Supplementary materials

A family of 3D UO_2^{2+}–5-X-1,3-dicarboxylate (X = –H, –NO_2, –NH_2, –OH) hybrid materials: structural relevance with a variation of substituent group and photochemical properties

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Figure S1. The experimental and the simulated XRD patterns based on the structural analysis for **2** and **4**.

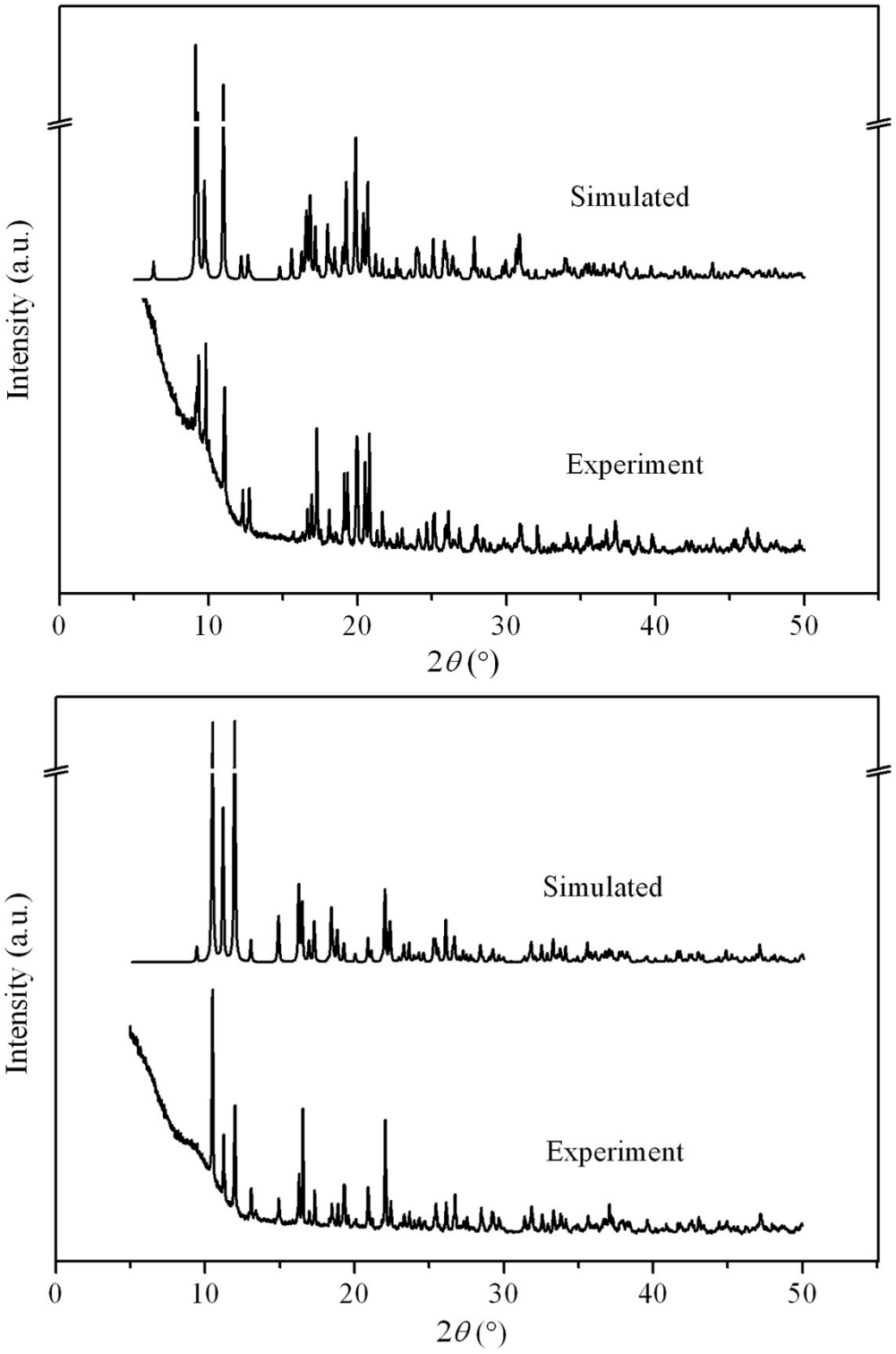

Figure S2. The IR spectrum for complexes **2** and **4** and the bulk products of compounds **1** and **3**.

