

Supplementary Materials

Theoretical Study of Complexes of Tetravalent Actinides with DOTA

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Table S1. Selected computed^a and experimental^b An-O and An-N bond distances (Å) of An^{IV}(DOTA) complexes. The averaged values are presented in Figure 2 of the paper.

Complex	An-O ₁	An-N ₁	An-O _w	An-O _{av}	An-N _{av}
Th(DOTA)	2.284	2.735		2.284	2.735
U(DOTA)	2.237	2.682		2.237	2.682
Np(DOTA)	2.227	2.664		2.227	2.664
Pu(DOTA)	2.216	2.672		2.216	2.672
Th(DOTA(H ₂ O))	2.3139 2.3074	2.7580 2.7596	2.490	2.311	2.759
Th(DOTA(DMSO)) ^b				2.36	2.75
U(DOTA)(H ₂ O)	2.2576 2.2575	2.7106 2.7097	2.499	2.258	2.710
U(DOTA(DMSO)) ^b				2.30	2.72
Np(DOTA)(H ₂ O)	2.2478 2.2489	2.6957 2.6926	2.470	2.248	2.694
Pu(DOTA)(H ₂ O)	2.2342 2.2389	2.6952 2.6972	2.497	2.237	2.696

^aFrom TPSSh-GD3BJ/ECP60MWB+TZ+6-311+G** calculations. For the molecular structure see Figure 1 of the paper.

^bFrom X-ray diffraction analysis of An^{IV}(DOTA)(DMSO) complexes (Inorg. Chem. 2019, 58, 8253-8256).

Table S2. Selected computed^a geometrical characteristics^b of the An(DOTA) and An(DOTA)(H₂O) complexes.^b

Complex	O-An-O	N-An-N	O···O	N···N	d _{An-OO}	d _{An-OO} ^c	d _{An-NN}	d _{An-NN} ^c
Th(DOTA)	150.7	102.1	4.418	4.254	0.578		1.720	
U(DOTA)	148.1	103.5	4.303	4.214	0.614		1.660	
Np(DOTA)	147.1	104.0	4.272	4.198	0.631		1.640	
Pu(DOTA)	148.6	103.0	4.266	4.181	0.600		1.664	
Th(DOTA(H ₂ O))	150.4	101.2	4.462	4.265	0.589	0.538	1.751	1.752
	155.7	101.1	4.525	4.260	0.486		1.752	
Th(DOTA(DMSO)) ^d						0.555(8)		1.75(1)
U(DOTA)(H ₂ O))	149.4	102.2	4.355	4.217	0.595	0.556	1.702	1.702
	153.5	102.2	4.395	4.218	0.517		1.703	
U(DOTA(DMSO)) ^d						0.565(7)		1.72(1)
Np(DOTA)(H ₂ O))	148.6	102.5	4.328	4.199	0.609	0.568	1.685	1.687
	152.9	102.4	4.372	4.202	0.528		1.689	
Pu(DOTA)(H ₂ O))	150.0	101.9	4.316	4.189	0.578	0.546	1.699	1.699
	153.5	101.8	4.358	4.184	0.514		1.699	

^aFrom TPSSh-GD3BJ/ECP60MWB+TZ+6-311+G** calculations. For the molecular structure see Figure 1 of the paper.

^bBond angles O-An-O and N-An-N according to the C₂ axis are given in deg., related O···O and N···N distances as well as the distance of An from the plane of the OO and NN shells (d_{An-OO}, d_{An-NN}) are given in Å.

^cAverage of the different d_{An-OO} and d_{An-NN} values in the An(DOTA)(H₂O) complexes (due to the symmetry decreased from C₄ to C₂). For the latter complexes these averaged values are presented in Figure 3 of the paper.

^dFrom X-ray diffraction analysis of An^{IV}(DOTA)(DMSO) complexes (Inorg. Chem. 2019, 58, 8253-8256).

Table S3a. Integral properties of the electron density distribution (ϵ) in the An(DOTA) and An(DOTA)(H₂O) complexes.^a

Complex	q_{An}	LI_{An}	CT_1	CT_2	DI				
					An-O	An-N	An-O _{av}	An-N _{av}	An-O _w
Th(DOTA)	2.75	25.556	1.25		0.53	0.23	0.53	0.23	
U(DOTA)	2.55	27.540	1.45		0.60	0.26	0.60	0.26	
Np(DOTA)	2.47	28.555	1.53		0.61	0.27	0.61	0.27	
Pu(DOTA)	2.39	29.603	1.61		0.63	0.27	0.63	0.27	
Th(DOTA)(H ₂ O)	2.79	25.521	1.15	0.06	0.49	0.22			0.26
					0.48	0.22	0.48	0.22	
U(DOTA)(H ₂ O)	2.58	27.508	1.36	0.06	0.55	0.24			0.26
					0.56	0.24	0.56	0.24	
Np(DOTA)(H ₂ O)	2.50	28.527	1.43	0.07	0.57	0.25			0.27
					0.57	0.25	0.57	0.25	
Pu(DOTA)(H ₂ O)	2.42	29.573	1.52	0.06	0.58	0.25			0.24
					0.59	0.25	0.59	0.25	

