

SUPPORTING INFORMATION

New Complexes of Actinides with Monobromoacetate Ions: Synthesis and Structures

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Table S1. Geometric parameters of coordination polyhedra of actinide atoms
in crystal structures of **I–IV**

Bond	d , Å	Ω , %*	Angle	ω , deg.
(CH ₃) ₄ N[UO ₂ (CH ₂ BrCOO) ₃] (I) Hexagonal bipyramid UO ₈ , V _{VDP} = 9.33 Å ^{3**}				
U–O1	1.761(4)	21.64	O1–U–O2	179.3(2)
U–O2	1.768(4)	22.01	O6–U–O7	67.59(14)
U–O6	2.455(4)	9.53	O8–U–O7	52.60(14)
U–O4	2.457(4)	9.46	O4–U–O3	52.64(12)
U–O8	2.459(4)	9.48	O8–U–O3	67.62(13)
U–O7	2.460(4)	9.45	O6–U–O5	62.40(13)
U–O3	2.475(4)	9.26	O4–U–O5	67.16(12)
U–O5	2.476(4)	9.17		
(CH ₃) ₄ N[NpO ₂ (CH ₂ BrCOO) ₂ (NO ₃)] (II) Hexagonal bipyramid NpO ₈ , V _{VDP} = 9.20 Å ³				
Np–O2	1.740(3)	22.25	O2–Np–O1	178.73(15)
Np–O1	1.743(3)	21.90	O5–Np–O4	69.11(10)
Np–O5	2.423(3)	9.86	O3–Np–O4	52.78(9)
Np–O3	2.445(3)	9.32	O5–Np–O6	53.31(9)
Np–O4	2.448(3)	9.46	O3–Np–O8	65.87(9)
Np–O6	2.454(3)	9.54	O6–Np–O7	68.27(11)
Np–O8	2.492(3)	8.85	O8–Np–O7	50.75(10)
Np–O7	2.515(3)	8.82		
(CH ₃) ₄ N[PuO ₂ (CH ₂ BrCOO) ₂ (NO ₃)] (III) Hexagonal bipyramid PuO ₈ , V _{VDP} = 8.96 Å ³				
Pu–O2	1.690(6)	22.47	O2–Pu–O1	179.9(3)
Pu–O1	1.727(6)	22.26	O4–Pu–O3	53.03(19)
Pu–O4	2.424(6)	9.65	O5–Pu–O6	52.9(2)
Pu–O3	2.432(5)	9.24	O6–Pu–O7	67.9(2)
Pu–O5	2.445(6)	9.43	O3–Pu–O8	65.1(2)
Pu–O6	2.449(5)	9.33	O7–Pu–O8	50.4(2)
Pu–O7	2.477(6)	9.00	O4–Pu–O5	70.9(2)
Pu–O8	2.488(6)	8.62		
(CH ₃) ₄ N[NpO ₂ (CH ₂ BrCOO)(NO ₃) ₂] (IV) Hexagonal bipyramid NpO ₈ , V _{VDP} = 9.21 Å ³				
Np–O1	1.744(3)	21.87	O1–Np–O2	178.39(15)
Np–O2	1.749(3)	22.11	O4–Np–O3	53.44(11)
Np–O4	2.413(3)	9.68	O3–Np–O9	68.75(12)
Np–O3	2.435(3)	9.44	O4–Np–O5	67.50(11)
Np–O9	2.471(4)	9.25	O5–Np–O6	51.51(12)
Np–O5	2.475(4)	9.13	O9–Np–O8	51.91(14)
Np–O6	2.478(3)	9.28	O6–Np–O8	66.89(13)
Np–O8	2.482(3)	9.23		

* 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.

** V_{VDP} is the volume of Voronoi–Dirichlet polyhedron of the actinide atom, Å³.