Electronic Supplementary Information

Thorium(IV) and Uranium(VI) Compounds with Cucurbit[10]uril: From One-Dimensional Nanotube to Supramolecular Framework

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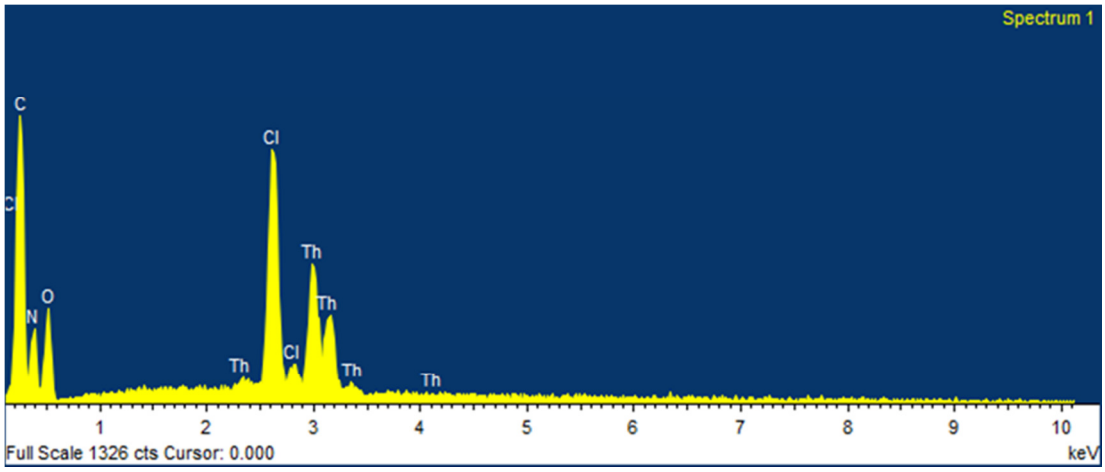
(a)



(b)

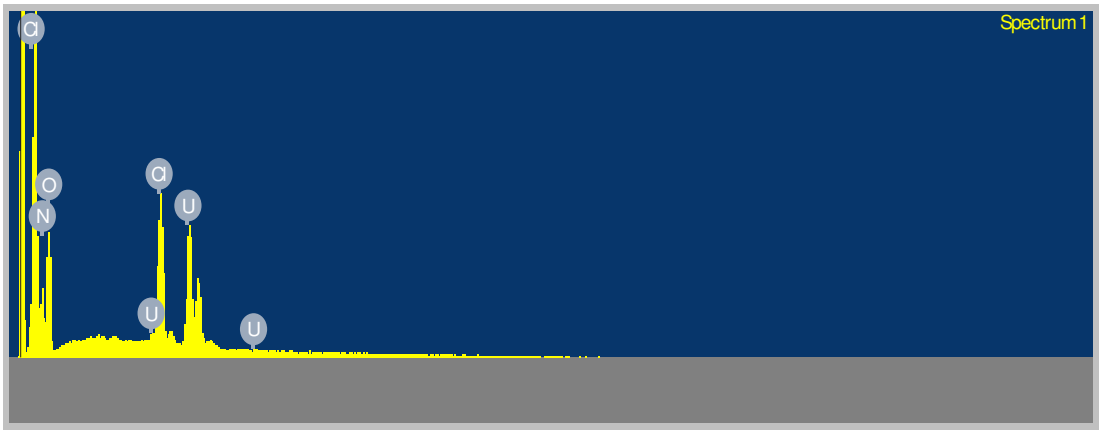
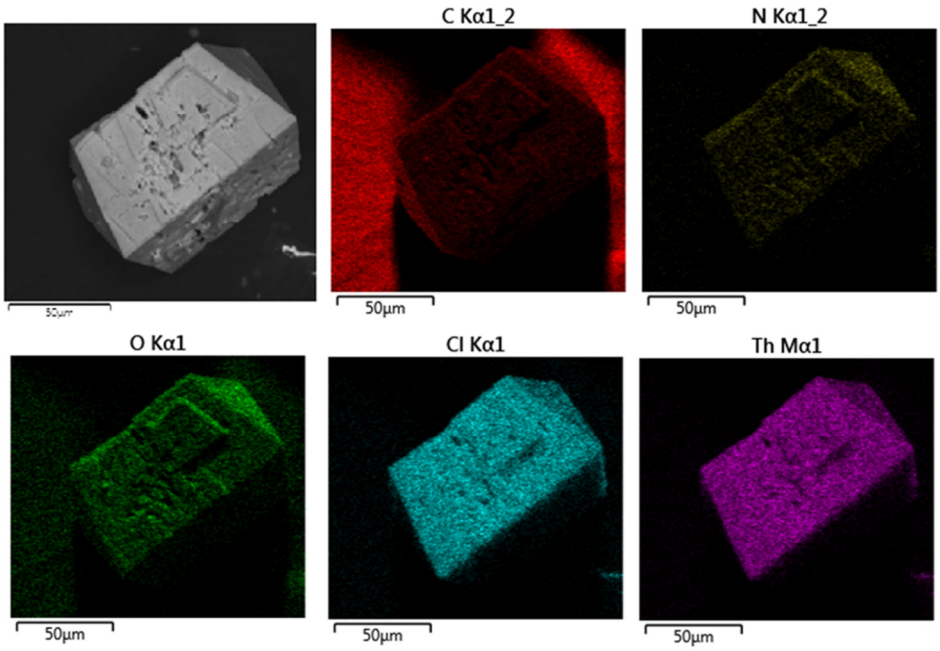
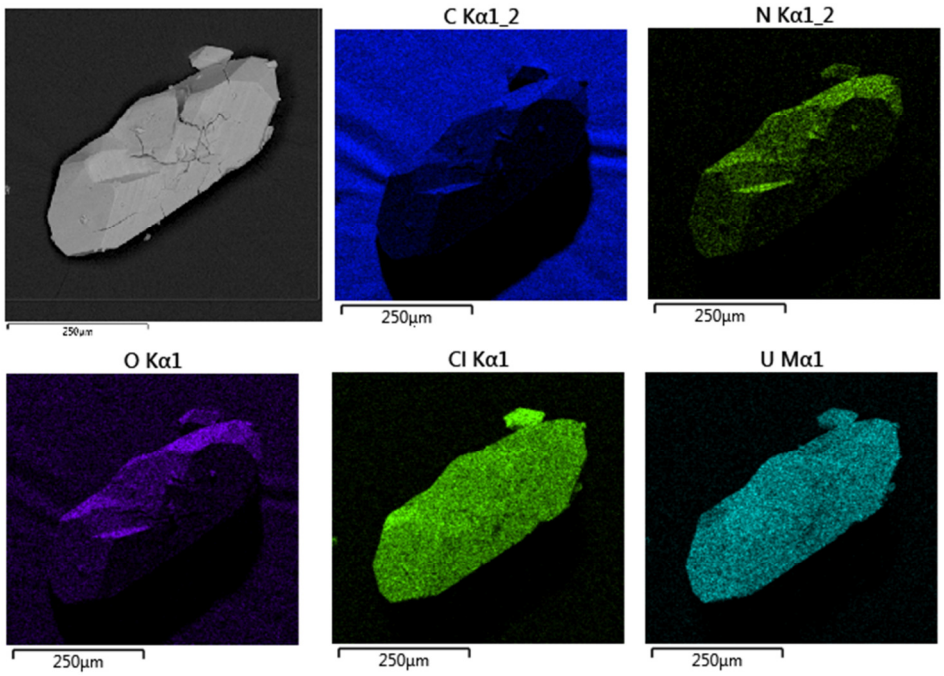


Fig. S1. EDS spectra of compounds **Q[10]-Th** (a) and **Q[10]-U** (b) showing the presence of key elements C, N, O, Cl and Th/U.