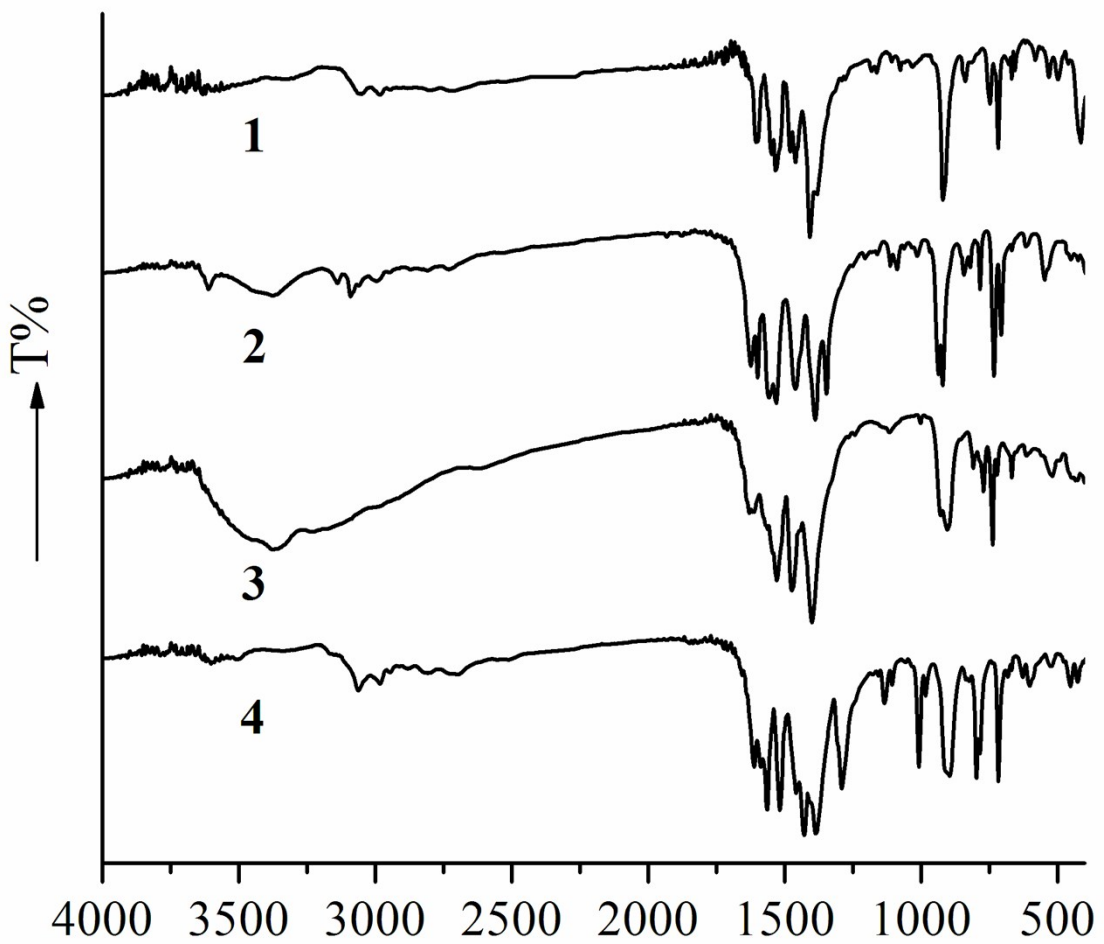

Figure S3. (a) 3D architecture of **1** viewed in [110] direction. (b) Schematic view of the net topology of **1** viewed in [110] direction. (c) 3D architecture of **1** viewed in [001] direction. (b) Schematic view of the net topology of **1** viewed in [001] direction.

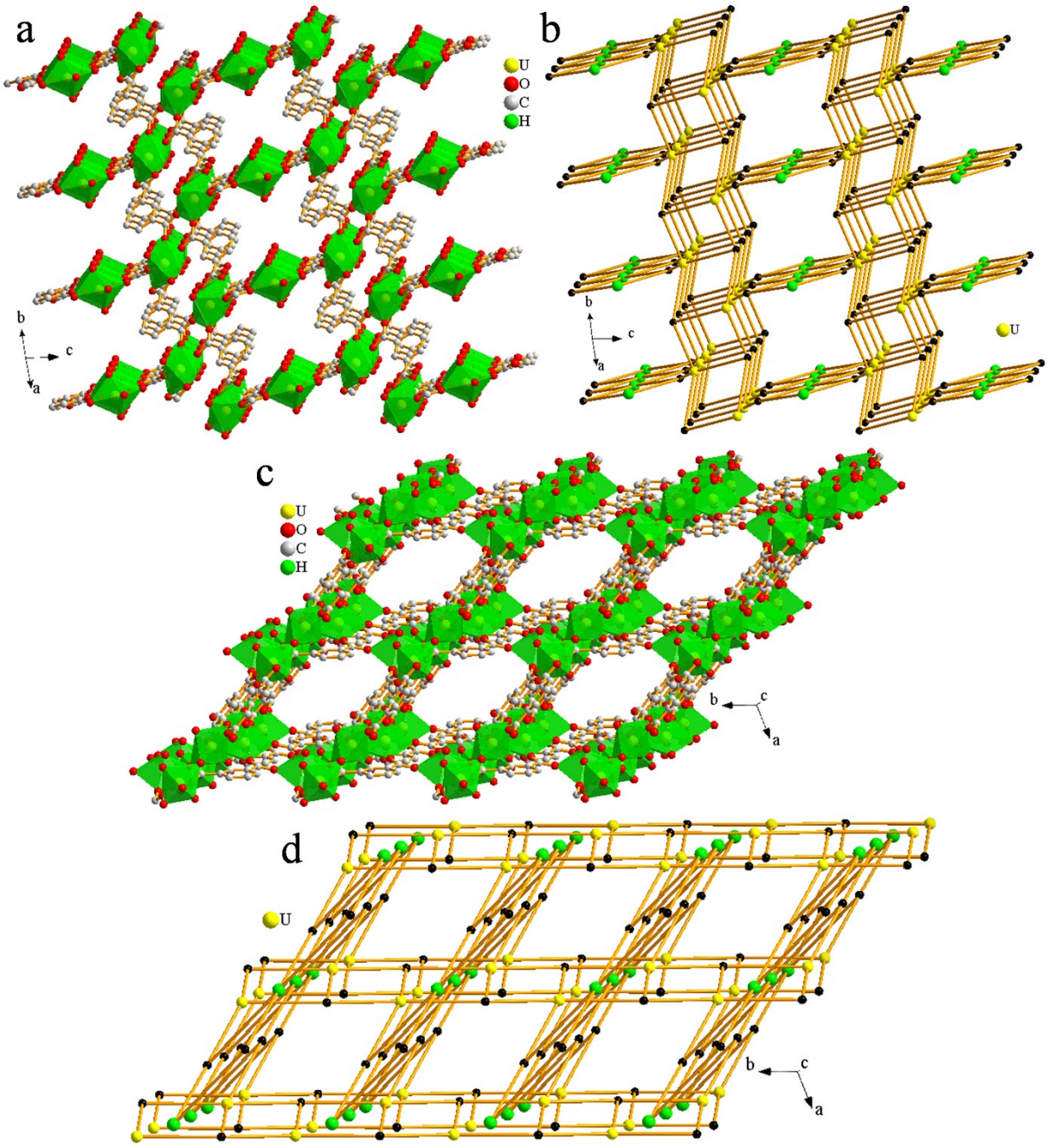

Figure S4. (a) 3D architecture of **2** viewed in [110] direction. (b) 3D architecture of **2** viewed in [001] direction.