^aFrom TPSSh-GD3BJ/ECP60MWB+TZ+6-311+G** calculations. An charge (q_{An}); localisation index on An (LI_{An}); charge transfer to An from DOTA (CT_1) and H₂O (CT_2); delocalisation indices (DI).

Table S3b. Selected results (au) from the DFT-based QTAIM analysis of An(DOTA) and An(DOTA)(H₂O) complexes.^a

An	$\rho(r)$		$\nabla^2\rho(r)$		$H(r)$		ϵ	
	An-O	An-N	An-O	An-N	An-O	An-N	An-O	An-N
Th(DOTA)	0.086	0.041	0.277	0.105	-0.016	-0.003	0.08	0.02
U(DOTA)	0.092	0.043	0.317	0.118	-0.017	-0.003	0.07	0.09
Np(DOTA)	0.093	0.043	0.338	0.126	-0.017	-0.003	0.04	0.09
Pu(DOTA)	0.094	0.042	0.353	0.121	-0.016	-0.003	0.02	0.06
Th(DOTA)(H ₂ O)	0.081	0.039	0.267	0.101	-0.014	-0.002	0.08	0.02
	0.080	0.039	0.263	0.101	-0.013	-0.002	0.08	0.03
data for OH ₂ O:	0.051		0.199		0.0		0.16	
U(DOTA)(H ₂ O)	0.087	0.041	0.305	0.112	-0.015	-0.003	0.09	0.07
	0.087	0.041	0.303	0.112	-0.015	-0.003	0.09	0.06
data for OH ₂ O:	0.047		0.198		0.0		0.12	
Np(DOTA)(H ₂ O)	0.088	0.041	0.324	0.118	-0.014	-0.003	0.01	0.09
	0.088	0.041	0.322	0.118	-0.014	-0.003	0.05	0.12
data for OH ₂ O:	0.049		0.205		0.0		0.06	
Pu(DOTA)(H ₂ O)	0.090	0.039	0.338	0.115	-0.014	-0.002	0.02	0.04
	0.088	0.040	0.332	0.116	-0.014	-0.002	0.03	0.05
data for OH ₂ O:	0.047		0.193		0.0		0.12	

^aFrom TPSSh-GD3BJ/ECP60MWB+TZ+6-311+G** calculations. Electron density ($\rho(r)$), Laplacian of this electron density ($\nabla^2\rho(r)$), total electronic energy density ($H(r)$) and ellipticity of electron density distribution at the An-O and An-N bond critical points.

Table S4. Comparison of selected computed An-O and An-N bond distances (Å) of An^{IV} and An^{III}(DOTA) complexes.^a

State	Complex	SCPP			LCPP		
		An-O _{av}	An-N _{av}	An-O _w	An-O _{av}	An-N _{av}	An-O _w
An ^{IV}	Th(DOTA)	2.284	2.735		2.295	2.748	
SAP	U(DOTA)	2.237	2.682		2.299	2.693	
	Np(DOTA)	2.227	2.664		2.287	2.673	
	Pu(DOTA)	2.216	2.672		2.275	2.656	
	Th(DOTA)(H ₂ O)	2.311	2.759	2.490	2.318	2.776	2.553
	U(DOTA)(H ₂ O)	2.258	2.710	2.499	2.325	2.722	2.500
	Np(DOTA)(H ₂ O)	2.248	2.694	2.470	2.314	2.704	2.478
	Pu(DOTA)(H ₂ O)	2.237	2.696	2.497	2.303	2.689	2.460
An ^{III}	U(DOTA) ⁻				2.459	2.825	
TSAP	Np(DOTA) ⁻				2.441	2.805	
	Pu(DOTA) ⁻				2.424	2.788	
	U(DOTA)(H ₂ O) ⁻				2.486	2.855	2.604
	Np(DOTA)(H ₂ O) ⁻				2.469	2.838	2.578
	Pu(DOTA)(H ₂ O) ⁻				2.453	2.822	2.555

^aFrom TPSSh-GD3BJ/ECP60MWB+TZ+6-311+G** (SCPP) and TPSSh-GD3BJ/ECP8xMWB+TZ+6-311+G** (LCPP) calculations. Data of the An^{III} complexes from Ref. ACS Omega, 2021, 6,13321-13330. For the molecular structure see Figure 1 of the paper.