(a)



(b)

Fig. S2. EDS element mappings of compounds **Q[10]-Th** (a) and **Q[10]-U** (b).

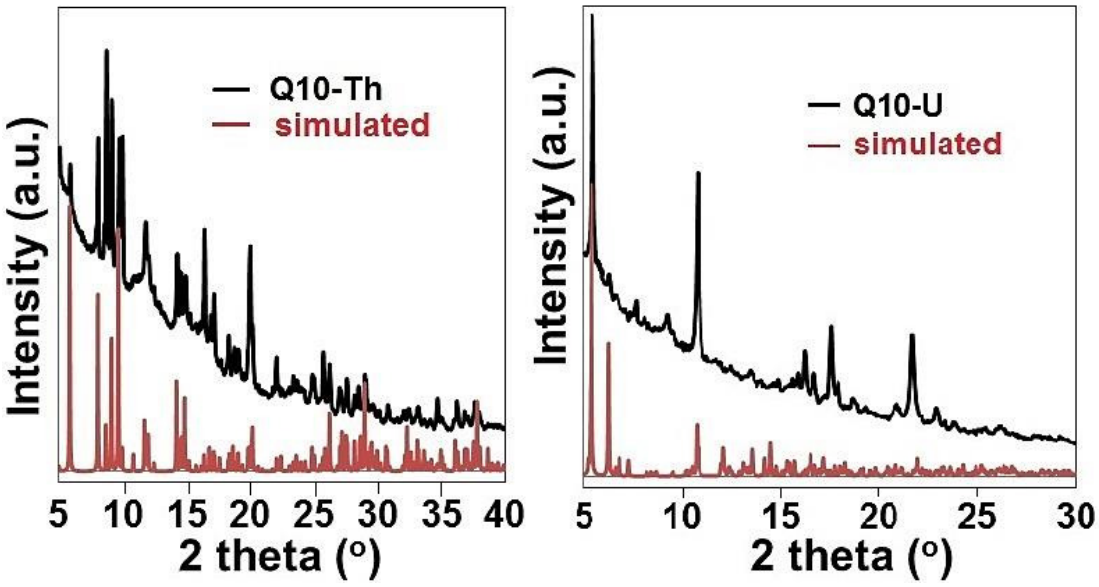


Fig. S3. Powder X-ray diffraction patterns for compounds **Q[10]-Th** and **Q[10]-U** with the measured patterns on top of the simulated patterns from the single crystal data.

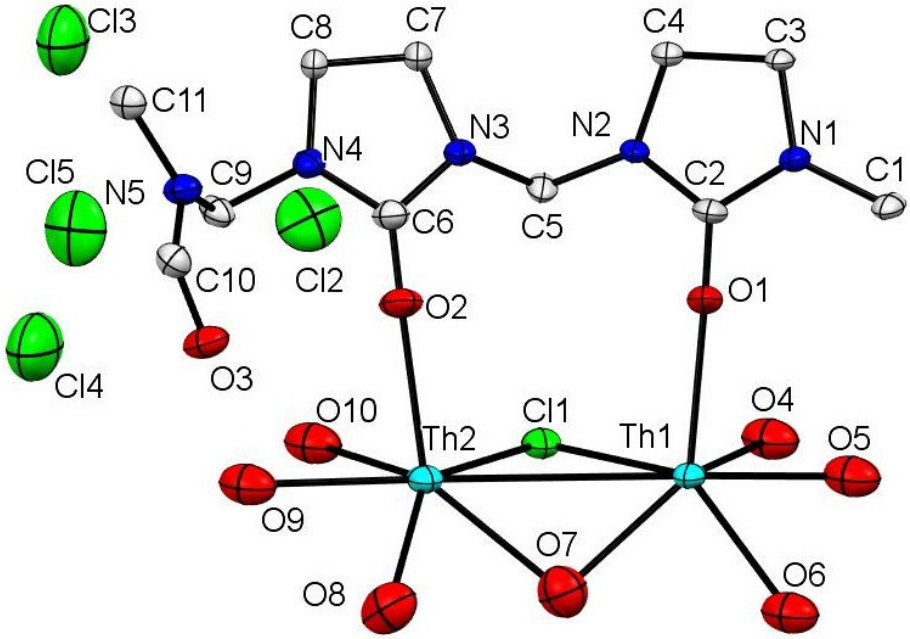


Fig. S4. ORTEP drawing (50% ellipsoid) of the asymmetric unit of compound **Q[10]-Th**.

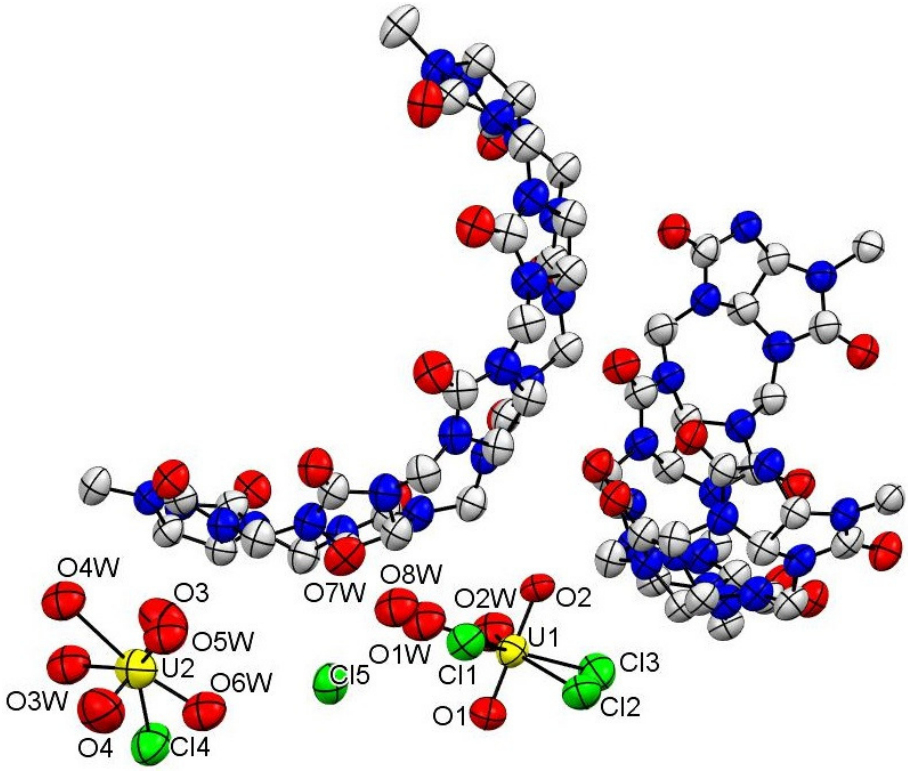


Fig. S5. ORTEP drawing (50% ellipsoid) of the asymmetric unit of compound **Q[10]-U**.

