Supporting information for

One-Dimensional Chain Structures of Hexanuclear Uranium(IV) Clusters Bridged by Formate Ligands

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S1. Powder X-ray diffraction (PXRD) of samples obtained from the reactions of compound 2.

Powder pattern of powder samples were collected from 5º to 50º, with a step of 0.02° using a Bruker D8 advance X–ray diffractometer with Cu–Kα radiation (λ = 1.54056 Å) equipped with a Lynxeye one-dimensional detector. Before PXRD measurement, sample for each reaction was fully grinded to avoid the strong diffraction from the preferential orientation in the crystal. Then, the powder sample was loaded on the glass tablet. The match between the experimental and simulated powder patterns indicates the examed sample of compound 2 is pure.
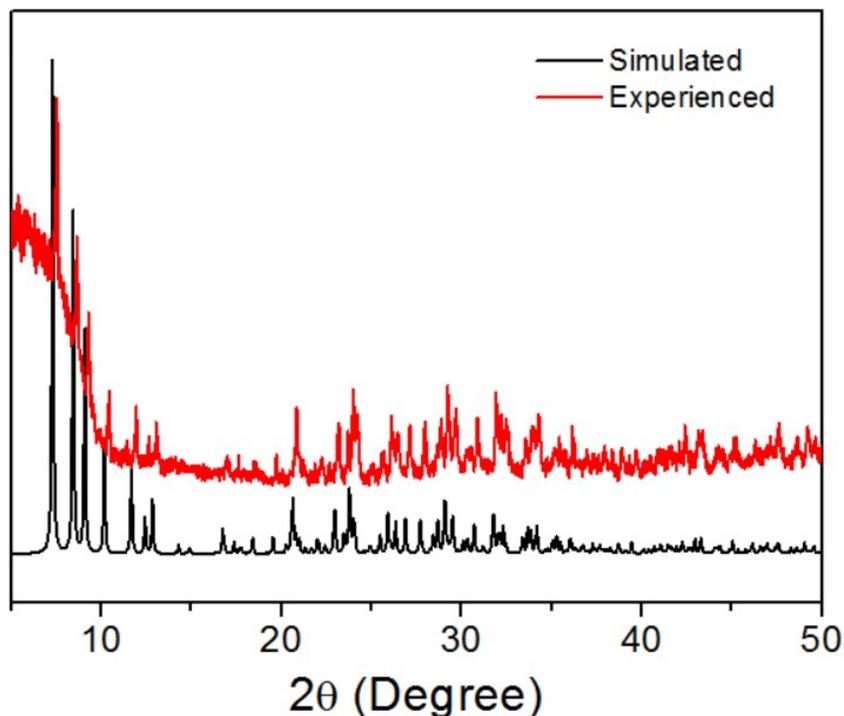

Figure S1. Simulated (black) and experimental (red) PXRD patterns for compound 2.

S2. Bond lengths between U(IV) and μ_3-O or μ_3-OH groups in three compounds (Table S1).

Compound 1a		Compound 1b		Compound 2	
U-O bond	bond length (Å)	U-O bond	bond length (Å)	U-O bond	bond length (Å)
O(6)-U(1)	2.222(6)	O(27)-U(1)	2.310(7)	O(1)-U(2)	2.219(4)
O(6)-U(2)	2.238(5)	O(27)-U(2)	2.243(8)	O(1)-U(3)	2.230(4)
O(6)-U(3)	2.240(5)	O(27)-U(5)	2.187(7)	O(1)-U(4)	2.288(4)
O(13)-U(2)	2.187(6)	O(31)-U(1)	2.275(7)	O(15)-U(1)	2.238(4)
O(13)-U(3)	2.244(6)	O(31)-U(3)	2.238(7)	O(15)-U(2)	2.255(4)
O(13)-U(4)	2.297(6)	O(31)-U(4)	2.204(7)	O(15)-U(3)	2.234(4)
O(3)-U(2)	2.419(6)	O(32)-U(2)	2.239(7)	O(7)-U(1)	2.432(4)
O(3)-U(3)	2.458(6)	O(32)-U(4)	2.233(7)	O(7)-U(2)	2.448(4)
O(3)-U(4)	2.427(6)	O(32)-U(6)	2.220(7)	O(7)-U(3)	2.464(4)
O(4)-U(1)	2.449(5)	O(33)-U(3)	2.222(7)	O(13)-U(2)	2.429(4)
O(4)-U(2)	2.444(6)	O(33)-U(5)	2.242(7)	O(13)-U(3)	2.390(4)
O(4)-U(3)	2.468(6)	O(33)-U(6)	2.227(7)	O(13)-U(4)	2.497(4)
		O(21)-U(1)	2.442(8)		
		O(21)-U(2)	2.452(7)		
		O(21)-U(4)	2.425(8)		
		O(22)-U(1)	2.424(8)		
		O(22)-U(3)	2.468(8)		
		O(22)-U(5)	2.408(7)		
		O(28)-U(3)	2.458(7)		
		O(28)-U(4)	2.455(8)		
		O(28)-U(6)	2.438(7)		
		O(30)-U(2)	2.479(7)		
		O(30)-U(5)	2.442(7)		
		O(30)-U(6)	2.460(7)		

