

Supporting information

Interpenetrated Uranyl-Organic Frameworks with *bor* and *pts* Topology: Structure, Spectroscopy and Computation

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Table S1. Selected bond lengths (Å) and angles (°) for compound **1**

U(2)-O(6)	1.767(5)	U(2)-O(10)	1.748(5)
U(2)-O(2)	2.470(4)	U(2)-O(3)	2.463(4)
U(2)-O(4)	2.481(4)	U(2)-O(5)	2.452(4)
U(2)-O(8)	2.403(4)	U(2)-O(5)	2.424(4)
O(2)-U(2)-O(4)	118.50(14)	O(6)-U(2)-O(9) ¹	91.35(2)
O(2)-U(2)-O(3)	70.71(13)	O(8)-U(2)-O(2)	53.20(5)
O(3)-U(2)-O(4)	170.41(13)	O(8)-U(2)-O(3)	123.91(4)
O(5)-U(2)-O(3)	52.66(13)	O(8)-U(2)-O(4)	65.36(11)
O(5)-U(2)-O(2)	123.25(13)	O(8)-U(2)-O(5)	175.26(5)
O(2)-U(2)-O(1)	53.7(3)	O(8)-U(2)-O(9)	118.18(3)
O(5)-U(2)-O(4)	118.24(13)	O(9)-U(2)-O(2)	171.38(5)
O(6)-U(2)-O(2)	88.60(3)	O(9)-U(2)-O(3)	117.91(3)
O(6)-U(2)-O(3)	88.74	O(9)-U(2)-O(4)	52.91(5)
O(6)-U(2)-O(4)	94.0(2)	O(9)-U(2)-O(5)	65.34(3)
O(6)-U(2)-O(5)	86.99(18)	O(10)-U(2)-O(2)	90.50(3)
O(10)-U(2)-O(3)	88.92(18)	O(10)-U(2)-O(4)	88.35(19)
O(10)-U(2)-O(5)	91.79(19)	O(10)-U(2)-O(6)	177.6(2)
O(10)-U(2)-O(8)	91.4(2)	O(10)-U(2)-O(9)	89.96(19)

Symmetry code: #1 1-y,+x-y,+z; #2 1+y-x,1-x,+z; #3 1/3+y-x,-1/3+y, 1/6+z

Table S2. Selected bond lengths (Å) and angles (°) for compound **2**

U(1)-O(3)	1.745(4)	U(1)-O(4)	1.756(4)
U(1)-O(1)	2.297(3)	U(1)-O(2) ¹	2.289(4)
U(1)-O(6)	2.468(3)	U(1)-O(5)	2.472(4)
U(1)-O(7)	2.415(4)		

O(3)-U(1)-O(4)	176.95(18)	O(3)-U(1)-O(2) ¹	90.96(19)
O(4)-U(1)-O(2) ¹	92.02(18)	O(3)-U(1)-O(1)	93.14(16)
O(4)-U(1)-O(1)	87.93(16)	O(2) ¹ -U(1)-O(1)	82.26(13)
O(2) ¹ -U(1)-O(7)	161.27(14)	O(1)-U(1)-O(7)	79.80(13)
O(3)-U(1)-O(6)	90.48(16)	O(4)-U(2)-O(6)	89.74(16)
O(2) ¹ -U(1)-O(6)	73.20(13)	O(1)-U(2)-O(6)	155.25(12)
O(7)-U(1)-O(6)	124.93(12)	O(3)-U(2)-O(5)	93.11(17)
O(4)-U(1)-O(5)	84.62(17)	O(2) ¹ -U(2)-O(5)	125.40(13)
O(1)-U(1)-O(5)	151.49(13)	O(7)-U(2)-O(5)	73.13(13)
O(6)-U(1)-O(5)	52.36(12)		

Symmetry code: #1 1/2-x, -1/2-y, -z; #2 1-x, +y, 1/2-z; #3 -1/2+x, -3/2+y, +z

Table S3. Optimized geometry parameters of model compounds in the gas phase, compared with experimental values of analogues. (Bond lengths in Å and angles in degree)

		U=O	U-O _c ^a	U-O _w ^a	O=U=O	O=U-O _c ^a	O=U-O _w ^a
1	Expt.	1.68~1.80	2.418~2.477	—	180.0	90.2~90.8	—
1_1U	Calc.	1.809	2.501	—	179.5	90.0	—
1_2U	Calc.	1.810	2.501	—	179.6	90.0	—
1_4U	Calc.	1.810	2.504	—	178.2	90.0	—
1_4U-Ph		1.807	2.506	—	178.2	90.0	—
2	Expt.	1.745~1.756	2.289~2.297	2.415~2.472	177.0	87.9~93.1	84.6~93.1
2_U1	Calc.	1.798	2.397	2.573	177.2	90.2	88.6
2_U2	Calc.	1.798	2.394	2.582	176.8	90.2	88.4
2_U1-U2	Calc.	1.798	2.395	2.577	177.0	90.2	88.4
2_2U1	Calc.	1.798	2.397	2.573	177.2	90.2	88.0
2_2U2	Calc.	1.798	2.395	2.582	176.8	90.2	88.4
2_2U1-2U2	Calc.	1.798	2.396	2.577	177.1	90.2	88.5

^a O_c and O_w correspond to the oxygen atom in carboxylic acid and water.

Table S4. Calculated absorptions of **2_U1-U2** at the TD-DFT level.