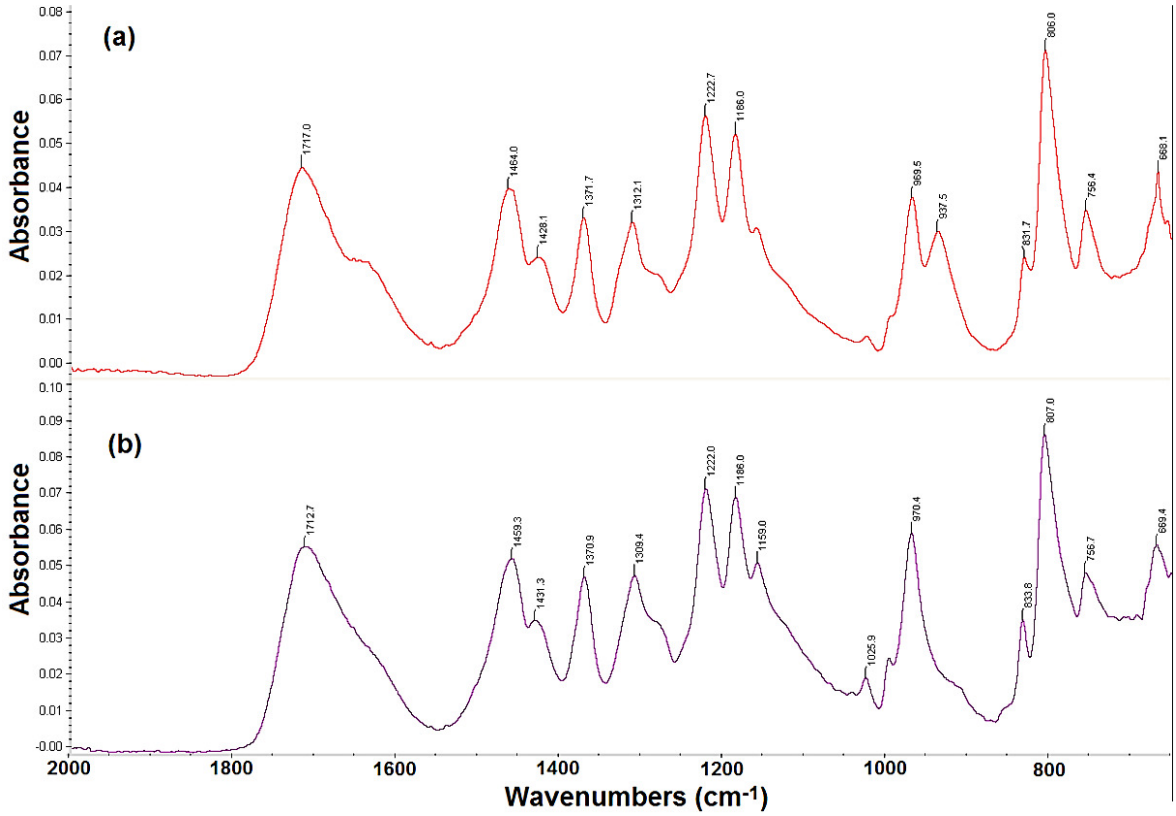


Fig. S6. FTIR spectra of compounds **Q[10]-Th** (b) and **Q[10]-U** (a) showing distinctive asymmetric uranyl vibrations at 937.5 cm^{-1} for **Q[10]-U**.

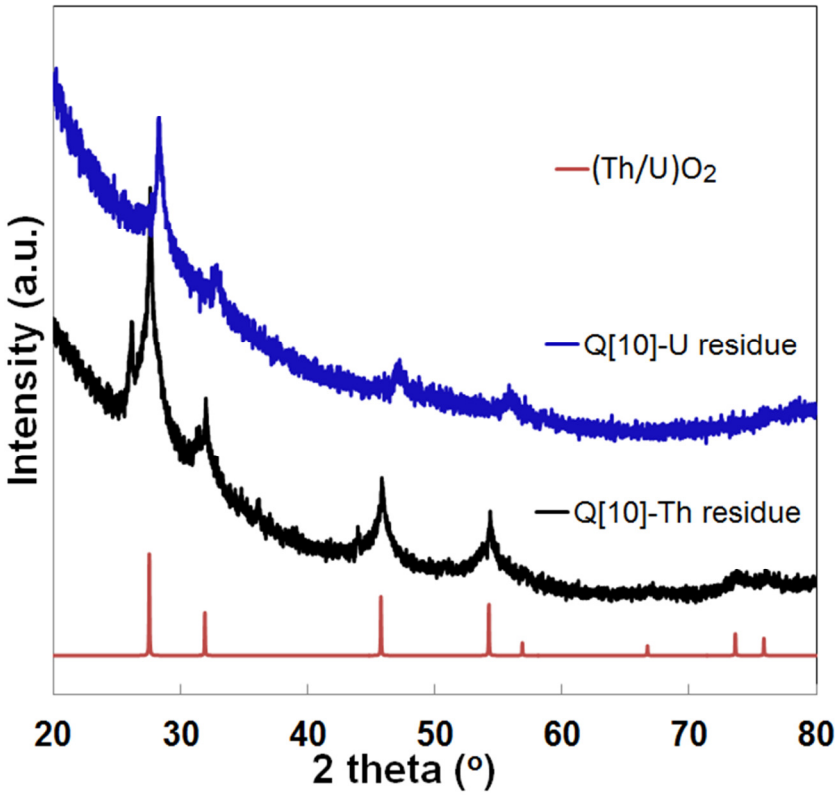


Fig. S7. Powder XRD patterns of the residues of compounds **Q[10]-Th** and **Q[10]-U** after TG test.

Table S1. Crystal data and structure refinement for **Q[10]-Th** and **Q[10]-U**.

