

## Supporting Information

### Theoretical study of actinide(III)-DOTA complexes

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Input Gaussian09 file of the SMD solvation calculation on Pu(DOTA)<sup>-</sup> using the PCM radii of Pu.

Cartesian coordinates of the M(DOTA)<sup>-</sup> and M(DOTA)(H<sub>2</sub>O)<sup>-</sup> complexes optimized at the TPSSh/TZ level.

Table S1. Benchmark results<sup>a</sup> on the Lu(DOTA)H<sub>2</sub>O<sup>-</sup> (SAP) and La(DOTA)H<sub>2</sub>O<sup>-</sup> (TSAP) models as compared to the X-ray diffraction data.

Bond		X-ray	B3PW91 6-311+G**	BH&HLYP	B3LYP	BP86	PBE	wB97XD	M062X	TPSSh				
										6-31G**	cc-pVTZ	6-31+G**	cc-pVDZ	
<b>Lu</b> <b>SAP</b>	<b>Lu-O1</b>	2.274	2.258	2.248	2.263	2.272	2.272	2.258	2.257	2.265	2.268	2.258	2.264	2.253
	<b>Lu-O2</b>	2.283	2.275	2.264	2.280	2.291	2.291	2.276	2.276	2.283	2.288	2.274	2.282	2.271
	<b>Lu-Ow</b>	2.416	2.382	2.366	2.389	2.387	2.391	2.375	2.352	2.377	2.356	2.380	2.376	2.356
	<b>Lu-N1</b>	2.597	2.723	2.739	2.762	2.729	2.727	2.728	2.688	2.690	2.693	2.708	2.689	2.703
	<b>Lu-N2</b>	2.630	2.729	2.745	2.770	2.735	2.733	2.730	2.689	2.693	2.695	2.712	2.691	2.706
<b>La</b> <b>TSAP</b>	<b>La-O1</b>	2.484	2.447	2.440	2.454	2.461	2.459	2.453	2.441	2.456	2.474	2.451	2.455	2.441
	<b>La-O2</b>	2.500	2.464	2.456	2.471	2.480	2.478	2.470	2.460	2.474	2.495	2.465	2.473	2.459
	<b>La-Ow*</b>	2.537	2.605	2.591	2.613	2.608	2.608	2.586	2.564	2.604	2.583	2.597	2.601	2.582
	<b>La-N1</b>	2.784	2.887	2.910	2.935	2.894	2.889	2.877	2.845	2.857	2.841	2.869	2.855	2.866
	<b>La-N2</b>	2.754	2.866	2.886	2.908	2.871	2.867	2.857	2.829	2.839	2.827	2.848	2.837	2.851
<b>Av<sup>b</sup></b>	<b>Lu</b>		0.057	0.070	0.069	0.055	0.054	0.059	0.048	0.041	0.046	0.051	0.041	0.055
	<b>La</b>		0.071	0.080	0.088	0.068	0.067	0.061	0.049	0.056	0.038	0.061	0.055	0.062

<sup>a</sup>Using the 4f-in-core pseudopotentials of the Stuttgart-Cologne group for La and Lu. The basis set of the light atoms was in most cases 6-311+G\*\*, exceptions given in the heading.

<sup>b</sup>Average of mean absolute deviations from the experimental bond distances.

Table S2. SO-CASPT2 energy levels (cm<sup>-1</sup>) of the ground-state multiplets in An(DOTA)(H<sub>2</sub>O)<sup>-</sup> molecules (An = U, Np, Pu).

U ( <sup>4</sup> I <sub>9/2</sub> ) <sup>a</sup>	Np ( <sup>5</sup> I <sub>4</sub> )	Pu ( <sup>6</sup> H <sub>5/2</sub> ) <sup>a</sup>
0	0	0
116	172	621
887	381	1052
1531	383	
1658	590	
	1175	
	1344	
	1489	
	1658	

<sup>a</sup>Doublet.

Table S3. Selected data<sup>a</sup> from analysis of the CASSCF wavefunctions of M(DOTA)(H<sub>2</sub>O)<sup>-</sup> complexes.

M	Wiberg bond indices			Topological data					
	M-N	M-O	M-OH <sub>2</sub>	ρ			∇ <sup>2</sup> ρ		
				M-O	M-OH <sub>2</sub>	M-N	M-O	M-OH <sub>2</sub>	M-N
Ac	0.10	0.25	0.15	0.048	0.030	0.025	0.19	0.13	0.09
U	0.09	0.21	0.13	0.051	0.034	0.027	0.21	0.17	0.10
Np	0.09	0.20	0.13	0.051	0.037	0.027	0.22	0.18	0.11
Pu	0.09	0.21	0.14	0.052	0.037	0.027	0.23	0.19	0.11
Am	0.09	0.21	0.14	0.052	0.038	0.028	0.24	0.20	0.11
Cm	0.09	0.20	0.14	0.053	0.038	0.028	0.25	0.20	0.11
Cf	0.07	0.18	0.14	0.053	0.040	0.028	0.24	0.20	0.10
La	0.09	0.25	0.15	0.050	0.034	0.027	0.19	0.15	0.09
Lu	0.09	0.22	0.15	0.055	0.039	0.023	0.29	0.22	0.10

<sup>a</sup>Wiberg bond indices of the M-ligand bonds; electron densities (ρ, au) and Laplacians of electron density (∇<sup>2</sup>ρ, au) at selected bond critical points (BCP). The different values of the M-O and M-N BCPs (because of the C<sub>2</sub> symmetry of DOTA) are averaged.

**Input Gaussian09 file of the SMD solvation calculation on Pu(DOTA)-  
using the PCM radii of Pu.**

```
%chk=Pu_DOTATSAP_SMD.chk  
%nproc=24  
%mem=28000MB  
# TPSSH/gen Int(Grid=Superfine) pseudo=read SCRF(SMD,Read) Pop=None
```

Pu-DOTA without H<sub>2</sub>O ligand, TSAP isomer

```
-1 1  
94 0.000000 0.000000 0.638334  
7 0.957849 1.882107 -1.166835  
7 -1.882107 0.957849 -1.166835  
7 -0.957849 -1.882107 -1.166835  
7 1.882107 -0.957849 -1.166835  
8 1.854081 1.389103 1.363695  
8 -1.389103 1.854081 1.363695  
8 -1.854081 -1.389103 1.363695  
8 1.389103 -1.854081 1.363695  
8 2.811986 3.447514 1.459351  
8 -3.447514 2.811986 1.459351  
8 -2.811986 -3.447514 1.459351  
8 3.447514 -2.811986 1.459351  
6 2.052228 2.611969 0.972434  
6 -2.611969 2.052228 0.972434  
6 -2.052228 -2.611969 0.972434  
6 2.611969 -2.052228 0.972434  
6 0.000000 2.221588 -2.236047  
6 -1.444548 2.251356 -1.739518  
6 -2.221588 0.000000 -2.236047  
6 -2.251356 -1.444548 -1.739518  
6 0.000000 -2.221588 -2.236047  
6 1.444548 -2.251356 -1.739518  
6 2.221588 0.000000 -2.236047  
6 2.251356 1.444548 -1.739518  
6 1.195058 3.031165 -0.251991  
6 -3.031165 1.195058 -0.251991  
6 -1.195058 -3.031165 -0.251991  
6 3.031165 -1.195058 -0.251991  
1 0.102779 1.475563 -3.032885  
1 0.243582 3.199346 -2.687895  
1 -1.544878 3.004705 -0.955420  
1 -2.106016 2.557889 -2.568382  
1 -1.475563 0.102779 -3.032885  
1 -3.199346 0.243582 -2.687895  
1 -3.004705 -1.544878 -0.955420  
1 -2.557889 -2.106016 -2.568382  
1 -0.102779 -1.475563 -3.032885  
1 -0.243582 -3.199346 -2.687895
```

1 1.544878 -3.004705 -0.955420  
1 2.106016 -2.557889 -2.568382  
1 1.475563 -0.102779 -3.032885  
1 3.199346 -0.243582 -2.687895  
1 3.004705 1.544878 -0.955420  
1 2.557889 2.106016 -2.568382  
1 1.682909 3.864851 -0.779104  
1 0.228725 3.367604 0.137046  
1 -3.864851 1.682909 -0.779104  
1 -3.367604 0.228725 0.137046  
1 -1.682909 -3.864851 -0.779104  
1 -0.228725 -3.367604 0.137046  
1 3.864851 -1.682909 -0.779104  
1 3.367604 -0.228725 0.137046

N C O H 0

6-31G(d,p)

\*\*\*\*

Pu 0

S 3 1.00

0.65609769D+01 -0.11962136

0.43739846D+01 0.78777152

0.29101337D+01 -1.17929153

S 2 1.00

0.56932013D+00 0.94235277

0.25405464D+00 0.36852651

S 1 1.00

0.73988463D-01 1.0

S 1 1.00

0.28837732D-01 1.0

P 3 1.00

0.37202910D+01 0.12119815

0.24801937D+01 -0.32571291

0.69446253D+00 0.45088197

P 2 1.00

0.34470180D+00 0.52984913

0.16360360D+00 0.17862426

P 1 1.00

0.67592645D-01 1.0

D 3 1.00

0.14436787D+01 -0.07919020

0.96245248D+00 0.10455122

0.40935068D+00 0.36548009

D 1 1.00

0.15000000D+00 1.0

D 1 1.00

0.50289521D-01 1.0

\*\*\*\*

Pu 0

ECP83MWB 4 83

G-Komponente

1

2 1.000000 0.000000

S-G

2

2 3.878850 101.511078

2 2.547456 -12.372693

P-G

2

2 3.029556 61.852609

2 2.026047 -0.872344

D-G

2

2 1.965746 27.691029

2 1.596316 1.101169

F-G

2

2 1.689032 -6.953746

2 0.892098 4.615700

ModifySph

Pu 1.807 1.0

## Cartesian coordinates

### Ac(DOTA)<sup>-</sup> SAP

Ac	0.00000000	0.00000000	0.83903000
N	0.21119100	2.14600200	-1.06815400
N	2.14600200	-0.21119100	-1.06815400
N	-0.21119100	-2.14600200	-1.06815400
N	-2.14600200	0.21119100	-1.06815400
O	-1.29932600	2.09398200	1.29999200
O	2.09398200	1.29932600	1.29999200
O	1.29932600	-2.09398200	1.29999200
O	-2.09398200	-1.29932600	1.29999200
O	4.25431300	1.87052400	0.95602700
O	1.87052400	-4.25431300	0.95602700
O	-4.25431300	-1.87052400	0.95602700
O	-1.87052400	4.25431300	0.95602700
C	-1.18045300	3.25569300	0.75159000
C	3.25569300	1.18045300	0.75159000
C	1.18045300	-3.25569300	0.75159000
C	-3.25569300	-1.18045300	0.75159000
C	1.56850000	2.17828500	-1.66473600
C	2.05308700	0.80739100	-2.13757300
C	2.17828500	-1.56850000	-1.66473600
C	0.80739100	-2.05308700	-2.13757300
C	-1.56850000	-2.17828500	-1.66473600
C	-2.05308700	-0.80739100	-2.13757300
C	-2.17828500	1.56850000	-1.66473600
C	-0.80739100	2.05308700	-2.13757300
C	0.00000000	3.36689200	-0.24268100
C	3.36689200	0.00000000	-0.24268100
C	0.00000000	-3.36689200	-0.24268100
C	-3.36689200	0.00000000	-0.24268100
H	0.89915600	3.49884500	0.36675600
H	-0.13403000	4.25213200	-0.88036800
H	4.25213200	0.13403000	-0.88036800
H	3.49884500	-0.89915600	0.36675600
H	0.13403000	-4.25213200	-0.88036800
H	-0.89915600	-3.49884500	0.36675600
H	-3.49884500	0.89915600	0.36675600
H	-4.25213200	-0.13403000	-0.88036800
H	2.25067200	2.57417600	-0.91296300
H	1.59891400	2.86890400	-2.52538700
H	3.03694400	0.93714500	-2.61991700
H	1.37603400	0.42480900	-2.90720500
H	2.86890400	-1.59891400	-2.52538700
H	2.57417600	-2.25067200	-0.91296300
H	0.93714500	-3.03694400	-2.61991700
H	0.42480900	-1.37603400	-2.90720500
H	-1.59891400	-2.86890400	-2.52538700
H	-2.25067200	-2.57417600	-0.91296300
H	-1.37603400	-0.42480900	-2.90720500
H	-3.03694400	-0.93714500	-2.61991700
H	-2.57417600	2.25067200	-0.91296300
H	-2.86890400	1.59891400	-2.52538700
H	-0.42480900	1.37603400	-2.90720500
H	-0.93714500	3.03694400	-2.61991700