	λ (nm) ^a	λ (nm) ^b	E (eV) ^b	<i>f</i> ^c	Configurations ^d	Weight > 0.1	Expt.
Band I	546	546	2.27	0.0738			493
Band II	544	544	2.28	0.3890	H-1→LUMO HOMO→LUMO	0.8188 0.1498	476
Band III	537	540	2.30	0.1070			462
		537	2.31	0.3590	H-3→LUMO	0.8890	
Band IV	524	532	2.33	0.1980	H-4→LUMO	0.9482	433~404
		525	2.36	0.2730	H-6→LUMO	0.9247	
		524	2.37	0.2610	H-1→L+2	0.9342	
		521	2.38	0.1620	H-1→L+4	0.8727	
		515	2.41	0.1480			
		509	2.44	0.0774			

		508	2.44	0.1630	H-7→LUMO	0.9199	
		504	2.46	0.0763			
Band V	483	499	2.48	0.4180	H-8→LUMO	0.8517	340~290
		488	2.54	0.4860	H-1→L+11	0.8072	
					H-5→L+9	0.1000	
		482	2.57	0.3980	H-9→LUMO	0.8532	
		482	2.57	0.1370			
		479	2.59	0.4740	H-8→L+4	0.7295	
					H-8→L+3	0.1292	
		478	2.59	0.0621			
Band VI	466	469	2.64	0.0903			238
		467	2.66	0.1190			
		464	2.67	0.2890	H-9→L+4	0.8055	
					H-9→L+3	0.1812	

^a The simulated absorption peak (nm).

^b Calculated absorption transitions in nm, eV and cm⁻¹.

^c Oscillator strength (*f*), which was multiplied by 100.

^d Orbitals 246 and 247 correspond to HOMO and LUMO, respectively. Additionally, we did not list configurations for the transition with the oscillator strength (*f**100) less than 0.16.

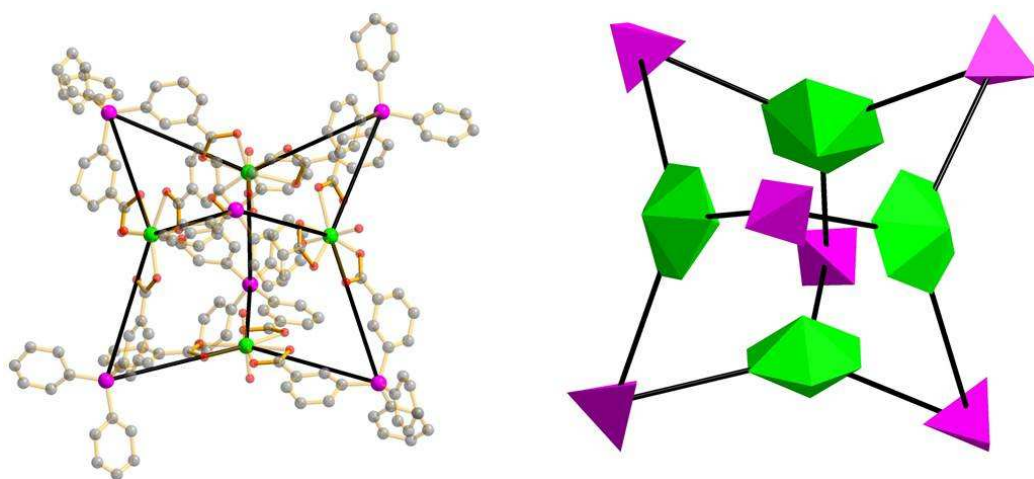


Figure S1. The minimal close loop of **1**, which consists of three uranyl units and three ligands.

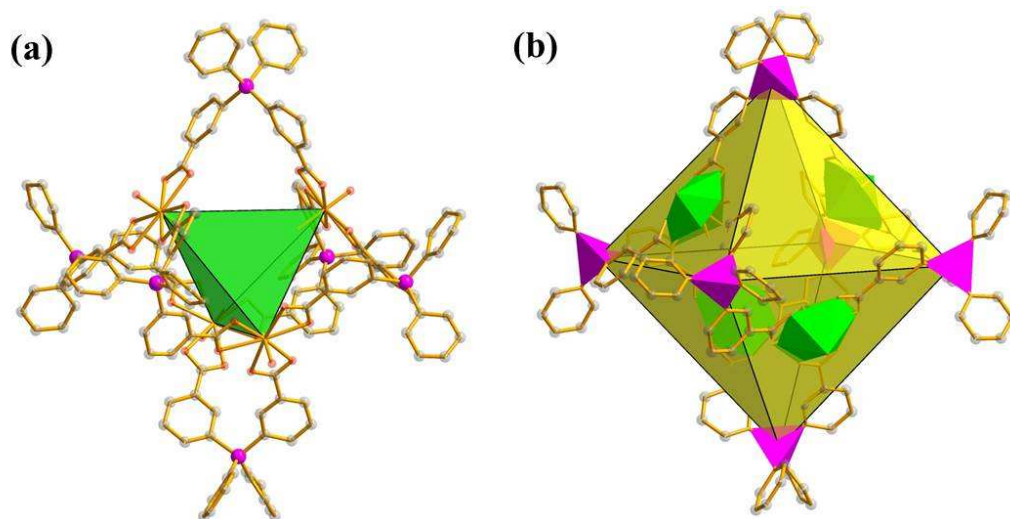


Figure S2. The octahedral cage in **1**. Four uranyl center occupy the vertices of the tetrahedron.

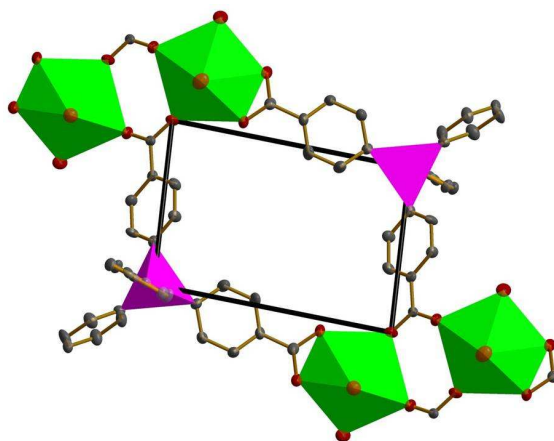


Figure S3. The minimal close loop of **2**, which consists of two dinuclear uranium units and two ligands.

