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Sequestered Plutonium: [Pu^{IV}-{5LIO(Me-3,2-HOPO)}$_2$]—The First Structurally Characterized Plutonium Hydroxypyridonate Complex

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In the paper by Raymond, Shuh et al., a technical problem at the Small Molecule Crystallography Beamline 11.3.1 of the Advanced Light Source at LBNL led to the spatial correction file not properly correcting for the geometry of the goniometer position during the initial data collection. This has been corrected, and the raw data from this crystal were re-integrated by using a new spatial correction file and the APEX-II software.[1] Absorption correction, unit-cell determination, and structure solution were performed as previously reported.

The result is that the new cell-edge lengths are 0.5–0.7 % (0.08–0.16 Å) smaller and the Pu–O bond lengths are 0.0–2.7 % (0.000–0.062 Å) shorter than their published values. The corrected average Pu–O(phenoxide) bond length for Pu1 is 2.262(42) Å, while that for Pu2 is slightly longer at 2.303(19) Å. The average Pu–O(amide) bond length for Pu1 is 2.394(24) Å, and for Pu2 it is 2.364(51) Å. The new data do not eliminate the disorder in the crystal, nor is the $R[I>2\sigma(I)]$ value significantly changed.

Table 1 summarizes selected Pu–O bond lengths and O-Pu-O angles, while Table 2 summarizes the shape measure results for each Pu center.[2] As before, the geometry that these most closely approach is that of the bicapped trigonal prism (C_{2v}). A revised CIF file for the re-refined structure is available.[3]

We thank Géza Szigethy for carrying out the correction.

[1] ApexII, Bruker Analytical X-ray Systems, Madison, WI, **2003**.
[2] Xu, Radkov, Ziegler, Raymond, *Inorg. Chem.* **2000**, *39*, 4156.
[3] CCDC 249885 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data request/cif.

Table 1. Selected bond lengths [Å] and angles [°] for the [Pu^{IV}-{5LIO(Me-3,2-HOPO)}$_2$] complex for each of the unique molecules within the unit cell. Standard deviations for the last decimal place are given in parentheses.

phenolic oxygens		amide oxygens	
Pu1–O1	2.217(16)	Pu1–O2	2.389(14)
Pu1–O3	2.237(16)	Pu1–O4	2.362(16)
Pu1–O5	2.293(14)	Pu1–O6	2.406(16)
Pu1–O7	2.304(12)	Pu1–O8	2.418(12)
Pu2–O15	2.284(17)	Pu2–O16	2.415(12)
Pu2–O17	2.296(11)	Pu2–O18	2.387(12)
Pu2–O19	2.329(12)	Pu2–O20	2.359(15)
Pu2–O21	2.303(13)	Pu2–O22	2.296(17)
O1-Pu1-O2	67.4(4)	O1-Pu1-O7	133.6(4)
O3-Pu1-O4	65.8(5)	O2-Pu1-O8	134.9(4)
O5-Pu1-O6	67.3(5)	O3-Pu1-O5	131.4(5)
O7-Pu1-O8	67.7(4)	O6-Pu1-O4	134.0(5)
O15-Pu2-O16	67.4(4)	O21-Pu2-O15	131.4(5)
O17-Pu2-O18	67.3(4)	O22-Pu2-O16	133.7(5)
O19-Pu2-O20	68.4(4)	O18-Pu2-O20	135.2(4)
O21-Pu2-O22	68.2(5)	O17-Pu2-O19	134.1(4)

Table 2. The shape measure (S) for the given geometry for D_{4d}, C_{2v}, and D_{2d} symmetry is calculated.

	D_{4d}	C_{2v}	D_{2d}
[Pu{5LIO(Me-3,2-HOPO}$_2$] for Pu1	15.36	13.53	16.38
[Pu{5LIO(Me-3,2-HOPO}$_2$] for Pu2	15.68	13.02	15.14