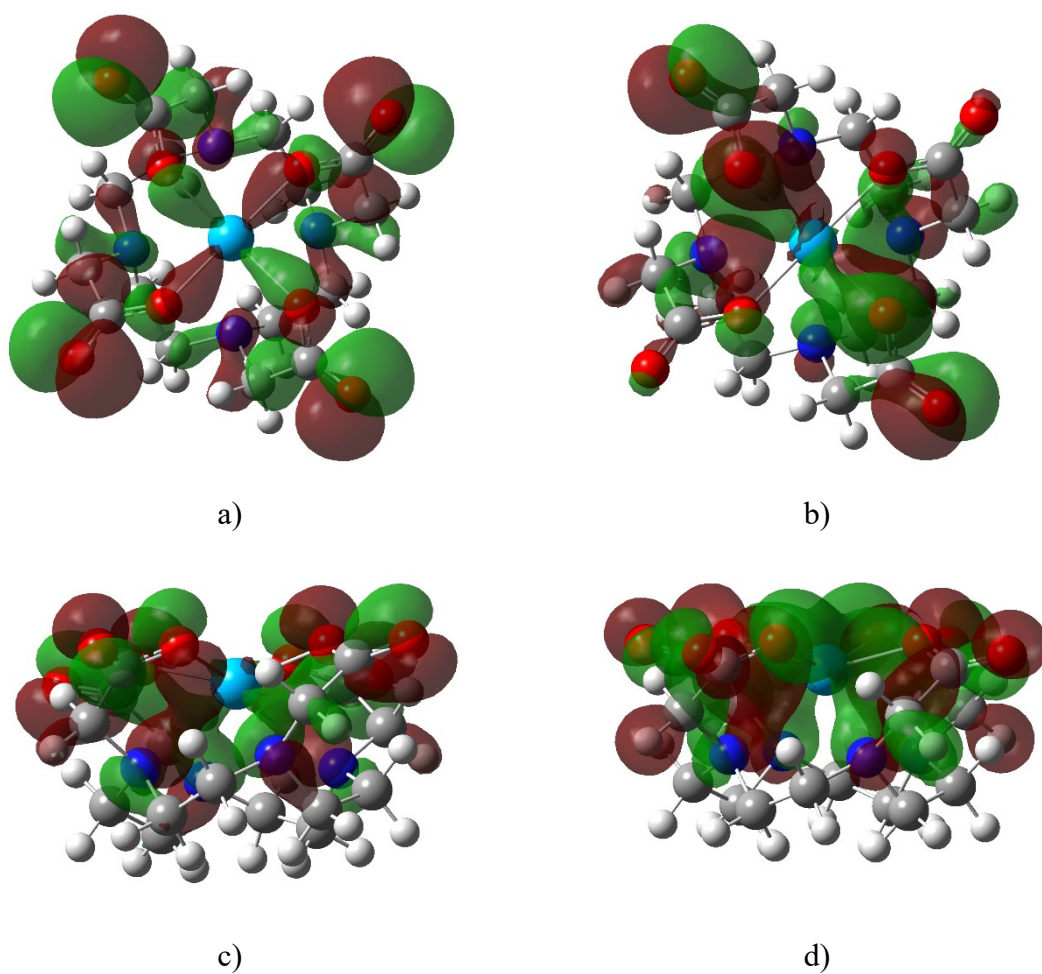


Figure S1. Selected molecular orbitals of Th(DOTA) with significant metal-ligand bonding. a) $\sigma_{O \rightarrow}$ with major $6d_{\pm 2}$; b) $\pi_{O \rightarrow Th}$ with major $5f_{\pm 3}$; c,d) mixed $O/N \rightarrow Th$ with major $6d_{\pm 2}$.

Cartesian coordinates

Th(DOTA)