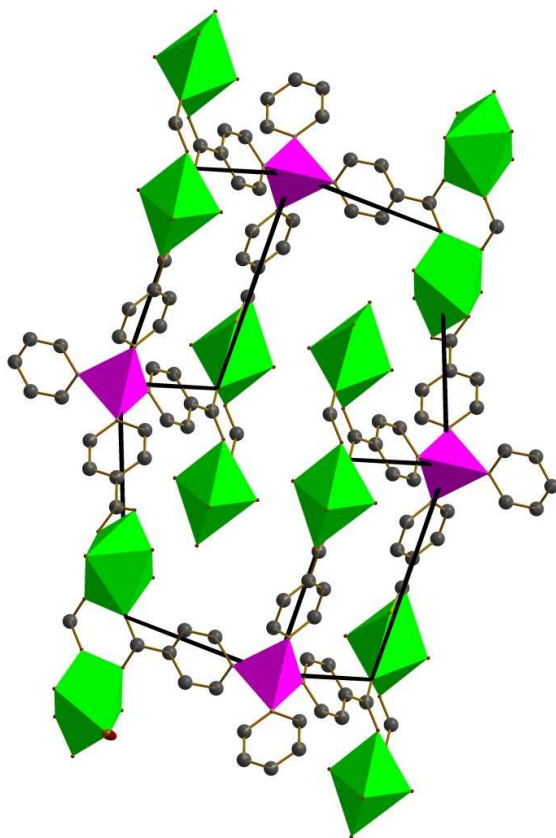


Figure S4. The big close loop of **2**, which is constituted by four dinuclear SBUs and four ligands.

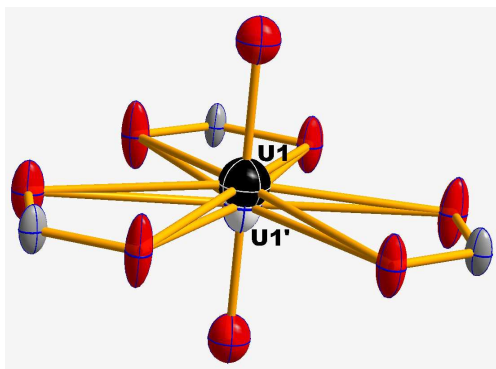


Figure S5. Disordered U1 atom was split to two components (68:32 atomic site occupancy ratios).

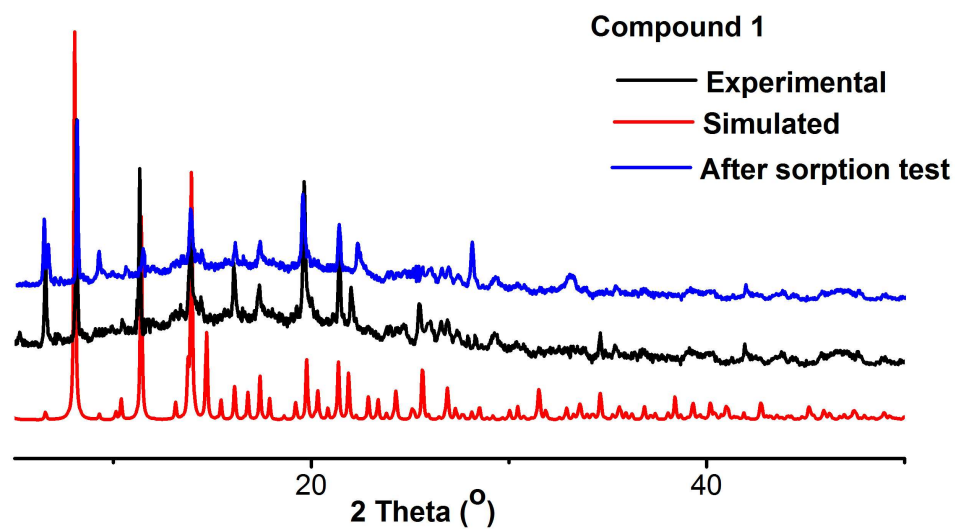


Figure S6. Simulated and experimental XRD patterns of 1.

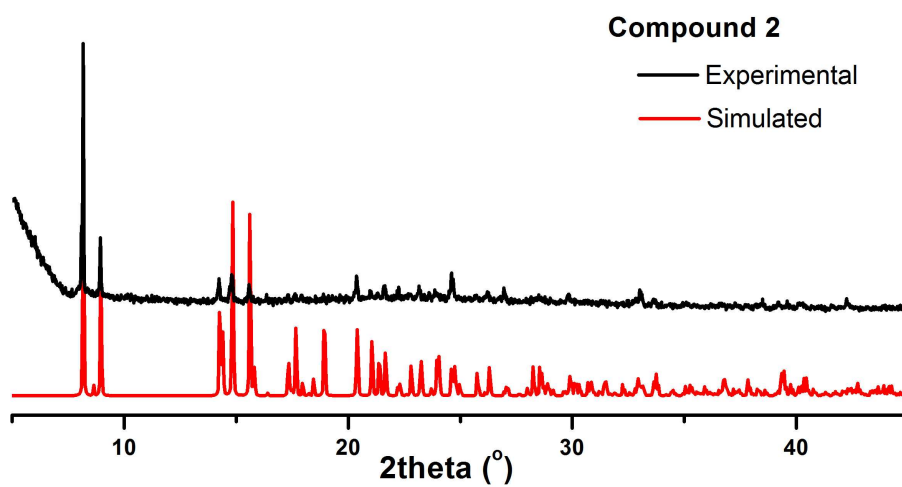


Figure S7. Simulated and experimental XRD patterns of 2.

