New Thorium(IV)-Arsonates with a $[Th_8O_{13}]^{6+}$ Octanuclear Core

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Supporting Information

Table S1. Bond-valence sums (without the contribution from O-H bonds) of the oxygen atoms in the sulfo-phenyl-arsonate ligands for Compounds **1**-**3**.

Table S2. Hydrogen bonds distances [Å] and angles [deg.] for compounds **1**-**3**.

Figure S1. Simulated and measured XRD powder patterns for compounds **1**-**3**.

Figure S2. Morphologies of compounds **1**(a), **2**(b) and **3**(c).

Figure S3. IR spectra of compounds **1**–**3**.

Figure S4. ORTEP representation of the selected unit in compound **1**. The thermal ellipsoids are drawn at 50% probability level. Symmetry codes for the generated atoms: (a) -z+1, x-1/2, -y+1/2; (b) y+1/2, -z+1/2, -x+1; (c) -y+3/2, z+1/2, x-1; (d) z+1, -x+3/2, y-1/2.

Table S1. Bond-valence sums (without the contribution from O-H bonds) of the oxygen atoms in the sulfo-phenyl-arsonate ligands for compounds **1**-**3**.

Compound **1**					
O1	1.988	O2	2.009	O3	1.995
O4	1.983	O5	1.792	O6	2.020
O7	1.949	O8	1.132	O9	1.913
O10	1.966	O11	1.703	O12	1.671
O13	1.301				
Compound **2**					
O1	2.065	O2	1.982	O3	2.057
O4	1.991	O5	1.990	O6	1.754
O7	2.031	O8	2.010	O9	2.008
O10	2.002	O11	1.731	O12	1.980
O13	2.029	O14	1.996	O15	1.964
O16	1.992	O17	2.002	O18	1.717
O19	1.936	O20	1.935	O21	1.111
O22	1.680	O23	1.676	O24	1.924
O25	1.920	O26	1.995	O27	1.097
O28	1.843	O29	1.708	O30	1.731
O31	2.029	O32	1.120	O33	2.017
O34	1.722	O35	1.985	O36	1.834
O37	1.611				
Compound **3**					
O1	1.983	O2	2.016	O3	2.003
O4	1.913	O5	1.930	O6	1.932
O7	2.004	O8	1.985	O9	1.157
O10	2.286	O11	1.898	O12	2.022
O13	2.127	O14	2.104	O15	2.054
O16	1.774	O17	2.112	O18	1.692
O19	1.972	O20	2.024	O21	2.029
O22	1.812	O23	1.968	O24	2.074
O25	1.997	O26	1.991	O27	1.192
O28	1.676	O29	1.588	O30	1.861
O31	1.961	O32	1.902	O33	1.170
O34	1.726	O35	1.788	O36	2.048
O37	2.129	O38	1.879	O39	0.808
O40	2.177	O41	1.504	O42	1.541
O43	1.892	O44	1.822	O45	1.154
O46	1.852	O47	1.689	O48	1.934
O49	2.053	O50	2.067	O51	2.046
O52	1.902	O53	1.917	O54	2.068
O55	1.976	O56	2.052	O57	1.976
O58	1.981	O59	2.054	O60	2.086

O61	2.170	O62	2.064	O63	2.096
O64	2.223	O65	1.827	O66	2.043
O67	1.964	O68	1.931	O69	1.036
O70	1.812	O71	1.994	O72	1.867
O73	1.803				

Table S2. Hydrogen bonds distances [Å] and angles [deg.] for compounds **1**-**3**.