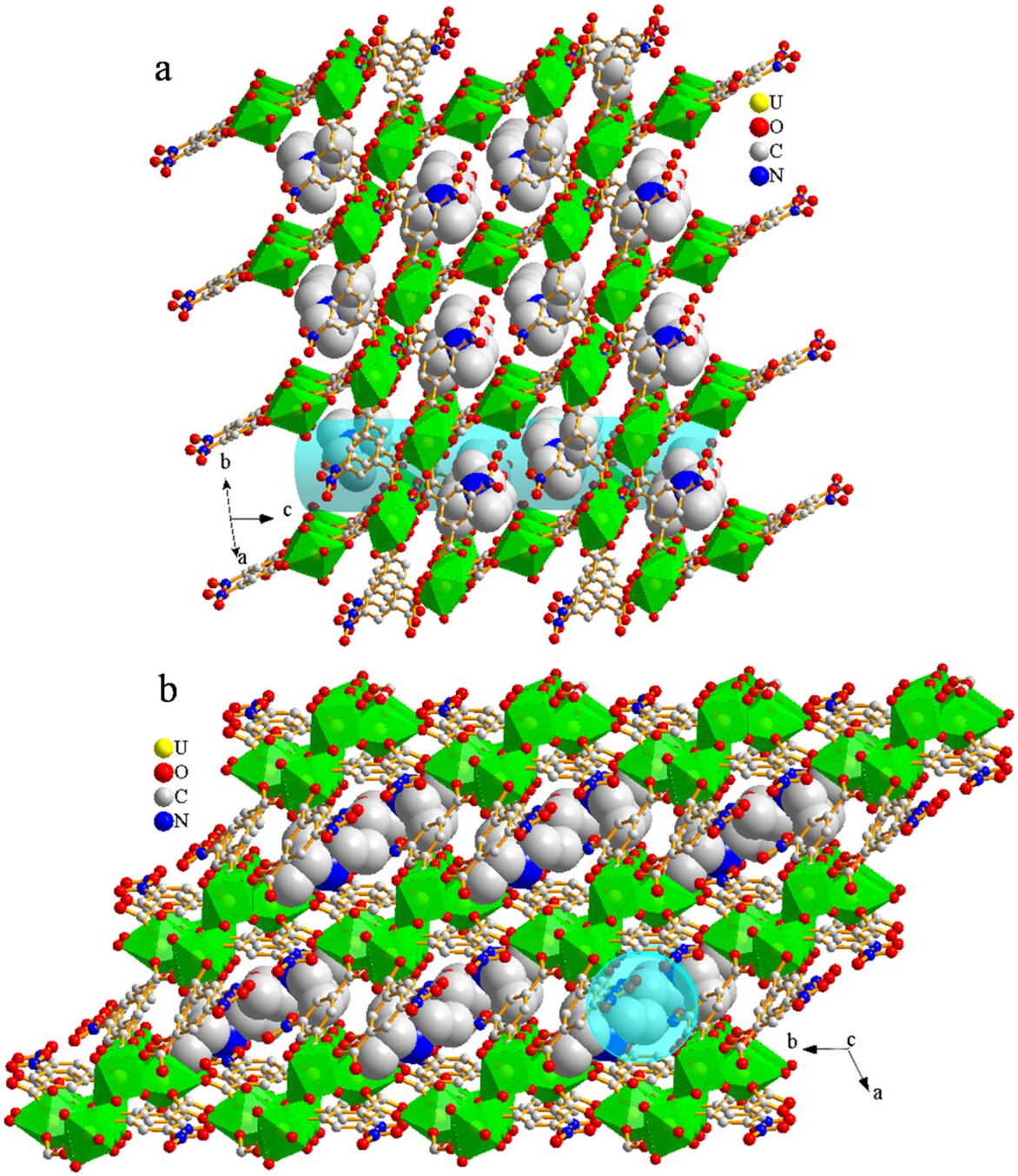

Figure S5. (a) 3D architecture of **3** viewed in [110] direction. (b) 3D architecture of **3** viewed in [001] direction.