Compound	**Q[10]-Th**	**Q[10]-U**
Empirical formula	$C_{30}H_{30}Cl_8N_{20}O_{20.5}Th_2$	$C_{30}H_{36}Cl_{2.5}N_{20}O_{16}U$
Formula weight	1746.42	1259.44
Temperature/K	100(2)	100(2)
Crystal system	orthorhombic	triclinic
Space group	*Immm*	*P*-1
a/Å	10.812(2)	17.212(3)
b/Å	21.943(4)	19.456(4)
c/Å	30.221(6)	21.391(4)
α/°	90	66.03(3)
β/°	90	86.24(3)
γ/°	90	72.18(3)
Volume/Å^3	7170(2)	6217(3)
Z	4	4
ρ_{calc}g/cm^3	1.618	1.345
μ/mm^{-1}	4.510	2.784
F(000)	3320.0	2474.0
Crystal size/mm^3	0.08 × 0.05 × 0.05	0.10 × 0.08 × 0.06
Synchrotron radiation, λ	0.7108	0.7108
2Θ range for data collection/°	2.294 to 49.992	2.406 to 50
Index ranges	$-12 \le h \le 12$, $-26 \le k \le 26$, $-35 \le l \le 35$	$-20 \le h \le 20$, $-23 \le k \le 23$, $-25 \le l \le 25$
Reflections collected	44391	67008
Independent reflections	3491 [R_{int} = 0.0600, R_{sigma} = 0.0218]	20452 [R_{int} = 0.1027, R_{sigma} = 0.0784]
Data/restraints/parameters	3491/0/221	20452/1350/1221
Goodness-of-fit on F^2	1.049	1.052
Final R indexes [I>=2σ (I)]	R_1 = 0.0578, wR_2 = 0.1766	R_1 = 0.1056, wR_2 = 0.3066
Final R indexes [all data]	R_1 = 0.0630, wR_2 = 0.1821	R_1 = 0.1206, wR_2 = 0.3225
Largest diff. peak/hole / e Å^{-3}	3.42/-1.06	2.88/-1.69

Table S2. Bond lengths for **Q[10]-Th**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Th1	Th1[1]	4.0333(15)	N1	C1	1.443(7)
Th1	Th2	3.6599(11)	N1	C2	1.364(8)
Th1	Cl1	2.720(3)	N1	C3	1.456(6)
Th1	O1[2]	2.415(5)	N2	C2	1.349(8)
Th1	O1	2.415(5)	N2	C4	1.445(6)
Th1	O4	2.553(15)	N2	C5	1.458(7)
Th1	O5	2.232(9)	N3	C5	1.459(8)
Th1	O6[1]	2.767(11)	N3	C6	1.368(8)
Th1	O6	2.767(11)	N3	C7	1.459(7)
Th1	O7	2.488(6)	N4	C6	1.354(8)
Th1	O7[2]	2.488(6)	N4	C8	1.440(6)
Th2	Cl1	2.785(3)	N4	C9	1.459(7)
Th2	O2[2]	2.430(5)	N5	C9	1.443(7)
Th2	O2	2.430(5)	N5	C10	1.365(7)
Th2	O7[2]	2.464(6)	N5	C11	1.441(7)
Th2	O7	2.464(6)	C1	N1[3]	1.443(7)
Th2	O8	2.459(11)	C3	N1[4]	1.456(7)
Th2	O8[2]	2.459(11)	C3	C4	1.556(11)
Th2	O9	2.475(17)	C4	N2[4]	1.445(6)
Th2	O10	2.568(17)	C7	N3[4]	1.459(7)
O1	C2	1.233(8)	C7	C8	1.535(11)
O2	C6	1.225(8)	C8	N4[4]	1.440(6)
O3	C10	1.208(11)	C10	N5[5]	1.364(7)
O5	Th1[1]	2.232(9)	C11	N5[4]	1.441(7)
O6	Th1[1]	2.767(10)	C11	C11[5]	1.536(16)

[1]1-X,2-Y,+Z; [2]1-X,+Y,+Z; [3]+X,2-Y,+Z; [4]-X,+Y,+Z; [5]+X,+Y,1-Z

Table S3. Bond angles for **Q[10]-Th**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Th2	Th1	Th1[1]	150.140(17)	O7	Th2	Th1	42.59(14)
Cl1	Th1	Th1[1]	160.77(5)	O7[2]	Th2	Cl1	77.18(13)
Cl1	Th1	Th2	49.09(5)	O7	Th2	Cl1	77.18(13)
Cl1	Th1	O6[1]	146.2(3)	O7[2]	Th2	O7	68.9(3)
Cl1	Th1	O6	146.2(3)	O7	Th2	O9	135.0(3)
O1	Th1	Th1[1]	91.72(11)	O7[2]	Th2	O9	135.0(3)
O1[2]	Th1	Th1[1]	91.72(11)	O7[2]	Th2	O10	133.1(3)
O1[2]	Th1	Th2	95.98(11)	O7	Th2	O10	133.1(3)
O1	Th1	Th2	95.98(11)	O8[2]	Th2	Th1	107.0(3)
O1	Th1	Cl1	83.43(12)	O8	Th2	Th1	107.0(3)
O1[2]	Th1	Cl1	83.43(12)	O8[2]	Th2	Cl1	140.7(3)
O1	Th1	O1[2]	149.5(3)	O8	Th2	Cl1	140.7(3)
O1	Th1	O4	74.97(15)	O8	Th2	O7	67.2(3)
O1[2]	Th1	O4	74.98(15)	O8	Th2	O7[2]	103.7(4)
O1[2]	Th1	O6[1]	130.3(3)	O8[2]	Th2	O7	103.7(4)
O1[2]	Th1	O6	67.9(3)	O8[2]	Th2	O7[2]	67.2(3)
O1	Th1	O6[1]	67.9(3)	O8	Th2	O8[2]	66.9(6)
O1	Th1	O6	130.3(3)	O8	Th2	O9	69.6(4)
O1	Th1	O7	134.97(19)	O8[2]	Th2	O9	69.6(4)
O1	Th1	O7[2]	68.0(2)	O8[2]	Th2	O10	122.7(4)
O1[2]	Th1	O7[2]	134.97(19)	O8	Th2	O10	122.7(4)
O1[2]	Th1	O7	68.0(2)	O9	Th2	Th1	175.8(4)
O4	Th1	Th1[1]	86.7(4)	O9	Th2	Cl1	136.6(4)
O4	Th1	Th2	123.2(4)	O9	Th2	O10	65.0(5)
O4	Th1	Cl1	74.1(4)	O10	Th2	Th1	119.2(3)
O4	Th1	O6[1]	113.0(4)	O10	Th2	Cl1	71.6(3)
O4	Th1	O6	113.0(4)	Th1	Cl1	Th2	83.33(7)
O5	Th1	Th1[1]	25.4(5)	C2	O1	Th1	172.1(6)
O5	Th1	Th2	175.5(5)	C6	O2	Th2	174.9(5)
O5	Th1	Cl1	135.4(5)	Th1	O5	Th1[1]	129.2(10)
O5	Th1	O1	85.12(17)	Th1	O6	Th1[1]	93.6(5)
O5	Th1	O1[2]	85.12(17)	Th2	O7	Th1	95.3(2)
O5	Th1	O4	61.3(6)	C1	N1	C3	120.6(6)
O5	Th1	O6[1]	61.8(5)	C2	N1	C1	121.8(6)
O5	Th1	O6	61.8(5)	C2	N1	C3	110.9(5)
O5	Th1	O7	135.3(3)	C2	N2	C4	111.8(5)
O5	Th1	O7[2]	135.3(3)	C2	N2	C5	122.1(5)
O6	Th1	Th1[1]	43.2(2)	C4	N2	C5	120.1(5)
O6[1]	Th1	Th1[1]	43.2(2)	C6	N3	C5	121.6(5)
O6[1]	Th1	Th2	114.6(2)	C6	N3	C7	110.8(5)
O6	Th1	Th2	114.6(2)	C7	N3	C5	120.5(6)
O6[1]	Th1	O6	64.0(6)	C6	N4	C8	112.2(5)
O7	Th1	Th1[1]	117.39(14)	C6	N4	C9	122.0(5)
O7[2]	Th1	Th1[1]	117.39(14)	C8	N4	C9	122.4(5)
O7	Th1	Th2	42.10(15)	C10	N5	C9	121.8(5)
O7[2]	Th1	Th2	42.10(15)	C10	N5	C11	112.5(6)
O7	Th1	Cl1	78.03(15)	C11	N5	C9	123.0(6)