S3. Bond valence sum (Σv, $v = e^{(R_0 - d)/a}$, d: bond distance) for μ_3-oxygen sites in compound 1a, 1b and 2 ($R_0 = 2.051$ Å and a = 0.51 for μ_3-O; $R_0 = 2.104$ Å and a = 0.37 for μ_3-OH).[1] (Table S2)

Compound 1a		Compound 1b		Compound 2	
μ_3-oxygen sites	Σv	μ_3-oxygen sites	Σv	μ_3-oxygen sites	Σv
O(6)	2.098	O(27)	2.064	O(1)	2.051
O(13)	2.068	O(31)	2.079	O(15)	2.061
O(3)H	1.229	O(32)	2.030	O(7)	1.185
O(4)H	1.187	O(33)	2.111	O(13)	1.223
		O(21)	1.211		
		O(22)	1.235		
		O(28)	1.176		
		O(30)	1.146		

[1] I. D. Brown, D. Altermatt, *Acta Crystallogr., Sect. B.*, 1985, **41**, 244-247.

S4. Magnetic susceptibility data of compound 2. (1) χ^{-1} - T plot for compound 2 under the applied filed of 0.1 T (Figure S3). (2) The inverse susceptibility data above 150 K was fitted to the C–W law (Figure S4). (3) χT-T plot for compound 2 under the applied filed of 0.1 T (Figure S5).
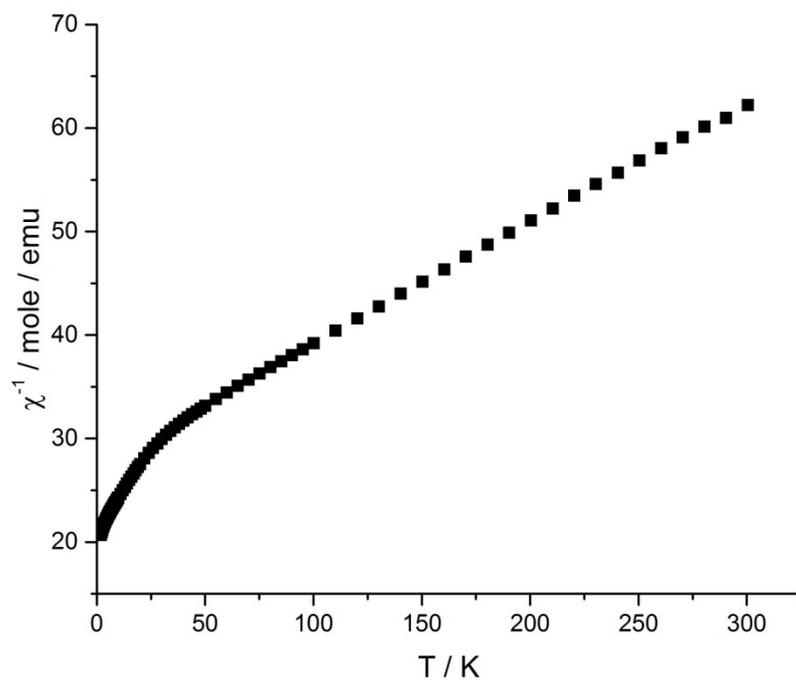

Figure S2. χ^{-1} - T plot for compound 2 under the applied filed of 0.1 T.