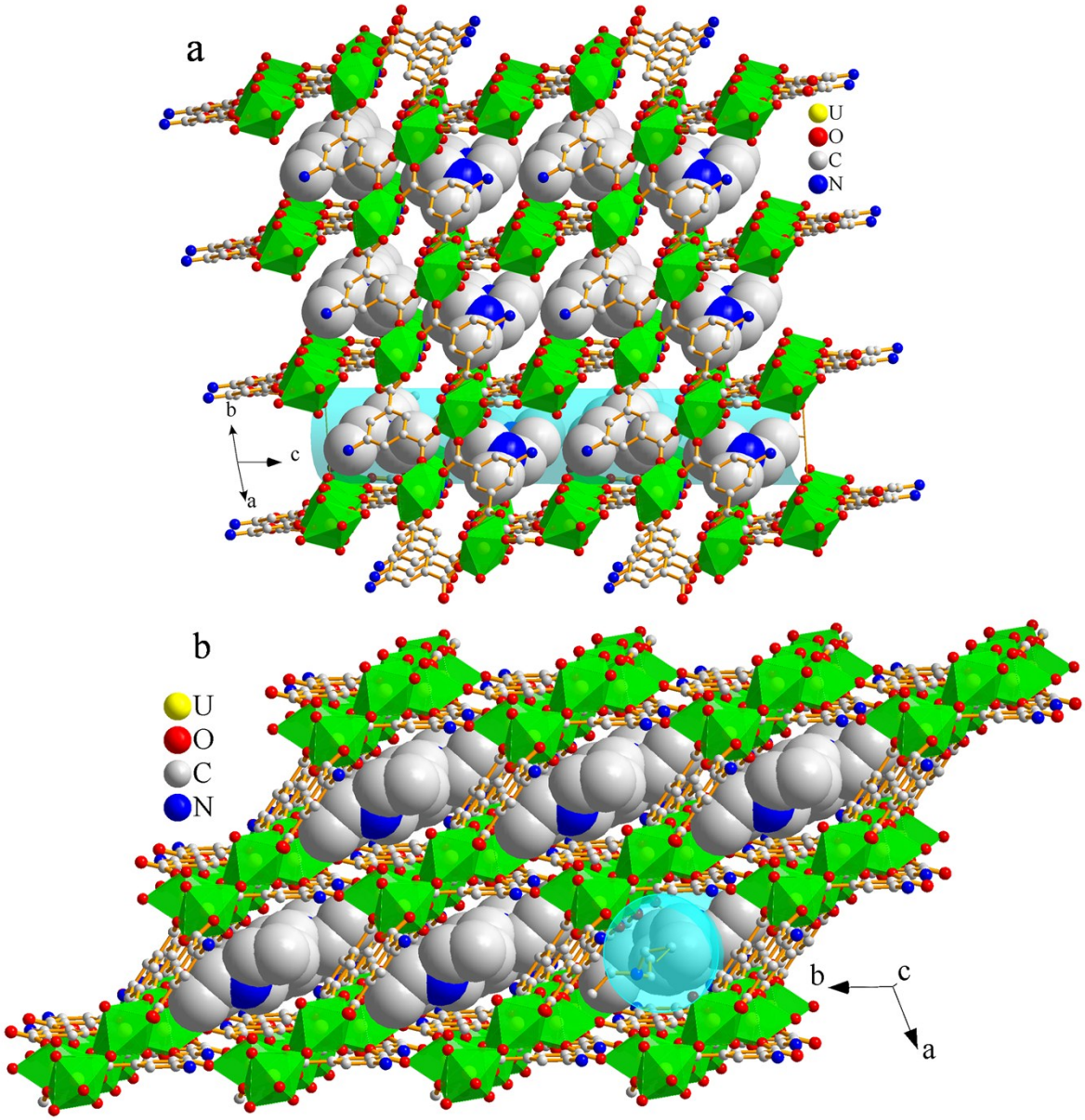

Figure S6. (a) 3D architecture of **4** viewed in [010] direction. (b) 3D architecture of **4** viewed in [001] direction. (c) Schematic view of the net topology of **4** viewed in [010] direction. (b) Schematic view of the net topology of **4** viewed in [001] direction.

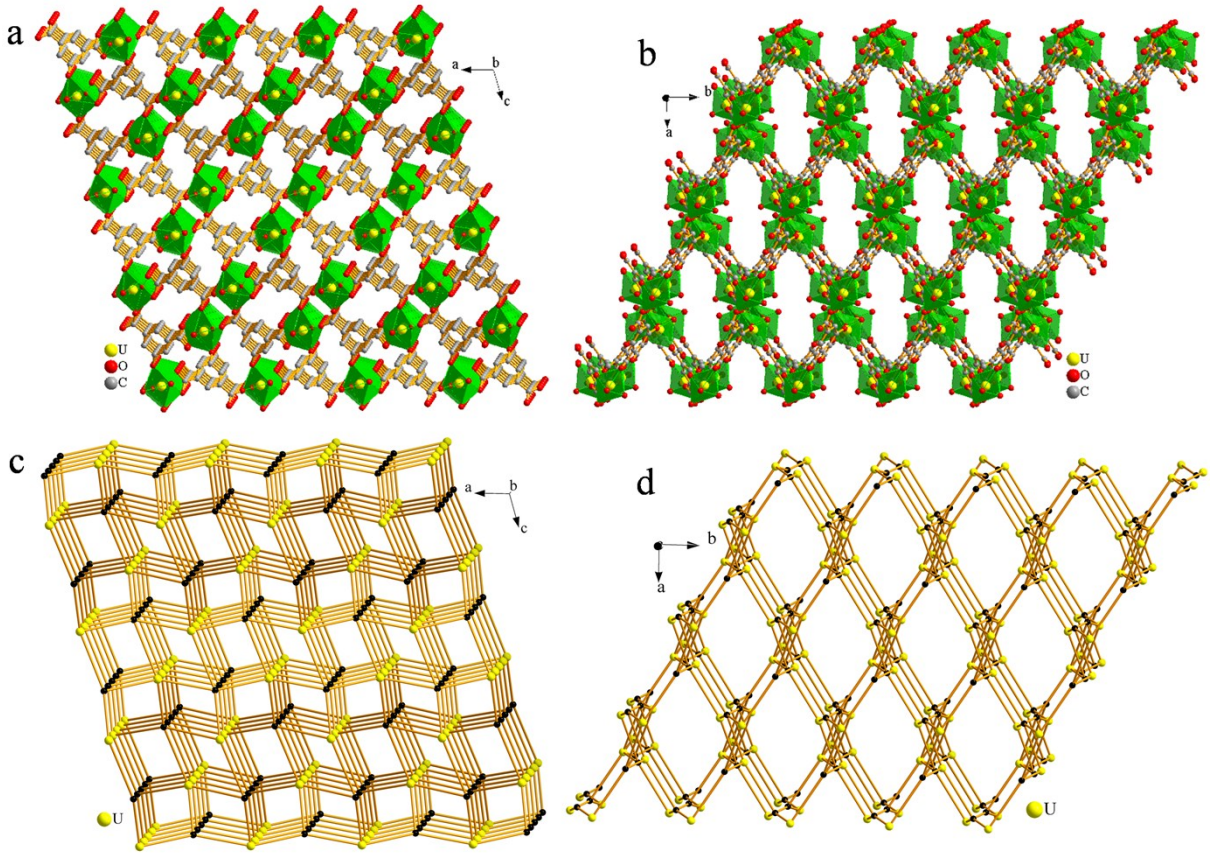

Figure S7. Solid-state reflectance spectra for **2** and **4**.