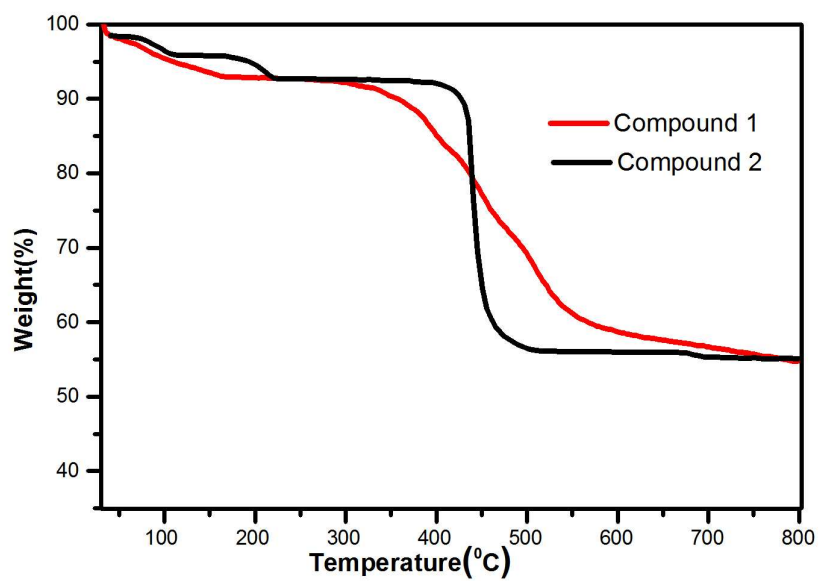


Figure S8. TG curve for compound 1 (red) and 2(black).

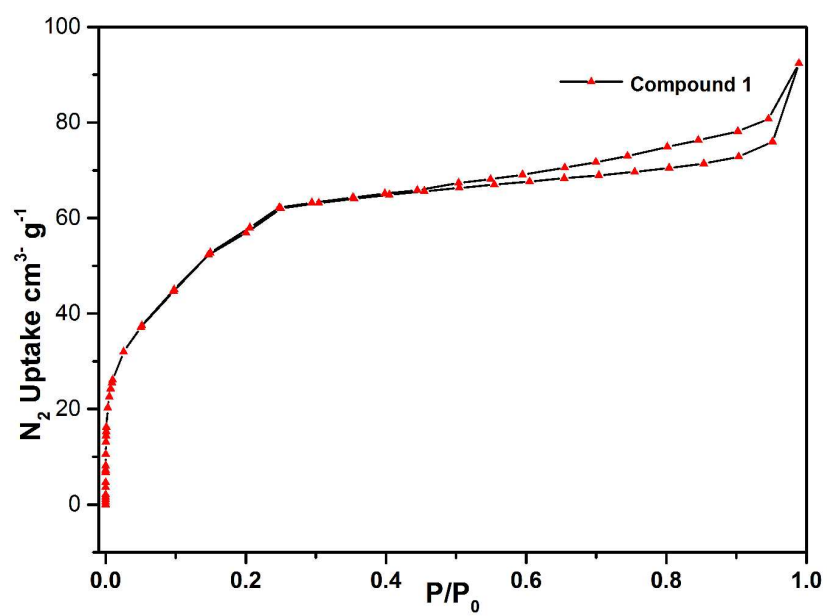


Figure S9. N₂ sorption isotherms of compound 1.