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
Compound **1**				
O(2W)-H(2WB)...O(6W)	0.85	2.17	2.67(5)	116.9
O(5W)-H(5WB)...O(2W)	0.85	2.23	2.68(3)	113.2
O(8W)-H(8WA)...O(1W)	0.85	1.92	2.77(7)	178.9
O(1W)-H(1WB)...O(10)#1	0.85	2.53	2.70(2)	92.3
O(2W)-H(2WA)...O(9)#1	0.85	2.19	2.715(15)	119.6
O(3W)-H(3WA)...O(8)#2	0.86	2.25	2.75(2)	117.0
O(4W)-H(4WA)...O(12)#1	0.85	1.89	2.74(3)	179.4
O(5W)-H(5WA)...O(12W)#3	0.85	1.82	2.67(11)	178.2
O(6W)-H(6WB)...O(7W)#4	0.85	1.82	2.58(10)	147.3
O(10W)-H(10B)...O(10W)#5	0.85	1.68	2.53(19)	179.6
Compound **2**				
O(21)-H(21A)...O(28)	0.82	1.94	2.743(7)	166.4
O(1W)-H(1WA)...O(11W)	0.85	2.32	2.673(10)	105.4
O(1W)-H(1WA)...O(10)	0.85	2.65	2.773(8)	89.1
O(1W)-H(1WB)...O(25)	0.85	2.36	2.729(7)	107.1
O(5W)-H(5WB)...O(13W)	0.85	2.39	2.765(14)	107.3
O(2W)-H(2WA)...O(9W)	0.85	2.21	2.733(10)	119.4
O(3W)-H(3WC)...O(8W)	0.85	2.27	2.710(8)	112.4
O(3W)-H(3WA)...O(5)	0.85	2.07	2.620(7)	122
O(12W)-H(12E)...O(11W)	0.85	1.90	2.72(2)	164.1
O(12W)-H(12D)...O(2W)	0.85	1.77	2.618(15)	177.6
O(13W)-H(13C)...O(5W)	0.85	2.30	2.765(13)	114.5
O(14W)-H(14B)...O(11)	0.85	1.79	2.645(17)	179.7
O(16W)-H(16B)...O(13W)	0.85	1.76	2.43(2)	133.4
O(32)-H(32B)...O(6W)#1	0.82	1.93	2.740(8)	170.7
O(3W)-H(3WA)...O(6)#2	0.85	2.08	2.706(6)	129.9
O(4W)-H(4WA)...O(20)#1	0.85	2.10	2.611(7)	118.5
O(5W)-H(5WA)...O(33)#1	0.85	2.22	2.714(6)	117.1
O(6W)-H(6WA)...O(7W)#3	0.85	2.23	2.777(9)	122
O(9W)-H(9WA)...O(16W)#4	0.85	1.85	2.70(2)	169.6
O(11W)-H(11A)...O(10W)#2	0.85	1.97	2.791(18)	162.1
O(16W)-H(16B)...O(15W)#4	0.85	2.07	2.70(3)	130.9
Compound **3**				
O(1W)-H(1WA)...O(6)	0.85	2.08	2.62(4)	120.8
O(1W)-H(1WA)...O(6W)	0.85	2.08	2.65(8)	123.2
O(4W)-H(4WA)...O(70)	0.85	2.12	2.73(3)	128.9
O(5W)-H(5WA)...O(46)	0.85	2.07	2.73(3)	133.3
O(33)-H(33B)...O(46)#1	0.82	1.95	2.68(3)	147.8
O(2W)-H(2WA)...O(39)#2	0.85	1.71	2.37(8)	133.5
O(3W)-H(3WA)...O(29)#3	0.85	1.86	2.65(4)	153.7
O(3W)-H(3WB)...O(11)#3	0.85	2.06	2.73(3)	134.5

O(4W)-H(4WB)...O(41)#4	0.85	1.72	2.56(3)	172.2

Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -y+3/2, z+1/2, x-1; #2 -z+3/4, -y+3/4, -x+3/4; #3 z+1, -x+3/2, y-1/2; #4 y+3/4, -x+5/4, -z-1/4; #5 x+0, -y+1, -z-1/2.

For **2**: #1 -x+1, -y+1, -z+1; #2 -x+2, -y+1, -z+1; #3 x, y+1, z; #4 -x+1, -y+1, -z.