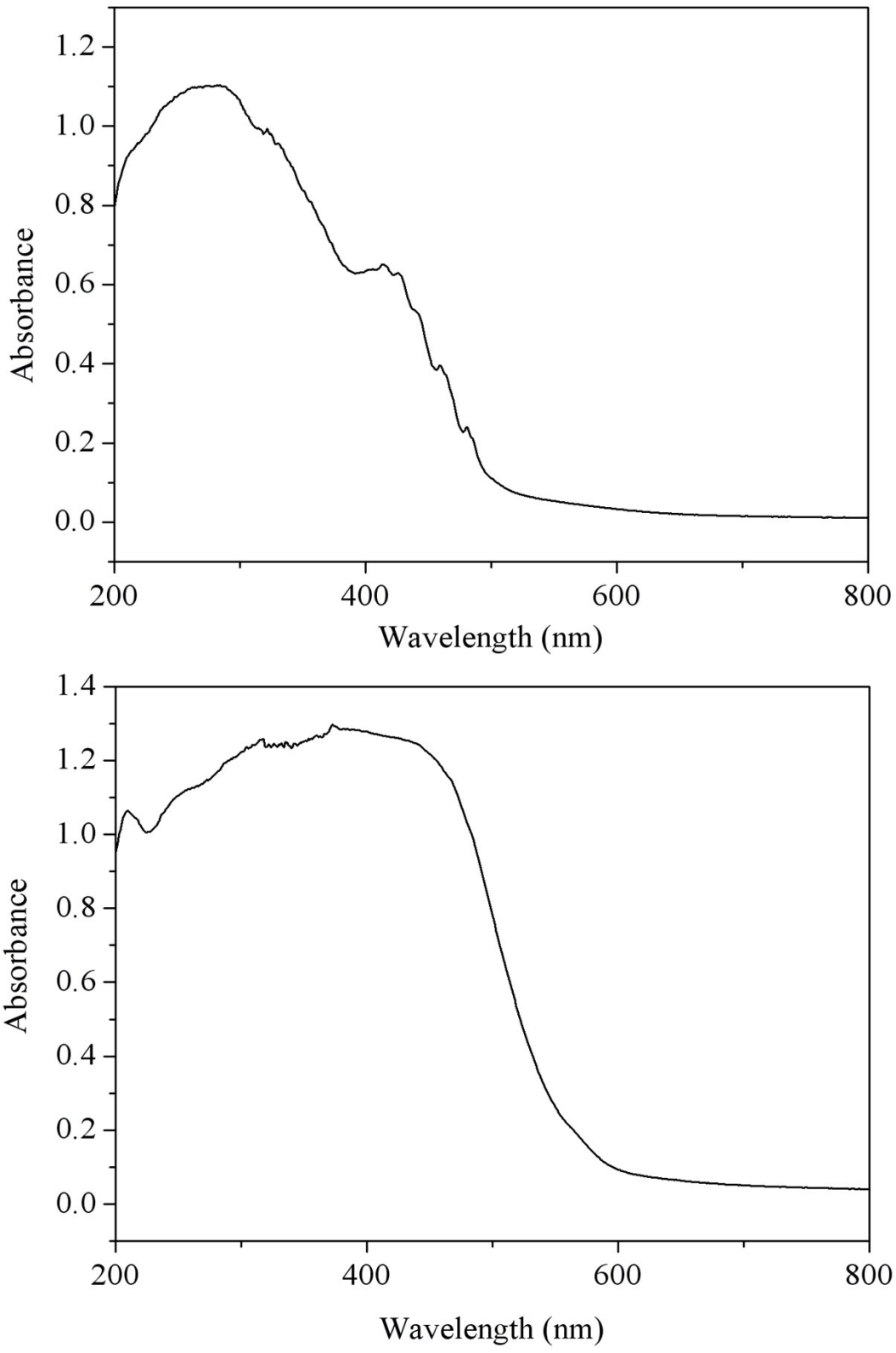

Figure S8. Absorption spectra of the RhB solution during the decomposition reaction with the use of complex **2** upon irradiation of 700 W xenon lamp.