O7[2]	Th1	Cl1	78.03(15)	N1	C1	N1[3]	112.8(7)
O7[2]	Th1	O4	135.6(3)	O1	C2	N1	123.8(6)
O7	Th1	O4	135.6(3)	O1	C2	N2	126.1(6)
O7	Th1	O6	74.9(3)	N2	C2	N1	110.0(5)
O7	Th1	O6[1]	109.5(3)	N1[4]	C3	N1	113.3(7)
O7[2]	Th1	O6[1]	74.9(3)	N1[4]	C3	C4	103.2(5)
O7[2]	Th1	O6	109.5(3)	N1	C3	C4	103.2(5)
O7[2]	Th1	O7	68.1(3)	N2[4]	C4	N2	115.2(7)
Cl1	Th2	Th1	47.59(5)	N2[4]	C4	C3	103.4(4)
O2	Th2	Th1	96.53(11)	N2	C4	C3	103.4(4)
O2[2]	Th2	Th1	96.53(11)	N2	C5	N3	111.8(5)
O2	Th2	Cl1	82.55(12)	O2	C6	N3	125.6(6)
O2[2]	Th2	Cl1	82.55(12)	O2	C6	N4	125.4(6)
O2[2]	Th2	O2	144.9(3)	N4	C6	N3	109.0(5)
O2[2]	Th2	O7[2]	136.61(19)	N3[4]	C7	N3	112.7(7)
O2	Th2	O7	136.61(19)	N3[4]	C7	C8	103.5(5)
O2[2]	Th2	O7	69.4(2)	N3	C7	C8	103.5(5)
O2	Th2	O7[2]	69.42(19)	N4	C8	N4[4]	115.3(7)
O2	Th2	O8[2]	70.1(3)	N4[4]	C8	C7	103.7(4)
O2[2]	Th2	O8[2]	135.3(3)	N4	C8	C7	103.7(4)
O2	Th2	O8	135.3(3)	N5	C9	N4	112.8(5)
O2[2]	Th2	O8	70.1(3)	O3	C10	N5	126.1(4)
O2	Th2	O9	84.66(16)	O3	C10	N5[5]	126.1(4)
O2[2]	Th2	O9	84.66(16)	N5[5]	C10	N5	107.9(8)
O2[2]	Th2	O10	72.58(13)	N5	C11	N5[4]	115.6(7)
O2	Th2	O10	72.58(13)	N5	C11	C11[5]	103.4(4)
O7[2]	Th2	Th1	42.59(14)	N5[4]	C11	C11[5]	103.4(4)

[1]1-X,2-Y,+Z; [2]1-X,+Y,+Z; [3]+X,2-Y,+Z; [4]-X,+Y,+Z; [5]+X,+Y,1-Z

Table S4. Bond lengths for **Q[10]-U**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
U1	Cl1	2.732(3)	C1	N20[1]	1.440(14)
U1	Cl2	2.758(4)	C4	C5	1.576(16)
U1	Cl3	2.788(4)	C10	C11	1.494(17)
U1	O1	1.796(9)	C15	C16	1.543(17)
U1	O1W	2.487(12)	C21	C22	1.479(17)
U1	O2	1.811(7)	C27	N3[1]	1.485(16)
U1	O2W	2.424(11)	C28	C29	1.561(16)
U2	Cl4	2.764(5)	O15	C32	1.256(13)
U2	O3	1.753(12)	O16	C38	1.221(13)
U2	O3W	2.539(12)	O17	C44	1.217(13)
U2	O4	1.710(14)	O18	C50	1.207(13)
U2	O4W	2.735(10)	O19	C56	1.223(14)
U2	O5W	2.383(11)	O20	C35	1.225(13)
U2	O6W	2.206(12)	O21	C41	1.224(12)
O5	C2	1.189(13)	O22	C47	1.242(12)
O6	C8	1.175(13)	O23	C53	1.196(13)
O7	C14	1.198(13)	O24	C59	1.206(12)
O8	C20	1.219(14)	N21	C31	1.468(14)
O9	C26	1.228(13)	N21	C32	1.331(14)
O10	C6	1.236(13)	N21	C33	1.436(12)
O11	C12	1.218(13)	N22	C32	1.389(15)
O12	C17	1.242(12)	N22	C34	1.486(13)
O13	C23	1.214(13)	N22	C36	1.432(15)
O14	C30	1.195(12)	N23	C33	1.451(14)
N1	C1	1.491(14)	N23	C35	1.393(14)
N1	C2	1.388(14)	N23	C60[2]	1.494(14)
N1	C4	1.454(13)	N24	C34	1.403(14)
N2	C2	1.383(14)	N24	C35	1.362(15)
N2	C3	1.448(15)	N24	C37	1.469(14)
N2	C5	1.422(14)	N25	C36	1.441(14)
N3	C4	1.452(13)	N25	C38	1.406(13)
N3	C6	1.362(14)	N25	C39	1.451(15)
N3	C27[1]	1.485(16)	N26	C38	1.346(15)
N4	C5	1.449(13)	N26	C40	1.432(13)
N4	C6	1.347(14)	N26	C42	1.473(13)
N4	C7	1.483(15)	N27	C37	1.499(12)
N5	C3	1.467(16)	N27	C39	1.435(14)
N5	C8	1.329(16)	N27	C41	1.369(13)
N5	C10	1.480(15)	N28	C40	1.481(13)
N6	C8	1.418(15)	N28	C41	1.362(14)
N6	C9	1.490(16)	N28	C43	1.427(13)
N6	C11	1.459(16)	N29	C42	1.458(13)
N7	C7	1.499(16)	N29	C44	1.367(13)
N7	C10	1.494(14)	N29	C45	1.446(14)
N7	C12	1.360(15)	N30	C44	1.373(14)
N8	C11	1.418(14)	N30	C46	1.434(13)
N8	C12	1.357(15)	N30	C48	1.459(11)