### Ac(DOTA)<sup>-</sup> TSAP

Ac	0.00000000	0.00000000	0.77812000
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N	-1.90426500	0.96913500	-1.18396300
N	-0.96913500	-1.90426500	-1.18396300
N	1.90426500	-0.96913500	-1.18396300
O	1.87793700	1.55394000	1.36670400
O	-1.55394000	1.87793700	1.36670400
O	-1.87793700	-1.55394000	1.36670400
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O	2.83641600	3.60495200	1.35481700
O	-3.60495200	2.83641600	1.35481700
O	-2.83641600	-3.60495200	1.35481700
O	3.60495200	-2.83641600	1.35481700
C	2.07969000	2.74472100	0.91199400
C	-2.74472100	2.07969000	0.91199400
C	-2.07969000	-2.74472100	0.91199400
C	2.74472100	-2.07969000	0.91199400
C	0.00000000	2.21111400	-2.25438900
C	-1.44264700	2.25434700	-1.75669900
C	-2.21111400	0.00000000	-2.25438900
C	-2.25434700	-1.44264700	-1.75669900
C	0.00000000	-2.21111400	-2.25438900
C	1.44264700	-2.25434700	-1.75669900
C	2.21111400	0.00000000	-2.25438900
C	2.25434700	1.44264700	-1.75669900
C	1.22608000	3.09654200	-0.33419200
C	-3.09654200	1.22608000	-0.33419200
C	-1.22608000	-3.09654200	-0.33419200
C	3.09654200	-1.22608000	-0.33419200
H	0.10153600	1.44935000	-3.03348400
H	0.23921400	3.17807900	-2.72934000
H	-1.53585200	3.00917600	-0.97388100
H	-2.09948500	2.56744600	-2.58638500
H	-1.44935000	0.10153600	-3.03348400
H	-3.17807900	0.23921400	-2.72934000
H	-3.00917600	-1.53585200	-0.97388100
H	-2.56744600	-2.09948500	-2.58638500
H	-0.10153600	-1.44935000	-3.03348400
H	-0.23921400	-3.17807900	-2.72934000
H	1.53585200	-3.00917600	-0.97388100
H	2.09948500	-2.56744600	-2.58638500
H	1.44935000	-0.10153600	-3.03348400
H	3.17807900	-0.23921400	-2.72934000
H	3.00917600	1.53585200	-0.97388100
H	2.56744600	2.09948500	-2.58638500
H	1.72119800	3.89211700	-0.90969200
H	0.26809400	3.47506800	0.03488700
H	-3.89211700	1.72119800	-0.90969200
H	-3.47506800	0.26809400	0.03488700
H	-1.72119800	-3.89211700	-0.90969200
H	-0.26809400	-3.47506800	0.03488700
H	3.89211700	-1.72119800	-0.90969200
H	3.47506800	-0.26809400	0.03488700

### Am(DOTA)- SAP

Am	0.00000000	0.00000000	0.68176800
N	0.21633300	2.11939100	-1.05553400
N	2.11939100	-0.21633300	-1.05553400
N	-0.21633300	-2.11939100	-1.05553400
N	-2.11939100	0.21633300	-1.05553400
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O	1.94483100	1.26978000	1.31725000
O	1.26978000	-1.94483100	1.31725000
O	-1.94483100	-1.26978000	1.31725000
O	4.11285100	1.85991600	1.08624000
O	1.85991600	-4.11285100	1.08624000
O	-4.11285100	-1.85991600	1.08624000
O	-1.85991600	4.11285100	1.08624000
C	-1.16315700	3.13189800	0.82499600
C	3.13189800	1.16315700	0.82499600
C	1.16315700	-3.13189800	0.82499600
C	-3.13189800	-1.16315700	0.82499600
C	1.57372000	2.17057100	-1.64953300
C	2.06072400	0.80283400	-2.12638900
C	2.17057100	-1.57372000	-1.64953300
C	0.80283400	-2.06072400	-2.12638900
C	-1.57372000	-2.17057100	-1.64953300
C	-2.06072400	-0.80283400	-2.12638900
C	-2.17057100	1.57372000	-1.64953300
C	-0.80283400	2.06072400	-2.12638900
C	0.00000000	3.30499000	-0.17938600
C	3.30499000	0.00000000	-0.17938600
C	0.00000000	-3.30499000	-0.17938600
C	-3.30499000	0.00000000	-0.17938600
H	0.90394800	3.42374900	0.42449100
H	-0.15809100	4.21114500	-0.78033300
H	4.21114500	0.15809100	-0.78033300
H	3.42374900	-0.90394800	0.42449100
H	0.15809100	-4.21114500	-0.78033300
H	-0.90394800	-3.42374900	0.42449100
H	-3.42374900	0.90394800	0.42449100
H	-4.21114500	-0.15809100	-0.78033300
H	2.25281700	2.56310700	-0.89312600
H	1.60071200	2.86838400	-2.50357700
H	3.05571200	0.92660100	-2.58610600
H	1.39563500	0.42779800	-2.91063400
H	2.86838400	-1.60071200	-2.50357700
H	2.56310700	-2.25281700	-0.89312600
H	0.92660100	-3.05571200	-2.58610600
H	0.42779800	-1.39563500	-2.91063400
H	-1.60071200	-2.86838400	-2.50357700
H	-2.25281700	-2.56310700	-0.89312600
H	-1.39563500	-0.42779800	-2.91063400
H	-3.05571200	-0.92660100	-2.58610600
H	-2.56310700	2.25281700	-0.89312600
H	-2.86838400	1.60071200	-2.50357700
H	-0.42779800	1.39563500	-2.91063400
H	-0.92660100	3.05571200	-2.58610600

### Am(DOTA)- TSAP

Am	0.00000000	0.00000000	0.63119600
N	0.95733000	1.88093700	-1.16633000
N	-1.88093700	0.95733000	-1.16633000
N	-0.95733000	-1.88093700	-1.16633000
N	1.88093700	-0.95733000	-1.16633000
O	1.82005100	1.39566900	1.36346800
O	-1.39566900	1.82005100	1.36346800
O	-1.82005100	-1.39566900	1.36346800
O	1.39566900	-1.82005100	1.36346800
O	2.80248100	3.43071700	1.46782900
O	-3.43071700	2.80248100	1.46782900
O	-2.80248100	-3.43071700	1.46782900
O	3.43071700	-2.80248100	1.46782900
C	2.03545300	2.60777800	0.97501400
C	-2.60777800	2.03545300	0.97501400
C	-2.03545300	-2.60777800	0.97501400
C	2.60777800	-2.03545300	0.97501400
C	0.00000000	2.21961600	-2.23657500
C	-1.44209400	2.25055900	-1.73947700
C	-2.21961600	0.00000000	-2.23657500
C	-2.25055900	-1.44209400	-1.73947700
C	0.00000000	-2.21961600	-2.23657500
C	1.44209400	-2.25055900	-1.73947700
C	2.21961600	0.00000000	-2.23657500
C	2.25055900	1.44209400	-1.73947700
C	1.20109100	3.03448900	-0.25970800
C	-3.03448900	1.20109100	-0.25970800
C	-1.20109100	-3.03448900	-0.25970800
C	3.03448900	-1.20109100	-0.25970800
H	0.10417300	1.47476100	-3.03226700
H	0.24504900	3.19714600	-2.68540500
H	-1.54123400	3.00407400	-0.95639200
H	-2.10567800	2.55464100	-2.56627000
H	-1.47476100	0.10417300	-3.03226700
H	-3.19714600	0.24504900	-2.68540500
H	-3.00407400	-1.54123400	-0.95639200
H	-2.55464100	-2.10567800	-2.56627000
H	-0.10417300	-1.47476100	-3.03226700
H	-0.24504900	-3.19714600	-2.68540500
H	1.54123400	-3.00407400	-0.95639200
H	2.10567800	-2.55464100	-2.56627000
H	1.47476100	-0.10417300	-3.03226700
H	3.19714600	-0.24504900	-2.68540500
H	3.00407400	1.54123400	-0.95639200
H	2.55464100	2.10567800	-2.56627000
H	1.70928800	3.85280500	-0.78921400
H	0.23952500	3.39385600	0.11704000
H	-3.85280500	1.70928800	-0.78921400
H	-3.39385600	0.23952500	0.11704000
H	-1.70928800	-3.85280500	-0.78921400
H	-0.23952500	-3.39385600	0.11704000
H	3.85280500	-1.70928800	-0.78921400
H	3.39385600	-0.23952500	0.11704000



**Cf(DOTA)- SAP**

Cf	0.00000000	0.00000000	0.63013800
N	0.21907800	2.10924900	-1.05504700
N	2.10924900	-0.21907800	-1.05504700
N	-0.21907800	-2.10924900	-1.05504700
N	-2.10924900	0.21907800	-1.05504700
O	-1.24943100	1.88289200	1.31483600
O	1.88289200	1.24943100	1.31483600
O	1.24943100	-1.88289200	1.31483600
O	-1.88289200	-1.24943100	1.31483600
O	4.05362500	1.84716200	1.14275900
O	1.84716200	-4.05362500	1.14275900
O	-4.05362500	-1.84716200	1.14275900
O	-1.84716200	4.05362500	1.14275900
C	-1.15016600	3.08167700	0.85043400
C	3.08167700	1.15016600	0.85043400
C	1.15016600	-3.08167700	0.85043400
C	-3.08167700	-1.15016600	0.85043400
C	1.57647200	2.16651500	-1.64759000
C	2.06286500	0.79969900	-2.12641300
C	2.16651500	-1.57647200	-1.64759000
C	0.79969900	-2.06286500	-2.12641300
C	-1.57647200	-2.16651500	-1.64759000
C	-2.06286500	-0.79969900	-2.12641300
C	-2.16651500	1.57647200	-1.64759000
C	-0.79969900	2.06286500	-2.12641300
C	0.00000000	3.28209000	-0.16253400
C	3.28209000	0.00000000	-0.16253400
C	0.00000000	-3.28209000	-0.16253400
C	-3.28209000	0.00000000	-0.16253400
H	0.90753500	3.40250100	0.43506400
H	-0.17414800	4.19386700	-0.75020000
H	4.19386700	0.17414800	-0.75020000
H	3.40250100	-0.90753500	0.43506400
H	0.17414800	-4.19386700	-0.75020000
H	-0.90753500	-3.40250100	0.43506400
H	-3.40250100	0.90753500	0.43506400
H	-4.19386700	-0.17414800	-0.75020000
H	2.25472300	2.55642900	-0.88894100
H	1.60352600	2.86751400	-2.49880200
H	3.06135100	0.92039600	-2.57919300
H	1.40101800	0.42796700	-2.91511200
H	2.86751400	-1.60352600	-2.49880200
H	2.55642900	-2.25472300	-0.88894100
H	0.92039600	-3.06135100	-2.57919300
H	0.42796700	-1.40101800	-2.91511200
H	-1.60352600	-2.86751400	-2.49880200
H	-2.25472300	-2.55642900	-0.88894100
H	-1.40101800	-0.42796700	-2.91511200
H	-3.06135100	-0.92039600	-2.57919300
H	-2.55642900	2.25472300	-0.88894100
H	-2.86751400	1.60352600	-2.49880200
H	-0.42796700	1.40101800	-2.91511200
H	-0.92039600	3.06135100	-2.57919300