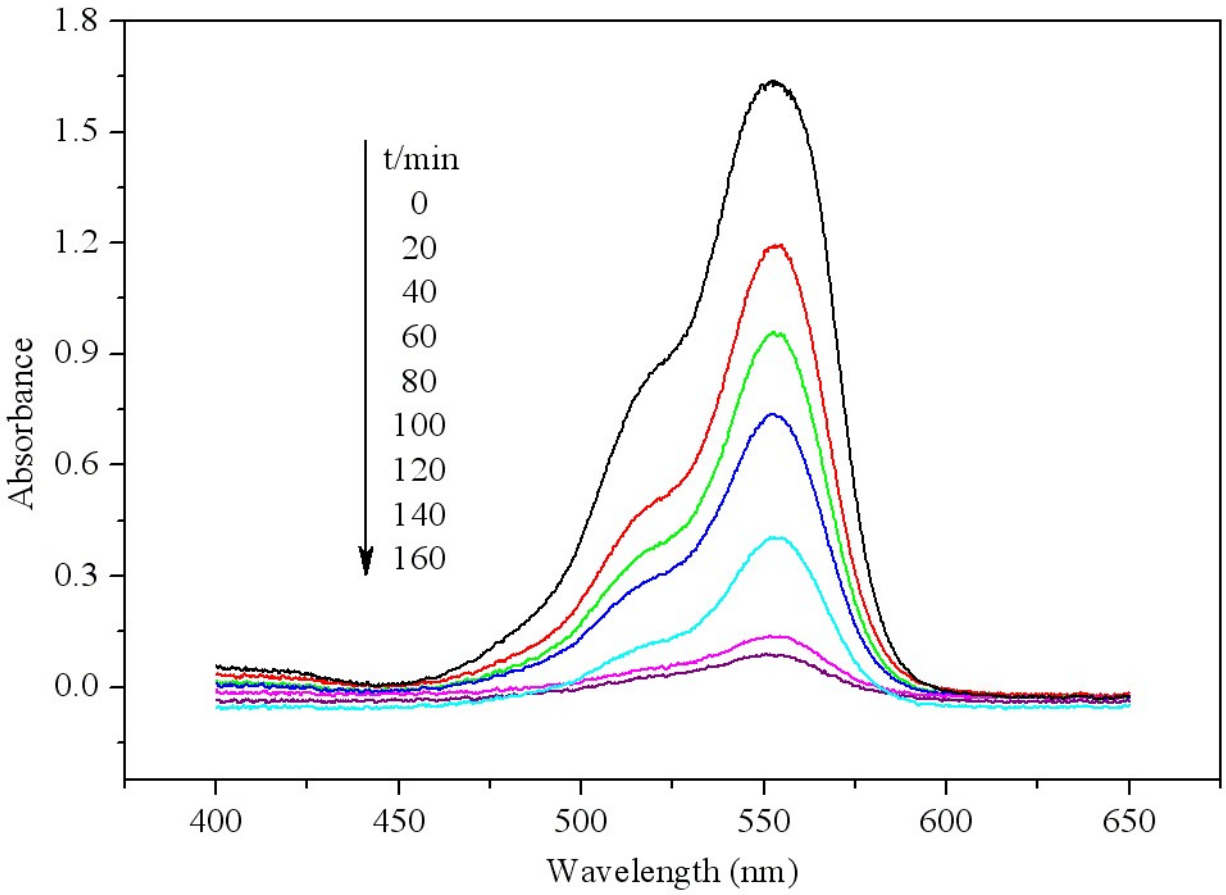

Figure S9. Absorption spectra of the RhB solution during the decomposition reaction with the use of complex **2** upon irradiation of 300 W xenon lamp.

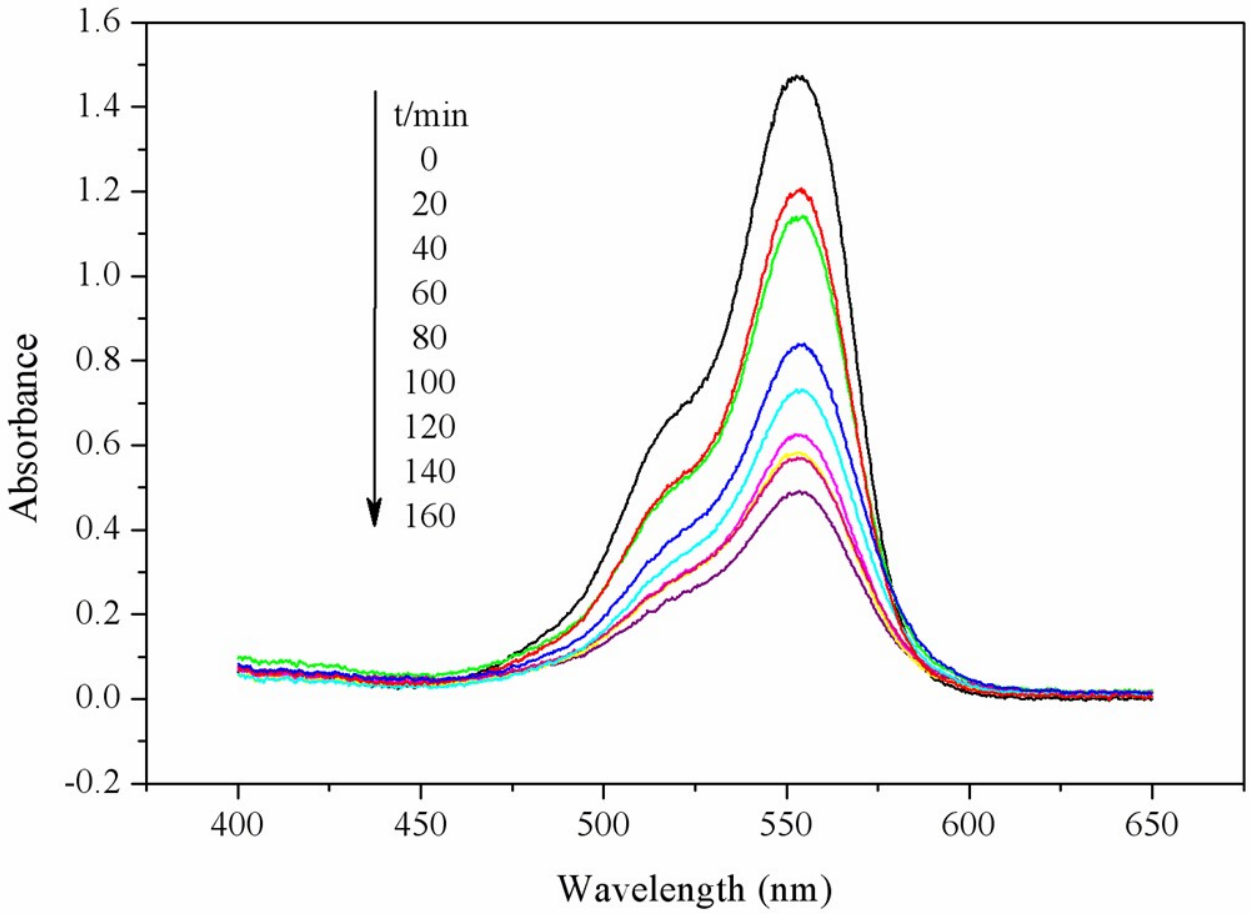

Table S1 Selected Interatomic Distances (Å) and Bond Angles (°) for **1**[a]

