

# Synthesis, Structures and Properties of Uranyl Hybrids Constructed by a Variety of Mono- and Poly-Carboxylic Acids

Weiting Yang,<sup>a,†</sup> Song Dang,<sup>a,†</sup> Hao Wang,<sup>a,b</sup> Tao Tian,<sup>a</sup> Qing-Jiang Pan,<sup>c</sup> and Zhong-Ming Sun<sup>a,\*</sup>

<sup>a</sup>State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, 5625 Renmin Street, Changchun, Jilin 130022, P.R. China. <sup>b</sup>Changchun University of Science & Technology, School of Chemistry and Environmental Engineering, Changchun 130022, China. <sup>c</sup>Key Laboratory of Functional Inorganic Material Chemistry of Education Ministry, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, China.

Table S1. Selected bonds and angles for compounds **1-8**.

<b>1</b>			
U(1)-O(1)	1.756(4)	U(1)-O(5)	2.352(3)
U(1)-O(2)	1.756(4)	U(1)-O(6)	2.426(3)
U(1)-O(3)	2.444(3)	U(1)-O(7)	2.486(4)
U(1)-O(4)	2.301(3)	O(1)-U(1)-O(2)	178.48(17)
<b>2</b>			
U(1)-O(1)	1.802(7)	U(2)-O(3)	1.776(7)
U(1)-O(2)	1.779(7)	U(2)-O(4)	1.782(8)
U(1)-O(10)#2	2.516(8)	U(2)-O(8)	2.486(8)
U(1)-O(13)	2.468(7)	U(2)-O(9)	2.489(9)
U(1)-O(17)	2.469(7)	U(2)-O(11)	2.336(7)
U(1)-O(18)	2.214(7)	U(2)-O(17)	2.418(7)
U(1)-O(18)#1	2.285(7)	U(2)-O(18)#1	2.235(8)
Zn(1)-O(12)	2.037(8)	Zn(1)-O(16)	2.004(8)
Zn(1)-O(14)	2.163(9)	Zn(1)-O(17)	2.069(7)
Zn(1)-O(15)	1.985(10)		
O(1)-U(1)-O(2)	173.8(3)	O(3)-U(2)-O(4)	177.5(4)
#1 -x+2,-y+2,-z+1	#2 -x+1,-y+1,-z+1		
<b>3</b>			
U(1)-O(1)	1.763(6)	U(1)-O(4)#2	2.393(6)
U(1)-O(2)	1.766(6)	U(1)-O(3)#2	2.462(6)
U(1)-O(7)#1	2.295(5)	U(1)-N(1)#2	2.501(6)
U(1)-O(6)	2.362(5)	O(1)-U(1)-O(2)	178.8(3)
#1 -x,-y,-z+1	#2 -x+1/2,y-1/2,-z+3/2		
<b>4</b>			
U(1)-O(1)	1.766(4)	U(1)-N(1)	2.544(4)
U(1)-O(2)	1.757(4)	U(1)-N(2)	2.553(5)
U(1)-O(3)	2.321(4)	U(1)-N(3)	2.466(4)
U(1)-O(4)	2.312(4)	O(1)-U(1)-O(2)	177.07(18)
<b>5</b>			
U(1)-O(1)	1.757(3)	U(1)-O(4)#1	2.5167(19)
U(1)-O(2)	1.759(3)	U(1)-O(4)	2.5167(19)
U(1)-O(3)#1	2.439(2)	U(1)-N(1)	2.612(2)
U(1)-O(3)	2.439(2)	U(1)-N(1)#1	2.612(2)
O(1)-U(1)-O(2)	180.000(1)		
#1 -x+1,y,-z+3/2			
<b>6</b>			
U(1)-O(1)	1.766(5)	U(1)-O(5)	2.434(7)
U(1)-O(2)	1.767(5)	U(1)-O(6)	2.456(6)
U(1)-O(3)	2.449(6)	U(1)-N(1)	2.638(6)
U(1)-O(4)	2.448(5)	U(1)-N(2)	2.666(8)
O(1)-U(1)-O(2)	179.6(2)		
<b>7</b>			

U(1)-O(1)	1.779(3)	Zn(1)-N(1)	2.126(3)
U(1)-O(2)	1.763(3)	Zn(1)-N(1)#1	2.126(3)
U(1)-O(3)	2.211(2)	Zn(1)-N(2)	2.161(3)
U(1)-O(5)	2.449(2)	Zn(1)-N(2)#1	2.161(3)
U(1)-O(6)	2.421(2)	Zn(1)-N(3)#1	2.179(3)
U(1)-O(7)	2.436(2)	Zn(1)-N(3)	2.179(3)
U(1)-O(8)	2.431(2)	O(1)-U(1)-O(2)	178.08(12)

