Supplementary Information

Six Uranyl-Organic Frameworks with Naphthalene-Dicarboxylic Acid and Bipyridyl-Based Spacers: Syntheses, Structures, and Properties

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Figure S1: IR spectra of complexes 1–6.



Figure S2: TG curve of complexes 1–6.



Figure S3: The simulated and experimental PXRD patterns of complexes 1–6.



Figure S4: The calculated UV-Vis absorption Spectroscopy of complexes 1–3.



Figure S5: The calculated UV-Vis absorption Spectroscopy of complexes 4–6.



Figure S6: The experimental UV-Vis absorption Spectroscopy of complexes 1–6.

U101	2.396(8)	U1–O2	2.411(8)	U1–07	2.408(8)
U1–O8	2.486(9)	U1–O11	2.467(9)	U1–O12	2.461(8)
U1–O15	1.685(9)	U1016	1.711(9)	U2–O3	2.470(9)
U2–O4	2.515(8)	U2–O5	1.629(9)	U2–O6	1.672(8)
U2–O9 ^{#2}	2.416(8)	U2O10 ^{#2}	2.514(9)	U2013 ^{#1}	2.393(8)
U2014 ^{#1}	2.477(8)				
O1–U1–O2	55.0(5)	01–U1–07	173.1(4)	O1–U1–O8	119.5(5)
01–U1–O11	67.9(3)	O1–U1–O12	119.3(5)	O1–U1–O15	88.0(8)
O1–U1–O16	91.4(7)	O2-U1-O7	118.1(4)	O2–U1–O8	64.6(5)
O2-U1-O11	122.9(5)	O2-U1-O12	173.3(4)	O2–U1–O15	86.0(7)
O2-U1-O16	93.9(7)	O7–U1–O8	53.6(4)	O7–U1–O11	119.0(4)
O7–U1–O12	67.6(5)	O7–U1–O15	91.3(7)	O7–U1–O16	89.4(6)
O8–U1–O11	172.4(4)	O8–U1–O12	121.2(5)	O8–U1–O15	90.9(7)
O8–U1–O16	89.7(7)	O11–U1–O12	51.5(5)	O11-U1-O15	91.2(6)
O11-U1-O16	88.2(7)	O12–U1–O15	90.3(7)	O12-U1-O16	89.7(7)
O15-U1-O16	179.3(6)	O3 –U2–O4	53.8(4)	O3 –U2–O5	94.8(9)
O3–U2–O6	87.3(6)	O3–U2–O9 ^{#2}	171.6(4)	O3 –U2–O10 ^{#2}	120.1(5)
O3–U2–O13 ^{#1}	67.2(4)	O3 –U2–O14 ^{#1}	119.6(4)	O4 –U2–O5	97.7(7)
O4–U2–O6	83.8(6)	O4–U2–O9 ^{#2}	118.0(4)	O4 –U2–O10 ^{#2}	67.1(4)
O4-U2-O13 ^{#1}	120.7(4)	O4-U2-O14 ^{#1}	169.3(5)	O5–U2–O6	177.8(8)
O5–U2–O9 ^{#2}	87.8(9)	O5–U2–O10 ^{#2}	83.6(8)	O5–U2–O13 ^{#1}	92.2(7)
O5–U2–O14 ^{#1}	91.2(7)	O6-U2-O9 ^{#2}	90.2(7)	O6–U2–O10 ^{#2}	95.6(7)
O6-U2-O13 ^{#1}	88.4(6)	O6-U2-O14 ^{#1}	87.5(6)	O9 ^{#2} -U2-O10 ^{#2}	52.2(4)
O9 ^{#2} -U2-O13 ^{#1}	120.7(4)	O9 ^{#2} -U2-O14 ^{#2}	68.2(4)	O10 ^{#2} –U2–O13 ^{#1}	171.8(5)
O10 ^{#2} -U2-O14 ^{#2}	120.3(4)	O13 ^{#1} -U2-O14 ^{#1}	52.5(4)		

Table S1: Selected interatomic distances (Å) and bond angles (°) for complex 1.

Symmetry transformations used to generate equivalent atoms: #1 = x-1, y, z; #2 =

x-1/2, *y*+1/2, *z*+1/2; #3 = *x*+1/2, *y*-1/2, *z*-1/2; #4 = *x*+1, *y*, *z*.