U1–O1	1.734(8)	U1–O6$^{\#2}$	2.304(10)	U2–O9$^{\#3}$	2.334(9)
U1–O2	1.717(11)	U1–O12	2.301(9)	U2–O10	2.457(9)
U1–O3	2.453(7)	U2–O7	1.730(13)	U2–O11	2.458(9)
U1–O4	2.449(8)	U2–O8	1.746(12)	U2–O13$^{\#4}$	2.314(13)
U1–O5$^{\#1}$	2.322(9)	U2–O9	2.321(8)		
O1–U1–O2	179.3(5)	O3–U1–O12	74.8(3)	O8–U2–O9$^{\#3}$	91.1(5)
O1–U1–O3	86.5(4)	O4–U1–O5$^{\#1}$	154.4(3)	O8–U2–O10	90.7(4)
O1–U1–O4	90.3(4)	O4–U1–O6$^{\#2}$	73.7(3)	O8–U2–O11	90.2(5)
O1–U1–O5$^{\#1}$	87.8(4)	O4–U1–O12	127.9(3)	O8–U2–O13$^{\#4}$	91.1(6)
O1–U1–O6$^{\#2}$	88.7(4)	O5$^{\#1}$–U1–O6$^{\#2}$	80.7(3)	O9–U2–O9$^{\#3}$	70.1(4)
O1–U1–O12	92.6(4)	O5$^{\#1}$–U1–O12	77.8(3)	O9–U2–O10	73.8(3)
O2–U1–O3	94.0(4)	O6$^{\#2}$–U1–O12	158.3(3)	O9–U2–O11	126.4(3)
O2–U1–O4	89.5(4)	O7–U2–O8	177.1(5)	O9–U2–O13$^{\#4}$	152.9(4)
O2–U1–O5$^{\#1}$	92.1(4)	O7–U2–O9	91.4(5)	O9$^{\#3}$–U2–O10	143.9(3)
O2–U1–O6$^{\#2}$	90.6(5)	O7–U2–O9$^{\#3}$	90.2(5)	O9$^{\#3}$–U2–O11	163.4(3)
O2–U1–O12	88.1(5)	O7–U2–O10	89.9(5)	O9$^{\#3}$–U2–O13$^{\#4}$	82.9(4)
O3–U1–O4	53.5(3)	O7–U2–O11	87.9(5)	O10–U2–O11	52.6(3)
O3–U1–O5$^{\#1}$	151.6(3)	O7–U2–O13$^{\#4}$	86.5(6)	O10–U2–O13$^{\#4}$	133.1(4)
O3–U1–O6$^{\#2}$	126.9(3)	O8–U2–O9	91.5(4)	O11–U2–O13$^{\#4}$	80.6(4)

[a] Symmetry codes: #1 = x, y–1, z; #2 = –x+2, –y+1, –z; #3 = –x, –y–1, –z+1; #4 = –x+1, –y, –z+1.

Table S2 Selected Interatomic Distances (Å) and Bond Angles (°) for **2**[a]

U1–O1	1.778(5)	U1–O6$^{\#2}$	2.362(4)	U2–O13	2.445(4)
U1–O2	1.779(5)	U1–O11	2.333(4)	U2–O14	2.492(4)
U1–O3	2.455(4)	U2–O9	1.781(5)	U2–O17	2.320(4)
U1–O4	2.472(4)	U2–O10	1.780(5)	U2–O17$^{\#4}$	2.350(4)
U1–O5$^{\#1}$	2.304(4)	U2–O12$^{\#3}$	2.331(4)		
O1–U1–O2	179.2(2)	O3–U1–O11	73.0(1)	O10–U2–O13	88.4(2)
O1–U1–O3	89.5(2)	O4–U1–O5$^{\#1}$	75.0(2)	O10–U2–O14	92.5(2)
O1–U1–O4	89.7(2)	O4–U1–O6$^{\#2}$	158.3(1)	O10–U2–O17	89.0(2)
O1–U1–O5$^{\#1}$	90.4(2)	O4–U1–O11	125.6(1)	O10–U2–O17$^{\#4}$	91.2(2)
O1–U1–O6$^{\#2}$	88.5(2)	O5$^{\#1}$–U1–O6$^{\#2}$	83.4(2)	O12$^{\#3}$–U2–O13	77.8(1)
O1–U1–O11	93.3(2)	O5$^{\#1}$–U1–O11	159.1(2)	O12$^{\#3}$–U2–O14	131.0(1)
O2–U1–O3	90.9(2)	O6$^{\#2}$–U1–O11	76.1(1)	O12$^{\#3}$–U2–O17	150.8(1)
O2–U1–O4	90.0(2)	O9–U2–O10	179.2(2)	O12$^{\#3}$–U2–O17$^{\#4}$	80.1(1)
O2–U1–O5$^{\#1}$	88.6(2)	O9–U2–O12$^{\#3}$	91.6(2)	O13–U2–O14	53.3(1)
O2–U1–O6$^{\#2}$	91.6(2)	O9–U2–O13	91.0(2)	O13–U2–O17	131.2(1)
O2–U1–O11	87.6(2)	O9–U2–O14	87.3(2)	O13–U2–O17$^{\#4}$	157.9(1)
O3–U1–O4	52.8(1)	O9–U2–O17	91.7(2)	O14–U2–O17	78.2(1)
O3–U1–O5$^{\#1}$	127.8(1)	O9–U2–O17$^{\#4}$	89.4(2)	O14–U2–O17$^{\#4}$	148.8(1)
O3–U1–O6$^{\#2}$	148.8(1)	O10–U2–O12$^{\#3}$	88.0(2)	O17–U2–O17$^{\#4}$	70.9(2)

Hydrogen bonding contacts

D–H	d(D–H)	d(H⋯A)	∠DHA	d (D⋯A)	A
O17–H171	0.66	2.15	156	2.764	O3$^{\#5}$
O18–H181	0.84	2.27	149	3.020	O8$^{\#6}$
O18–H182	0.84	2.09	176	2.927	O17$^{\#7}$
N3–H31	0.86	1.91	168	2.761	O18

[a] Symmetry codes: #1 = –x+1, –y+1, –z+2; #2 = x, y+1, z; #3 = –x+2, –y+2, –z+1; #4 = –x+3, –y+3, –z+1; #5 = x+1, y+1, z; #6 = –x+1, –y+1, –z+1; #7 = x–1, y–1, z.