#1 -x+2,y,-z+1/2

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**8**

U(1)-O(1)	1.791(3)	Zn(1)-O(4)#1	1.911(3)
U(1)-O(2)	1.794(3)	Zn(1)-O(7)	2.041(3)
U(1)-O(3)	2.363(3)	Zn(1)-N(1)	2.026(4)
U(1)-O(4)	2.267(3)	Zn(1)-N(3)	2.005(4)
U(1)-O(4) #1	2.228(3)		
U(1)-O(5)	2.511(3)		
U(1)-O(6)	2.530(3)	O(2)-U(1)-O(1)	175.04(14)

#1 -x+1,-y+1,-z+1

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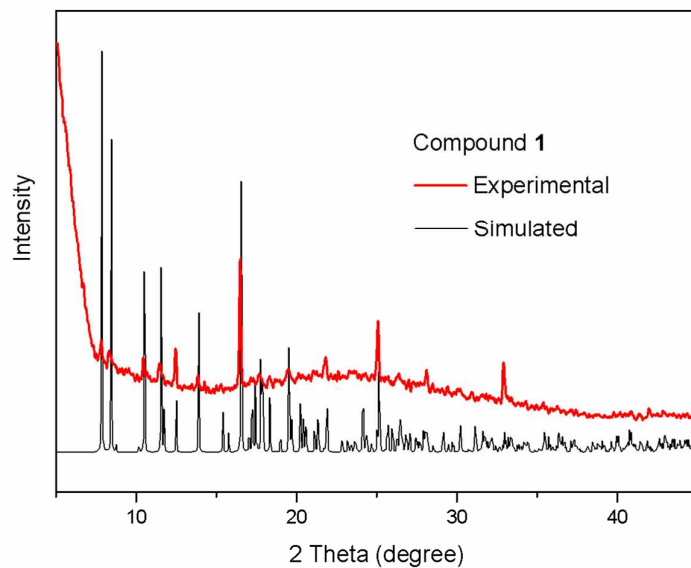


Figure S1. Simulated and experimental XRD patterns of compound 1.

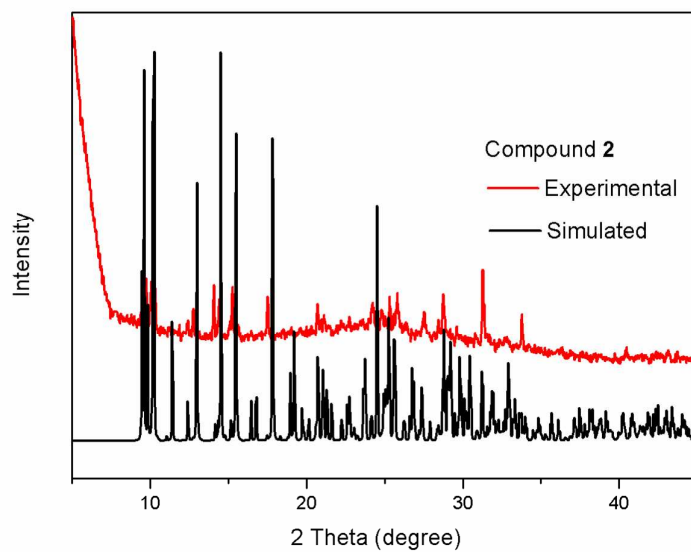


Figure S2. Simulated and experimental XRD patterns of compound 2.

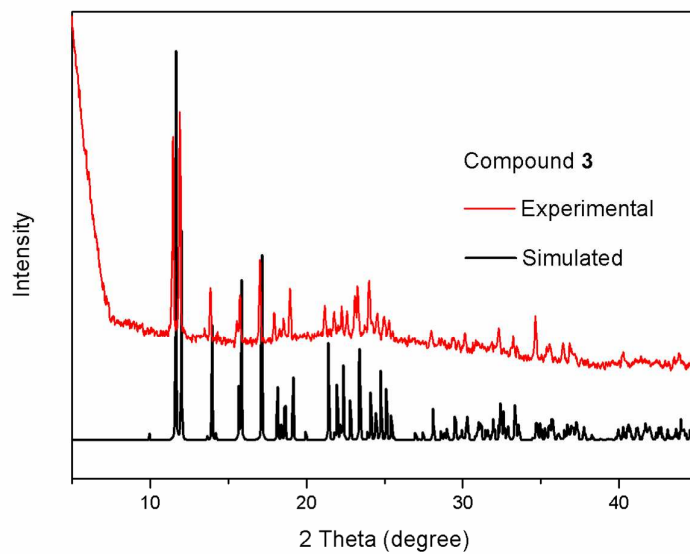


Figure S3. Simulated and experimental XRD patterns of compound 3.