U1–O1	2.433(8)	U1–O2	2.473(8)	U1–O5	2.308(7)
U1O6 ^{#1}	2.335(7)	U1–O9	2.321(7)	U1012	1.766(2)
U1–O13	1.670(2)	U2–O3	2.437(8)	U2–O4	2.437(8)
U2–O7 ^{#3}	2.475(8)	U2–O8 ^{#3}	2.479(8)	U2–O11 ^{#2}	2.460(7)
U2–O14 ^{#2}	2.429(8)	U2–O15	1.689(2)	U2–O16	1.722(2)
O1–U1–O2	52.0(3)	01–U1–O5	127.6(3)	O1-U1-O6 ^{#1}	147.3(3)
O1–U1–O9	70.9(3)	O1–U1–O12	91.0(4)	O1–U1–O13	88.2(4)
O2–U1–O5	75.8(3)	O2–U1–O6 ^{#1}	160.4(3)	O2–U1–O9	122.8(3)
O2-U1-O12	88.5(4)	O2–U1–O13	90.2(4)	$O5 - U1 - O6^{#1}$	85.0(3)
O5–U1–O9	161.3(3)	O5–U1–O12	92.0(4)	O5–U1–O13	87.7(4)
O6 ^{#1} -U1-O9	76.4(3)	O6 ^{#1} -U1-O12	88.2(4)	O6 ^{#1} -U1-O13	93.1(4)
O9-U1-O12	89.7(4)	O9–U1–O13	91.0(4)	O12–U1–O13	178.4(4)
O3 –U2–O4	52.5(3)	O3–U2–O7 ^{#3}	121.3(3)	O3–U2–O8 ^{#3}	173.2(3)
O3-U2-O11 ^{#2}	118.8(3)	O3–U2–O14 ^{#2}	67.1(3)	O3–U2–O15	89.7(4)
O3–U2–O16	90.8(4)	O4–U2–O7 ^{#3}	68.8(3)	O4-U2-O8 ^{#3}	121.4(3)
O4-U2-O11 ^{#2}	171.3(3)	O4-U2-O14 ^{#2}	119.4(3)	O4–U2–O15	91.1(4)
O4-U2-O16	90.0(4)	O7 ^{#3} –U2–O8 ^{#3}	52.6(3)	O7 ^{#3} -U2-O11 ^{#2}	119.9(3)
O7 ^{#3} -U2-O14 ^{#2}	171.5(3)	O7 ^{#3} -U2-O15	90.2(4)	O7 ^{#3} -U2-O16	90.3(4)
O8 ^{#3} -U2-O11 ^{#2}	67.3(3)	O8 ^{#3} -U2-O14 ^{#2}	119.2(3)	O8 ^{#3} –U2–O15	87.5(4)
O8 ^{#3} -U2-O16	92.1(4)	O11 ^{#2} -U2-O14 ^{#2}	51.9(3)	O11 ^{#2} –U2–O15	88.1(4)
O11 ^{#2} -U2-O16	90.8(4)	O14 ^{#2} -U2-O15	91.8(4)	O14 ^{#2} -U2-O16	87.5(4)
O15-U2-O16	178.9(5)				

Table S2: Selected interatomic distances (Å) and bond angles (°) for complex 2.

Symmetry transformations used to generate equivalent atoms: #1 = -x+2, -y+1, -z+1; #2 = -x+2, -y+2, -z+1; #3 = -x+1, y+1/2, -z+1/2; #4 = -x+1, y-1/2, -z+1/2.

