

Electronic supplementary information

for

Bis(nitrate)diaquauranyl(VI) synthon to generate $[1\times 2+1\times 1]$ and $[1\times 1+1\times 1]$ cocrystalized 3d...5f self-assemblies

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Table S1

Bond angles (°) in the coordination environments of uranium(VI) in **1–4**.
 Symmetry codes: A (for **1**), 1-x, 1-y, 1-z; A (for **2**), 1-x, -y, 1-z;
 A (for **3**), -x, 1-y, 2-z; D (for **4**), 0.5-x, 0.5-y, 1-z

Compound	Bond angles	
1	O(5)–U(1)–O(5A)	180
	O(7)–U(1)–O(7A)	180
	O(8)–U(1)–O(8A)	180
	O(9)–U(1)–O(9A)	180
	O(5)–U(1)–O(7)	50.71(9)
	O(5)–U(1)–O(7A)	129.29(9)
	O(5)–U(1)–O(8)	90.62(11)
	O(5)–U(1)–O(8A)	89.38(11)
	O(5)–U(1)–O(9)	64.68(9)
	O(5)–U(1)–O(9A)	115.32(9)
	O(7)–U(1)–O(8)	91.42(11)
	O(7)–U(1)–O(8A)	88.58(11)
	O(7)–U(1)–O(9)	115.34(9)
	O(7)–U(1)–O(9A)	64.66(9)
	O(8)–U(1)–O(9)	91.55(11)
	O(8)–U(1)–O(9A)	88.45(11)
2	O(5)–U(1)–O(5A)	180
	O(7)–U(1)–O(7A)	180
	O(8)–U(1)–O(8A)	180
	O(9)–U(1)–O(9A)	180
	O(5)–U(1)–O(7)	51.15(5)
	O(5)–U(1)–O(7A)	128.85(5)
	O(5)–U(1)–O(8)	92.07(7)
	O(5)–U(1)–O(8A)	87.93(7)
	O(5)–U(1)–O(9)	63.96(6)
	O(5)–U(1)–O(9A)	116.04(6)
	O(7)–U(1)–O(8)	85.84(7)
	O(7)–U(1)–O(8A)	94.16(7)
	O(7)–U(1)–O(9)	114.60(6)
	O(7)–U(1)–O(9A)	65.40(6)
	O(8)–U(1)–O(9)	89.43(7)
	O(8)–U(1)–O(9A)	90.57(7)
3	O(5)–U(1)–O(5A)	180
	O(7)–U(1)–O(7A)	180
	O(8)–U(1)–O(8A)	180.
	O(9)–U(1)–O(9A)	180.
	O(5)–U(1)–O(7)	51.04(7)
	O(5)–U(1)–O(7A)	128.96(7)
	O(5)–U(1)–O(8)	92.13(8)
	O(5)–U(1)–O(8A)	87.87(8)
	O(5)–U(1)–O(9)	64.22(7)
	O(5)–U(1)–O(9A)	115.78(7)
	O(7)–U(1)–O(8)	86.54(8)
	O(7)–U(1)–O(8A)	93.46(8)
	O(7)–U(1)–O(9)	114.88(7)
	O(7)–U(1)–O(9A)	65.12(7)
	O(8)–U(1)–O(9)	89.72(9)
	O(8)–U(1)–O(9A)	90.28(9)

4	O(3)-U(1)-O(3D)	180
	O(4)-U(1)-O(4D)	180
	O(6)-U(1)-O(6D)	180
	O(7)-U(1)-O(7D)	180
	O(3)-U(1)-O(4)	50.55(7)
	O(3)-U(1)-O(4D)	129.45(7)
	O(3)-U(1)-O(6)	93.95(9)
	O(3)-U(1)-O(6D)	86.05(9)
	O(3)-U(1)-O(7)	65.60(7)
	O(3)-U(1)-O(7D)	114.40(7)
	O(4)-U(1)-O(6)	88.74(10)
	O(4)-U(1)-O(6D)	91.26(10)
	O(4)-U(1)-O(7)	115.58(7)
	O(4)-U(1)-O(7D)	64.42(7)
	O(6)-U(1)-O(7)	87.74(9)
	O(6)-U(1)-O(7D)	92.26(9)