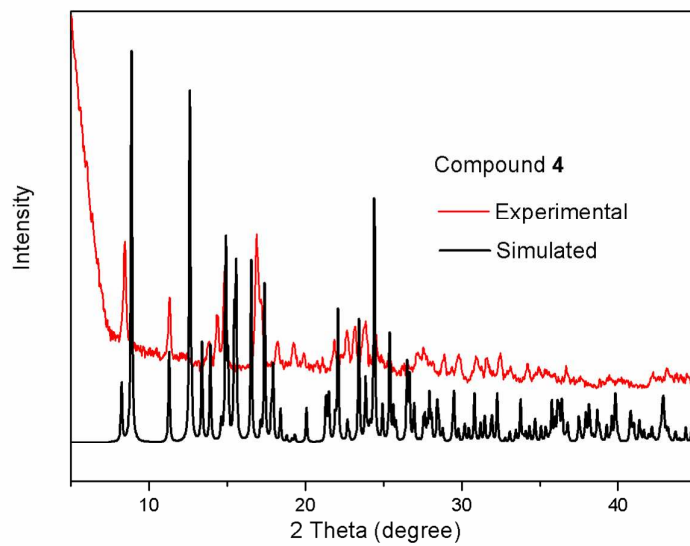


Figure S4. Simulated and experimental XRD patterns of compound 4.

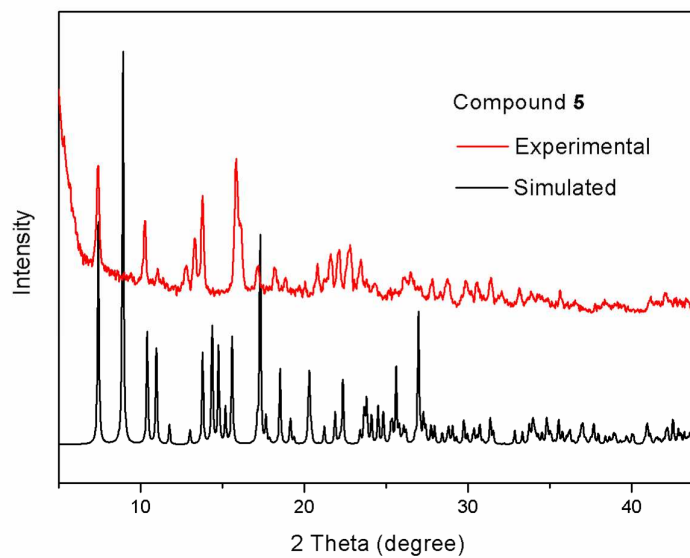


Figure S5. Simulated and experimental XRD patterns of compound **5**.

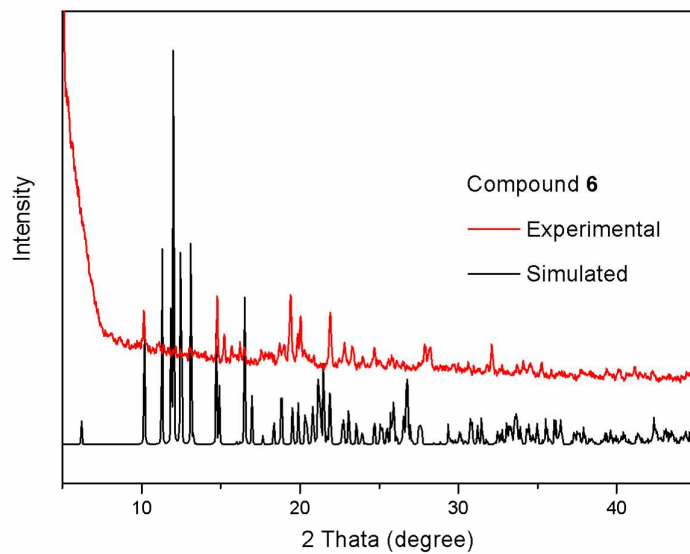


Figure S6. Simulated and experimental XRD patterns of compound **6**.