			,		
U1-O3 ^{#1}	2.460(7)	U1O4 ^{#1}	2.439(7)	U1–O7 ^{#2}	2.347(6)
U1–O8	2.396(6)	U1O12 ^{#3}	2.303(6)	U1–O15	1.737(7)
U1016	1.744(7)	U2–O1	2.488(7)	U2–O2	2.434(7)
U2–O5	2.505(8)	U2–O6	2.459(7)	U2–O9	2.481(7)
U2–O10	2.439(7)	U2–O13	1.733(9)	U2–O14	1.735(8)
$O3^{\#1}$ -U1-O4 $^{\#1}$	52.5(2)	$O3^{\#1}$ -U1-O7 $^{\#2}$	157.7(2)	O3 ^{#1} -U1-O8	73.3(2)
O3 ^{#1} -U1-O12 ^{#3}	125.2(3)	O3 ^{#1} –U1–O15	94.3(3)	O3 ^{#1} -U1-O16	85.3(3)
$O4^{\#1}$ – $U1$ – $O7^{\#2}$	149.5(3)	O4 ^{#1} -U1-O8	125.8(3)	O4 ^{#1} -U1-O12 ^{#3}	72.7(3)
O4 ^{#1} -U1-O15	91.1(3)	O4 ^{#1} -U1-O16	90.1(3)	O7 ^{#2} –U1–O8	84.7(2)
O7 ^{#2} -U1-O12 ^{#3}	76.8(3)	O7 ^{#2} –U2–O15	89.8(3)	O7 ^{#2} -U1-O16	90.3(3)
O8–U1–O12 ^{#3}	161.0(3)	O8–U1–O15	86.4(3)	O8–U1–O16	91.1(3)
O12 ^{#3} -U1-O15	89.3(3)	O12 ^{#3} -U1-O16	93.1(3)	O15–U1–O16	177.5(3)
O1–U2–O2	52.1(3)	O1–U2–O5	116.2(3)	O1–U2–O6	68.2(3)
O1–U2–O9	118.5(2)	O1–U2–O10	171.3(3)	O1–U2–O13	92.0(4)
O1–U2–O14	87.4(4)	O2–U2–O5	171.1(3)	O2–U2–O6	129.7(3)
O2–U2–O9	66.7(3)	O2–U2–O10	119.3(3)	O2 –U2–O13	88.0(4)
O2–U2–O14	91.6(4)	O5–U2–O6	51.4(3)	O5–U2–O9	122.2(3)
O5–U2–O10	69.5(3)	O5–U2–O13	91.0(4)	O5–U2–O14	89.4(4)
O6–U2–O9	172.9(3)	O6-U2-O10	120.5(3)	O6-U2-O13	87.1(4)
O6 –U2–O14	92.8(4)	O9–U2–O10	52.8(3)	O9–U2–O13	90.3(4)
O9–U2–O14	89.9(4)	O10-U2-O13	92.7(3)	O10-U2-O14	89.7(4)
O13–U2–O14	180.0(4)				

Table S3: Selected interatomic distances (Å) and bond angles (°) for complex 3.

Symmetry transformations used to generate equivalent atoms: #1 = -x, -y+1, -z; #2 = -x+1, -y+1, -z-1; #3 = x-1, y-1, z-1; #4 = x-1, y-1, z-1.

		and and the test (
U101	2.345(5)	U1–O2 ^{#1}	2.326(5)	U1–O5	1.753(6)
U106	1.735(6)	U1–O7	2.470(5)	U1–O8	2.476(5)
U1O13 ^{#2}	2.326(5)	U2–O3 ^{#3}	2.464(5)	U2–O4 ^{#3}	2.471(5)
U2–O9	2.470(5)	U2–O10	2.450(5)	U2–O11	2.458(5)
U2–O12	2.440(5)	U2–O15	1.731(6)	U2–O16	1.734(7)
O1-U1-O2 ^{#1}	84.4(2)	O1–U1–O5	86.7(2)	O1–U1–O6	93.8(2)
O1–U1–O7	148.7(3)	O1–U1–O8	158.7(3)	O1-U1-O13 ^{#2}	76.9(3)
O2 ^{#1} -U1-O5	91.2(2)	O2 ^{#1} -U1-O6	87.1(2)	O2 ^{#1} -U1-O7	127.0(3)
O2 ^{#1} -U1-O8	75.1(3)	O2 ^{#1} -U1-O13 ^{#2}	161.1(2)	O5 –U1–O6	178.1(3)
O5–U1–O7	92.0(2)	O5–U1–O8	88.4(3)	O5–U1–O13 ^{#2}	90.2(3)
O6-U1-O7	88.6(2)	O6–U1–O8	90.5(2)	O6-U1-O13 ^{#2}	91.7(2)
O7–U1–O8	52.2(3)	O7–U1–O13 ^{#2}	71.8(3)	O8–U1–O13 ^{#2}	123.8(3)
O3 ^{#3} -U2-O4 ^{#3}	52.0(3)	O3 ^{#3} –U2–O9	68.3(3)	O3 ^{#3} –U2– O10	120.6(3)
O3 ^{#3} -U2- O11	121.1(3)	O3 ^{#3} –U2 –O12	173.4(3)	O3 ^{#3} -U2-O15	89.5(3)
O3 ^{#3} -U2-O16	89.8(3)	$O4^{#3}-U2-O9$	120.4(3)	O4 ^{#3} -U2-O10	172.5(3)
O4 ^{#3} -U2-O11	69.1(3)	O4 ^{#3} -U2-O12	121.5(3)	O4 ^{#3} -U2-O15	90.0(3)
O4 ^{#3} -U2-O16	89.6(3)	O9–U2–O10	52.2(3)	O9–U2– O11	170.5(3)
O9–U2–O12	118.2(3)	O9–U2–O15	89.3(3)	O9–U2–O16	90.3(3)
O10-U2-O11	118.4(3)	O10-U2-O12	66.0(3)	O10-U2-O15	90.6(3)
O10-U2-O16	89.7(3)	O11-U2-O12	52.5(3)	O11–U2–O15	89.7(3)
O11-U2-O16	90.7(3)	O12–U2–O15	91.7(3)	O12–U2–O16	89.0(3)
O15–U2–O16	179.3(3)				

