

**Table S1.** Uranium coordination environments, **1a-c**

Atoms	U(1)			U(2)		
	<b>1a</b> (anions 1,2)	<b>1b</b>	<b>1c</b>	<b>1a</b> (anions 1,2)	<b>1b</b>	<b>1c</b>
Distances (Å)						
U-O(0)	2.344(3), 2.339(3)	2.337(3)	2.336(3)	2.347(3), 2.353(3)	2.363(3)	2.333(3)
U-O(101)	1.795(3), 1.793(3)	1.786(4)	1.797(3)	1.793(3), 1.792(3)	1.793(4)	1.782(3)
U-O(102)	1.806(3), 1.784(3)	1.801(4)	1.802(3)	1.784(3), 1.794(3)	1.797(4)	1.788(3)
U-O(21)	2.434(3), 2.494(3)	2.489(3)	2.564(3)	2.487(3), 2.473(3)	2.564(3)	2.566(3)
U-O(71)	2.596(3), 2.613(3)	2.508(4)	2.441(3)	2.590(3), 2.532(3)	2.516(4)	2.461(3)
U-O(11)	2.244(3), 2.208(3)	2.250(4)	2.277(3)	2.310(3), 2.320(3)	2.291(4)	2.273(3)
U-O(81)	2.311(3), 2.304(3)	2.283(3)	2.274(3)	2.238(3), 2.257(3)	2.205(4)	2.281(3)
O(21)...O(31)	2.493(5), 2.470(5)	2.512(5)	2.538(4)	2.517(6), 2.526(5)	2.561(5)	2.525(4)
U...U	4.4890(4), 4.4647(3)	4.4955(7)	4.4724(4)			
Angle (degrees)						
O(0)-U-O(101)	85.1(1), 84.5(1)	85.7(2)	85.6(1)	84.5(1), 84.9(1)	84.8(2)	85.5(1)
O(0)-U-O(102)	94.6(1), 95.49(5)	94.3(1)	95.9(1)	94.3(1), 94.7(1)	93.3(1)	96.4(1)
O(0)-U-O(21)	70.1(1), 69.3(1)	68.3(1)	66.81(9)	69.2(1), 69.0(1)	65.9(1)	66.92(9)
O(0)-U-O(71)	64.9(1), 65.9(1)	67.4(1)	69.10(9)	66.0(1), 67.0(1)	68.1(1)	68.7(1)
O(0)-U-O(11)	145.4(1), 142.1(1)	142.5(1)	139.0(1)	143.2(1), 143.0(1)	138.8(1)	139.5(1)
O(0)-U-O(81)	136.9(1), 137.1(1)	139.9(1)	141.3(1)	137.8(1), 140.2(1)	141.7(1)	141.59(9)
O(101)-U-O(102)	177.9(1), 177.8(1)	178.9(2)	178.4(1)	178.8(2), 179.6(1)	177.0(2)	178.1(1)
O(101)-U-O(21)	93.7(1), 94.8(1)	93.1(2)	93.1(1)	92.6(1), 93.0(1)	91.3(2)	94.1(1)
O(101)-U-O(71)	92.6(1), 92.1(1)	91.4(2)	94.0(1)	94.4(1), 93.4(1)	93.8(2)	93.0(1)
O(101)-U-O(11)	89.8(1), 87.6(1)	88.7(2)	89.9(1)	90.4(1), 91.2(1)	90.3(2)	89.8(1)

O(101)-U-O(81)	90.2(1), 88.7(1)	89.5(1)	90.0(1)	O(201)-U-O(41)	87.8(1), 89.3(1)	89.0(2)	89.4(1)
O(102)-U-O(21)	88.1(1), 87.3(1)	88.0(1)	87.1(1)	O(202)-U-O(61)	87.2(1), 86.9(1)	85.8(1)	86.5(1)
O(102)-U-O(71)	85.4(1), 85.9(1)	87.6(2)	86.9(1)	O(202)-U-O(31)	84.9(1), 86.4(1)	87.6(2)	87.8(1)
O(102)-U-O(11)	91.7(1), 93.7(1)	92.0(2)	88.6(1)	O(202)-U-O(51)	90.7(1), 89.2(1)	89.6(2)	88.7(1)
O(102)-U-O(81)	88.7(1), 89.8(1)	89.8(1)	89.1(1)	O(202)-U-O(41)	93.0(1), 90.9(1)	94.0(2)	89.2(1)
O(21)-U-O(71)	133.8(1), 133.6(1)	134.9(1)	134.56(9)	O(61)-U-O(31)	133.7(1), 134.6(1)	133.0(1)	134.21(9)
O(21)-U-O(11)	76.2(1), 74.6(1)	75.1(1)	72.8(1)	O(61)-U-O(51)	74.7(1), 74.6(1)	73.3(1)	73.4(1)
O(71)-U-O(81)	72.6(1), 72.1(1)	73.0(1)	72.9(1)	O(31)-U-O(41)	73.4(1), 74.2(1)	74.8(1)	73.7(1)
O(21)-U-O(81)	153.0(1), 153.6(1)	151.8(1)	151.9(1)	O(61)-U-O(41)	152.8(1), 150.8(1)	152.2(1)	151.49(9)
O(71)-U-O(11)	149.6(1), 151.6(1)	149.9(1)	151.88(9)	O(31)-U-O(51)	150.8(1), 150.0(1)	153.2(1)	151.8(1)
O(11)-U-O(81)	77.1(1), 79.5(1)	77.0(1)	79.2(1)	O(51)-U-O(41)	78.1(1), 76.3(1)	78.8(1)	78.3(1)
U(1)-O(0)-O(2)	146.2(2), 144.2(1)	146.1(2)	146.6(1)				
U(1)-O(21)-C(21)	126.1(3), 126.2(3)	125.9(3)	129.4(2)	U(2)-O(61)-C(61)	130.2(3), 130.1(3)	129.8(3)	128.7(2)
U(1)-O(71)-C(71)	130.1(3), 130.8(3)	133.2(3)	132.3(3)	U(2)-O(31)-C(31)	124.4(3), 126.6(3)	126.2(4)	129.3(2)
U(1)-O(11)-C(11)	136.4(3), 137.6(3)	139.3(3)	132.7(3)	U(2)-O(51)-C(51)	127.7(3), 129.1(3)	128.6(4)	134.0(3)
U(1)-O(81)-C(81)	130.7(3), 127.5(3)	131.1(3)	132.7(3)	U(2)-O(41)-C(41)	141.4(3), 135.9(2)	143.5(4)	130.2(2)

