804(14)	O(1)-P(1)-C(1)	107.21(10)
P(2)-O(8)	1.496(6)	P(2)-O(10)	1.487(11)		
P(2)-O(9)	1.506(5)	P(2)-O(12)	1.534(11)		
P(2)-O(7)	1.558(5)	P(2)-O(11)	1.537(11)		
P(2)-C(4)	1.805(7)	P(2)-C(4)	1.789(14)		
O(1)-U(1)-O(2)	177.6(3)	O(1)-U(1)-O(2)	176.6(5)		
O(3)-U(2)-O(3)#3	179.998(1)	O(3)-U(2)-O(4)	177.8(6)		

Symmetry codes: **DPTP-U1**, #1 -x+1,-y,-z+2; #2 x,y-1,z; #3 -x+1,-y,-z+1; #4 -x+1,-y+1,-z+1. **DPTP-U2**, #1 -x+2,-y+1,-z+1; #2 x+1,y,z; #3 -x+2,-y,-z; #4 -x+2,-y+1,-z. **DPTP**, #1 -x,y,-z+1/2.

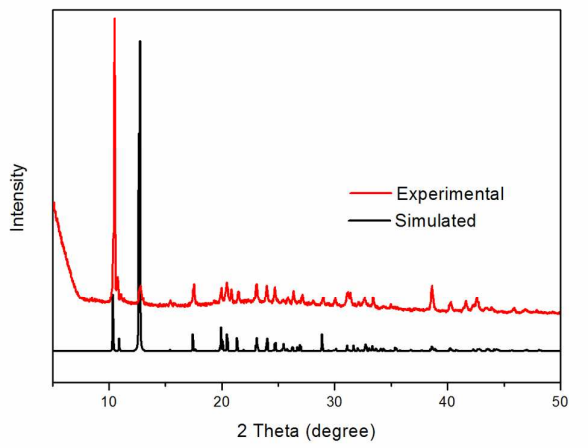

Figure S1. Simulated and experimental XRD patterns of **DPTP** ligand.

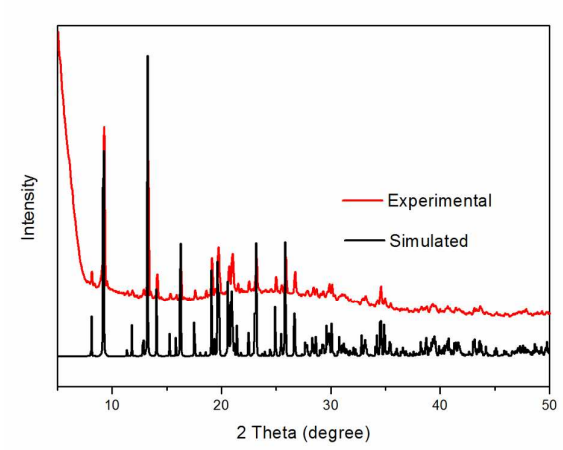

Figure S2. Simulated and experimental XRD patterns of **DPTP-U1**.

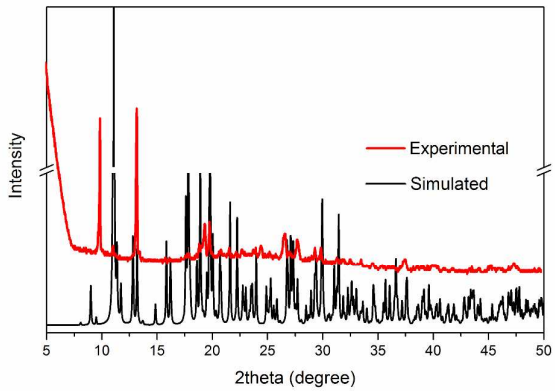

Figure S3. Simulated and experimental XRD patterns of **DPTP-U2**.

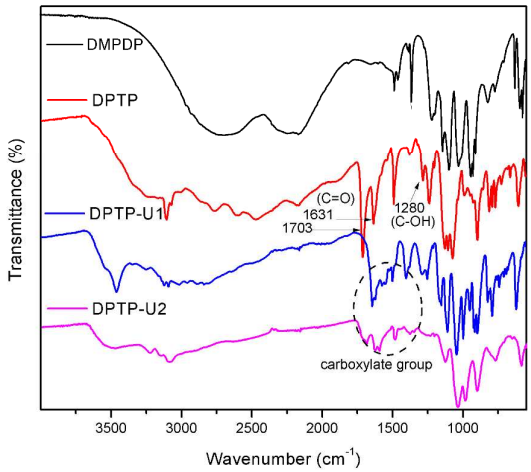

Figure S4. FT-IR spectra of DMPDP and DPTP ligands as well as **DPTP-U1** and **DPTP-U2**.

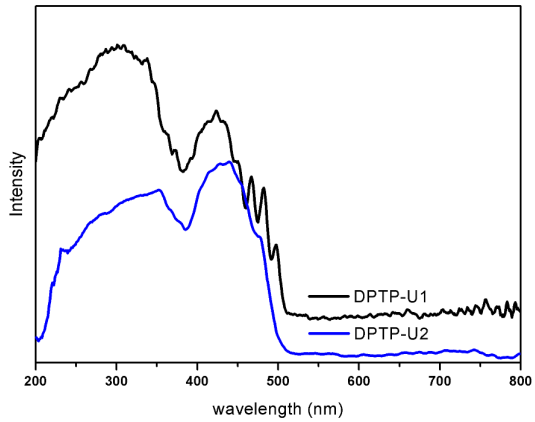

Figure S5. Solid state absorption spectra of **DPTP-U1** and **DPTP-U2**.