Table S4: Selected interatomic distances (Å) and bond angles (°) for complex 4.

Symmetry transformations used to generate equivalent atoms: #1 = -x-1, -y, -z; #2 = -x-1, -y+1, -z; #3 = x-1, -y+1/2, z-1/2; #4 = x+1, -y+1/2, z+1/2.

Table 55. Selected interationic distances (A) and bond angles (7) for complex 5.								
U101	2.466(7)	U102		2.4	93(8)	U1-	-O3 ^{#1}	2.475(8)
U1-O4 ^{#1}	2.459(9)	U1–O5	2.4	40(8)	U1-	-06	2.497(9)	
U109	1.915(2)	U1–O10		1.6	525(1)	U2-	-011	2.490(8)
U2–O12	2.454(9)	U2O13 ^{#1}		2.4	62(9)	U2-	O14 ^{#1}	2.456(8)
U2015	2.487(8)	U2–O16		2.4	36(1)	U2-	-019	1.661(1)
U2–O20	1.902(2)							
O1–U1–O2	51.8(3)	O1–U1–O3	O1–U1–O3 ^{#1}		65.7(3) O1–U1–O4 ^{#1}			117.7(3)
O1–U1–O5	118.5(3)	O1–U1–O6		170.	6(3)	01–L	J1–O9	88.7(5)
O1–U1–O10	91.9(5)	O2 –U1–O3	$8^{\#1}$	116.	8(3)	02–L	J1-O4 ^{#1}	169.5(3)
O2–U1–O5	67.1(3)	O2–U1–O6		118.	9(3)	02–L	J1–O9	92.7(5)
O2–U1–O10	87.4(5)	O3 ^{#1} –U1–O	$4^{#1}$	52.	8(3)	O3 ^{#1}	-U1-O5	175.1(4)
O3 ^{#1} -U1-O6	123.5(3)	O3 ^{#1} –U1–O	9	94.	4(5)	O3 ^{#1} -	-U1–O10	86.2(5)
O4 ^{#1} -U1-O5	123.4(3)	O4 ^{#1} –U1–O	6	71.	6(3)	O4 ^{#1} -	-U1–O9	87.1(5)
O4 ^{#1} -U1-O10	92.9(6)	O5–U1–O6		52.	1(4)	05–L	J1–O9	88.2(6)
O5 –U1–O10	91.1(6)	O6–U1–O 9)	91.8(6) O6–U1–O10		J1–O10	87.5(6)	
O9–U1–O10	179.3(4)	O11–U2–O	12	52.1(3) O11–U2–O13 ^{#1}		119.0(3)		
O11-U2-O14 ^{#1}	66.8(3)	O11–U2–O	15	120.0(3) O11–U2–O16		U2–O16	172.0(3)	
O11–U2–O19	93.3(6)	O11–U2–O20		88.	2(5)	O12–	U2013 ^{#1}	170.3(3)
O12-U2-O14 ^{#1}	118.1(3)	O12–U2–O15		68.	8(3)	O12–	U2–O16	120.4(3)
O12–U2–O19	86.6(5)	O12–U2–O20		94.	4(5)	O13#	-U2-O14 ^{#1}	52.5(3)
O13 ^{#1} –U2–O15	120.6(3)	O13 ^{#1} –U2–	016	68.	6(3)	O13#	^l –U2–O19	90.4(6)
O13 ^{#1} -U2-O20	88.7(5)	O14 ^{#1} –U2–	015	173.1(3) O14 ^{#1} –U2–O 16		–U2–O 16	121.0(3)	
O14 ^{#1} –U2–O19	87.5(5)	O14 ^{#1} –U2–	O20	92.	92.8(5) O15-U2-O16		52.1(3)	
O15–U2–O19	92.4(6)	O15–U2–O	20	87.	1(5)	O16-U2-O19		89.1(7)
O16-U2-O20	89.6(6)	O19–U2–O	20	178.	6(5)			
Hydrogen bonding	g contacts							
D-H	d(D–H)	$d(H \cdots A)$	d(D···	·A)	∠DI	ΗA	А	
O7–H7	0.95	1.93	2.88		179		O3 ^{#3}	
O17–H17	0.95	1.76	2.71		180		O11 ^{#4}	
O21-H211	0.85	2.38	3.17		156		O17 ^{#5}	
O21-H212	0.85	2.55	3.06		120		O8 ^{#6}	
O22-H221	0.84	2.23	3.07		180		O20	
O22–H222	0.84	2.16	3.00		178		O2	
N1–H1A	0.86	2.70	3.27		125		O2 ^{#7}	
N2–H2B	0.86	2.94	3.37		113		O8 ^{#8}	
N2–H2B	0.86	1.98	2.77		153		O21	