N8	C13	1.453(14)	N31	C43	1.445(11)
N9	C9	1.451(15)	N31	C45	1.434(12)
N9	C14	1.347(16)	N31	C47	1.357(13)
N9	C15	1.429(13)	N32	C46	1.441(13)
N10	C14	1.402(15)	N32	C47	1.364(12)
N10	C16	1.430(15)	N32	C49	1.443(12)
N10	C18	1.423(16)	N33	C48	1.478(14)
N11	C13	1.432(15)	N33	C50	1.376(13)
N11	C15	1.465(13)	N33	C51	1.445(13)
N11	C17	1.405(15)	N34	C50	1.352(14)
N12	C16	1.443(12)	N34	C52	1.437(13)
N12	C17	1.333(14)	N34	C54	1.453(13)
N12	C19	1.437(14)	N35	C49	1.462(13)
N13	C18	1.466(15)	N35	C51	1.477(12)
N13	C20	1.430(16)	N35	C53	1.361(14)
N13	C21	1.412(13)	N36	C52	1.466(13)
N14	C20	1.347(16)	N36	C53	1.371(13)
N14	C22	1.448(14)	N36	C55	1.410(15)
N14	C24	1.477(16)	N37	C54	1.434(14)
N15	C19	1.425(14)	N37	C56	1.364(15)
N15	C21	1.484(14)	N37	C57	1.407(14)
N15	C23	1.397(13)	N38	C56	1.343(14)
N16	C22	1.476(13)	N38	C58	1.427(14)
N16	C23	1.365(15)	N38	C60	1.492(14)
N16	C25	1.463(15)	N39	C55	1.438(15)
N17	C24	1.426(15)	N39	C57	1.482(12)
N17	C26	1.355(14)	N39	C59	1.363(14)
N17	C28	1.444(13)	N40	C31[2]	1.454(14)
N18	C26	1.371(14)	N40	C58	1.439(12)
N18	C27	1.504(15)	N40	C59	1.374(14)
N18	C29	1.439(13)	C31	N40[2]	1.454(14)
N19	C25	1.496(14)	C33	C34	1.567(15)
N19	C28	1.409(14)	C39	C40	1.557(14)
N19	C30	1.404(14)	C45	C46	1.571(12)
N20	C1[1]	1.440(14)	C51	C52	1.566(14)
N20	C29	1.453(14)	C57	C58	1.550(16)
N20	C30	1.378(14)	C60	N23[2]	1.494(14)

[1]2-X,1-Y,1-Z; [2]1-X,-Y,1-Z

Table S5. Bond angles for **Q[10]-U**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
Cl1	U1	Cl2	76.99(12)	N14	C22	N16	113.4(9)
Cl1	U1	Cl3	151.13(12)	N14	C22	C21	105.3(9)
Cl2	U1	Cl3	74.59(14)	N16	C22	C21	105.5(10)
O1	U1	Cl1	92.2(3)	O13	C23	N15	124.9(11)
O1	U1	Cl2	87.5(3)	O13	C23	N16	126.8(10)
O1	U1	Cl3	91.6(3)	N16	C23	N15	108.3(9)
O1	U1	O1W	86.4(4)	N17	C24	N14	111.5(10)
O1	U1	O2	179.1(4)	N16	C25	N19	110.0(9)
O1	U1	O2W	89.1(4)	O9	C26	N17	127.4(11)
O1W	U1	Cl1	69.0(3)	O9	C26	N18	124.6(11)
O1W	U1	Cl2	145.2(3)	N17	C26	N18	107.9(9)
O1W	U1	Cl3	139.8(3)	N3[1]	C27	N18	109.4(10)
O2	U1	Cl1	88.8(2)	N17	C28	C29	103.4(8)
O2	U1	Cl2	92.6(2)	N19	C28	N17	114.1(10)
O2	U1	Cl3	87.6(2)	N19	C28	C29	102.7(9)
O2	U1	O1W	94.0(4)	N18	C29	N20	113.9(10)
O2	U1	O2W	90.3(4)	N18	C29	C28	102.2(8)
O2W	U1	Cl1	137.0(3)	N20	C29	C28	103.3(9)
O2W	U1	Cl2	146.0(3)	O14	C30	N19	128.0(10)
O2W	U1	Cl3	71.7(3)	O14	C30	N20	126.5(10)
O2W	U1	O1W	68.2(4)	N20	C30	N19	105.3(9)
O3	U2	Cl4	94.6(5)	C32	N21	C31	122.8(9)
O3	U2	O3W	82.0(6)	C32	N21	C33	113.3(9)
O3	U2	O4W	87.5(6)	C33	N21	C31	121.8(8)
O3	U2	O5W	94.7(5)	C32	N22	C34	110.3(8)
O3	U2	O6W	100.5(6)	C32	N22	C36	124.0(9)
O3W	U2	Cl4	69.8(2)	C36	N22	C34	119.9(10)
O3W	U2	O4W	69.7(3)	C33	N23	C60[2]	119.7(9)
O4	U2	Cl4	88.4(6)	C35	N23	C33	113.3(9)
O4	U2	O3	170.9(8)	C35	N23	C60[2]	118.6(9)
O4	U2	O3W	91.1(7)	C34	N24	C37	122.9(10)
O4	U2	O4W	84.6(6)	C35	N24	C34	114.3(9)
O4	U2	O5W	87.8(7)	C35	N24	C37	119.3(9)
O4	U2	O6W	88.5(7)	C36	N25	C39	121.1(9)
O4W	U2	Cl4	138.7(3)	C38	N25	C36	124.2(9)
O5W	U2	Cl4	144.5(3)	C38	N25	C39	110.7(9)
O5W	U2	O3W	145.5(3)	C38	N26	C40	113.0(8)
O5W	U2	O4W	75.9(4)	C38	N26	C42	120.8(9)
O6W	U2	Cl4	72.4(3)	C40	N26	C42	119.9(10)
O6W	U2	O3W	142.1(4)	C39	N27	C37	123.3(8)
O6W	U2	O4W	147.7(4)	C41	N27	C37	120.2(8)
O6W	U2	O5W	72.3(4)	C41	N27	C39	113.6(8)
C2	N1	C1	120.8(8)	C41	N28	C40	113.8(8)
C2	N1	C4	112.2(9)	C41	N28	C43	122.1(9)
C4	N1	C1	120.8(9)	C43	N28	C40	121.8(9)
C2	N2	C3	118.5(9)	C44	N29	C42	122.8(9)
C2	N2	C5	114.3(9)	C44	N29	C45	112.4(8)