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

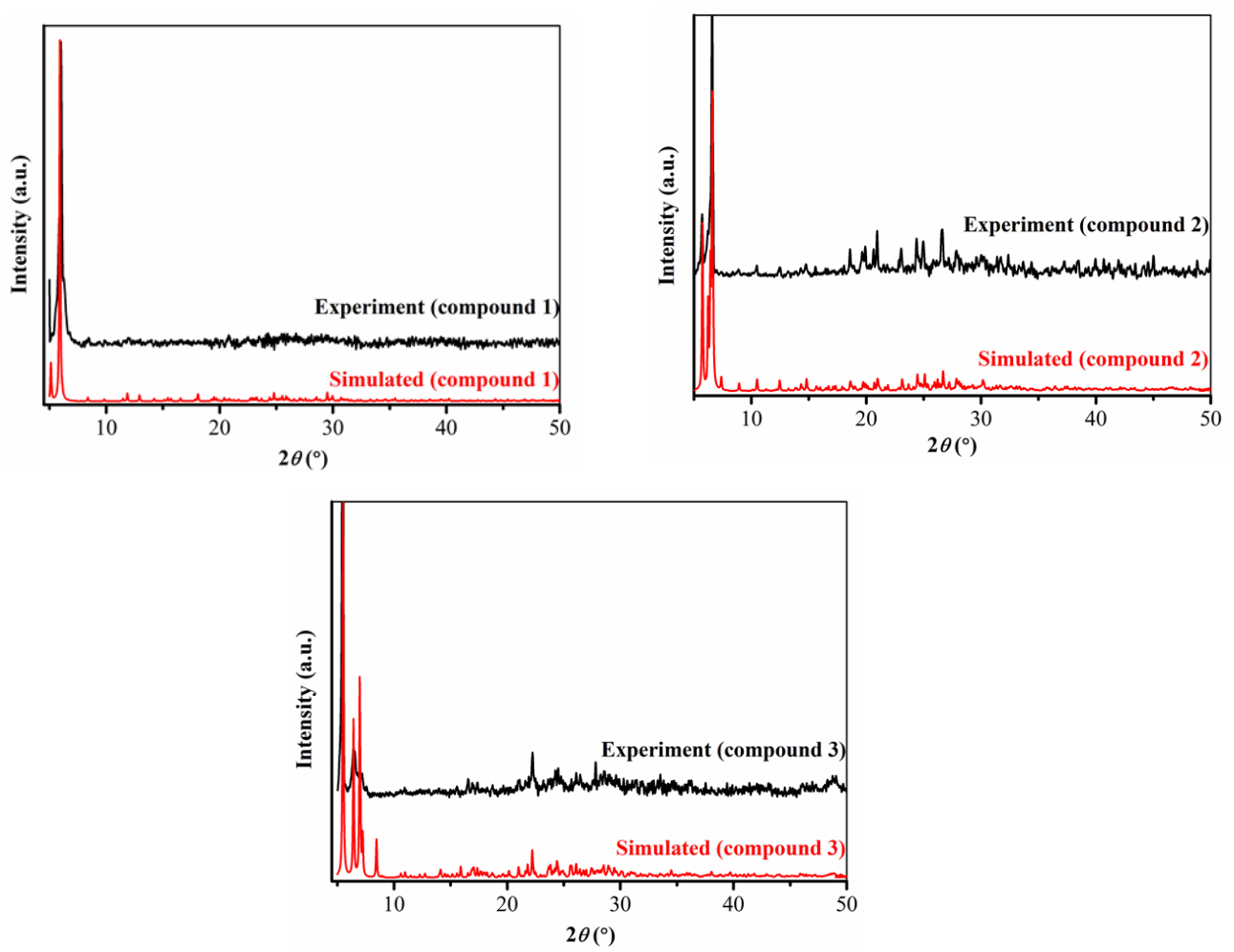

Figure S1. Simulated and measured XRD powder patterns for compounds **1**-**3**.

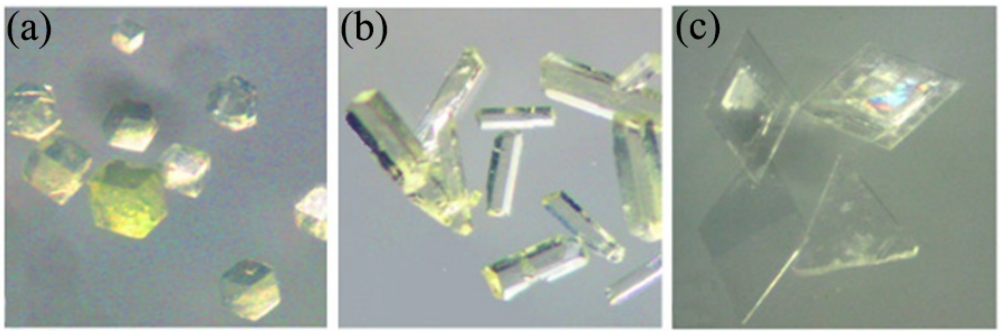

Figure S2. Morphologies of compounds **1**(a), **2**(b) and **3**(c).