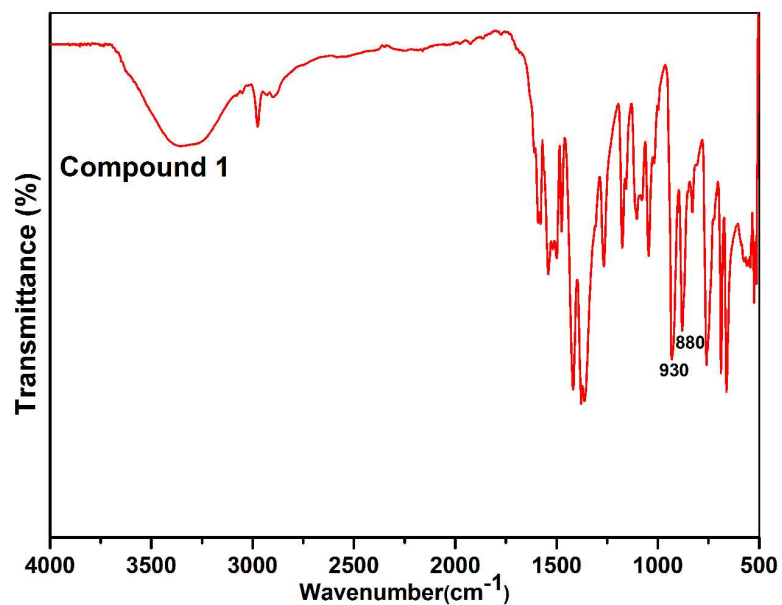


Figure S10. FT-IR spectra of 1

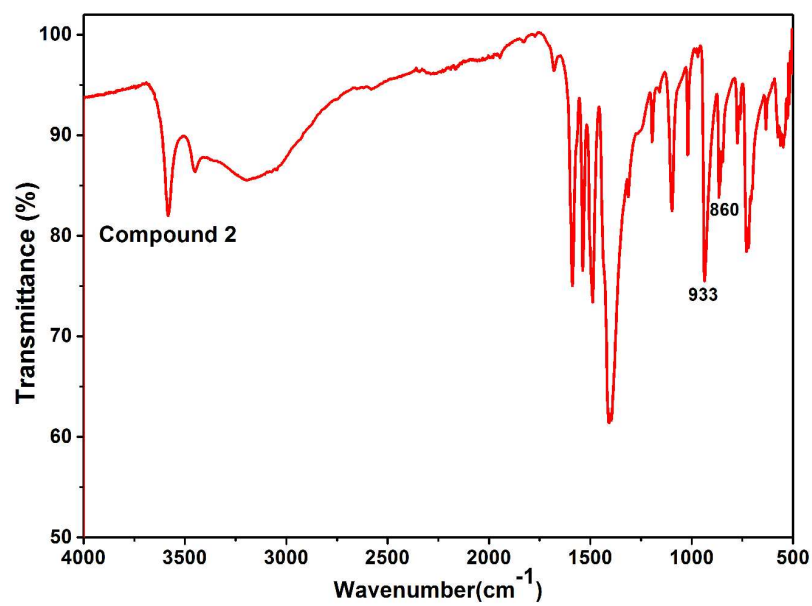


Figure S11. FT-IR spectra of 2

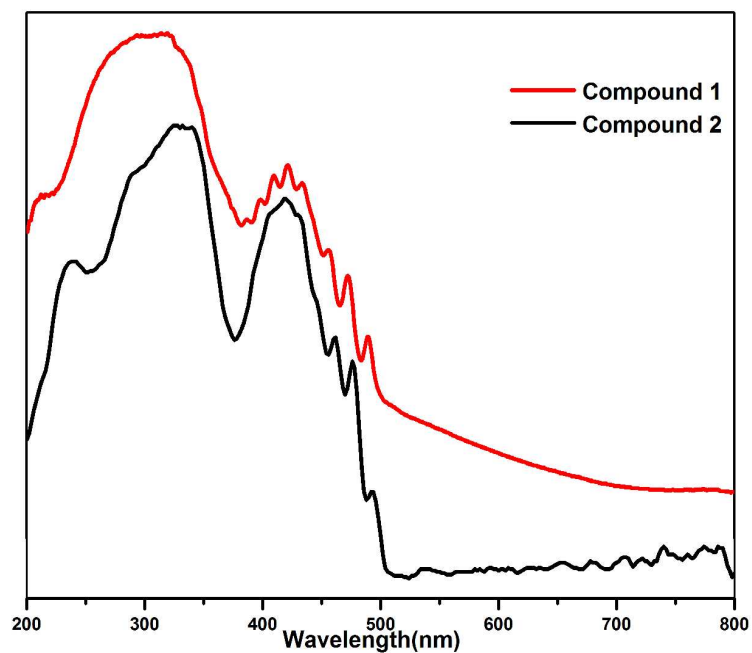


Figure S12. Solid state absorption spectra of **1** and **2**

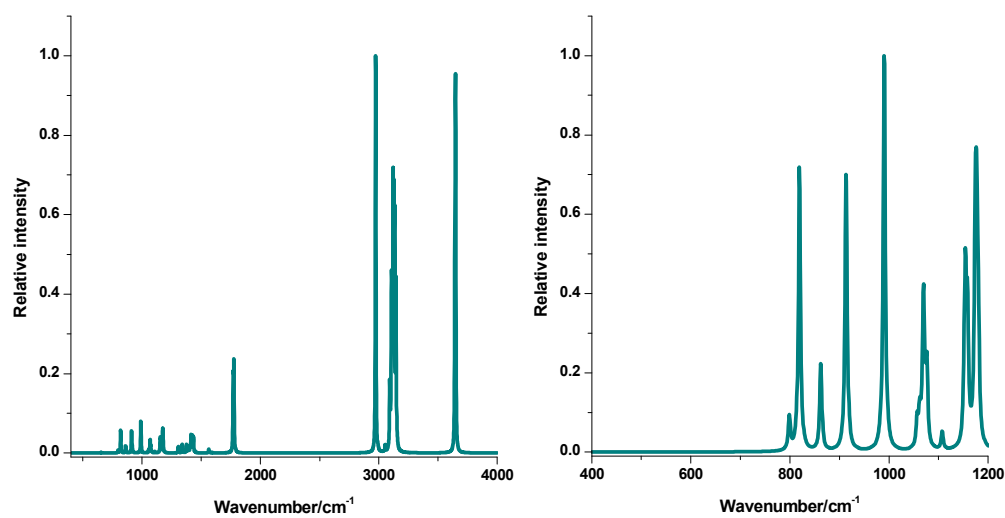


Figure S13. Theoretically simulated vibrational spectra of the model compound **1_1U**: the one spreading the region from 400 to 4000 cm^{-1} was presented on the left side, and the one between 400 and 1200 cm^{-1} on the right side where the U=O stretches were marked.

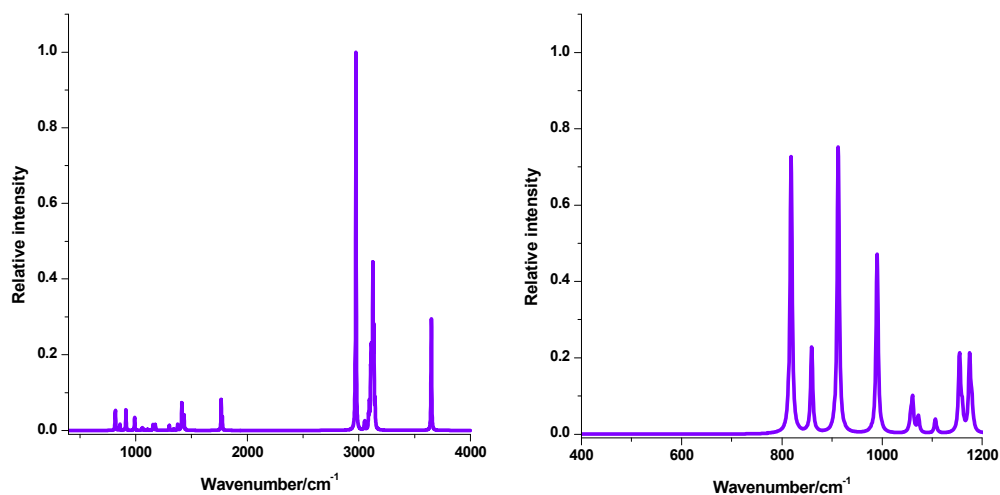


Figure S14. Theoretically simulated vibrational spectra of the model compound **1_2U**: the one spreading the region from 400 to 4000 cm⁻¹ was presented on the left side, and the one between 400 and 1200 cm⁻¹ on the right side where the U=O stretches were marked.