**Cf(DOTA)- TSAP**

Cf	0.00000000	0.00000000	0.58355300
N	0.95272200	1.87246500	-1.16291200
N	-1.87246500	0.95272200	-1.16291200
N	-0.95272200	-1.87246500	-1.16291200
N	1.87246500	-0.95272200	-1.16291200
O	1.78718700	1.33653900	1.35500300
O	-1.33653900	1.78718700	1.35500300
O	-1.78718700	-1.33653900	1.35500300
O	1.33653900	-1.78718700	1.35500300
O	2.77970200	3.36265100	1.51323500
O	-3.36265100	2.77970200	1.51323500
O	-2.77970200	-3.36265100	1.51323500
O	3.36265100	-2.77970200	1.51323500
C	2.01168400	2.55623600	0.99559300
C	-2.55623600	2.01168400	0.99559300
C	-2.01168400	-2.55623600	0.99559300
C	2.55623600	-2.01168400	0.99559300
C	0.00000000	2.22234700	-2.23299000
C	-1.44157500	2.24879700	-1.73558700
C	-2.22234700	0.00000000	-2.23299000
C	-2.24879700	-1.44157500	-1.73558700
C	0.00000000	-2.22234700	-2.23299000
C	1.44157500	-2.24879700	-1.73558700
C	2.22234700	0.00000000	-2.23299000
C	2.24879700	1.44157500	-1.73558700
C	1.19326900	3.01226800	-0.23837700
C	-3.01226800	1.19326900	-0.23837700
C	-1.19326900	-3.01226800	-0.23837700
C	3.01226800	-1.19326900	-0.23837700
H	0.10487900	1.48343200	-3.03434600
H	0.24695300	3.20332600	-2.67298400
H	-1.54230100	3.00130900	-0.95175800
H	-2.10797500	2.55059300	-2.56071900
H	-1.48343200	0.10487900	-3.03434600
H	-3.20332600	0.24695300	-2.67298400
H	-3.00130900	-1.54230100	-0.95175800
H	-2.55059300	-2.10797500	-2.56071900
H	-0.10487900	-1.48343200	-3.03434600
H	-0.24695300	-3.20332600	-2.67298400
H	1.54230100	-3.00130900	-0.95175800
H	2.10797500	-2.55059300	-2.56071900
H	1.48343200	-0.10487900	-3.03434600
H	3.20332600	-0.24695300	-2.67298400
H	3.00130900	1.54230100	-0.95175800
H	2.55059300	2.10797500	-2.56071900
H	1.71328300	3.83426800	-0.75019600
H	0.23100300	3.37151600	0.13559800
H	-3.83426800	1.71328300	-0.75019600
H	-3.37151600	0.23100300	0.13559800
H	-1.71328300	-3.83426800	-0.75019600
H	-0.23100300	-3.37151600	0.13559800
H	3.83426800	-1.71328300	-0.75019600
H	3.37151600	-0.23100300	0.13559800

### Cm(DOTA)- SAP

Cm	0.00000000	0.00000000	0.66276300
N	0.21729700	2.11575800	-1.05516100
N	2.11575800	-0.21729700	-1.05516100
N	-0.21729700	-2.11575800	-1.05516100
N	-2.11575800	0.21729700	-1.05516100
O	-1.26275800	1.92252000	1.31663800
O	1.92252000	1.26275800	1.31663800
O	1.26275800	-1.92252000	1.31663800
O	-1.92252000	-1.26275800	1.31663800
O	4.09182400	1.85528000	1.10703200
O	1.85528000	-4.09182400	1.10703200
O	-4.09182400	-1.85528000	1.10703200
O	-1.85528000	4.09182400	1.10703200
C	-1.15859400	3.11391500	0.83447600
C	3.11391500	1.15859400	0.83447600
C	1.15859400	-3.11391500	0.83447600
C	-3.11391500	-1.15859400	0.83447600
C	1.57469100	2.16914500	-1.64865700
C	2.06152000	0.80174600	-2.12620900
C	2.16914500	-1.57469100	-1.64865700
C	0.80174600	-2.06152000	-2.12620900
C	-1.57469100	-2.16914500	-1.64865700
C	-2.06152000	-0.80174600	-2.12620900
C	-2.16914500	1.57469100	-1.64865700
C	-0.80174600	2.06152000	-2.12620900
C	0.00000000	3.29673900	-0.17301600
C	3.29673900	0.00000000	-0.17301600
C	0.00000000	-3.29673900	-0.17301600
C	-3.29673900	0.00000000	-0.17301600
H	0.90522800	3.41589400	0.42867100
H	-0.16372500	4.20502800	-0.76914300
H	4.20502800	0.16372500	-0.76914300
H	3.41589400	-0.90522800	0.42867100
H	0.16372500	-4.20502800	-0.76914300
H	-0.90522800	-3.41589400	0.42867100
H	-3.41589400	0.90522800	0.42867100
H	-4.20502800	-0.16372500	-0.76914300
H	2.25347300	2.56076800	-0.89145100
H	1.60168500	2.86809800	-2.50168900
H	3.05778200	0.92442000	-2.58341100
H	1.39762000	0.42787600	-2.91207400
H	2.86809800	-1.60168500	-2.50168900
H	2.56076800	-2.25347300	-0.89145100
H	0.92442000	-3.05778200	-2.58341100
H	0.42787600	-1.39762000	-2.91207400
H	-1.60168500	-2.86809800	-2.50168900
H	-2.25347300	-2.56076800	-0.89145100
H	-1.39762000	-0.42787600	-2.91207400
H	-3.05778200	-0.92442000	-2.58341100
H	-2.56076800	2.25347300	-0.89145100
H	-2.86809800	1.60168500	-2.50168900
H	-0.42787600	1.39762000	-2.91207400
H	-0.92442000	3.05778200	-2.58341100

### Cm(DOTA)- TSAP

Cm	0.00000000	0.00000000	0.61364800
N	0.95568300	1.87788000	-1.16490700
N	-1.87788000	0.95568300	-1.16490700
N	-0.95568300	-1.87788000	-1.16490700
N	1.87788000	-0.95568300	-1.16490700
O	1.80850500	1.37426400	1.36081100
O	-1.37426400	1.80850500	1.36081100
O	-1.80850500	-1.37426400	1.36081100
O	1.37426400	-1.80850500	1.36081100
O	2.79453400	3.40630300	1.48436500
O	-3.40630300	2.79453400	1.48436500
O	-2.79453400	-3.40630300	1.48436500
O	3.40630300	-2.79453400	1.48436500
C	2.02708900	2.58918000	0.98270700
C	-2.58918000	2.02708900	0.98270700
C	-2.02708900	-2.58918000	0.98270700
C	2.58918000	-2.02708900	0.98270700
C	0.00000000	2.22064000	-2.23509700
C	-1.44191700	2.24995200	-1.73789700
C	-2.22064000	0.00000000	-2.23509700
C	-2.24995200	-1.44191700	-1.73789700
C	0.00000000	-2.22064000	-2.23509700
C	1.44191700	-2.24995200	-1.73789700
C	2.22064000	0.00000000	-2.23509700
C	2.24995200	1.44191700	-1.73789700
C	1.19821400	3.02644000	-0.25168500
C	-3.02644000	1.19821400	-0.25168500
C	-1.19821400	-3.02644000	-0.25168500
C	3.02644000	-1.19821400	-0.25168500
H	0.10442900	1.47794600	-3.03286000
H	0.24575000	3.19943900	-2.68070000
H	-1.54163800	3.00310500	-0.95454600
H	-2.10651200	2.55319900	-2.56409900
H	-1.47794600	0.10442900	-3.03286000
H	-3.19943900	0.24575000	-2.68070000
H	-3.00310500	-1.54163800	-0.95454600
H	-2.55319900	-2.10651200	-2.56409900
H	-0.10442900	-1.47794600	-3.03286000
H	-0.24575000	-3.19943900	-2.68070000
H	1.54163800	-3.00310500	-0.95454600
H	2.10651200	-2.55319900	-2.56409900
H	1.47794600	-0.10442900	-3.03286000
H	3.19943900	-0.24575000	-2.68070000
H	3.00310500	1.54163800	-0.95454600
H	2.55319900	2.10651200	-2.56409900
H	1.71046100	3.84628600	-0.77480300
H	0.23635600	3.38550100	0.12422900
H	-3.84628600	1.71046100	-0.77480300
H	-3.38550100	0.23635600	0.12422900
H	-1.71046100	-3.84628600	-0.77480300
H	-0.23635600	-3.38550100	0.12422900
H	3.84628600	-1.71046100	-0.77480300
H	3.38550100	-0.23635600	0.12422900

**La(DOTA)<sup>-</sup> SAP**

La	0.00000000	0.00000000	0.83681500
N	0.21458700	2.13002800	-0.96307600
N	2.13002800	-0.21458700	-0.96307600
N	-0.21458700	-2.13002800	-0.96307600
N	-2.13002800	0.21458700	-0.96307600
O	-1.27669600	1.99555200	1.40464000
O	1.99555200	1.27669600	1.40464000
O	1.27669600	-1.99555200	1.40464000
O	-1.99555200	-1.27669600	1.40464000
O	4.16254300	1.86172900	1.14261000
O	1.86172900	-4.16254300	1.14261000
O	-4.16254300	-1.86172900	1.14261000
O	-1.86172900	4.16254300	1.14261000
C	-1.16773200	3.17627900	0.89603300
C	3.17627900	1.16773200	0.89603300
C	1.16773200	-3.17627900	0.89603300
C	-3.17627900	-1.16773200	0.89603300
C	1.57187400	2.17324800	-1.55776400
C	2.05719600	0.80424700	-2.03325000
C	2.17324800	-1.57187400	-1.55776400
C	0.80424700	-2.05719600	-2.03325000
C	-1.57187400	-2.17324800	-1.55776400
C	-2.05719600	-0.80424700	-2.03325000
C	-2.17324800	1.57187400	-1.55776400
C	-0.80424700	2.05719600	-2.03325000
C	0.00000000	3.32853500	-0.10634300
C	3.32853500	0.00000000	-0.10634300
C	0.00000000	-3.32853500	-0.10634300
C	-3.32853500	0.00000000	-0.10634300
H	0.90250600	3.45336100	0.49896600
H	-0.15061100	4.22747300	-0.72047400
H	4.22747300	0.15061100	-0.72047400
H	3.45336100	-0.90250600	0.49896600
H	0.15061100	-4.22747300	-0.72047400
H	-0.90250600	-3.45336100	0.49896600
H	-3.45336100	0.90250600	0.49896600
H	-4.22747300	-0.15061100	-0.72047400
H	2.25221800	2.56660900	-0.80296200
H	1.60122900	2.86861700	-2.41425900
H	3.04750300	0.93033000	-2.50309400
H	1.38679400	0.42640400	-2.81132600
H	2.86861700	-1.60122900	-2.41425900
H	2.56660900	-2.25221800	-0.80296200
H	0.93033000	-3.04750300	-2.50309400
H	0.42640400	-1.38679400	-2.81132600
H	-1.60122900	-2.86861700	-2.41425900
H	-2.25221800	-2.56660900	-0.80296200
H	-1.38679400	-0.42640400	-2.81132600
H	-3.04750300	-0.93033000	-2.50309400
H	-2.56660900	2.25221800	-0.80296200
H	-2.86861700	1.60122900	-2.41425900
H	-0.42640400	1.38679400	-2.81132600
H	-0.93033000	3.04750300	-2.50309400

**La(DOTA)<sup>-</sup> TSAP**

La	0.00000000	0.00000000	0.77544600
N	0.96200400	1.88992100	-1.08397900
N	-1.88992100	0.96200400	-1.08397900
N	-0.96200400	-1.88992100	-1.08397900
N	1.88992100	-0.96200400	-1.08397900
O	1.83902400	1.44811200	1.44903400
O	-1.44811200	1.83902400	1.44903400
O	-1.83902400	-1.44811200	1.44903400
O	1.44811200	-1.83902400	1.44903400
O	2.80421500	3.49345900	1.52741400
O	-3.49345900	2.80421500	1.52741400
O	-2.80421500	-3.49345900	1.52741400
O	3.49345900	-2.80421500	1.52741400
C	2.04746100	2.65623800	1.04331200
C	-2.65623800	2.04746100	1.04331200
C	-2.04746100	-2.65623800	1.04331200
C	2.65623800	-2.04746100	1.04331200
C	0.00000000	2.21603000	-2.15407400
C	-1.44215200	2.25197000	-1.65660200
C	-2.21603000	0.00000000	-2.15407400
C	-2.25197000	-1.44215200	-1.65660200
C	0.00000000	-2.21603000	-2.15407400
C	1.44215200	-2.25197000	-1.65660200
C	2.21603000	0.00000000	-2.15407400
C	2.25197000	1.44215200	-1.65660200
C	1.20998000	3.05695100	-0.19782600
C	-3.05695100	1.20998000	-0.19782600
C	-1.20998000	-3.05695100	-0.19782600
C	3.05695100	-1.20998000	-0.19782600
H	0.10284100	1.46435500	-2.94319500
H	0.24253400	3.18942500	-2.61388500
H	-1.53852900	3.00586500	-0.87346100
H	-2.10308600	2.56042000	-2.48446400
H	-1.46435500	0.10284100	-2.94319500
H	-3.18942500	0.24253400	-2.61388500
H	-3.00586500	-1.53852900	-0.87346100
H	-2.56042000	-2.10308600	-2.48446400
H	-0.10284100	-1.46435500	-2.94319500
H	-0.24253400	-3.18942500	-2.61388500
H	1.53852900	-3.00586500	-0.87346100
H	2.10308600	-2.56042000	-2.48446400
H	1.46435500	-0.10284100	-2.94319500
H	3.18942500	-0.24253400	-2.61388500
H	3.00586500	1.53852900	-0.87346100
H	2.56042000	2.10308600	-2.48446400
H	1.71501700	3.86770600	-0.74244400
H	0.24942300	3.42416800	0.17476100
H	-3.86770600	1.71501700	-0.74244400
H	-3.42416800	0.24942300	0.17476100
H	-1.71501700	-3.86770600	-0.74244400
H	-0.24942300	-3.42416800	0.17476100
H	3.86770600	-1.71501700	-0.74244400
H	3.42416800	-0.24942300	0.17476100