C5	N2	C3	124.6(10)	C45	N29	C42	120.3(9)
C4	N3	C27[1]	117.9(10)	C44	N30	C46	114.1(8)
C6	N3	C4	111.9(9)	C44	N30	C48	123.1(9)
C6	N3	C27[1]	118.8(9)	C46	N30	C48	121.8(9)
C5	N4	C7	116.6(10)	C45	N31	C43	122.7(9)
C6	N4	C5	114.5(9)	C47	N31	C43	120.4(8)
C6	N4	C7	120.7(9)	C47	N31	C45	112.6(7)
C3	N5	C10	122.8(11)	C46	N32	C49	119.0(8)
C8	N5	C3	120.3(9)	C47	N32	C46	112.2(8)
C8	N5	C10	113.0(10)	C47	N32	C49	121.7(8)
C8	N6	C9	119.4(10)	C50	N33	C48	121.7(8)
C8	N6	C11	112.7(10)	C50	N33	C51	110.7(8)
C11	N6	C9	122.0(10)	C51	N33	C48	119.1(9)
C10	N7	C7	122.9(10)	C50	N34	C52	112.9(9)
C12	N7	C7	121.3(9)	C50	N34	C54	123.5(8)
C12	N7	C10	112.0(10)	C52	N34	C54	119.2(9)
C11	N8	C13	125.8(10)	C49	N35	C51	119.3(9)
C12	N8	C11	113.8(9)	C53	N35	C49	124.5(8)
C12	N8	C13	119.5(9)	C53	N35	C51	113.6(8)
C14	N9	C9	120.4(9)	C53	N36	C52	112.5(9)
C14	N9	C15	112.1(10)	C53	N36	C55	122.2(9)
C15	N9	C9	122.1(11)	C55	N36	C52	120.2(8)
C14	N10	C16	112.5(10)	C56	N37	C54	123.6(9)
C14	N10	C18	123.5(9)	C56	N37	C57	111.7(9)
C18	N10	C16	121.3(10)	C57	N37	C54	122.5(10)
C13	N11	C15	124.8(10)	C56	N38	C58	113.5(10)
C17	N11	C13	122.3(9)	C56	N38	C60	118.3(9)
C17	N11	C15	109.8(9)	C58	N38	C60	121.5(9)
C17	N12	C16	112.9(9)	C55	N39	C57	120.9(9)
C17	N12	C19	118.6(8)	C59	N39	C55	120.3(9)
C19	N12	C16	120.4(9)	C59	N39	C57	113.2(8)
C20	N13	C18	120.6(8)	C58	N40	C31[2]	124.7(8)
C21	N13	C18	123.9(10)	C59	N40	C31[2]	121.0(8)
C21	N13	C20	109.7(10)	C59	N40	C58	112.7(9)
C20	N14	C22	110.9(10)	N40[2]	C31	N21	113.0(8)
C20	N14	C24	122.3(9)	O15	C32	N21	127.7(12)
C22	N14	C24	124.8(10)	O15	C32	N22	122.4(10)
C19	N15	C21	126.6(8)	N21	C32	N22	109.9(9)
C23	N15	C19	121.2(8)	N21	C33	N23	114.8(9)
C23	N15	C21	110.7(9)	N21	C33	C34	104.0(8)
C23	N16	C22	111.2(9)	N23	C33	C34	100.9(8)
C23	N16	C25	121.3(9)	N22	C34	C33	101.9(8)
C25	N16	C22	125.4(10)	N24	C34	N22	114.5(8)
C24	N17	C28	122.9(9)	N24	C34	C33	104.6(9)
C26	N17	C24	122.5(9)	O20	C35	N23	126.2(11)
C26	N17	C28	112.7(9)	O20	C35	N24	127.7(11)
C26	N18	C27	120.2(8)	N24	C35	N23	106.0(9)
C26	N18	C29	113.0(9)	N22	C36	N25	114.0(9)
C29	N18	C27	119.3(10)	N24	C37	N27	111.7(8)
C28	N19	C25	121.8(10)	O16	C38	N25	123.9(11)
C30	N19	C25	116.2(8)	O16	C38	N26	127.3(10)
C30	N19	C28	114.2(9)	N26	C38	N25	108.7(9)
C1[1]	N20	C29	122.9(10)	N25	C39	C40	103.4(8)

C30	N20	C1[1]	117.4(9)	N27	C39	N25	115.2(10)
C30	N20	C29	112.9(9)	N27	C39	C40	104.3(8)
N20[1]	C1	N1	112.0(8)	N26	C40	N28	113.4(8)
O5	C2	N1	125.8(11)	N26	C40	C39	103.9(9)
O5	C2	N2	127.4(11)	N28	C40	C39	101.1(8)
N2	C2	N1	106.8(9)	O21	C41	N27	126.2(9)
N2	C3	N5	113.2(9)	O21	C41	N28	126.8(9)
N1	C4	C5	103.2(9)	N28	C41	N27	107.0(9)
N3	C4	N1	112.9(9)	N29	C42	N26	111.5(8)
N3	C4	C5	103.7(8)	N28	C43	N31	113.2(9)
N2	C5	N4	115.3(10)	O17	C44	N29	126.7(10)
N2	C5	C4	102.8(8)	O17	C44	N30	125.8(9)
N4	C5	C4	101.0(8)	N29	C44	N30	107.5(9)
O10	C6	N3	125.5(11)	N29	C45	C46	103.5(8)
O10	C6	N4	126.0(11)	N31	C45	N29	113.9(9)
N4	C6	N3	108.3(9)	N31	C45	C46	103.1(8)
N4	C7	N7	110.3(10)	N30	C46	N32	116.9(9)
O6	C8	N5	127.7(11)	N30	C46	C45	101.9(8)
O6	C8	N6	126.3(12)	N32	C46	C45	102.6(7)
N5	C8	N6	106.0(10)	O22	C47	N31	124.6(8)
N9	C9	N6	112.4(9)	O22	C47	N32	126.3(9)
N5	C10	N7	111.2(10)	N31	C47	N32	109.0(8)
N5	C10	C11	105.0(10)	N30	C48	N33	112.4(8)
C11	C10	N7	102.0(9)	N32	C49	N35	112.7(8)
N6	C11	C10	102.5(9)	O18	C50	N33	123.6(10)
N8	C11	N6	112.9(10)	O18	C50	N34	127.2(10)
N8	C11	C10	105.1(9)	N34	C50	N33	109.2(9)
O11	C12	N7	125.7(11)	N33	C51	N35	113.3(8)
O11	C12	N8	127.6(11)	N33	C51	C52	103.7(8)
N7	C12	N8	106.7(9)	N35	C51	C52	101.8(8)
N11	C13	N8	111.8(9)	N34	C52	N36	114.3(9)
O7	C14	N9	127.5(12)	N34	C52	C51	102.6(8)
O7	C14	N10	125.0(13)	N36	C52	C51	103.7(7)
N9	C14	N10	107.6(9)	O23	C53	N35	124.5(10)
N9	C15	N11	114.2(9)	O23	C53	N36	127.2(11)
N9	C15	C16	104.8(10)	N35	C53	N36	108.3(9)
N11	C15	C16	103.7(8)	N37	C54	N34	114.1(8)
N10	C16	N12	115.7(10)	N36	C55	N39	115.0(10)
N10	C16	C15	102.3(9)	O19	C56	N37	125.4(11)
N12	C16	C15	103.6(9)	O19	C56	N38	126.5(12)
O12	C17	N11	122.7(11)	N38	C56	N37	108.1(10)
O12	C17	N12	128.0(11)	N37	C57	N39	114.4(8)
N12	C17	N11	109.3(8)	N37	C57	C58	104.7(9)
N10	C18	N13	112.1(9)	N39	C57	C58	100.9(8)
N15	C19	N12	113.4(9)	N38	C58	N40	115.2(9)
O8	C20	N13	125.8(12)	N38	C58	C57	101.2(8)
O8	C20	N14	126.2(13)	N40	C58	C57	104.7(8)
N14	C20	N13	108.0(9)	O24	C59	N39	126.5(11)
N13	C21	N15	112.0(10)	O24	C59	N40	126.0(11)
N13	C21	C22	105.8(9)	N39	C59	N40	107.4(8)
C22	C21	N15	104.3(8)	N23[2]	C60	N38	111.0(8)

[1]2-X,1-Y,1-Z; [2]1-X,-Y,1-Z

Table S6. Potential Hydrogen Bonds for **Q[10]-U**.