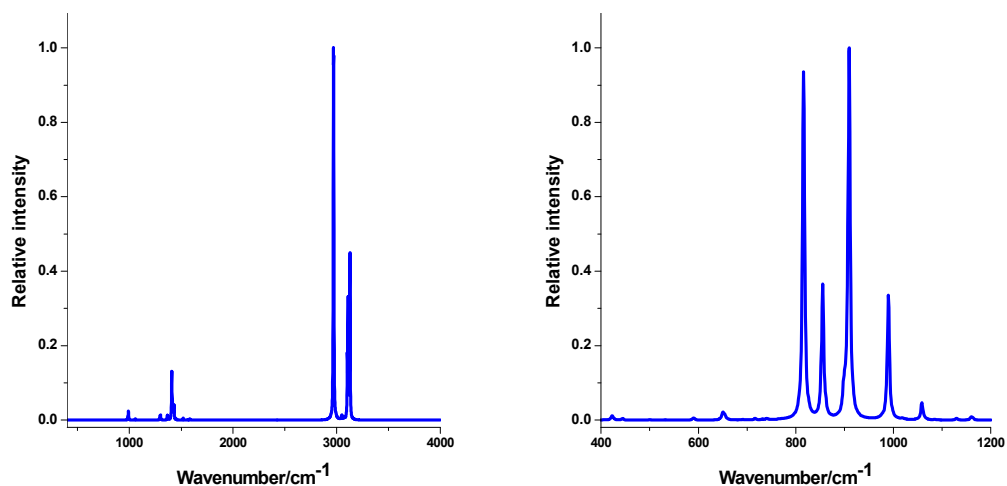


Figure S15. Theoretically simulated vibrational spectra of the model compound **1_4U**: the one spreading the region from 400 to 4000 cm⁻¹ was presented on the left side, and the one between 400 and 1200 cm⁻¹ on the right side where the U=O stretches were marked.

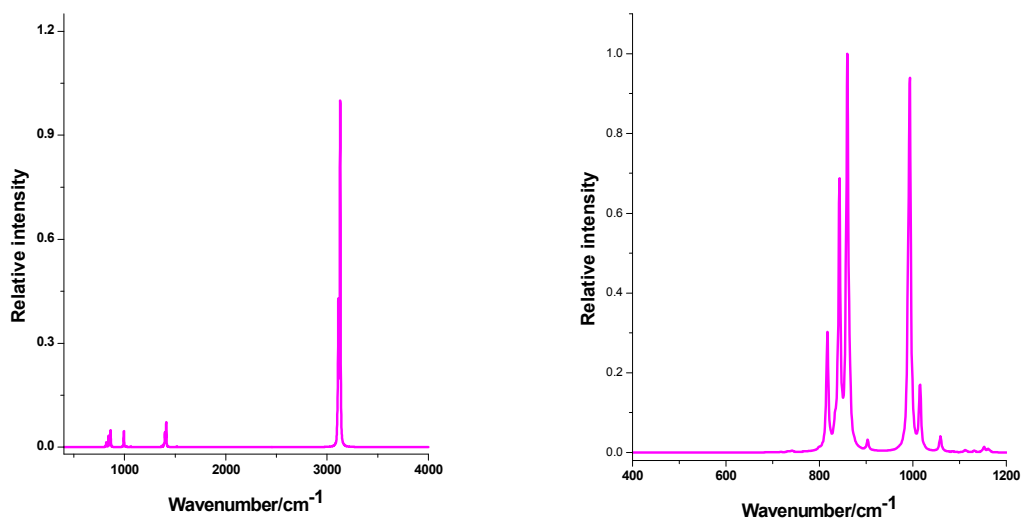


Figure S16. Theoretically simulated vibrational spectra of the model compound **1_4U-Ph**: the one spreading the region from 400 to 4000 cm^{-1} was presented on the left side, and the one between 400 and 1200 cm^{-1} on the right side where the U=O stretches were marked.

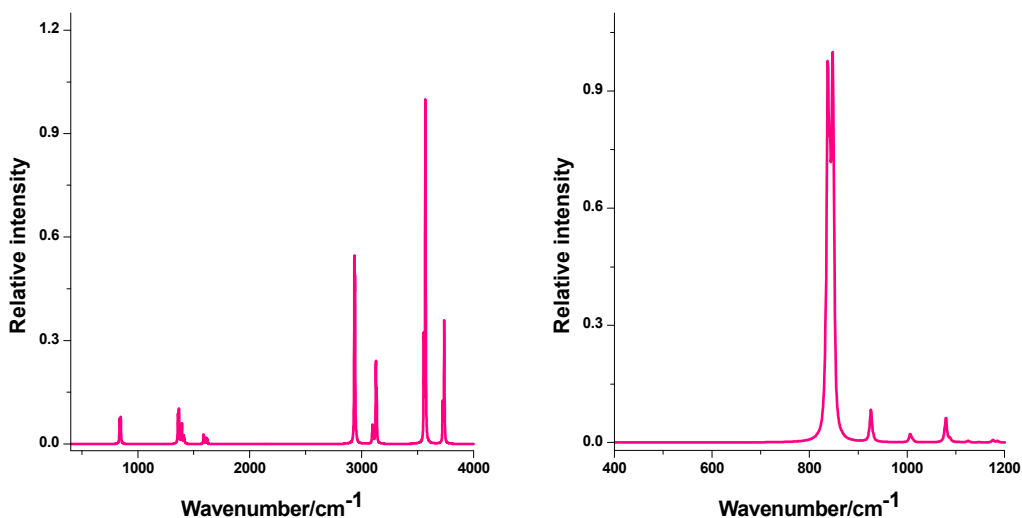


Figure S17. Theoretically simulated vibrational spectra of the model compound **2_2U1-2U2**: the one spreading the region from 400 to 4000 cm^{-1} was presented on the left side, and the one between 400 and 1200 cm^{-1} on the right side where the U=O stretches were marked.