**Lu(DOTA)- SAP**

Lu	0.00000000	0.00000000	0.59892600
N	0.22654700	2.08408500	-0.99154400
N	2.08408500	-0.22654700	-0.99154400
N	-0.22654700	-2.08408500	-0.99154400
N	-2.08408500	0.22654700	-0.99154400
O	-1.19341400	1.73965000	1.35512500
O	1.73965000	1.19341400	1.35512500
O	1.19341400	-1.73965000	1.35512500
O	-1.73965000	-1.19341400	1.35512500
O	3.91176300	1.80723100	1.33794100
O	1.80723100	-3.91176300	1.33794100
O	-3.91176300	-1.80723100	1.33794100
O	-1.80723100	3.91176300	1.33794100
C	-1.11347100	2.96571300	0.96492900
C	2.96571300	1.11347100	0.96492900
C	1.11347100	-2.96571300	0.96492900
C	-2.96571300	-1.11347100	0.96492900
C	1.58359400	2.15471100	-1.58099700
C	2.06486500	0.78974600	-2.06511300
C	2.15471100	-1.58359400	-1.58099700
C	0.78974600	-2.06486500	-2.06511300
C	-1.58359400	-2.15471100	-1.58099700
C	-2.06486500	-0.78974600	-2.06511300
C	-2.15471100	1.58359400	-1.58099700
C	-0.78974600	2.06486500	-2.06511300
C	0.00000000	3.23179500	-0.06954700
C	3.23179500	0.00000000	-0.06954700
C	0.00000000	-3.23179500	-0.06954700
C	-3.23179500	0.00000000	-0.06954700
H	0.91641500	3.36745900	0.50966400
H	-0.21795000	4.15081700	-0.63049600
H	4.15081700	0.21795000	-0.63049600
H	3.36745900	-0.91641500	0.50966400
H	0.21795000	-4.15081700	-0.63049600
H	-0.91641500	-3.36745900	0.50966400
H	-3.36745900	0.91641500	0.50966400
H	-4.15081700	-0.21795000	-0.63049600
H	2.26096300	2.53694000	-0.81734800
H	1.61150300	2.86398600	-2.42496800
H	3.07013400	0.90059400	-2.50523700
H	1.40772700	0.42654500	-2.86191300
H	2.86398600	-1.61150300	-2.42496800
H	2.53694000	-2.26096300	-0.81734800
H	0.90059400	-3.07013400	-2.50523700
H	0.42654500	-1.40772700	-2.86191300
H	-1.61150300	-2.86398600	-2.42496800
H	-2.26096300	-2.53694000	-0.81734800
H	-1.40772700	-0.42654500	-2.86191300
H	-3.07013400	-0.90059400	-2.50523700
H	-2.53694000	2.26096300	-0.81734800
H	-2.86398600	1.61150300	-2.42496800
H	-0.42654500	1.40772700	-2.86191300
H	-0.90059400	3.07013400	-2.50523700

**Lu(DOTA)- TSAP**

Lu	0.00000000	0.00000000	0.55770900
N	0.19072100	2.06901000	-1.09753300
N	-2.06901000	0.19072100	-1.09753300
N	-0.19072100	-2.06901000	-1.09753300
N	2.06901000	-0.19072100	-1.09753300
O	1.13590500	1.75149100	1.37824000
O	-1.75149100	1.13590500	1.37824000
O	-1.13590500	-1.75149100	1.37824000
O	1.75149100	-1.13590500	1.37824000
O	1.33566200	3.98401800	1.67630400
O	-3.98401800	1.33566200	1.67630400
O	-1.33566200	-3.98401800	1.67630400
O	3.98401800	-1.33566200	1.67630400
C	0.90970700	2.99116300	1.09357000
C	-2.99116300	0.90970700	1.09357000
C	-0.90970700	-2.99116300	1.09357000
C	2.99116300	-0.90970700	1.09357000
C	-0.82198800	2.06843800	-2.16809500
C	-2.16610000	1.55347200	-1.66915700
C	-2.06843800	-0.82198800	-2.16809500
C	-1.55347200	-2.16610000	-1.66915700
C	0.82198800	-2.06843800	-2.16809500
C	2.16610000	-1.55347200	-1.66915700
C	2.06843800	0.82198800	-2.16809500
C	1.55347200	2.16610000	-1.66915700
C	0.00000000	3.19108300	-0.14159000
C	-3.19108300	0.00000000	-0.14159000
C	0.00000000	-3.19108300	-0.14159000
C	3.19108300	0.00000000	-0.14159000
H	-0.45538200	1.43153800	-2.98040000
H	-0.95243800	3.07897300	-2.59066600
H	-2.53881700	2.21262200	-0.88339500
H	-2.90199100	1.58087300	-2.48962500
H	-1.43153800	-0.45538200	-2.98040000
H	-3.07897300	-0.95243800	-2.59066600
H	-2.21262200	-2.53881700	-0.88339500
H	-1.58087300	-2.90199100	-2.48962500
H	0.45538200	-1.43153800	-2.98040000
H	0.95243800	-3.07897300	-2.59066600
H	2.53881700	-2.21262200	-0.88339500
H	2.90199100	-1.58087300	-2.48962500
H	1.43153800	0.45538200	-2.98040000
H	3.07897300	0.95243800	-2.59066600
H	2.21262200	2.53881700	-0.88339500
H	1.58087300	2.90199100	-2.48962500
H	0.21210600	4.15927900	-0.61653200
H	-1.03070500	3.18074900	0.21929100
H	-4.15927900	0.21210600	-0.61653200
H	-3.18074900	-1.03070500	0.21929100
H	-0.21210600	-4.15927900	-0.61653200
H	1.03070500	-3.18074900	0.21929100
H	4.15927900	-0.21210600	-0.61653200
H	3.18074900	1.03070500	0.21929100

### Np(DOTA)- SAP

Np	0.00000000	0.00000000	0.72397600
N	0.21448000	2.12705200	-1.05702200
N	2.12705200	-0.21448000	-1.05702200
N	-0.21448000	-2.12705200	-1.05702200
N	-2.12705200	0.21448000	-1.05702200
O	-1.28232400	1.99142000	1.31679700
O	1.99142000	1.28232400	1.31679700
O	1.28232400	-1.99142000	1.31679700
O	-1.99142000	-1.28232400	1.31679700
O	4.15637100	1.86787000	1.04343000
O	1.86787000	-4.15637100	1.04343000
O	-4.15637100	-1.86787000	1.04343000
O	-1.86787000	4.15637100	1.04343000
C	-1.17131300	3.16962800	0.80440300
C	3.16962800	1.17131300	0.80440300
C	1.17131300	-3.16962800	0.80440300
C	-3.16962800	-1.17131300	0.80440300
C	1.57187000	2.17324500	-1.65190300
C	2.05887600	0.80476200	-2.12745700
C	2.17324500	-1.57187000	-1.65190300
C	0.80476200	-2.05887600	-2.12745700
C	-1.57187000	-2.17324500	-1.65190300
C	-2.05887600	-0.80476200	-2.12745700
C	-2.17324500	1.57187000	-1.65190300
C	-0.80476200	2.05887600	-2.12745700
C	0.00000000	3.32273500	-0.19445600
C	3.32273500	0.00000000	-0.19445600
C	0.00000000	-3.32273500	-0.19445600
C	-3.32273500	0.00000000	-0.19445600
H	0.90165200	3.44236000	0.41305600
H	-0.14772800	4.22368800	-0.80594100
H	4.22368800	0.14772800	-0.80594100
H	3.44236000	-0.90165200	0.41305600
H	0.14772800	-4.22368800	-0.80594100
H	-0.90165200	-3.44236000	0.41305600
H	-3.44236000	0.90165200	0.41305600
H	-4.22368800	-0.14772800	-0.80594100
H	2.25161100	2.56723900	-0.89689500
H	1.59936300	2.86887500	-2.50791200
H	3.05098700	0.93069700	-2.59291900
H	1.39096900	0.42735400	-2.90800700
H	2.86887500	-1.59936300	-2.50791200
H	2.56723900	-2.25161100	-0.89689500
H	0.93069700	-3.05098700	-2.59291900
H	0.42735400	-1.39096900	-2.90800700
H	-1.59936300	-2.86887500	-2.50791200
H	-2.25161100	-2.56723900	-0.89689500
H	-1.39096900	-0.42735400	-2.90800700
H	-3.05098700	-0.93069700	-2.59291900
H	-2.56723900	2.25161100	-0.89689500
H	-2.86887500	1.59936300	-2.50791200
H	-0.42735400	1.39096900	-2.90800700
H	-0.93069700	3.05098700	-2.59291900

### Np(DOTA)- TSAP

Np	0.00000000	0.00000000	0.66966500
N	0.96075900	1.88735800	-1.17023000
N	-1.88735800	0.96075900	-1.17023000
N	-0.96075900	-1.88735800	-1.17023000
N	1.88735800	-0.96075900	-1.17023000
O	1.84373100	1.44011800	1.36659400
O	-1.44011800	1.84373100	1.36659400
O	-1.84373100	-1.44011800	1.36659400
O	1.44011800	-1.84373100	1.36659400
O	2.81310800	3.48343900	1.43633400
O	-3.48343900	2.81310800	1.43633400
O	-2.81310800	-3.48343900	1.43633400
O	3.48343900	-2.81310800	1.43633400
C	2.05081600	2.64714600	0.95887000
C	-2.64714600	2.05081600	0.95887000
C	-2.05081600	-2.64714600	0.95887000
C	2.64714600	-2.05081600	0.95887000
C	0.00000000	2.21754900	-2.24054900
C	-1.44238400	2.25185600	-1.74345900
C	-2.21754900	0.00000000	-2.24054900
C	-2.25185600	-1.44238400	-1.74345900
C	0.00000000	-2.21754900	-2.24054900
C	1.44238400	-2.25185600	-1.74345900
C	2.21754900	0.00000000	-2.24054900
C	2.25185600	1.44238400	-1.74345900
C	1.20762000	3.05148700	-0.27812800
C	-3.05148700	1.20762000	-0.27812800
C	-1.20762000	-3.05148700	-0.27812800
C	3.05148700	-1.20762000	-0.27812800
H	0.10351000	1.46821500	-3.03191800
H	0.24348500	3.19239900	-2.69618000
H	-1.54004000	3.00565600	-0.96044000
H	-2.10400500	2.55812400	-2.57121600
H	-1.46821500	0.10351000	-3.03191800
H	-3.19239900	0.24348500	-2.69618000
H	-3.00565600	-1.54004000	-0.96044000
H	-2.55812400	-2.10400500	-2.57121600
H	-0.10351000	-1.46821500	-3.03191800
H	-0.24348500	-3.19239900	-2.69618000
H	1.54004000	-3.00565600	-0.96044000
H	2.10400500	-2.55812400	-2.57121600
H	1.46821500	-0.10351000	-3.03191800
H	3.19239900	-0.24348500	-2.69618000
H	3.00565600	1.54004000	-0.96044000
H	2.55812400	2.10400500	-2.57121600
H	1.70928800	3.86526700	-0.82088200
H	0.24683900	3.41362100	0.09870700
H	-3.86526700	1.70928800	-0.82088200
H	-3.41362100	0.24683900	0.09870700
H	-1.70928800	-3.86526700	-0.82088200
H	-0.24683900	-3.41362100	0.09870700
H	3.86526700	-1.70928800	-0.82088200
H	3.41362100	-0.24683900	0.09870700