Th	0.00000000	0.00000000	0.69619299
N	0.16465566	-2.12057412	-1.02329701
N	-2.12057412	-0.16465566	-1.02329701
N	-0.16465566	2.12057412	-1.02329701
N	2.12057412	0.16465566	-1.02329701
O	1.52836698	-1.59508899	1.27411899
O	-1.59508899	-1.52836698	1.27411899
O	-1.52836698	1.59508899	1.27411899
O	1.59508899	1.52836698	1.27411899
O	-3.59778566	-2.64886061	1.10196299
O	-2.64886061	3.59778566	1.10196299
O	3.59778566	2.64886061	1.10196299
O	2.64886061	-3.59778566	1.10196299
C	1.70566598	-2.84609330	0.81347399
C	-2.84609330	-1.70566598	0.81347399
C	-1.70566598	2.84609330	0.81347399
C	2.84609330	1.70566598	0.81347399
C	-1.17424860	-2.42718945	-1.63146901
C	-1.88368766	-1.16729558	-2.11253901
C	-2.42718945	1.17424860	-1.63146901
C	-1.16729558	1.88368766	-2.11253901
C	1.17424860	2.42718945	-1.63146901
C	1.88368766	1.16729558	-2.11253901
C	2.42718945	-1.17424860	-1.63146901
C	1.16729558	-1.88368766	-2.11253901
C	0.59139781	-3.26531358	-0.13960901
C	-3.26531358	-0.59139781	-0.13960901
C	-0.59139781	3.26531358	-0.13960901
C	3.26531358	0.59139781	-0.13960901
H	-0.27314439	-3.53385256	0.46914399
H	0.90583545	-4.12519226	-0.73647601
H	-4.12519226	-0.90583545	-0.73647601
H	-3.53385256	0.27314439	0.46914399
H	-0.90583545	4.12519226	-0.73647601
H	0.27314439	3.53385256	0.46914399
H	3.53385256	-0.27314439	0.46914399
H	4.12519226	0.90583545	-0.73647601
H	-1.76964542	-2.94198469	-0.88238401
H	-1.05328030	-3.11365939	-2.47923201
H	-2.84173001	-1.44611229	-2.56970701
H	-1.28963312	-0.67630971	-2.88513001
H	-3.11365939	1.05328030	-2.47923201
H	-2.94198469	1.76964542	-0.88238401
H	-1.44611229	2.84173001	-2.56970701
H	-0.67630971	1.28963312	-2.88513001
H	1.05328030	3.11365939	-2.47923201
H	1.76964542	2.94198469	-0.88238401
H	1.28963312	0.67630971	-2.88513001
H	2.84173001	1.44611229	-2.56970701
H	2.94198469	-1.76964542	-0.88238401
H	3.11365939	-1.05328030	-2.47923201
H	0.67630971	-1.28963312	-2.88513001
H	1.44611229	-2.84173001	-2.56970701

Th(DOTA)(H₂O)

Th	0.00000000	0.00000000	0.61476500
N	0.20048400	2.12316700	-1.13664200
N	2.11868400	-0.22082200	-1.13701100
N	-0.20048400	-2.12316700	-1.13664200
N	-2.11868400	0.22082200	-1.13701100
O	-1.22082000	1.86713000	1.20408600
O	1.86301400	1.28333900	1.10104400
O	1.22082000	-1.86713000	1.20408600
O	-1.86301400	-1.28333900	1.10104400
O	4.04429500	1.99171700	0.93526800
O	1.91615400	-4.05227500	1.04225400
O	-4.04429500	-1.99171700	0.93526800
O	-1.91615400	4.05227500	1.04225400
C	-1.15385000	3.12212400	0.73132700
C	3.12075300	1.20841600	0.65327800
C	1.15385000	-3.12212400	0.73132700
C	-3.12075300	-1.20841600	0.65327800
C	1.56658200	2.17261600	-1.75838700
C	2.03071400	0.79900400	-2.23191300
C	2.19347300	-1.59649400	-1.73072200
C	0.83495000	-2.08130300	-2.21798400
C	-1.56658200	-2.17261600	-1.75838700
C	-2.03071400	-0.79900400	-2.23191300
C	-2.19347300	1.59649400	-1.73072200
C	-0.83495000	2.08130300	-2.21798400
C	0.00000000	3.32183600	-0.24780200
C	3.33052600	0.01908800	-0.27832500
C	0.00000000	-3.32183600	-0.24780200
C	-3.33052600	-0.01908800	-0.27832500
H	0.90886800	3.42677600	0.34651500
H	-0.16338600	4.22691800	-0.83902900
H	4.22393300	0.16974900	-0.89070500
H	3.45823500	-0.86773100	0.34435700
H	0.16338600	-4.22691800	-0.83902900
H	-0.90886800	-3.42677600	0.34651500
H	-3.45823500	0.86773100	0.34435700
H	-4.22393300	-0.16974900	-0.89070500
H	2.25469500	2.58120800	-1.02416800
H	1.56288600	2.85753900	-2.61662800
H	3.01069400	0.90080200	-2.71710800
H	1.33910200	0.41384600	-2.98303600
H	2.90080700	-1.60795000	-2.57063000
H	2.58643800	-2.26365600	-0.96782200
H	0.94603300	-3.07998100	-2.66046400
H	0.46199400	-1.42269100	-3.00401400
H	-1.56288600	-2.85753900	-2.61662800
H	-2.25469500	-2.58120800	-1.02416800
H	-1.33910200	-0.41384600	-2.98303600
H	-3.01069400	-0.90080200	-2.71710800
H	-2.58643800	2.26365600	-0.96782200
H	-2.90080700	1.60795000	-2.57063000
H	-0.46199400	1.42269100	-3.00401400
H	-0.94603300	3.07998100	-2.66046400
O	0.00000000	0.00000000	3.10515000
H	0.41713000	-0.69606000	3.63521800
H	-0.41713000	0.69606000	3.63521800