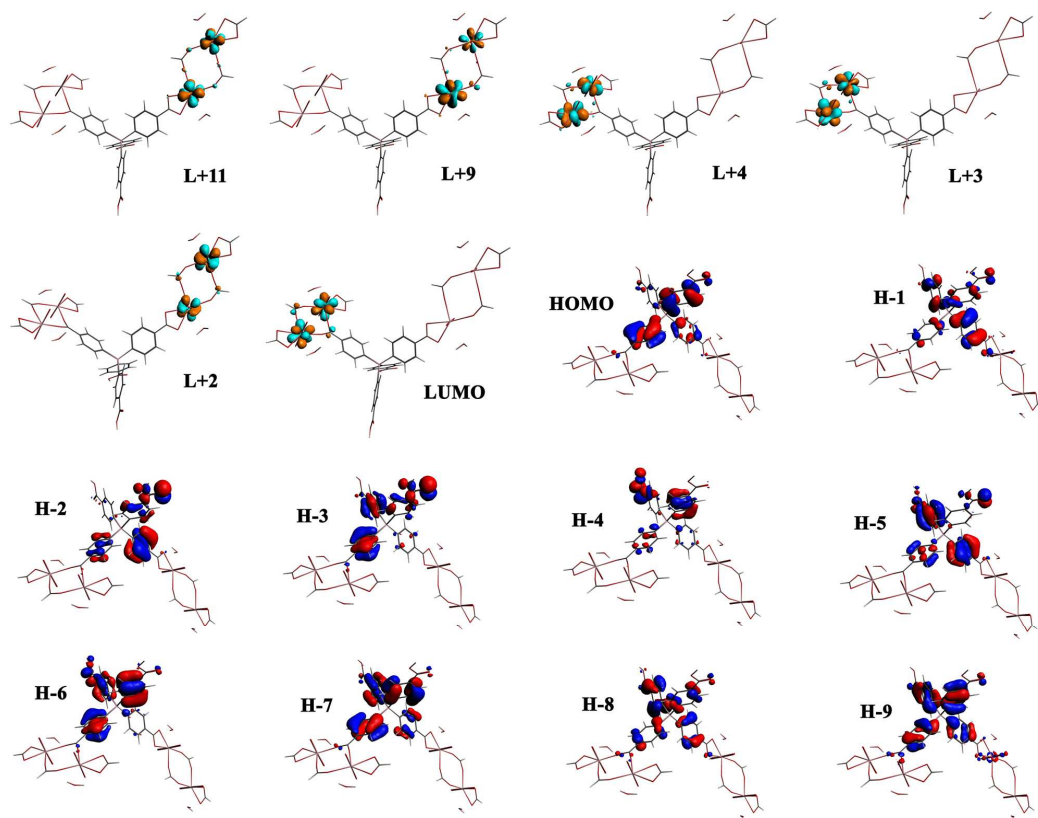


Figure S18. Diagrams of partial frontier molecular orbitals of **2_U1-U2** that are involved in relative more intense absorption transitions (see Table S4) from the TD-DFT calculation.

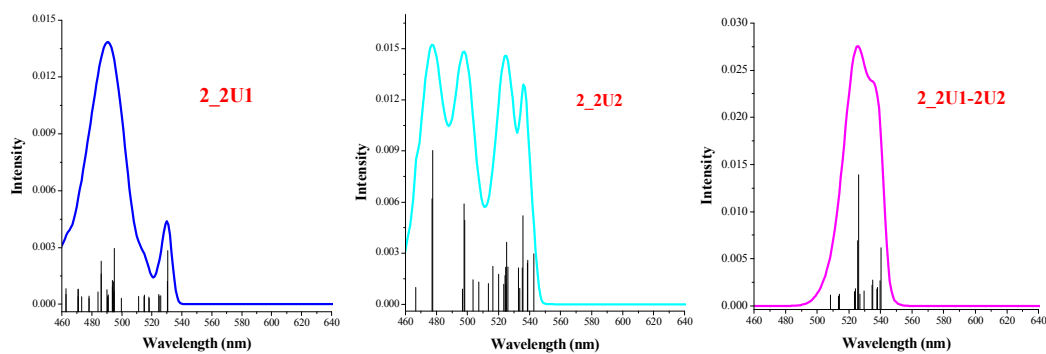


Figure S19. Simulated absorption spectra of model compounds **2_2U1** (left), **2_2U2** (middle) and **2_2U1-2U2** (right) under the TD-DFT calculations, where 120 low-lying excited states were computed for the first two complexes while only 80 states for the last one to save computational cost.

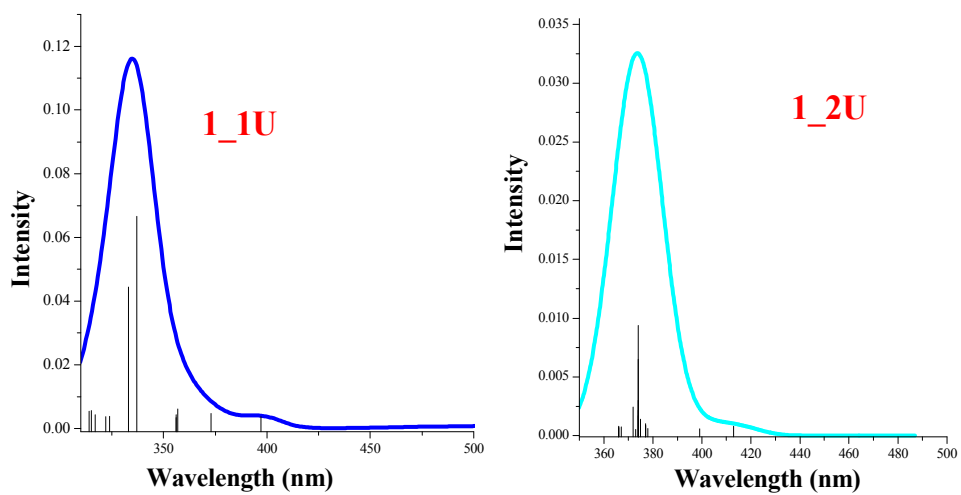


Figure S20. Simulated absorption spectra of model compounds **1_1U** (left) and **1_2U** (right) under the TD-DFT calculations, where 120 low-lying excited states were computed.