**Pu(DOTA)<sup>-</sup> SAP**

Pu	0.00000000	0.00000000	0.70206200
N	0.21537000	2.12309900	-1.05604700
N	2.12309900	-0.21537000	-1.05604700
N	-0.21537000	-2.12309900	-1.05604700
N	-2.12309900	0.21537000	-1.05604700
O	-1.27634700	1.96766200	1.31736500
O	1.96766200	1.27634700	1.31736500
O	1.27634700	-1.96766200	1.31736500
O	-1.96766200	-1.27634700	1.31736500
O	4.13407800	1.86453100	1.06481300
O	1.86453100	-4.13407800	1.06481300
O	-4.13407800	1.86453100	1.06481300
O	-1.86453100	4.13407800	1.06481300
C	-1.16756000	3.15030900	0.81496700
C	3.15030900	1.16756000	0.81496700
C	1.16756000	-3.15030900	0.81496700
C	-3.15030900	-1.16756000	0.81496700
C	1.57273000	2.17196300	-1.65055400
C	2.05982700	0.80387200	-2.12671100
C	2.17196300	-1.57273000	-1.65055400
C	0.80387200	-2.05982700	-2.12671100
C	-1.57273000	-2.17196300	-1.65055400
C	-2.05982700	-0.80387200	-2.12671100
C	-2.17196300	1.57273000	-1.65055400
C	-0.80387200	2.05982700	-2.12671100
C	0.00000000	3.31356600	-0.18634400
C	3.31356600	0.00000000	-0.18634400
C	0.00000000	-3.31356600	-0.18634400
C	-3.31356600	0.00000000	-0.18634400
H	0.90269400	3.43230100	0.41960200
H	-0.15257500	4.21733200	-0.79237700
H	4.21733200	0.15257500	-0.79237700
H	3.43230100	-0.90269400	0.41960200
H	0.15257500	-4.21733200	-0.79237700
H	-0.90269400	-3.43230100	0.41960200
H	-3.43230100	0.90269400	0.41960200
H	-4.21733200	-0.15257500	-0.79237700
H	2.25216900	2.56539400	-0.89495500
H	1.59977400	2.86861300	-2.50563500
H	3.05345500	0.92872400	-2.58911800
H	1.39343200	0.42764100	-2.90921100
H	2.86861300	-1.59977400	-2.50563500
H	2.56539400	-2.25216900	-0.89495500
H	0.92872400	-3.05345500	-2.58911800
H	0.42764100	-1.39343200	-2.90921100
H	-1.59977400	-2.86861300	-2.50563500
H	-2.25216900	-2.56539400	-0.89495500
H	-1.39343200	-0.42764100	-2.90921100
H	-3.05345500	-0.92872400	-2.58911800
H	-2.56539400	2.25216900	-0.89495500
H	-2.86861300	1.59977400	-2.50563500
H	-0.42764100	1.39343200	-2.90921100
H	-0.92872400	3.05345500	-2.58911800

**Pu(DOTA)<sup>-</sup> TSAP**

Pu	0.00000000	0.00000000	0.64965000
N	0.95899000	1.88404600	-1.16793300
N	-1.88404600	0.95899000	-1.16793300
N	-0.95899000	-1.88404600	-1.16793300
N	1.88404600	-0.95899000	-1.16793300
O	1.83176500	1.41757400	1.36568000
O	-1.41757400	1.83176500	1.36568000
O	-1.83176500	-1.41757400	1.36568000
O	1.41757400	-1.83176500	1.36568000
O	2.80930900	3.45604500	1.45140000
O	-3.45604500	2.80930900	1.45140000
O	-2.80930900	-3.45604500	1.45140000
O	3.45604500	-2.80930900	1.45140000
C	2.04348200	2.62690100	0.96706600
C	-2.62690100	2.04348200	0.96706600
C	-2.04348200	-2.62690100	0.96706600
C	2.62690100	-2.04348200	0.96706600
C	0.00000000	2.21846200	-2.23822000
C	-1.44222300	2.25112800	-1.74113700
C	-2.21846200	0.00000000	-2.23822000
C	-2.25112800	-1.44222300	-1.74113700
C	0.00000000	-2.21846200	-2.23822000
C	1.44222300	-2.25112800	-1.74113700
C	2.21846200	0.00000000	-2.23822000
C	2.25112800	1.44222300	-1.74113700
C	1.20411600	3.04274100	-0.26831100
C	-3.04274100	1.20411600	-0.26831100
C	-1.20411600	-3.04274100	-0.26831100
C	3.04274100	-1.20411600	-0.26831100
H	0.10383400	1.47132700	-3.03173300
H	0.24429700	3.19463600	-2.69046600
H	-1.54064800	3.00490800	-0.95821100
H	-2.10480000	2.55622800	-2.56845900
H	-1.47132700	0.10383400	-3.03173300
H	-3.19463600	0.24429700	-2.69046600
H	-3.00490800	-1.54064800	-0.95821100
H	-2.55622800	-2.10480000	-2.56845900
H	-0.10383400	-1.47132700	-3.03173300
H	-0.24429700	-3.19463600	-2.69046600
H	1.54064800	-3.00490800	-0.95821100
H	2.10480000	-2.55622800	-2.56845900
H	1.47132700	-0.10383400	-3.03173300
H	3.19463600	-0.24429700	-2.69046600
H	3.00490800	1.54064800	-0.95821100
H	2.55622800	2.10480000	-2.56845900
H	1.70869800	3.85914500	-0.80428500
H	0.24291700	3.40303300	0.10887700
H	-3.85914500	1.70869800	-0.80428500
H	-3.40303300	0.24291700	0.10887700
H	-1.70869800	-3.85914500	-0.80428500
H	-0.24291700	-3.40303300	0.10887700
H	3.85914500	-1.70869800	-0.80428500
H	3.40303300	-0.24291700	0.10887700

**U(DOTA)- SAP**

U	0.00000000	0.00000000	0.74804400
N	0.21342100	2.13109700	-1.05837400
N	2.13109700	-0.21342100	-1.05837400
N	-0.21342100	-2.13109700	-1.05837400
N	-2.13109700	0.21342100	-1.05837400
O	-1.28938800	2.01646100	1.31450000
O	2.01646100	1.28938800	1.31450000
O	1.28938800	-2.01646100	1.31450000
O	-2.01646100	-1.28938800	1.31450000
O	4.18076400	1.86940400	1.02233100
O	1.86940400	-4.18076400	1.02233100
O	-4.18076400	-1.86940400	1.02233100
O	-1.86940400	4.18076400	1.02233100
C	-1.17489400	3.19034900	0.79294700
C	3.19034900	1.17489400	0.79294700
C	1.17489400	-3.19034900	0.79294700
C	-3.19034900	-1.17489400	0.79294700
C	1.57080000	2.17464200	-1.65386300
C	2.05764300	0.80573200	-2.12870900
C	2.17464200	-1.57080000	-1.65386300
C	0.80573200	-2.05764300	-2.12870900
C	-1.57080000	-2.17464200	-1.65386300
C	-2.05764300	-0.80573200	-2.12870900
C	-2.17464200	1.57080000	-1.65386300
C	-0.80573200	2.05764300	-2.12870900
C	0.00000000	3.33260900	-0.20368600
C	3.33260900	0.00000000	-0.20368600
C	0.00000000	-3.33260900	-0.20368600
C	-3.33260900	0.00000000	-0.20368600
H	0.90066700	3.45332200	0.40525900
H	-0.14271000	4.23030000	-0.82121200
H	4.23030000	0.14271000	-0.82121200
H	3.45332200	-0.90066700	0.40525900
H	0.14271000	-4.23030000	-0.82121200
H	-0.90066700	-3.45332200	0.40525900
H	-3.45332200	0.90066700	0.40525900
H	-4.23030000	-0.14271000	-0.82121200
H	2.25099600	2.56947000	-0.89974600
H	1.59834500	2.86901100	-2.51099500
H	3.04810400	0.93257200	-2.59748200
H	1.38796100	0.42700100	-2.90701500
H	2.86901100	-1.59834500	-2.51099500
H	2.56947000	-2.25099600	-0.89974600
H	0.93257200	-3.04810400	-2.59748200
H	0.42700100	-1.38796100	-2.90701500
H	-1.59834500	-2.86901100	-2.51099500
H	-2.25099600	-2.56947000	-0.89974600
H	-1.38796100	-0.42700100	-2.90701500
H	-3.04810400	-0.93257200	-2.59748200
H	-2.56947000	2.25099600	-0.89974600
H	-2.86901100	1.59834500	-2.51099500
H	-0.42700100	1.38796100	-2.90701500
H	-0.93257200	3.04810400	-2.59748200

**U(DOTA)- TSAP**

U	0.00000000	0.00000000	0.69239600
N	0.96268000	1.89112600	-1.17231300
N	-1.89112600	0.96268000	-1.17231300
N	-0.96268000	-1.89112600	-1.17231300
N	1.89112600	-0.96268000	-1.17231300
O	1.85450000	1.46609000	1.36838000
O	-1.46609000	1.85450000	1.36838000
O	-1.85450000	-1.46609000	1.36838000
O	1.46609000	-1.85450000	1.36838000
O	2.82214500	3.51106600	1.41612300
O	-3.51106600	2.82214500	1.41612300
O	-2.82214500	-3.51106600	1.41612300
O	3.51106600	-2.82214500	1.41612300
C	2.05963800	2.66918300	0.94871600
C	-2.66918300	2.05963800	0.94871600
C	-2.05963800	-2.66918300	0.94871600
C	2.66918300	-2.05963800	0.94871600
C	0.00000000	2.21612400	-2.24271700
C	-1.44254300	2.25245300	-1.74569000
C	-2.21612400	0.00000000	-2.24271700
C	-2.25245300	-1.44254300	-1.74569000
C	0.00000000	-2.21612400	-2.24271700
C	1.44254300	-2.25245300	-1.74569000
C	2.21612400	0.00000000	-2.24271700
C	2.25245300	1.44254300	-1.74569000
C	1.21146800	3.06151100	-0.28901600
C	-3.06151100	1.21146800	-0.28901600
C	-1.21146800	-3.06151100	-0.28901600
C	3.06151100	-1.21146800	-0.28901600
H	0.10318400	1.46402400	-3.03138000
H	0.24267400	3.18925000	-2.70253900
H	-1.53939900	3.00678900	-0.96306700
H	-2.10304600	2.55979500	-2.57405800
H	-1.46402400	0.10318400	-3.03138000
H	-3.18925000	0.24267400	-2.70253900
H	-3.00678900	-1.53939900	-0.96306700
H	-2.55979500	-2.10304600	-2.57405800
H	-0.10318400	-1.46402400	-3.03138000
H	-0.24267400	-3.18925000	-2.70253900
H	1.53939900	-3.00678900	-0.96306700
H	2.10304600	-2.55979500	-2.57405800
H	1.46402400	-0.10318400	-3.03138000
H	3.18925000	-0.24267400	-2.70253900
H	3.00678900	1.53939900	-0.96306700
H	2.55979500	2.10304600	-2.57405800
H	1.70972700	3.87232800	-0.83942400
H	0.25126000	3.42559000	0.08777800
H	-3.87232800	1.70972700	-0.83942400
H	-3.42559000	0.25126000	0.08777800
H	-1.70972700	-3.87232800	-0.83942400
H	-0.25126000	-3.42559000	0.08777800
H	3.87232800	-1.70972700	-0.83942400
H	3.42559000	-0.25126000	0.08777800