Donor---H...Acceptor	D - H	H...A	D...A	D - H...A
O1W---H1WA...Cl1	0.93	2.61	2.964(13)	103
O1W---H1WA...Cl5	0.93	2.45	3.233(13)	142'
O1W---H1WB...Cl5	0.93	2.26	3.084(13)	147
O2W---H2WA...Cl3	0.87	2.61	3.066(13)	114
O2W---H2WA...Cl4	0.87	2.48	3.112(13)	130'
O4W---H4WA...O3W	1.03	2.49	2.878(17)	101
O4W---H4WB...O3W	1.03	2.50	2.878(17)	101
O6W---H6WA...Cl4	1.05	2.59	2.969(14)	101
O6W---H6WA...O15	1.05	1.92	2.635(16)	122'
C1---H1B...O5	0.97	2.51	2.886(16)	103
C1---H1B...O14	0.97	2.38	2.807(16)	106'
C3---H3B...O5	0.97	2.39	2.819(17)	106
C3---H3B...O6	0.97	2.43	2.822(17)	104'
C4---H4...Cl3	0.98	2.61	3.522(13)	155
C5---H5...O3	0.98	2.42	2.945(18)	113
C7---H7A...O10	0.97	2.52	2.898(17)	103
C7---H7A...O11	0.97	2.50	2.885(17)	103'
C7---H7B...Cl5	0.97	2.69	3.588(14)	154
C9---H9A...O6	0.97	2.48	2.882(17)	105
C9---H9A...O7	0.97	2.45	2.846(17)	104'
C11---H11...Cl1	0.98	2.70	3.475(14)	136
C13---H13B...O11	0.97	2.44	2.839(15)	104
C13---H13B...O12	0.97	2.45	2.860(16)	105'
C18---H18B...O7	0.97	2.51	2.893(17)	103

C18---H18B...O8	0.97	2.53	2.931(17)	105'
C18---H18B...O8	0.97	2.34	3.136(17)	139"
C19---H19B...O12	0.97	2.40	2.835(14)	106
C19---H19B...O13	0.97	2.43	2.846(14)	106'
C19---H19B...O23	0.97	2.53	3.363(15)	144"
C24---H24A...O8	0.97	2.52	2.880(17)	102
C24---H24A...O9	0.97	2.52	2.890(17)	103'
C25---H25A...O13	0.97	2.50	2.876(14)	103
C25---H25A...O14	0.97	2.44	2.860(15)	106'
C27---H27A...O9	0.97	2.49	2.877(19)	104
C27---H27A...O10	0.97	2.50	2.888(18)	104'
C31---H31A...O11	0.97	2.32	3.154(16)	144
C31---H31B...O15	0.97	2.54	2.921(16)	104
C31---H31B...O24	0.97	2.44	2.848(15)	105'
C33---H33...O11	0.98	2.37	3.208(14)	143
C34---H34...Cl5	0.98	2.77	3.322(12)	117
C36---H36B...O15	0.97	2.50	2.898(17)	105
C36---H36B...O16	0.97	2.54	2.920(18)	103’
C37---H37A...O20	0.97	2.45	2.863(14)	105
C37---H37A...O21	0.97	2.47	2.877(13)	105'
C39---H39...Cl1	0.98	2.59	3.537(13)	105
C42---H42A...O16	0.97	2.50	2.880(15)	103
C42---H42A...O17	0.97	2.53	2.911(17)	103'
C43---H43A...O21	0.97	2.47	2.870(14)	105
C43---H43A...O22	0.97	2.43	2.830(14)	105'
C45---H45...Cl2	0.98	2.79	3.706(11)	156
C46---H46...Cl3	0.98	2.81	3.540(11)	132

C48---H48B...O17	0.97	2.52	2.897(14)	103
C48---H48B...O18	0.97	2.49	2.872(14)	103'
C49---H49A...O12	0.97	2.52	3.461(13)	164
C49---H49A...O22	0.97	2.51	2.905(13)	104'
C49---H49A...O23	0.97	2.55	2.897(14)	101"
C52---H52...O13	0.98	2.24	3.158(13)	155
C54---H54A...O18	0.97	2.54	2.916(14)	103
C54---H54A...O19	0.97	2.51	2.886(17)	103'
C55---H55A...O23	0.97	2.50	2.890(16)	104
C55---H55A...O24	0.97	2.41	2.832(15)	106'
C55---H55B...O13	0.97	2.56	3.411(17)	146
C55---H55B...O23	0.97	2.47	3.154(18)	128'
C57---H57...O12	0.98	2.59	3.207(14)	121
C60---H60A...O19	0.97	2.41	2.828(15)	105
C60---H60A...O20	0.97	2.47	2.883(17)	105’

Table S7. Raman band assignments for compounds **Q[10]-Th** and **Q[10]-U**.

Raman band position, cm^{-1}		Band assignment
Q10-U	**Q10-Th**	
1742 m	1741 m-s	ν (C=O)
–	1660 w	ν (C=O) (metal coordinated)
1428 and 1378 m	1434 and 1377 m	δ CH_2 + δ CH deformation vibrations; plus ν_{as} C–N (in N–C–N)
–	1396 m	ν (C=O) (metal coordinated)
1316 w	1313 vw	ν C–N + νC–C + δ CH + ω CH_2
1280 w	1273 vw	ν_s C–N (in N–C–N) + τ CH_2
1222–1191 m	1223–1199 m	ν C–C +ν C–N + τ CH_2 + δ CH
1135 w	1126 w	ν (HC–CH) + δ CH + ρ CH_2
1040 m-w	1043 m-s, 1020 sh, w	ν C–N + ρ CH_2 + γ CH
982 vw	980 w	ν (HC–CH) + δ CH
915 w-m	930 and 910 sh, w-m	ρ CH_2
855 vs	–	ν_s $(UO_2)^{2+}$ symmetric stretch
835 vs	838 vs	δ C–N–C (ring R10 deformation) + ρ CH_2 (rocking)
752 m	745 m-s	δ C–N–C out-of-plane ring R10 deformation
	730 sh, m	δ (C=O) (metal coordinated) in-plane deformation
704 vw	690 vw	ρ CH_2 + ω CH
658 w-m	659 m-s	τ HC–CH + ring deformation δ C=O (C–CO–C) in-plane deformation vibration
441 vs	450 vs	σ N–C–N, ring R10 scissoring
369 w-m	373 vw	Out-of-plane R10 deformation
251 and 201 m, br		δ$(UO_2)^{2+}$deformation vibration
	261–223 m, br	ν (MO) stretching vibration
< 200	< 200	Lattice modes

ν stretching
δ in-plane bending (rocking - ρ, and scissoring - sciss)
γ out-of plane bending (wagging - ω,and twisting - τ)