U(DOTA)

U	0.00000000	0.00000000	0.63437400
N	-1.05758000	1.82249900	-1.02549200
N	1.82249900	1.05758000	-1.02549200
N	1.05758000	-1.82249900	-1.02549200
N	-1.82249900	-1.05758000	-1.02549200
O	-2.02273600	0.73262800	1.24837300
O	0.73262800	2.02273600	1.24837300
O	2.02273600	-0.73262800	1.24837300
O	-0.73262800	-2.02273600	1.24837300
O	2.09311600	3.82160000	1.23262700
O	3.82160000	-2.09311600	1.23262700
O	-2.09311600	-3.82160000	1.23262700
O	-3.82160000	2.09311600	1.23262700
C	-2.70920000	1.78829000	0.85604100
C	1.78829000	2.70920000	0.85604100
C	2.70920000	-1.78829000	0.85604100
C	-1.78829000	-2.70920000	0.85604100
C	0.00000000	2.67632400	-1.62678500
C	1.18583500	1.85128900	-2.10691800
C	2.67632400	0.00000000	-1.62678500
C	1.85128900	-1.18583500	-2.10691800
C	0.00000000	-2.67632400	-1.62678500
C	-1.18583500	-1.85128900	-2.10691800
C	-2.67632400	0.00000000	-1.62678500
C	-1.85128900	1.18583500	-2.10691800
C	-1.93586500	2.64721000	-0.14965400
C	2.64721000	1.93586500	-0.14965400
C	1.93586500	-2.64721000	-0.14965400
C	-2.64721000	-1.93586500	-0.14965400
H	-1.28854200	3.29951900	0.44185100
H	-2.62692700	3.25952600	-0.73949900
H	3.25952600	2.62692700	-0.73949900
H	3.29951900	1.28854200	0.44185100
H	2.62692700	-3.25952600	-0.73949900
H	1.28854200	-3.29951900	0.44185100
H	-3.29951900	-1.28854200	0.44185100
H	-3.25952600	-2.62692700	-0.73949900
H	0.31664300	3.39711800	-0.87401500
H	-0.40220400	3.24946800	-2.47428100
H	1.92718800	2.52051200	-2.56612400
H	0.86191200	1.15439700	-2.88419400
H	3.24946800	0.40220400	-2.47428100
H	3.39711800	-0.31664300	-0.87401500
H	2.52051200	-1.92718800	-2.56612400
H	1.15439700	-0.86191200	-2.88419400
H	0.40220400	-3.24946800	-2.47428100
H	-0.31664300	-3.39711800	-0.87401500
H	-0.86191200	-1.15439700	-2.88419400
H	-1.92718800	-2.52051200	-2.56612400
H	-3.39711800	0.31664300	-0.87401500
H	-3.24946800	-0.40220400	-2.47428100
H	-1.15439700	0.86191200	-2.88419400
H	-2.52051200	1.92718800	-2.56612400

U(DOTA)(H₂O)