Computational Details

To simulate the experimental compounds **1** and **2**, some molecular models, as shown in Figure 9 in the text, were calculated. Models including one to four uranyl coordination structural units around the H_4L^1 ligand were used for **1**, while those containing two types of uranyl structural units (U1 and U2) were taken into account for **2**. Thus, geometries of ten uranyl model compounds were fully optimized by the relativistic density functional theory. The PBE functional of the generalized gradient approximation (GGA) was applied. All these optimizations were accomplished carried out by the Priroda code,^{1, 2} where a scalar relativistic four-component all-electron approach and all-electron correlation-consistent double- ζ polarized quality basis sets were used.¹ Subsequent analytical frequency calculations were used to confirm the nature of the stationary points on the potential energy surface. Also, we have simulated vibrational spectra of complexes with the Lorentzian broadening based on the frequency data. Population-based Mayer³ bond orders were calculated.

The electronic structures and absorption spectra in the aqueous solution were examined explored with the ADF 2014 code⁴⁻⁶ while employing the above optimized geometries. An integration parameter of 6.0 was applied. The solvent effects of water were taken into account with the Conductor-Like Screening Model, COSMO.^{7, 8} Klamt radii were used for the main group atoms ($\text{H} = 1.30 \text{ \AA}$, $\text{C} = 2.00 \text{ \AA}$, $\text{O} = 1.72 \text{ \AA}$ and $\text{P} = 2.16 \text{ \AA}$)⁹ and for the uranium atom ($1.70 \text{ \AA}$)¹⁰⁻¹⁴. The ZORA scalar relativistic approach of van Lenthe et al¹⁵⁻¹⁸ was employed, associated with the Slater-type TZP basis sets. The time-dependent density functional theory (TD-DFT) with the PBE functional was performed to explore electronic absorption spectra in water. 120 spin-allowed excited states were calculated for most model compounds, with the exception of **2_2U1-2U2** whose 80 excited states were studied for its large number of atoms (149).

References:

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Fonseca Guerra, C.; Franchini, M.; Ghysels, A.; Giammona, A.; van Gisbergen, S. J. A.; Götz, A. W.; Groeneveld, J. A.; Gritsenko, O. V.; Grüning, M.; Gusarov, S.; Harris, F. E.; van den Hoek, P.; Jacob, C. R.; Jacobsen, H.; Jensen, L.; Kaminski, J. W.; van Kesse, G.; Kootstra, F.; Kovalenko, A.; Krykunov, M. V.; van Lenthe, E.; McCormack, D. A.; Michalak, A.; Mitoraj, M.; Morton, S. M.; Neugebauer, J.; Nicu, V. P.; Noodleman, L.; Osinga, V. P.; Patchkovskii, S.; Pavanello, M.; Philipsen, P. H. T.; Post, D.; Pye, C. C.; Ravenek, W.; Rodríguez, J. I.; Ros, P.; Schipper, P. R. T.; van Schoot, H.; Schreckenbach, G.; Seldenthuis, J. S.; Seth, M.; Snijders, J. G.; Solà, M.; Swart, M.; Swerhone, D.; te Velde, G.; Vernooijs, P.; Versluis, L.; Visscher, L.; Visser, O.; Wang, F.; Wesolowski, T. A.; van Wezenbeek, E. M.; Wiesenekker, G.; Wolff, S. K.; Woo, T. K.; Yakovlev, A. L. *ADF*, ADF2014.06; SCM, Theoretical Chemistry, Vrije Universiteit: Amsterdam, The Netherlands, 2014.

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Cartesian coordinates of optimized model compounds

1_1U

| _U 13.51288072 7.90531152 9.17035045
O 11.40075329 9.18790335 8.91386527
O 13.44048227 5.40002287 9.45051306
O 15.70996595 9.07183541 9.15370215
O 13.92066345 10.34815284 8.91192440
O 11.18955443 6.99901968 9.14452439
O 15.45998013 6.31841814 9.43371366
O 13.42365311 8.10737093 10.96559775
O 13.60666920 7.68805117 7.37626232
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C 14.70447229 5.30234671 9.49082895
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C 9.16209743 8.29696390 8.88131740
C 15.32814138 3.92926963 9.58187809
C 16.06829019 11.45331328 8.98352634
C 16.71963386 3.78194721 9.55811882
C 14.51378517 2.79560492 9.66238546
H 17.32779651 4.68885316 9.50006097
C 17.28724718 2.50892578 9.60386676
C 15.06783840 1.50216579 9.68779942
H 13.43178077 2.96624961 9.70155794
H 18.37505377 2.39312761 9.59025334
C 16.46987574 1.37615026 9.65963300
Si 13.91784703 0.00561369 9.69912076
H 16.92756404 0.38225959 9.68510975
C 14.91835572 -1.60895056 9.88963775
C 12.68639647 0.15077502 11.14525956
C 12.94560420 -0.11593507 8.06202313
C 14.94447314 -2.34123814 11.08972327
C 15.67925356 -2.08760454 8.80891829
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