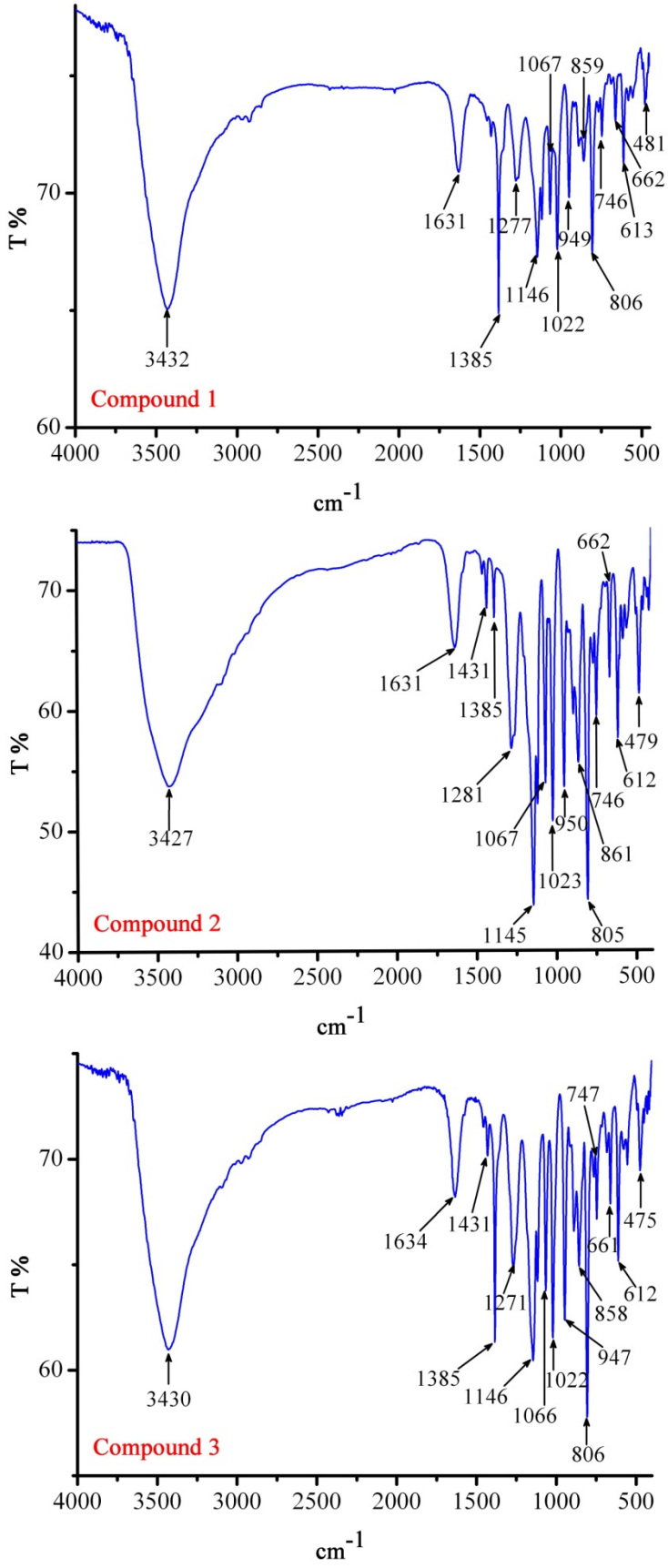

Figure S3. IR spectra of compounds **1**–**3**.

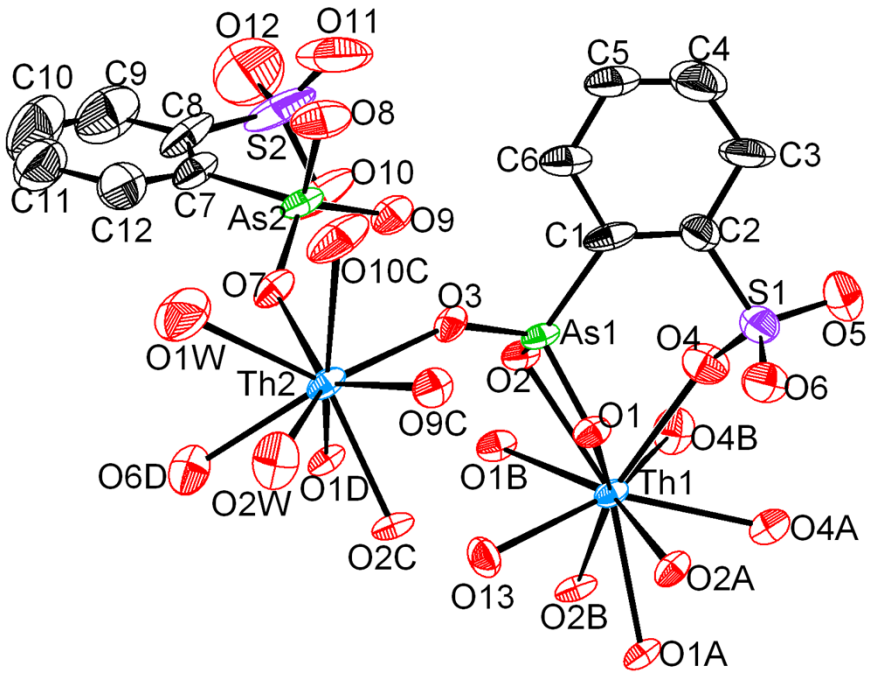

Figure S4. ORTEP representation of the selected unit in compound **1**. The thermal ellipsoids are drawn at 50% probability level. Symmetry codes for the generated atoms: (a) -z+1, x-1/2, -y+1/2; (b) y+1/2, -z+1/2, -x+1; (c) -y+3/2, z+1/2, x-1; (d) z+1, -x+3/2, y-1/2.