**Ac(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

Ac	0.00000000	0.00000000	0.74158700
N	0.00000000	2.16359800	-1.19474000
N	2.16059400	-0.00983700	-1.19701900
N	0.00000000	-2.16359800	-1.19474000
N	-2.16059400	0.00983700	-1.19701900
O	-1.48107300	1.99020300	1.20364600
O	1.97552200	1.54013800	1.12357500
O	1.48107300	-1.99020300	1.20364600
O	-1.97552200	-1.54013800	1.12357500
O	4.09208100	2.26926700	0.80633500
O	2.20498100	-4.10689100	0.88351700
O	-4.09208100	-2.26926700	0.80633500
O	-2.20498100	4.10689100	0.88351700
C	-1.45531600	3.15604000	0.65422200
C	3.14682000	1.50667600	0.59298600
C	1.45531600	-3.15604000	0.65422200
C	-3.14682000	-1.50667600	0.59298600
C	1.34370300	2.31018600	-1.80393600
C	1.94555500	0.98349400	-2.27155400
C	2.32621400	-1.36236800	-1.77869800
C	1.01365600	-1.98327200	-2.25605300
C	-1.34370300	-2.31018600	-1.80393600
C	-1.94555500	-0.98349400	-2.27155400
C	-2.32621400	1.36236800	-1.77869800
C	-1.01365600	1.98327200	-2.25605300
C	-0.30871300	3.36022700	-0.36645600
C	3.36380000	0.33504200	-0.39488500
C	0.30871300	-3.36022700	-0.36645600
C	-3.36380000	-0.33504200	-0.39488500
H	0.58520800	3.57375300	0.22737000
H	-0.53309400	4.22955800	-1.00119300
H	4.22156200	0.55441100	-1.04722900
H	3.60172400	-0.53992400	0.21784800
H	0.53309400	-4.22955800	-1.00119300
H	-0.58520800	-3.57375300	0.22737000
H	-3.60172400	0.53992400	0.21784800
H	-4.22156200	-0.55441100	-1.04722900
H	1.99461300	2.77349000	-1.06365500
H	1.30454800	2.99098500	-2.67257000
H	2.90128400	1.20077600	-2.77977500
H	1.28965200	0.53075100	-3.02109300
H	3.02537400	-1.33756700	-2.63343400
H	2.77704800	-1.99483200	-1.01406200
H	1.24409300	-2.95486700	-2.72639000
H	0.57413600	-1.35628600	-3.03750700
H	-1.30454800	-2.99098500	-2.67257000
H	-1.99461300	-2.77349000	-1.06365500
H	-1.28965200	-0.53075100	-3.02109300
H	-2.90128400	-1.20077600	-2.77977500
H	-2.77704800	1.99483200	-1.01406200
H	-3.02537400	1.33756700	-2.63343400
H	-0.57413600	1.35628600	-3.03750700
H	-1.24409300	2.95486700	-2.72639000
O	0.00000000	0.00000000	3.46755400
H	0.40550300	-0.66734700	4.03282000
H	-0.40550300	0.66734700	4.03282000

**Ac(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

Ac	0.00000000	0.00000000	0.68851700
N	-0.97828200	-1.90858900	-1.31895600
N	1.90077100	-0.98029900	-1.29900700
N	0.97828200	1.90858900	-1.31895600
N	-1.90077100	0.98029900	-1.29900700
O	-1.95529700	-1.54117600	1.18699400
O	1.58259600	-1.87893500	1.27504200
O	1.95529700	1.54117600	1.18699400
O	-1.58259600	1.87893500	1.27504200
O	-2.87181700	-3.61145700	1.20550000
O	3.65611100	-2.78349700	1.26584600
O	2.87181700	3.61145700	1.20550000
O	-3.65611100	2.78349700	1.26584600
C	-2.12796100	-2.74073000	0.75465800
C	2.77114700	-2.06102500	0.80987900
C	2.12796100	2.74073000	0.75465800
C	-2.77114700	2.06102500	0.80987900
C	0.00000000	-2.22261300	-2.37669200
C	1.43695400	-2.26816900	-1.86107400
C	2.19572900	-0.01917800	-2.37960300
C	2.25195200	1.42934200	-1.90072500
C	0.00000000	2.22261300	-2.37669200
C	-1.43695400	2.26816900	-1.86107400
C	-2.19572900	0.01917800	-2.37960300
C	-2.25195200	-1.42934200	-1.90072500
C	-1.25761400	-3.09948500	-0.47808500
C	3.09920100	-1.22830800	-0.45752100
C	1.25761400	3.09948500	-0.47808500
C	-3.09920100	1.22830800	-0.45752100
H	-0.09064100	-1.46482000	-3.16101300
H	-0.23547800	-3.19142400	-2.85075200
H	1.51567900	-3.01327400	-1.06713500
H	2.10160900	-2.59657600	-2.67937400
H	1.42279300	-0.12380600	-3.14706400
H	3.15519400	-0.26585800	-2.86711800
H	3.01683500	1.52753500	-1.12884400
H	2.55985800	2.07149200	-2.74443800
H	0.09064100	1.46482000	-3.16101300
H	0.23547800	3.19142400	-2.85075200
H	-1.51567900	3.01327400	-1.06713500
H	-2.10160900	2.59657600	-2.67937400
H	-1.42279300	0.12380600	-3.14706400
H	-3.15519400	0.26585800	-2.86711800
H	-3.01683500	-1.52753500	-1.12884400
H	-2.55985800	-2.07149200	-2.74443800
H	-1.75147000	-3.89042900	-1.06206900
H	-0.30882000	-3.49039300	-0.09790500
H	3.88942000	-1.73242700	-1.03334200
H	3.48150000	-0.26538800	-0.10582800
H	1.75147000	3.89042900	-1.06206900
H	0.30882000	3.49039300	-0.09790500
H	-3.88942000	1.73242700	-1.03334200
H	-3.48150000	0.26538800	-0.10582800
O	0.00000000	0.00000000	3.38759500
H	-0.57928000	0.52752600	3.94913900
H	0.57928000	-0.52752600	3.94913900



**Am(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

Am	0.00000000	0.00000000	0.60751900
N	0.00000000	2.13609800	-1.16950500
N	2.13682800	-0.01393000	-1.17122000
N	0.00000000	-2.13609800	-1.16950500
N	-2.13682800	0.01393000	-1.17122000
O	-1.44507200	1.84427200	1.23468600
O	1.84246100	1.51475400	1.13270700
O	1.44507200	-1.84427200	1.23468600
O	-1.84246100	-1.51475400	1.13270700
O	3.96632800	2.25801400	0.92727100
O	2.19080400	-3.96513600	1.02781000
O	-3.96632800	-2.25801400	0.92727100
O	-2.19080400	3.96513600	1.02781000
C	-1.43721000	3.03365600	0.73811300
C	3.03783600	1.48984100	0.66214300
C	1.43721000	-3.03365600	0.73811300
C	-3.03783600	-1.48984100	0.66214300
C	1.34218500	2.30615200	-1.77566100
C	1.95212000	0.98507800	-2.24632100
C	2.32240900	-1.36228500	-1.75488300
C	1.01326300	-1.98433800	-2.23506100
C	-1.34218500	-2.30615200	-1.77566100
C	-1.95212000	-0.98507800	-2.24632100
C	-2.32240900	1.36228500	-1.75488300
C	-1.01326300	1.98433800	-2.23506100
C	-0.31744000	3.29908900	-0.29615500
C	3.30956200	0.33103900	-0.32420000
C	0.31744000	-3.29908900	-0.29615500
C	-3.30956200	-0.33103900	-0.32420000
H	0.58155000	3.50923500	0.28995400
H	-0.57400400	4.18251800	-0.89753400
H	4.18670200	0.56528700	-0.94414300
H	3.52940300	-0.54679500	0.29017200
H	0.57400400	-4.18251800	-0.89753400
H	-0.58155000	-3.50923500	0.28995400
H	-3.52940300	0.54679500	0.29017200
H	-4.18670200	-0.56528700	-0.94414300
H	1.98793700	2.77096800	-1.03202000
H	1.29556700	2.99150600	-2.63955400
H	2.91971500	1.20215300	-2.73073200
H	1.31016500	0.53896700	-3.01232000
H	3.02717700	-1.32951700	-2.60386300
H	2.77199200	-1.99374800	-0.98849300
H	1.23739800	-2.96529800	-2.68790400
H	0.57911100	-1.36542300	-3.02640800
H	-1.29556700	-2.99150600	-2.63955400
H	-1.98793700	-2.77096800	-1.03202000
H	-1.31016500	-0.53896700	-3.01232000
H	-2.91971500	-1.20215300	-2.73073200
H	-2.77199200	1.99374800	-0.98849300
H	-3.02717700	1.32951700	-2.60386300
H	-0.57911100	1.36542300	-3.02640800
H	-1.23739800	2.96529800	-2.68790400
O	0.00000000	0.00000000	3.15393200
H	0.45580600	-0.64319200	3.70742100
H	-0.45580600	0.64319200	3.70742100

**Am(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

Am	0.00000000	0.00000000	0.56663700
N	0.96572600	1.88444700	-1.29334800
N	-1.87657800	0.97133600	-1.26879500
N	-0.96572600	-1.88444700	-1.29334800
N	1.87657800	-0.97133600	-1.26879500
O	1.91668500	1.39352200	1.17515900
O	-1.42677000	1.82913700	1.28201400
O	-1.91668500	-1.39352200	1.17515900
O	1.42677000	-1.82913700	1.28201400
O	2.85102600	3.45017100	1.30716200
O	-3.48726500	2.75118500	1.39274400
O	-2.85102600	-3.45017100	1.30716200
O	3.48726500	-2.75118500	1.39274400
C	2.09537000	2.61438400	0.81126800
C	-2.63782400	2.02327800	0.88154700
C	-2.09537000	-2.61438400	0.81126800
C	2.63782400	-2.02327800	0.88154700
C	0.00000000	2.22704400	-2.35210000
C	-1.43474400	2.26547500	-1.83457500
C	-2.20284900	0.02255200	-2.35052100
C	-2.24730300	-1.42621100	-1.87566200
C	0.00000000	-2.22704400	-2.35210000
C	1.43474400	-2.26547500	-1.83457500
C	2.20284900	-0.02255200	-2.35052100
C	2.24730300	1.42621100	-1.87566200
C	1.23278300	3.04215500	-0.40264100
C	-3.03924900	1.21070500	-0.37579900
C	-1.23278300	-3.04215500	-0.40264100
C	3.03924900	-1.21070500	-0.37579900
H	0.09037700	1.48205900	-3.14928200
H	0.24359700	3.20349300	-2.80523900
H	-1.51565200	3.01102000	-1.04164400
H	-2.10806200	2.58422700	-2.64873900
H	-1.44666200	0.13149500	-3.13452400
H	-3.17300700	0.27594100	-2.81192400
H	-3.01199000	-1.53204500	-1.10510200
H	-2.54490800	-2.07293200	-2.71874400
H	-0.09037700	-1.48205900	-3.14928200
H	-0.24359700	-3.20349300	-2.80523900
H	1.51565200	-3.01102000	-1.04164400
H	2.10806200	-2.58422700	-2.64873900
H	1.44666200	-0.13149500	-3.13452400
H	3.17300700	-0.27594100	-2.81192400
H	3.01199000	1.53204500	-1.10510200
H	2.54490800	2.07293200	-2.71874400
H	1.73176200	3.85672300	-0.94774700
H	0.28133500	3.41027300	-0.00835900
H	-3.84837300	1.73066600	-0.90888800
H	-3.40794600	0.24589700	-0.01703700
H	-1.73176200	-3.85672300	-0.94774700
H	-0.28133500	-3.41027300	-0.00835900
H	3.84837300	-1.73066600	-0.90888800
H	3.40794600	-0.24589700	-0.01703700
O	0.00000000	0.00000000	3.10033300
H	0.53408900	-0.58342700	3.64992200
H	-0.53408900	0.58342700	3.64992200

**Cf(DOTA)(H<sub>2</sub>O)- SAP**

Cf	0.00000000	0.00000000	0.56938900
N	0.20826600	2.11518100	-1.16648700
N	2.11588300	-0.22320500	-1.16761500
N	-0.20826600	-2.11518100	-1.16648700
N	-2.11588300	0.22320500	-1.16761500
O	-1.24662300	1.91691800	1.23006100
O	1.92627600	1.31511300	1.12731000
O	1.24662300	-1.91691800	1.23006100
O	-1.92627600	-1.31511300	1.12731000
O	4.11456500	1.85489500	0.97584500
O	1.78593100	-4.10346100	1.08241700
O	-4.11456500	-0.785489500	0.97584500
O	-1.78593100	4.10346100	1.08241700
C	-1.12834400	3.11172300	0.76104000
C	3.12423000	1.17912400	0.68379400
C	1.12834400	-3.11172300	0.76104000
C	-3.12423000	-1.17912400	0.68379400
C	1.56071700	2.16185000	-1.77078600
C	2.04105000	0.78937500	-2.24282100
C	2.17574500	-1.58194000	-1.75205500
C	0.81297200	-2.07209800	-2.23367900
C	-1.56071700	-2.16185000	-1.77078600
C	-2.04105000	-0.78937500	-2.24282100
C	-2.17574500	1.58194000	-1.75205500
C	-0.81297200	2.07209800	-2.23367900
C	0.00000000	3.29283000	-0.28045600
C	3.30576400	0.00751300	-0.30636100
C	0.00000000	-3.29283000	-0.28045600
C	-3.30576400	-0.00751300	-0.30636100
H	0.91757800	3.41929500	0.30032200
H	-0.18554800	4.20097500	-0.87090600
H	4.20747700	0.16637600	-0.91474400
H	3.43793300	-0.88966600	0.30473500
H	0.18554800	-4.20097500	-0.87090600
H	-0.91757800	-3.41929500	0.30032200
H	-3.43793300	0.88966600	0.30473500
H	-4.20747700	-0.16637600	-0.91474400
H	2.24704300	2.56105200	-1.02535400
H	1.57977500	2.85100900	-2.63253000
H	3.02926200	0.90998600	-2.71911000
H	1.36365100	0.41041200	-3.01453200
H	2.88270800	-1.61600700	-2.59896400
H	2.56032100	-2.25455300	-0.98522500
H	0.93691700	-3.07256900	-2.68231400
H	0.44327700	-1.41522000	-3.02725800
H	-1.57977500	-2.85100900	-2.63253000
H	-2.24704300	-2.56105200	-1.02535400
H	-1.36365100	-0.41041200	-3.01453200
H	-3.02926200	-0.90998600	-2.71911000
H	-2.56032100	2.25455300	-0.98522500
H	-2.88270800	1.61600700	-2.59896400
H	-0.44327700	1.41522000	-3.02725800
H	-0.93691700	3.07256900	-2.68231400
O	0.00000000	0.00000000	3.05573100
H	0.40614700	-0.67905800	3.60450000
H	-0.40614700	0.67905800	3.60450000