**Table S2.** Ligand conformational descriptors, **1a-c, 2**

	<b>1a</b> (cations 1,2)	<b>1b</b>	<b>1c</b>	<b>2</b>	<b>1a</b> (cations 1,2)	<b>1b</b>	<b>1c</b>	<b>2</b>
Aromatic ring C <sub>6</sub> interplanar dihedral angles to the associated equatorial (phenolic-O) <sub>4</sub> planes (degrees)								
Ring 1	43.9(1), 44.7(1)	43.2(2)	45.7(1)	50.2(2)	48.4(2), 50.1(1)	52.0(2)	45.1(1)	48.3(3)
8	49.4(1), 40.6(1)	49.7(2)	44.3(1)	45.8(2)	41.2(1), 44.7(1)	41.4(2)	48.4(1)	52.4(2)
2	65.4(1), 65.2(1)	69.3(2)	61.5(1)	64.5(2)	57.9(2), 59.8(1)	60.5(2)	61.4(1)	65.52(3)
7	60.6(1), 57.9(1)	62.5(2)	44.2(1)	63.9(2)	65.2(1), 65.1(1)	67.8(2)	64.0(1)	61.9(2)
$\chi^2(\text{O}_4)$	34, 261	100	10.5	2.8	$\chi^2(\text{O}_4)$	251	10.3	16.1
$\delta\text{O}_{\text{max}}$ (Å)	0.014(4), 0.041(4)	0.023(5)	0.007(4)	0.008(8)	$\delta\text{O}_{\text{max}}$ (Å)	0.048(5)	0.007(4)	0.020(8)
$\delta\text{O}(0)$ (Å)	0.408(5), 0.486(5)	0.337(5)	0.414(4)	0.532(9)	$\delta\text{O}(0)$ (Å)	0.382(5)	0.423(4)	0.556(9)
$\delta\text{U}(1)$ (Å)	0.090(1), 0.071(1)	0.050(1)	0.100(1)	0.096(2)	$\delta\text{U}(2)$ (Å)	0.065(1)	0.095(1)	0.023(1)
O <sub>4</sub> /O <sub>4</sub>	16.5(1), 17.8(1)	19.2(1)	17.83(9)	6.2(2)				
Aromatic ring C <sub>6</sub> interplanar dihedral angles to the (phenolic-O) <sub>8</sub> 'plane' (degrees)								
Ring 1	39.9(1), 41.0(1)	38.1(1)	41.0(1)	47.7(2)	44.7(2), 47.1(1)	45.7(2)	40.2(1)	47.0(2)
8	47.2(1), 46.4(1)	44.7(2)	42.2(1)	47.5(2)	37.9(1), 41.0(1)	38.0(2)	45.8(1)	41.2(2)
2	59.4(1), 58.8(1)	59.1(2)	55.0(1)	58.6(2)	51.4(1), 51.8(1)	49.9(2)	55.6(1)	57.2(2)
7	53.3(1), 51.3(1)	51.1(1)	56.0(1)	55.7(2)	59.7(1), 58.7(1)	57.7(2)	56.2(1)	58.2(2)
$\chi^2(\text{O}_8)$	2x10 <sup>4</sup> , 2x10 <sup>4</sup>	2x10 <sup>4</sup>	3x10 <sup>4</sup>	853				
$\delta\text{O}_{\text{max}}$ (Å)	0.276(4), 0.280(4)	0.293(4)	0.273(3)	0.107(8)				
$\delta\text{O}(0)$ (Å)	0.827(4), 0.867(4)	0.803(3)						
$\delta\text{U}(1)$ Å)	0.170(1), 0.114(1)	0.126(1)	0.157(1)	0.123(2)	$\delta\text{U}(2)$ Å)	0.111(2)	0.162(1)	0.039(2)
C <sub>6</sub> /C <sub>6</sub> interplanar dihedral angles								
2/3	75.4(2), 76.1(2)	80.0(2)	80.1(2)	84.5(3)	77.7(2), 76.5(2)	78.1(2)	82.9(2)	79.4(3)