U	0.00000000	0.00000000	0.56337000
N	0.21315400	2.09782000	-1.13843200
N	2.09613200	-0.23024400	-1.13979900
N	-0.21315400	-2.09782000	-1.13843200
N	-2.09613200	0.23024400	-1.13979900
O	-1.21146100	1.80953300	1.15879000
O	1.80879000	1.24793200	1.08024300
O	1.21146100	-1.80953300	1.15879000
O	-1.80879000	-1.24793200	1.08024300
O	3.97949800	1.85452100	1.08032700
O	1.79877100	-3.98489900	1.16118300
O	-3.97949800	-1.85452100	1.08032700
O	-1.79877100	3.98489900	1.16118300
C	-1.11646600	3.06093700	0.76289800
C	3.06248200	1.15017300	0.70347700
C	1.11646600	-3.06093700	0.76289800
C	-3.06248200	-1.15017300	0.70347700
C	1.56693200	2.15320200	-1.74850100
C	2.02998800	0.78214800	-2.22349700
C	2.16665800	-1.58805600	-1.73516100
C	0.80429200	-2.06099600	-2.21739900
C	-1.56693200	-2.15320200	-1.74850100
C	-2.02998800	-0.78214800	-2.22349700
C	-2.16665800	1.58805600	-1.73516100
C	-0.80429200	2.06099600	-2.21739900
C	0.00000000	3.28286600	-0.26415300
C	3.28981300	0.00265700	-0.28485100
C	0.00000000	-3.28286600	-0.26415300
C	-3.28981300	-0.00265700	-0.28485100
H	0.91530100	3.42977400	0.31452900
H	-0.20422900	4.18400500	-0.85344600
H	4.18583600	0.18956900	-0.88789600
H	3.44204500	-0.89690200	0.31706800
H	0.20422900	-4.18400500	-0.85344600
H	-0.91530100	-3.42977400	0.31452900
H	-3.44204500	0.89690200	0.31706800
H	-4.18583600	-0.18956900	-0.88789600
H	2.25532600	2.55467400	-1.00669700
H	1.57551600	2.84409100	-2.60407100
H	3.01553300	0.88326500	-2.70100100
H	1.34420600	0.40695500	-2.98741300
H	2.87223400	-1.60613500	-2.57863200
H	2.55685000	-2.26491400	-0.97573400
H	0.90768900	-3.05780600	-2.66991200
H	0.43558400	-1.39393100	-3.00070200
H	-1.57551600	-2.84409100	-2.60407100
H	-2.25532600	-2.55467400	-1.00669700
H	-1.34420600	-0.40695500	-2.98741300
H	-3.01553300	-0.88326500	-2.70100100
H	-2.55685000	2.26491400	-0.97573400
H	-2.87223400	1.60613500	-2.57863200
H	-0.43558400	1.39393100	-3.00070200
H	-0.90768900	3.05780600	-2.66991200
O	0.00000000	0.00000000	3.06207800
H	0.43698200	-0.65666500	3.61697600
H	-0.43698200	0.65666500	3.61697600

Np(DOTA)

Np	0.00000000	-0.00000000	0.61805206
N	-0.79562340	1.94253101	-1.02178194
N	1.94253101	0.79562340	-1.02178194
N	0.79562340	-1.94253101	-1.02178194
N	-1.94253101	-0.79562340	-1.02178194
O	-1.89479620	0.98638208	1.24854906
O	0.98638208	1.89479620	1.24854906
O	1.89479620	-0.98638208	1.24854906
O	-0.98638208	-1.89479620	1.24854906
O	2.57287855	3.49583136	1.24096006
O	3.49583136	-2.57287855	1.24096006
O	-2.57287855	-3.49583136	1.24096006
O	-3.49583136	2.57287855	1.24096006
C	-2.43440163	2.12454912	0.85923406
C	2.12454912	2.43440163	0.85923406
C	2.43440163	-2.12454912	0.85923406
C	-2.12454912	-2.43440163	0.85923406
C	0.36455264	2.64888474	-1.62347094
C	1.42571155	1.67055747	-2.10419494
C	2.64888474	-0.36455264	-1.62347094
C	1.67055747	-1.42571155	-2.10419494
C	-0.36455264	-2.64888474	-1.62347094
C	-1.42571155	-1.67055747	-2.10419494
C	-2.64888474	0.36455264	-1.62347094
C	-1.67055747	1.42571155	-2.10419494
C	-1.55423539	2.87565420	-0.14301694
C	2.87565420	1.55423539	-0.14301694
C	1.55423539	-2.87565420	-0.14301694
C	-2.87565420	-1.55423539	-0.14301694
H	-0.82522964	3.43290759	0.45042706
H	-2.15667481	3.57684517	-0.73099894
H	3.57684517	2.15667481	-0.73099894
H	3.43290759	0.82522964	0.45042706
H	2.15667481	-3.57684517	-0.73099894
H	0.82522964	-3.43290759	0.45042706
H	-3.43290759	-0.82522964	0.45042706
H	-3.57684517	-2.15667481	-0.73099894
H	0.77644183	3.32041896	-0.87125294
H	0.04135731	3.27129083	-2.47001694
H	2.25420853	2.23088987	-2.56011894
H	1.01045274	1.02619114	-2.88334294
H	3.27129083	-0.04135731	-2.47001694
H	3.32041896	-0.77644183	-0.87125294
H	2.23088987	-2.25420853	-2.56011894
H	1.02619114	-1.01045274	-2.88334294
H	-0.04135731	-3.27129083	-2.47001694
H	-0.77644183	-3.32041896	-0.87125294
H	-1.01045274	-1.02619114	-2.88334294
H	-2.25420853	-2.23088987	-2.56011894
H	-3.32041896	0.77644183	-0.87125294
H	-3.27129083	0.04135731	-2.47001694
H	-1.02619114	1.01045274	-2.88334294
H	-2.23088987	2.25420853	-2.56011894