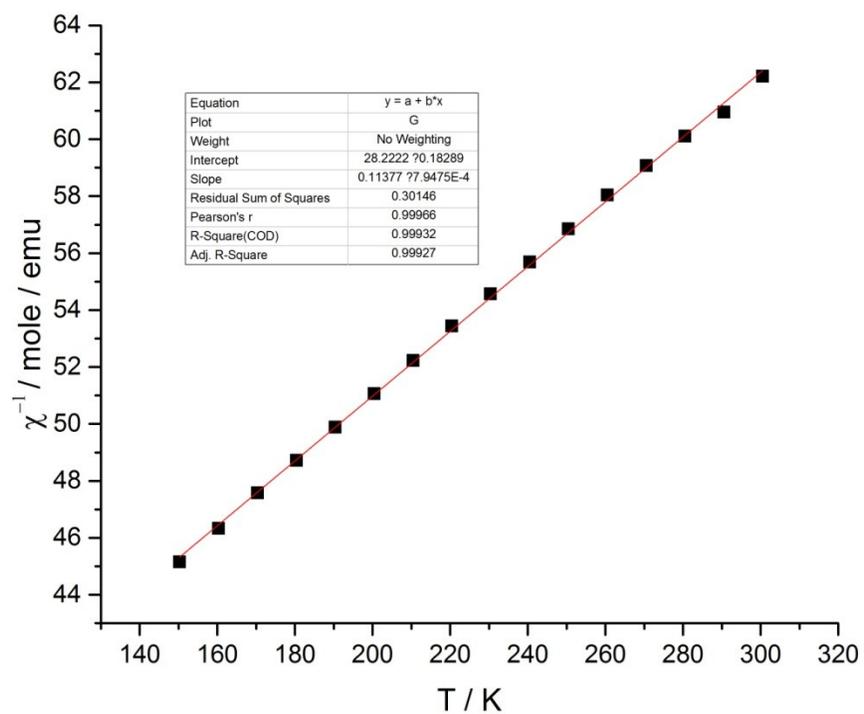| Equation	y = a + b*x
Plot	G
Weight	No Weighting
Intercept	28.2222 ?0.18289
Slope	0.11377 ?7.9475E-4
Residual Sum of Squares	0.30146
Pearson's r	0.99966
R-Square(COD)	0.99932
Adj. R-Square	0.99927

Figure S3. The inverse susceptibility data above 150 K was fitted to the C–W law (χ = C/(T - theta)), resulting in values of 8.790 emuK/mol and -248.07 K for the Curie and Weiss constants, respectively.
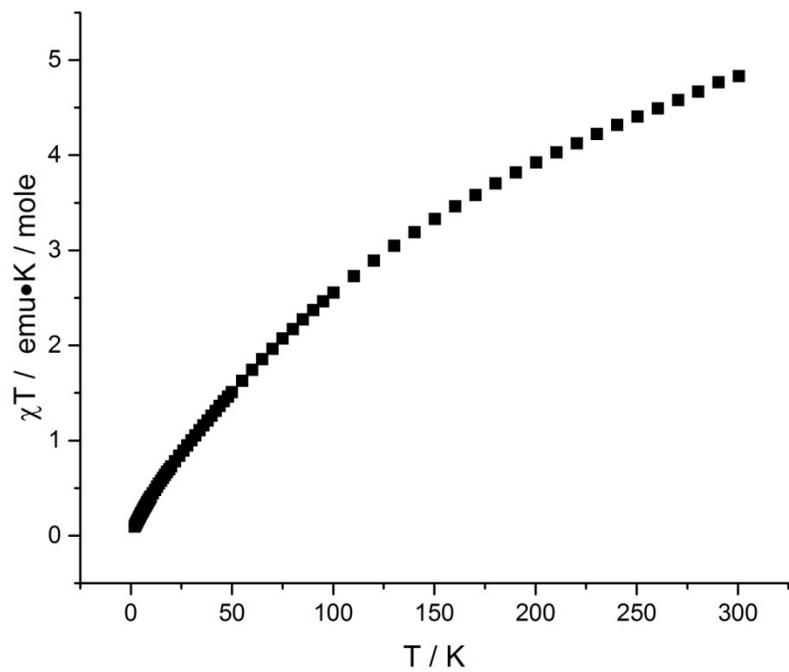
Figure S4. χT-T plot for compound 2 under the applied filed of 0.1 T.