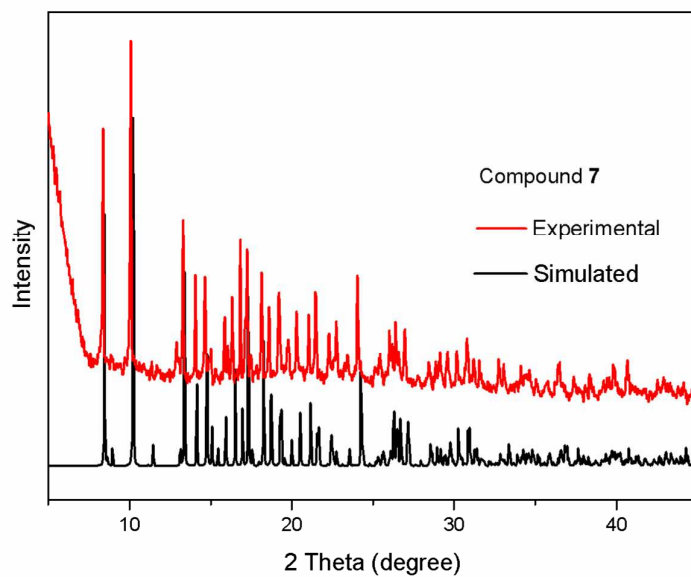


Figure S7. Simulated and experimental XRD patterns of compound 7.

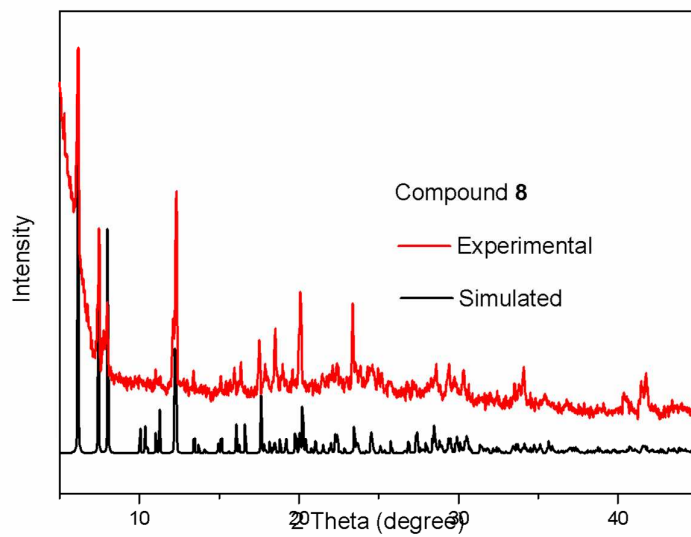


Figure S8. Simulated and experimental XRD patterns of compound 8.

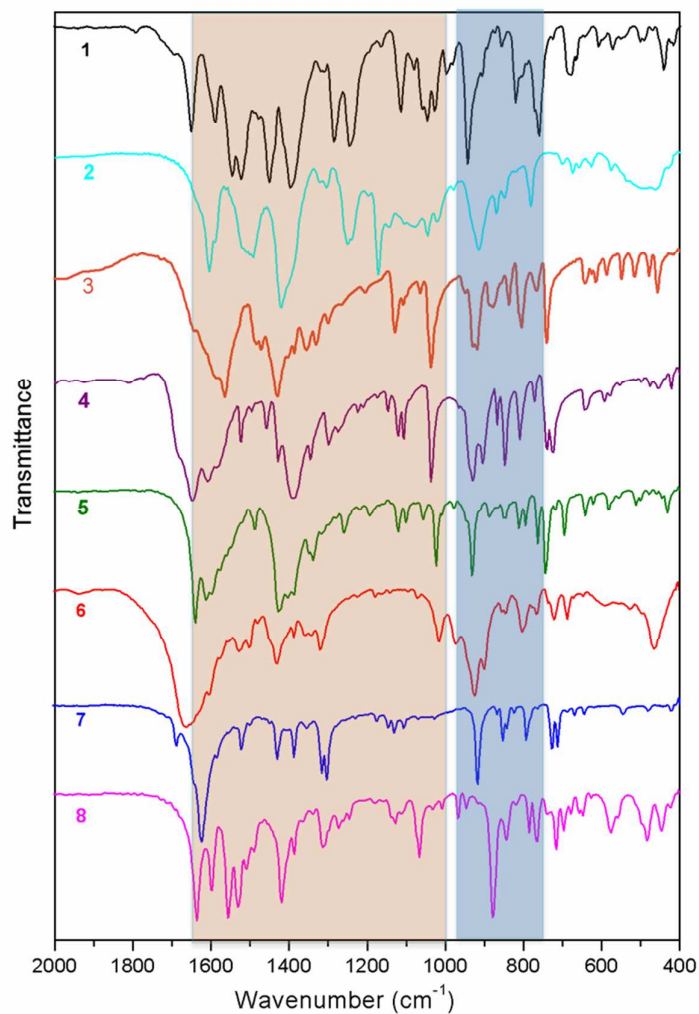


Figure S9. The IR spectra of compounds **1** – **8** with the range of 400 – 2000  $\text{cm}^{-1}$ . The adsorption of organic ligands are indicated in orange range, while U=O stretching modes are shown in blue range.