Np(DOTA)(H₂O)

Np	0.00000000	0.00000000	0.55281300
N	0.21356800	2.08882700	-1.13274600
N	2.08815100	-0.23181100	-1.13621900
N	-0.21356800	-2.08882700	-1.13274600
N	-2.08815100	0.23181100	-1.13621900
O	-1.21515100	1.79036200	1.16143900
O	1.79726500	1.24455600	1.08059300
O	1.21515100	-1.79036200	1.16143900
O	-1.79726500	-1.24455600	1.08059300
O	3.96110700	1.87009500	1.07115500
O	1.79792800	-3.96516700	1.17635600
O	-3.96110700	-1.87009500	1.07115500
O	-1.79792800	3.96516700	1.17635600
C	-1.11726800	3.04294400	0.77064600
C	3.04907500	1.15587800	0.69900100
C	1.11726800	-3.04294400	0.77064600
C	-3.04907500	-1.15587800	0.69900100
C	1.56554100	2.14945700	-1.74491700
C	2.02595800	0.77898800	-2.22135500
C	2.16439900	-1.58884000	-1.73068500
C	0.80310700	-2.06136500	-2.21260200
C	-1.56554100	-2.14945700	-1.74491700
C	-2.02595800	-0.77898800	-2.22135500
C	-2.16439900	1.58884000	-1.73068500
C	-0.80310700	2.06136500	-2.21260200
C	0.00000000	3.26977100	-0.25299600
C	3.28101400	0.00406800	-0.28108100
C	0.00000000	-3.26977100	-0.25299600
C	-3.28101400	-0.00406800	-0.28108100
H	0.91433600	3.41403800	0.32769200
H	-0.20359700	4.17341500	-0.83859100
H	4.17732600	0.18819200	-0.88449300
H	3.43206200	-0.89232900	0.32560700
H	0.20359700	-4.17341500	-0.83859100
H	-0.91433600	-3.41403800	0.32769200
H	-3.43206200	0.89232900	0.32560700
H	-4.17732600	-0.18819200	-0.88449300
H	2.25567400	2.55134400	-1.00504200
H	1.57048800	2.84148000	-2.59954100
H	3.01220400	0.87671500	-2.69806100
H	1.33933900	0.40551400	-2.98535300
H	2.87117700	-1.60536000	-2.57316600
H	2.55508200	-2.26496200	-0.97085500
H	0.90298200	-3.06105900	-2.65937800
H	0.43638800	-1.39740300	-2.99941900
H	-1.57048800	-2.84148000	-2.59954100
H	-2.25567400	-2.55134400	-1.00504200
H	-1.33933900	-0.40551400	-2.98535300
H	-3.01220400	-0.87671500	-2.69806100
H	-2.55508200	2.26496200	-0.97085500
H	-2.87117700	1.60536000	-2.57316600
H	-0.43638800	1.39740300	-2.99941900
H	-0.90298200	3.06105900	-2.65937800
O	0.00000000	0.00000000	3.02261000
H	0.44937600	-0.65062500	3.57467900
H	-0.44937600	0.65062500	3.57467900

Pu(DOTA)

