SUPPLEMENTARY MATERIAL

New itaconate-containing uranyl complex unit and coordination modes of itaconate ions

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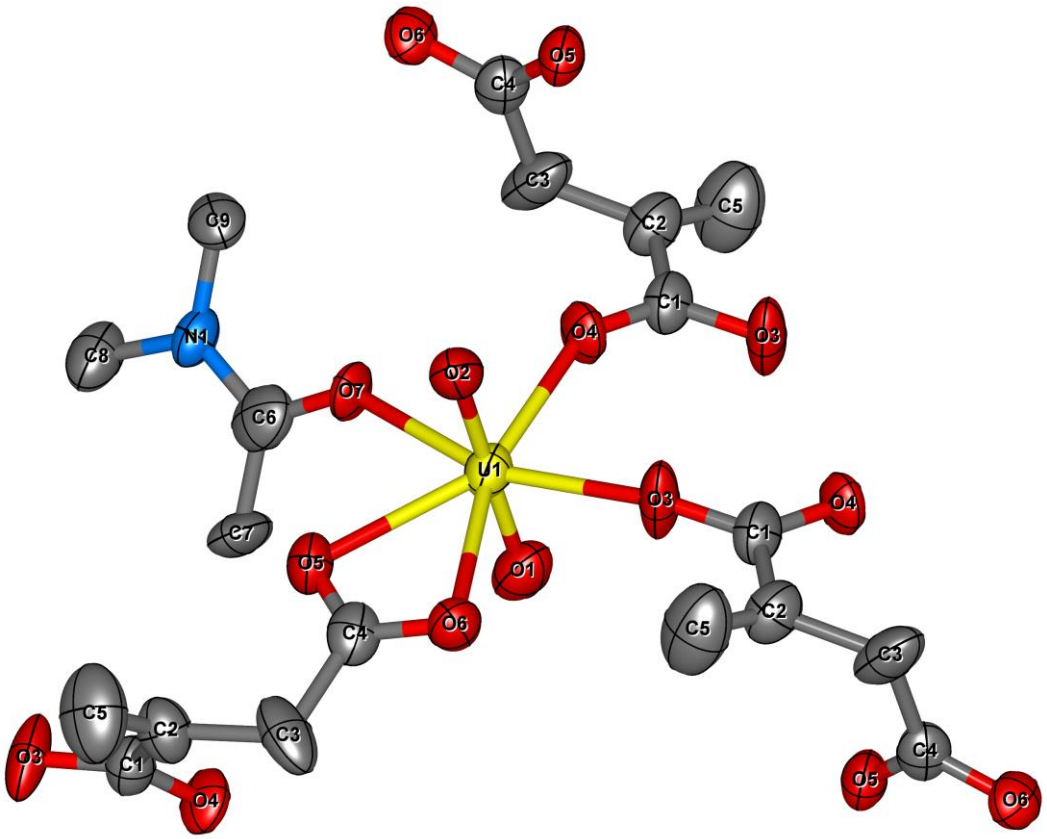

Fig. S1. ORTEP image (displacement ellipsoids are shown at 50% probability level) of the uranyl complex unit in the structure of $[UO_2(C_5H_4O_4)(C_4H_9NO)]$ (**I**). Uranium, oxygen, nitrogen and carbon atoms are depicted with yellow, red, blue and grey colors respectively. Hydrogen atoms are omitted.

Table S1. Coordinates of basic atoms in the structure of $[UO_2(C_5H_4O_4)(Dma)]$ (**I**)

Atom	x	y	z
U1	0.38556(7)	0.58094(5)	0.29838(4)
O1	0.3178(17)	0.6876(10)	0.3703(9)
O2	0.4620(15)	0.4759(9)	0.2259(8)
O3	0.6163(17)	0.5695(11)	0.4250(9)
O4	0.7146(16)	0.5494(9)	0.5965(8)
O5	0.8327(14)	0.8087(9)	0.6364(8)
O6	1.0732(14)	0.7883(8)	0.7372(8)
O7	0.1179(12)	0.5453(10)	0.2083(7)
N1	–0.1264(16)	0.5328(12)	0.0975(10)
C1	0.727(2)	0.5825(13)	0.5067(13)
C2	0.882(2)	0.6399(15)	0.4952(14)
C3	1.011(3)	0.6590(16)	0.5931(14)
C4	0.967(2)	0.7587(14)	0.6592(12)
C5	0.917(3)	0.657(2)	0.4063(17)
C6	–0.010(3)	0.5942(15)	0.1531(15)
C7	–0.033(2)	0.7142(12)	0.1545(15)
C8	–0.273(3)	0.5772(15)	0.0327(16)
C9	–0.116(3)	0.4143(12)	0.0974(14)
H1	1.1179	0.6729	0.5719
H2	1.0225	0.5923	0.6374
H3	0.8456	0.6334	0.3444
H4	1.0163	0.6937	0.4009
H5	–0.1303	0.7313	0.1842
H6	–0.0474	0.7427	0.0824
H7	0.0632	0.7481	0.1978
H8	–0.3017	0.5340	–0.0321
H9	–0.2543	0.6534	0.0147
H10	–0.3637	0.5740	0.0717
H11	–0.0009	0.3920	0.1146
H12	–0.1650	0.3863	0.0276
H13	–0.1748	0.3844	0.1502

Table S2. Basic bond lengths and valence angles in the structure of $[UO_2(C_5H_4O_4)(Dma)]$ (**I**)

Pentagonal bipyramid UO_7				
Bond	*d*, Å	Ω, % *	Angle	ω, deg.
U1−O1	1.752(13)	21.73	O1−U1−O2	177.6(5)
U1−O2	1.774(12)	21.42	O3−U1−O4	83.5(4)
U1−O3	2.284(12)	13.22	O4−U1−O7	75.8(4)
U1−O4	2.344(10)	12.64	O5−U1−O7	71.2(4)
U1−O5	2.458(10)	9.44	O5−U1−O6	52.8(4)
U1−O6	2.465(11)	9.47	O3−U1−O6	76.7(4)
U1−O7	2.35 (9)	12.09		

Itaconate anion			
Bond	*d*, Å	Angle	ω, deg.
C1−O3	1.28(2)	O3−C1−O4	123.6(17)
C1−O4	1.251(19)	O5−C4−O6	120.4(16)
C4−O5	1.262(19)	O3−C1−C2	118.7(15)
C4−O6	1.261(18)	O4−C1−C2	117.8(15)
C1−C2	1.50(3)	O5−C4−C3	122.3(15)
C2−C3	1.52(3)	O6−C4−C3	117.2(16)
C3−C4	1.57(3)	C1−C2−C5	121.5(19)
C2−C5	1.26(3)	C1−C2−C3	118.7(15)
		C5−C2−C3	119.0(2)
		C2−C3−C4	111.8(18)

N,N-dimethylacetamide molecule			
Bond	*d*, Å	Angle	ω, deg.
N1−C6	1.32(2)	C6−N1−C8	123.6(16)
N1−C8	1.45(2)	C6−N1−C9	121.9(16)
N1−C9	1.450(19)	C8−N1−C9	114.6(14)
C6−O7	1.31(3)	N1−C6−O7	118.4(17)
C6−C7	1.48(2)	N1−C6−C7	119.0(2)
		O7−C6−C7	122.5(18)

* Ω is the solid angle (in percent of 4π steradian), at which the shared face of the Voronoi-Dirichlet polyhedra of adjacent atoms is seen from the nucleus of any of them.