Table S5: Selected interatomic distances (Å) and bond angles (°) for complex 5.

Symmetry transformations used to generate equivalent atoms: #1 = x+1/2, -y-2, z; #2 = x-1/2, -y-2, z; #3 = x+1/2, -y+1/2, z; #4 = x, y+1, z; #5 = x-1/2, -y+1/2, z; #6 = x-1/2, -y+1/2, z; #7 = -x-3/2, y-1/2, z+1/2; #8 = -x-1/2, y+1/2, z+1/2.

Table 56: Selected interatomic distances (A) and bond angles (*) for complex 6.							
U1–O1	2.46	8(5) U1-	-02	2.405(5)	U1O3 ^{#1}	2.480(5)	
U1-O4 ^{#1}	2.44	1(5) U1-	-05	2.496(5)	U1–O6	2.436(5)	
U1–O9	1.743	3(6) U1-	-O10	1.721(6)			
O1–U1–O2	61.	6(3) 01-	-U1-O3	118.1(3)	O1–U1–O4	67.8(3)	
01–U1–O5	121.4	4(4) 01-	-U1-O6	173.4(3)	O1–U1–O9	87.0(6)	
O1–U1–O10	94.:	5(6) O2-	-U1-O3 ^{#1}	167.6(3)	O2 –U1–O4 ^{#1}	116.5(3)	
O2 –U1–O5	70.0	O(3) O2	-U1-O6	122.4(3)	O2 –U1–O9	93.3(5)	
O2–U1–O10 87.1(5) O3 ^{#1}		^{#1} -U1-O4 ^{#1}	53.4(3)	O3 ^{#1} -U1-O5	120.5(3)		
O3 ^{#1} –U1–O6 62.3(3)		3(3) 03-	93–U1–O9 92.9(5)		O3–U1–O10	87.0(5)	
O4 ^{#1} -U1-O5 171.6(4)		6(4) O4	^{#1} –U1–O6	120.6(3)	O4 ^{#1} -U1-O9	92.7(3)	
O4 ^{#1} –U1–O10 88		6(5) O5-	-U1-O6	53.4(3)	O5–U1–O9	92.1(5)	
O5–U1–O10 86.5(5)		5(5) 06	-U1-O9	87.5(5)	O6-U1-O10	90.1(5)	
O9–U1–O10 178.3(6)		3(6)					
Hydrogen bonding contacts							
D–H	d(D–H)	d(H···A	a) $d(D \cdots A)$	∠DHA	А		
C33–H33A	0.93	2.48	3.14	128	O5		
C36–H36A	0.93	2.23	3.08	152	O3 ^{#3}		
C25-H25A	0.93	2.55	3.47	171	O3 ^{#4}		

Table S6: Selected interatomic distances (Å) and bond angles (°) for complex 6.

Symmetry transformations used to generate equivalent atoms: #1 = x, -y+1/2, z+1/2;#2 = x, -y+1/2, z-1/2; #3 = x, y+1, z; #4 = -x+1, -y, -z+1.

Table S7: The number of active sites for complexes **1–6.** (Based on the volume of the complex **3**)

Complexes	1	2	3	4	5	6
Volume	11201(4)	5263.0(5)	2472.5(9)	5221.9(19)	6006(2)	3044.6(15)
The number of active sites in the unit cell	16	10	4	10	8	4
The number of active sites (Based on the volume of the complex 3)	3.5	5	4	5	3	2