Pu	-0.00000000	0.00000000	0.63215592
N	0.49638031	-2.03094232	-1.03217608
N	-2.03094232	-0.49638031	-1.03217608
N	-0.49638031	2.03094232	-1.03217608
N	2.03094232	0.49638031	-1.03217608
O	1.72979435	-1.24797028	1.23184292
O	-1.24797028	-1.72979435	1.23184292
O	-1.72979435	1.24797028	1.23184292
O	1.24797028	1.72979435	1.23184292
O	-3.06534544	-3.06029763	1.24820792
O	-3.06029763	3.06534544	1.24820792
O	3.06534544	3.06029763	1.24820792
O	3.06029763	-3.06534544	1.24820792
C	2.08831105	-2.45812860	0.84960592
C	-2.45812860	-2.08831105	0.84960592
C	-2.08831105	2.45812860	0.84960592
C	2.45812860	2.08831105	0.84960592
C	-0.75304280	-2.56101724	-1.63343108
C	-1.65391328	-1.43653056	-2.11594008
C	-2.56101724	-0.75304280	-1.63343108
C	-1.43653056	1.65391328	-2.11594008
C	0.75304280	2.56101724	-1.63343108
C	1.65391328	1.43653056	-2.11594008
C	2.56101724	-0.75304280	-1.63343108
C	1.43653056	-1.65391328	-2.11594008
C	1.10903313	-3.06646184	-0.15563108
C	-3.06646184	-1.10903313	-0.15563108
C	-1.10903313	3.06646184	-0.15563108
C	3.06646184	1.10903313	-0.15563108
H	0.30653919	-3.51248195	0.43699992
H	1.60229064	-3.84802537	-0.74424008
H	-3.84802537	-1.60229064	-0.74424008
H	-3.51248195	-0.30653919	0.43699992
H	-1.60229064	3.84802537	-0.74424008
H	-0.30653919	3.51248195	0.43699992
H	3.51248195	0.30653919	0.43699992
H	3.84802537	1.60229064	-0.74424008
H	-1.26114468	-3.16273770	-0.88096508
H	-0.52372182	-3.22669157	-2.47784708
H	-2.55765431	-1.86518409	-2.57230008
H	-1.14561950	-0.86172958	-2.89391108
H	-3.22669157	0.52372182	-2.47784708
H	-3.16273770	1.26114468	-0.88096508
H	-1.86518409	2.55765431	-2.57230008
H	-0.86172958	1.14561950	-2.89391108
H	0.52372182	3.22669157	-2.47784708
H	1.26114468	3.16273770	-0.88096508
H	1.14561950	0.86172958	-2.89391108
H	2.55765431	1.86518409	-2.57230008
H	3.16273770	-1.26114468	-0.88096508
H	3.22669157	-0.52372182	-2.47784708
H	0.86172958	-1.14561950	-2.89391108
H	1.86518409	-2.55765431	-2.57230008

Pu(DOTA)(H₂O)

Pu	0.00000000	0.00000000	0.55804800
N	0.21656200	2.08321100	-1.14138500
N	2.07948400	-0.22879500	-1.14113000
N	-0.21656200	-2.08321100	-1.14138500
N	-2.07948400	0.22879500	-1.14113000
O	-1.21469100	1.78389600	1.13595800
O	1.78366800	1.25179000	1.07214800
O	1.21469100	-1.78389600	1.13595800
O	-1.78366800	-1.25179000	1.07214800
O	3.95028300	1.85929700	1.08607500
O	1.78882800	-3.95915100	1.17717200
O	-3.95028300	-1.85929700	1.08607500
O	-1.78882800	3.95915100	1.17717200
C	-1.11427800	3.03959900	0.75593200
C	3.03761400	1.15358500	0.69950700
C	1.11427800	-3.03959900	0.75593200
C	-3.03761400	-1.15358500	0.69950700
C	1.56757300	2.14842500	-1.75226200
C	2.02671300	0.77933800	-2.22776200
C	2.15805700	-1.58423500	-1.73720000
C	0.79760100	-2.05214400	-2.22201900
C	-1.56757300	-2.14842500	-1.75226200
C	-2.02671300	-0.77933800	-2.22776200
C	-2.15805700	1.58423500	-1.73720000
C	-0.79760100	2.05214400	-2.22201900
C	0.00000000	3.26696600	-0.26791300
C	3.26967300	0.00468000	-0.28228100
C	0.00000000	-3.26696600	-0.26791300
C	-3.26967300	-0.00468000	-0.28228100
H	0.91314100	3.41695600	0.31312400
H	-0.20605900	4.16801100	-0.85683500
H	4.16805600	0.18945600	-0.88247700
H	3.41901600	-0.89249400	0.32352200
H	0.20605900	-4.16801100	-0.85683500
H	-0.91314100	-3.41695600	0.31312400
H	-3.41901600	0.89249400	0.32352200
H	-4.16805600	-0.18945600	-0.88247700
H	2.25705600	2.55011700	-1.01163800
H	1.57176700	2.84199600	-2.60577900
H	3.01592200	0.87335900	-2.69930300
H	1.34264300	0.40735600	-2.99428900
H	2.86659800	-1.59798400	-2.57831400
H	2.54773200	-2.26273700	-0.97916100
H	0.89519000	-3.04979800	-2.67428400
H	0.43179600	-1.38285100	-3.00432200
H	-1.57176700	-2.84199600	-2.60577900
H	-2.25705600	-2.55011700	-1.01163800
H	-1.34264300	-0.40735600	-2.99428900
H	-3.01592200	-0.87335900	-2.69930300
H	-2.54773200	2.26273700	-0.97916100
H	-2.86659800	1.59798400	-2.57831400
H	-0.43179600	1.38285100	-3.00432200
H	-0.89519000	3.04979800	-2.67428400
O	0.00000000	0.00000000	3.05524600
H	0.43907600	-0.65423900	3.61128600
H	-0.43907600	0.65423900	3.61128600