**Cf(DOTA)(H<sub>2</sub>O)- TSAP**

Cf	0.00000000	0.00000000	0.53381600
N	-1.88608000	0.94086100	-1.28908600
N	-0.94800000	-1.87800700	-1.26342200
N	1.88608000	-0.94086100	-1.28908600
N	0.94800000	1.87800700	-1.26342200
O	-1.36219300	1.87655600	1.16359000
O	-1.79062300	-1.38993000	1.27106900
O	1.36219300	-1.87655600	1.16359000
O	1.79062300	1.38993000	1.27106900
O	-3.42105300	2.79660900	1.34547100
O	-2.69875600	-3.45253000	1.43426900
O	3.42105300	-2.79660900	1.34547100
O	2.69875600	3.45253000	1.43426900
C	-2.59181500	2.04918300	0.82673600
C	-1.97856300	-2.61149500	0.89911600
C	2.59181500	-2.04918300	0.82673600
C	1.97856300	2.61149500	0.89911600
C	-2.22784100	-0.02326500	-2.34866400
C	-2.24842500	-1.45743900	-1.83089400
C	0.00000000	-2.20495300	-2.34500800
C	1.44866500	-2.22996000	-1.87056500
C	2.22784100	0.02326500	-2.34866400
C	2.24842500	1.45743900	-1.83089400
C	0.00000000	2.20495300	-2.34500800
C	-1.44866500	2.22996000	-1.87056500
C	-3.03563000	1.19241900	-0.38403500
C	-1.17450500	-3.03163600	-0.35608700
C	3.03563000	-1.19241900	-0.38403500
C	1.17450500	3.03163600	-0.35608700
H	-1.48814400	0.07525900	-3.14998200
H	-3.20930100	0.21260300	-2.79494400
H	-2.99375100	-1.54731800	-1.03877000
H	-2.55625800	-2.13690100	-2.64394800
H	-0.11788900	-1.45574400	-3.13458400
H	-0.24508700	-3.18120800	-2.79781800
H	1.56455300	-2.99280100	-1.09964300
H	2.10054700	-2.51835300	-2.71270200
H	1.48814400	-0.07525900	-3.14998200
H	3.20930100	-0.21260300	-2.79494400
H	2.99375100	1.54731800	-1.03877000
H	2.55625800	2.13690100	-2.64394800
H	0.11788900	1.45574400	-3.13458400
H	0.24508700	3.18120800	-2.79781800
H	-1.56455300	2.99280100	-1.09964300
H	-2.10054700	2.51835300	-2.71270200
H	-3.85973200	1.69076400	-0.91510000
H	-3.39135600	0.23646400	0.00978000
H	-1.69649700	-3.84877100	-0.87465600
H	-0.20622600	-3.39127000	0.00151900
H	3.85973200	-1.69076400	-0.91510000
H	3.39135600	-0.23646400	0.00978000
H	1.69649700	3.84877100	-0.87465600
H	0.20622600	3.39127000	0.00151900
O	0.00000000	0.00000000	3.01144000
H	0.59383800	0.52650900	3.55686500
H	-0.59383800	-0.52650900	3.55686500

**Cm(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

Cm	0.00000000	0.00000000	0.59329400
N	0.20590900	2.12219600	-1.16813500
N	2.12209900	-0.22014600	-1.16947800
N	-0.20590900	-2.12219600	-1.16813500
N	-2.12209900	0.22014600	-1.16947800
O	-1.25686900	1.95325700	1.23319300
O	1.95957600	1.32599300	1.13162500
O	1.25686900	-1.95325700	1.23319300
O	-1.95957600	-1.32599300	1.13162500
O	4.14605600	1.86359800	0.94537100
O	1.79685700	-4.13713500	1.04672200
O	-4.14605600	-1.86359800	0.94537100
O	-1.79685700	4.13713500	1.04672200
C	-1.13650800	3.14060900	0.74625800
C	3.15090100	1.18774200	0.67070800
C	1.13650800	-3.14060900	0.74625800
C	-3.15090100	-1.18774200	0.67070800
C	1.55828500	2.16519000	-1.77354000
C	2.03902700	0.79217800	-2.24463800
C	2.17934500	-1.57960100	-1.75356500
C	0.81662100	-2.07222500	-2.23423900
C	-1.55828500	-2.16519000	-1.77354000
C	-2.03902700	-0.79217800	-2.24463800
C	-2.17934500	1.57960100	-1.75356500
C	-0.81662100	2.07222500	-2.23423900
C	0.00000000	3.30633100	-0.28992500
C	3.31846600	0.01088300	-0.31691400
C	0.00000000	-3.30633100	-0.28992500
C	-3.31846600	-0.01088300	-0.31691400
H	0.91570900	3.42992600	0.29475200
H	-0.17543000	4.21207000	-0.88720700
H	4.21642500	0.16343700	-0.93248100
H	3.45204700	-0.88477600	0.29639400
H	0.17543000	-4.21207000	-0.88720700
H	-0.91570900	-3.42992600	0.29475200
H	-3.45204700	0.88477600	0.29639400
H	-4.21642500	-0.16343700	-0.93248100
H	2.24514000	2.56544600	-1.02916700
H	1.57745900	2.85280600	-2.63661500
H	3.02470300	0.91466300	-2.72571700
H	1.35925100	0.41082100	-3.01300500
H	2.88477600	-1.61403100	-2.60185400
H	2.56561200	-2.25160800	-0.98712200
H	0.94397000	-3.07111300	-2.68545800
H	0.44479900	-1.41496400	-3.02644000
H	-1.57745900	-2.85280600	-2.63661500
H	-2.24514000	-2.56544600	-1.02916700
H	-1.35925100	-0.41082100	-3.01300500
H	-3.02470300	-0.91466300	-2.72571700
H	-2.56561200	2.25160800	-0.98712200
H	-2.88477600	1.61403100	-2.60185400
H	-0.44479900	1.41496400	-3.02644000
H	-0.94397000	3.07111300	-2.68545800
O	0.00000000	0.00000000	3.11742400
H	0.39680000	-0.68239200	3.66923700
H	-0.39680000	0.68239200	3.66923700

**Cm(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

Cm	0.00000000	0.00000000	0.55401700
N	0.96360600	1.88139900	-1.29129000
N	-1.87337200	0.97022200	-1.26634300
N	-0.96360600	-1.88139900	-1.29129000
N	1.87337200	-0.97022200	-1.26634300
O	1.90761900	1.37488600	1.17167500
O	-1.40642500	1.82028300	1.27930400
O	-1.90761900	-1.37488600	1.17167500
O	1.40642500	-1.82028300	1.27930400
O	2.84511500	3.42879900	1.32094000
O	-3.46354700	2.74719700	1.40735400
O	-2.84511500	-3.42879900	1.32094000
O	3.46354700	-2.74719700	1.40735400
C	2.08945100	2.59795300	0.81676200
C	-2.62045700	2.01718800	0.88873900
C	-2.08945100	-2.59795300	0.81676200
C	2.62045700	-2.01718800	0.88873900
C	0.00000000	2.22762700	-2.35048600
C	-1.43450900	2.26498700	-1.83304800
C	-2.20356000	0.02278700	-2.34788300
C	-2.24635100	-1.42581000	-1.87306700
C	0.00000000	-2.22762700	-2.35048600
C	1.43450900	-2.26498700	-1.83304800
C	2.20356000	-0.02278700	-2.34788300
C	2.24635100	1.42581000	-1.87306700
C	1.22937000	3.03499600	-0.39504300
C	-3.03177500	1.20926500	-0.36787100
C	-1.22937000	-3.03499600	-0.39504300
C	3.03177500	-1.20926500	-0.36787100
H	0.09064500	1.48424400	-3.14919400
H	0.24468400	3.20499100	-2.80103900
H	-1.51597200	3.01092500	-1.04055700
H	-2.10890300	2.58213200	-2.64686700
H	-1.44960100	0.13212400	-3.13403300
H	-3.17506200	0.27681300	-2.80603700
H	-3.01065600	-1.53237700	-1.10222500
H	-2.54323000	-2.07336000	-2.71569400
H	-0.09064500	-1.48424400	-3.14919400
H	-0.24468400	-3.20499100	-2.80103900
H	1.51597200	-3.01092500	-1.04055700
H	2.10890300	-2.58213200	-2.64686700
H	1.44960100	-0.13212400	-3.13403300
H	3.17506200	-0.27681300	-2.80603700
H	3.01065600	1.53237700	-1.10222500
H	2.54323000	2.07336000	-2.71569400
H	1.73040300	3.85161300	-0.93510100
H	0.27770400	3.40146500	-0.00008200
H	-3.84195900	1.73297500	-0.89558800
H	-3.40058000	0.24450500	-0.00946200
H	-1.73040300	-3.85161300	-0.93510100
H	-0.27770400	-3.40146500	-0.00008200
H	3.84195900	-1.73297500	-0.89558800
H	3.40058000	-0.24450500	-0.00946200
O	0.00000000	0.00000000	3.06712800
H	0.52870300	-0.58964100	3.61515700
H	-0.52870300	0.58964100	3.61515700

**La(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

La	0.00000000	0.00000000	0.73506000
N	0.20205800	2.13667600	-1.09497500
N	2.13457500	-0.21382900	-1.09677800
N	-0.20205800	-2.13667600	-1.09497500
N	-2.13457500	0.21382900	-1.09677800
O	-1.27401200	2.02011000	1.30069000
O	2.01956600	1.33848200	1.20996400
O	1.27401200	-2.02011000	1.30069000
O	-2.01956600	-1.33848200	1.20996400
O	4.20362100	1.87181200	0.97642300
O	1.80571600	-4.20282500	1.06624400
O	-4.20362100	-1.87181200	0.97642300
O	-1.80571600	4.20282500	1.06624400
C	-1.14720900	3.19787100	0.79187100
C	3.20136000	1.19895300	0.72318900
C	1.14720900	-3.19787100	0.79187100
C	-3.20136000	-1.19895300	0.72318900
C	1.55390700	2.17115700	-1.70249800
C	2.03340700	0.79688200	-2.17195300
C	2.18523800	-1.57451500	-1.67974000
C	0.82231800	-2.07016200	-2.15886500
C	-1.55390700	-2.17115700	-1.70249800
C	-2.03340700	-0.79688200	-2.17195300
C	-2.18523800	1.57451500	-1.67974000
C	-0.82231800	2.07016200	-2.15886500
C	0.00000000	3.33563300	-0.23743500
C	3.34483900	0.01847100	-0.26531400
C	0.00000000	-3.33563300	-0.23743500
C	-3.34483900	-0.01847100	-0.26531400
H	0.91298000	3.46096700	0.35179500
H	-0.16074300	4.23417000	-0.85007300
H	4.23337300	0.16554200	-0.89615700
H	3.48812200	-0.87606200	0.34798700
H	0.16074300	-4.23417000	-0.85007300
H	-0.91298000	-3.46096700	0.35179500
H	-3.48812200	0.87606200	0.34798700
H	-4.23337300	-0.16554200	-0.89615700
H	2.24244800	2.57242700	-0.96017600
H	1.57456000	2.85617700	-2.56805300
H	3.01287300	0.92219900	-2.66544000
H	1.34706600	0.41101300	-2.93191900
H	2.88774000	-1.61089100	-2.53088300
H	2.57408300	-2.24572900	-0.91405400
H	0.95587800	-3.06461100	-2.61856300
H	0.44642400	-1.41007600	-2.94654100
H	-1.57456000	-2.85617700	-2.56805300
H	-2.24244800	-2.57242700	-0.96017600
H	-1.34706600	-0.41101300	-2.93191900
H	-3.01287300	-0.92219900	-2.66544000
H	-2.57408300	2.24572900	-0.91405400
H	-2.88774000	1.61089100	-2.53088300
H	-0.44642400	1.41007600	-2.94654100
H	-0.95587800	3.06461100	-2.61856300
O	0.00000000	0.00000000	3.35876900
H	0.37854800	-0.68729800	3.91796800
H	-0.37854800	0.68729800	3.91796800