Table S3 Selected Interatomic Distances (Å) and Bond Angles (°) for **3**[a]

U1–O1	1.702(9)	U1–O6$^{\#2}$	2.314(7)	U2–O10	2.441(9)
U1–O2	1.727(9)	U1–O12	2.326(8)	U2–O11$^{\#3}$	2.335(9)
U1–O3	2.463(8)	U2–O7	1.744(10)	U2–O13	2.329(8)
U1–O4	2.439(7)	U2–O8	1.725(11)	U2–O13$^{\#4}$	2.319(8)
U1–O5$^{\#1}$	2.335(9)	U2–O9	2.474(8)		
O1–U1–O2	179.0(4)	O3–U1–O12	74.9(3)	O8–U2–O10	89.7(4)
O1–U1–O3	86.0(3)	O4–U1–O5$^{\#1}$	73.5(3)	O8–U2–O11$^{\#3}$	92.1(4)
O1–U1–O4	91.1(3)	O4–U1–O6$^{\#2}$	153.6(3)	O8–U2–O13	92.6(4)
O1–U1–O5$^{\#1}$	90.5(4)	O4–U1–O12	127.3(3)	O8–U2–O13$^{\#4}$	89.6(4)
O1–U1–O6$^{\#2}$	89.7(4)	O5$^{\#1}$–U1–O6$^{\#2}$	79.1(3)	O9–U2–O10	52.3(3)
O1–U1–O12	93.0(3)	O5$^{\#1}$–U1–O12	158.8(3)	O9–U2–O11$^{\#3}$	80.8(3)
O2–U1–O3	93.1(4)	O6$^{\#2}$–U1–O12	79.9(3)	O9–U2–O13	164.9(3)
O2–U1–O4	88.1(3)	O7–U2–O8	177.7(4)	O9–U2–O13$^{\#4}$	125.7(3)
O2–U1–O5$^{\#1}$	89.9(4)	O7–U2–O9	90.4(4)	O10–U2–O11$^{\#3}$	133.0(3)
O2–U1–O6$^{\#2}$	91.3(4)	O7–U2–O10	90.7(4)	O10–U2–O13	142.7(3)
O2–U1–O12	88.0(4)	O7–U2–O11$^{\#3}$	86.0(4)	O10–U2–O13$^{\#4}$	73.4(3)
O3–U1–O4	52.9(3)	O7–U2–O13	88.5(4)	O11$^{\#3}$–U2–O13	84.1(3)
O3–U1–O5$^{\#1}$	126.1(3)	O7–U2–O13$^{\#4}$	92.6(4)	O11$^{\#3}$–U2–O13$^{\#4}$	153.5(3)
O3–U1–O6$^{\#2}$	153.4(3)	O8–U2–O9	88.1(4)	O13–U2–O13$^{\#4}$	69.4(4)

Hydrogen bonding contacts

D–H	d(D–H)	d(H⋯A)	∠DHA	d (D⋯A)	A
N1–H12	0.86	2.51	145	3.248	O7$^{\#5}$
N1–H13	0.86	2.58	142	3.308	O11$^{\#6}$
N2–H22	0.86	2.62	118	3.115	O2$^{\#7}$
O13–H132	0.84	2.46	180	3.304	O3$^{\#8}$

[a] Symmetry codes: #1 = –x–3, –y–3, –z+1; #2 = x, y+1, z; #3 = –x–2, –y–2, –z; #4 = –x–1, –y–1, –z; #5 = x–1, y–1, z; #6 = x, y–1, z; #7 = –x+1, –y+1, –z+1; #8 = –x+1, –y+1, –z.

Table S4 Selected Interatomic Distances (Å) and Bond Angles (°) for **4**[a]

U–O1	1.766(13)	U–O4$^{\#1}$	2.450(8)	U–O9	2.323(9)
U–O2	1.763(13)	U–O5$^{\#2}$	2.478(10)		
U–O3	2.250(8)	U–O6$^{\#2}$	2.347(11)		
O1–U–O2	179.7(5)	O2–U–O4$^{\#1}$	89.8(5)	O3–U–O7$^{\#3}$	82.7(3)
O1–U–O3	89.4(4)	O2–U–O5$^{\#1}$	88.2(6)	O4$^{\#1}$–U–O5$^{\#2}$	52.5(3)
O1–U–O4$^{\#1}$	90.2(5)	O2–U–O6$^{\#2}$	91.0(5)	O4$^{\#1}$–U–O6$^{\#2}$	124.8(3)
O1–U–O5$^{\#1}$	92.0(5)	O2–U–O7$^{\#3}$	90.0(5)	O4$^{\#1}$–U–O7$^{\#3}$	156.8(3)
O1–U–O6$^{\#2}$	89.3(5)	O3–U–O4$^{\#1}$	74.2(3)	O5$^{\#2}$–U–O6$^{\#2}$	72.3(3)
O1–U–O7$^{\#3}$	90.0(5)	O3–U–O5$^{\#1}$	126.7(3)	O5$^{\#2}$–U–O7$^{\#3}$	150.6(3)
O2–U–O3	90.3(5)	O3–U–O6$^{\#2}$	131.0(4)	O6$^{\#2}$–U–O7$^{\#3}$	78.4(4)
Hydrogen bonding contacts					
D–H	d(D–H)	d(H···A)	∠DHA	d (D···A)	A
O6–H61	0.84	2.01	177	2.847	O5$^{\#4}$
O8–H81	0.84	2.09	160	2.898	O3

[a] Symmetry codes: #1 = –x+0.5, y+0.5, –z+0.5; #2 = x, 1–y, z–0.5; #3 = –x, y, –z+0.5; #4= –x+0.5, –y+0.5, –z+1.