1/2	80.2(2), 79.5(2)	80.3(3)	75.7(2)	76.3(3)	3/4	81.5(2), 82.9(2)	78.6(2)	75.9(1)	73.1(3)
7/8	77.5(2), 74.2(2)	73.2(2)	75.9(2)	77.9(3)	5/6	72.2(2), 74.5(2)	73.2(2)	75.8(2)	74.8(3)
1/8	81.7(2), 78.8(2)	79.2(2)	78.4(2)	79.1(3)	4/5	75.7(2), 83.4(2)	78.3(2)	78.7(2)	78.8(3)
1/4	23.8(2), 24.1(2)	17.6(2)	29.8(2)	37.1(3)	5/8	29.9(2), 31.4(2)	26.0(2)	23.1(2)	35.4(3)
2/7	64.1(2), 67.4(2)	59.8(2)	59.2(2)	65.6(3)	3/6	68.8(2), 62.8(2)	61.5(2)	62.6(2)	61.9(3)

In **1a**, the two O<sub>8</sub> planes of the independent cations are virtually parallel (interplanar dihedral angle 0.93(5)<sup>o</sup>). The ring numbering 1-8 in **1a-c** is transposed to 3-8, 1, 2 in **2**.

**Table S3.** Uranium atom environments, **2**.

$r$  is the U-O distance (Å); other entries in each matrix are the angles (degrees) subtended by the relevant atoms at the head of the row and column  $\theta$  (degrees) is the U-O-X angle.

(a) U(1)

Atom	$r$	O(1)	O(3)	O(11)	O(41)	O(21)	O(31)	$\theta$
O(0)	2.223(6)	78.1(2)	100.3(2)	69.6(2)	71.2(2)	141.9(2)	142.3(2)	
O(1)	1.839(6)		178.4(3)	92.4(2)	91.8(2)	93.3(2)	92.3(2)	
O(3)	1.781(6)			87.6(3)	87.2(3)	88.2(3)	88.6(3)	
O(11)	2.459(6)				138.8(2)	73.8(2)	147.9(2)	130.0(5)
O(41)	2.398(6)					146.8(2)	72.7(2)	133.2(5)
O(21)	2.299(6)						74.2(2)	139.4(6)
O(31)	2.340(6)							135.4(6)

(b) U(2)

Atom	$r$	O(2)	O(4)	O(51)	O(81)	O(61)	O(71)	$\theta$
O(0)	2.235(5)	77.0(2)	100.6(3)	67.5(2)	68.8(2)	136.3(2)	140.6(2)	
O(2)	1.846(6)		177.6(3)	91.0(2)	90.7(2)	90.8(2)	89.2(2)	
O(4)	1.791(6)			89.9(2)	88.6(2)	90.8(3)	92.8(2)	
O(51)	2.522(5)				134.6(2)	71.1(2)	150.7(2)	131.9(5)
O(81)	2.451(6)					154.2(2)	74.7(2)	128.2(5)
O(61)	2.282(6)						79.6(2)	132.4(5)
O(71)	2.187(5)							138.8(5)

(c) U(3)

Atom	$r$	O(1)	O(2)	O(5)	O(6)	O(10)	O(20)	$\theta$
O(0)	2.262(6)	65.5(2)	65.7(2)	94.4(3)	92.3(3)	145.2(2)	137.3(2)	
O(1)	2.492(6)		131.1(2)	88.7(2)	93.2(2)	80.0(2)	157.1(2)	
O(2)	2.445(6)			92.2(2)	89.8(2)	148.7(2)	71.6(2)	
O(5)	1.772(6)				175.3(3)	90.9(3)	87.9(3)	
O(6)	1.778(6)					85.2(2)	88.7(3)	
O(10)	2.418(6)						77.4(2)	119.5(4)
O(20)	2.388(8)							125.4(5)

U(1)...U(2,3), U(2)...U(3) are 4.2952(6), 3.5786(5), 3.5742(5) Å. U(2)-O(0)-U(1,3), U(1)-O(0)-U(3) are 148.9(3), 105.3(2), 105.9(2)°. U(1,2)-O(1,2)-U(3) are 110.5(2), 112.1(3)°. Deviations of O(0; 1-4; 11-81; 10,20) from the  $U_3$  plane are: -0.001(6); -0.012(6), 0.058(6), 0.022(6); -2.288(6), -1.401(6), 1.404(6), 2.256(6), 2.317(6), 1.537(6), -1.313(6), -2.276(6); 0.170(7), -0.048(8) Å.