**La(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

La	0.00000000	0.00000000	0.68245000
N	-1.90144900	0.95168100	-1.22503300
N	-0.95622300	-1.89473300	-1.20277800
N	1.90144900	-0.95168100	-1.22503300
N	0.95622300	1.89473300	-1.20277800
O	-1.45450600	1.91885000	1.25111100
O	-1.83350200	-1.49177200	1.34997900
O	1.45450600	-1.91885000	1.25111100
O	1.83350200	1.49177200	1.34997900
O	-3.53130900	2.81225000	1.36295500
O	-2.71614300	-3.57171000	1.43747400
O	3.53130900	-2.81225000	1.36295500
O	2.71614300	3.57171000	1.43747400
C	-2.67396400	2.07813700	0.87210900
C	-2.00629500	-2.70154700	0.93604500
C	2.67396400	-2.07813700	0.87210900
C	2.00629500	2.70154700	0.93604500
C	-2.22554800	-0.02162700	-2.28338900
C	-2.25256300	-1.45752800	-1.76701000
C	0.00000000	-2.20067900	-2.28420100
C	1.44889400	-2.23505400	-1.80767100
C	2.22554800	0.02162700	-2.28338900
C	2.25256300	1.45752800	-1.76701000
C	0.00000000	2.20067900	-2.28420100
C	-1.44889400	2.23505400	-1.80767100
C	-3.07165500	1.21109800	-0.34942600
C	-1.18652100	-3.07139100	-0.32668400
C	3.07165500	-1.21109800	-0.34942600
C	1.18652100	3.07139100	-0.32668400
H	-1.47740000	0.07621600	-3.07650200
H	-3.20190800	0.20999000	-2.74344400
H	-2.99706700	-1.54504300	-0.97369800
H	-2.56839900	-2.13059500	-2.58295500
H	-0.11489600	-1.43966100	-3.06245700
H	-0.24156300	-3.16958700	-2.75501900
H	1.55942100	-2.99894200	-1.03680900
H	2.09733600	-2.52953500	-2.65091500
H	1.47740000	-0.07621600	-3.07650200
H	3.20190800	-0.20999000	-2.74344400
H	2.99706700	1.54504300	-0.97369800
H	2.56839900	2.13059500	-2.58295500
H	0.11489600	1.43966100	-3.06245700
H	0.24156300	3.16958700	-2.75501900
H	-1.55942100	2.99894200	-1.03680900
H	-2.09733600	2.52953500	-2.65091500
H	-3.88423800	1.70115700	-0.90591900
H	-3.43803900	0.25662900	0.03977700
H	-1.69460300	-3.87958100	-0.87299900
H	-0.21843800	-3.43584700	0.02829500
H	3.88423800	-1.70115700	-0.90591900
H	3.43803900	-0.25662900	0.03977700
H	1.69460300	3.87958100	-0.87299900
H	0.21843800	3.43584700	0.02829500
O	0.00000000	0.00000000	3.28624500
H	0.56061000	0.55269100	3.84174300
H	-0.56061000	-0.55269100	3.84174300

**Lu(DOTA)(H<sub>2</sub>O)- SAP**

Lu	0.00000000	0.00000000	0.57098100
N	0.21642300	2.08977100	-1.10853600
N	2.09217100	-0.23399600	-1.10845400
N	-0.21642300	-2.08977100	-1.10853600
N	-2.09217100	0.23399600	-1.10845400
O	-1.20459400	1.79139800	1.25664800
O	1.80576300	1.26777800	1.15677300
O	1.20459400	-1.79139800	1.25664800
O	-1.80576300	-1.26777800	1.15677300
O	3.99327000	1.82675100	1.13354000
O	1.75030800	-3.97995800	1.24960700
O	-3.99327000	-1.82675100	1.13354000
O	-1.75030800	3.97995800	1.24960700
C	-1.09829500	3.01164700	0.85474800
C	3.02673500	1.14714900	0.77748000
C	1.09829500	-3.01164700	0.85474800
C	-3.02673500	-1.14714900	0.77748000
C	1.56862200	2.14865100	-1.70900600
C	2.04486600	0.77801600	-2.18443800
C	2.16226900	-1.58952700	-1.69499700
C	0.79948600	-2.06994200	-2.18002200
C	-1.56862200	-2.14865100	-1.70900600
C	-2.04486600	-0.77801600	-2.18443800
C	-2.16226900	1.58952700	-1.69499700
C	-0.79948600	2.06994200	-2.18002200
C	0.00000000	3.24854000	-0.20204200
C	3.26160200	-0.00214500	-0.22215200
C	0.00000000	-3.24854000	-0.20204200
C	-3.26160200	0.00214500	-0.22215200
H	0.92338000	3.39111000	0.36444600
H	-0.22269300	4.16152300	-0.77184400
H	4.17305600	0.18447900	-0.80772800
H	3.39710000	-0.90507100	0.37860700
H	0.22269300	-4.16152300	-0.77184400
H	-0.92338000	-3.39111000	0.36444600
H	-3.39710000	0.90507100	0.37860700
H	-4.17305600	-0.18447900	-0.80772800
H	2.25397200	2.54344400	-0.96020400
H	1.58804700	2.84388100	-2.56572100
H	3.04090800	0.89012200	-2.64648500
H	1.37396200	0.40781900	-2.96607000
H	2.87473000	-1.62162500	-2.53719100
H	2.54139100	-2.26506500	-0.92782200
H	0.91067800	-3.07525200	-2.62137200
H	0.43738100	-1.41339300	-2.97742000
H	-1.58804700	-2.84388100	-2.56572100
H	-2.25397200	-2.54344400	-0.96020400
H	-1.37396200	-0.40781900	-2.96607000
H	-3.04090800	-0.89012200	-2.64648500
H	-2.54139100	2.26506500	-0.92782200
H	-2.87473000	1.62162500	-2.53719100
H	-0.43738100	1.41339300	-2.97742000
H	-0.91067800	3.07525200	-2.62137200
O	0.00000000	0.00000000	2.94748300
H	0.42753100	-0.67169000	3.48800700
H	-0.42753100	0.67169000	3.48800700

**Lu(DOTA)(H<sub>2</sub>O)- TSAP**

Lu	0.00000000	0.00000000	0.54515400
N	1.86822000	-0.92995200	-1.23317700
N	0.93767700	1.85772200	-1.20572900
N	-1.86822000	0.92995200	-1.23317700
N	-0.93767700	-1.85772200	-1.20572900
O	1.25054100	-1.80523700	1.17840500
O	1.73187500	1.26956600	1.27897300
O	-1.25054100	1.80523700	1.17840500
O	-1.73187500	-1.26956600	1.27897300
O	3.28281400	-2.75067000	1.47826900
O	2.65012300	3.31190500	1.57256800
O	-3.28281400	2.75067000	1.47826900
O	-2.65012300	-3.31190500	1.57256800
C	2.49339500	-2.00020700	0.90543500
C	1.93469900	2.50922800	0.97668200
C	-2.49339500	2.00020700	0.90543500
C	-1.93469900	-2.50922800	0.97668200
C	2.22828500	0.02261200	-2.29441300
C	2.24198400	1.45413200	-1.77570100
C	0.00000000	2.20594200	-2.28770400
C	-1.44666100	2.22410400	-1.81325700
C	-2.22828500	-0.02261200	-2.29441300
C	-2.24198400	-1.45413200	-1.77570100
C	0.00000000	-2.20594200	-2.28770400
C	1.44666100	-2.22410400	-1.81325700
C	2.99524700	-1.17675500	-0.30169700
C	1.16517900	2.98936000	-0.27418500
C	-2.99524700	1.17675500	-0.30169700
C	-1.16517900	-2.98936000	-0.27418500
H	1.49739500	-0.07685600	-3.10394600
H	3.21470600	-0.21770400	-2.72754000
H	2.98823000	1.54599400	-0.98478900
H	2.54252800	2.14060500	-2.58539500
H	0.11882800	1.46723300	-3.08725300
H	0.25013000	3.18801800	-2.72505700
H	-1.56534200	2.98618200	-1.04200100
H	-2.10392500	2.50833600	-2.65252900
H	-1.49739500	0.07685600	-3.10394600
H	-3.21470600	0.21770400	-2.72754000
H	-2.98823000	-1.54599400	-0.98478900
H	-2.54252800	-2.14060500	-2.58539500
H	-0.11882800	-1.46723300	-3.08725300
H	-0.25013000	-3.18801800	-2.72505700
H	1.56534200	-2.98618200	-1.04200100
H	2.10392500	-2.50833600	-2.65252900
H	3.82294800	-1.70106100	-0.80143200
H	3.35519100	-0.22045900	0.08511800
H	1.71611700	3.80621000	-0.76257000
H	0.19962300	3.36033800	0.07641100
H	-3.82294800	1.70106100	-0.80143200
H	-3.35519100	0.22045900	0.08511800
H	-1.71611700	-3.80621000	-0.76257000
H	-0.19962300	-3.36033800	0.07641100
O	0.00000000	0.00000000	2.92300000
H	-0.62209000	-0.49923300	3.46166100
H	0.62209000	0.49923300	3.46166100

**Np(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

Np	0.00000000	0.00000000	0.64083200
N	0.00000000	2.14423700	-1.17435200
N	2.14368200	-0.01288800	-1.17671700
N	0.00000000	-2.14423700	-1.17435200
N	-2.14368200	0.01288800	-1.17671700
O	-1.45883400	1.88871900	1.23096700
O	1.88357200	1.52597900	1.13391100
O	1.45883400	-1.88871900	1.23096700
O	-1.88357200	-1.52597900	1.13391100
O	4.00721900	2.26028600	0.89271900
O	2.19307100	-4.01050900	0.98919200
O	-4.00721900	-2.26028600	0.89271900
O	-2.19307100	4.01050900	0.98919200
C	-1.44303100	3.07080000	0.71759600
C	3.07171100	1.49503200	0.64505000
C	1.44303100	-3.07080000	0.71759600
C	-3.07171100	-1.49503200	0.64505000
C	1.34276600	2.30748800	-1.78143100
C	1.95030900	0.98481900	-2.25157200
C	2.32357300	-1.36255600	-1.75992500
C	1.01350100	-1.98483600	-2.23883200
C	-1.34276600	-2.30748800	-1.78143100
C	-1.95030900	-0.98481900	-2.25157200
C	-2.32357300	1.36255600	-1.75992500
C	-1.01350100	1.98483600	-2.23883200
C	-0.31418600	3.31671500	-0.31267400
C	3.32538700	0.33154600	-0.34194100
C	0.31418600	-3.31671500	-0.31267400
C	-3.32538700	-0.33154600	-0.34194100
H	0.58353800	3.52569200	0.27619500
H	-0.55975700	4.19700400	-0.92332900
H	4.19732800	0.56012000	-0.97137000
H	3.54914600	-0.54558800	0.27233500
H	0.55975700	-4.19700400	-0.92332900
H	-0.58353800	-3.52569200	0.27619500
H	-3.54914600	0.54558800	0.27233500
H	-4.19732800	-0.56012000	-0.97137000
H	1.98993900	2.77152900	-1.03852700
H	1.29814200	2.99175900	-2.64643600
H	2.91459700	1.20212100	-2.74260400
H	1.30440400	0.53690100	-3.01304200
H	3.02652100	-1.33190900	-2.61068500
H	2.77378400	-1.99392500	-0.99393100
H	1.23965400	-2.96339100	-2.69599800
H	0.57757300	-1.36419600	-3.02772800
H	-1.29814200	-2.99175900	-2.64643600
H	-1.98993900	-2.77152900	-1.03852700
H	-1.30440400	-0.53690100	-3.01304200
H	-2.91459700	-1.20212100	-2.74260400
H	-2.77378400	1.99392500	-0.99393100
H	-3.02652100	1.33190900	-2.61068500
H	-0.57757300	1.36419600	-3.02772800
H	-1.23965400	2.96339100	-2.69599800
O	0.00000000	0.00000000	3.23702300
H	0.44405900	-0.64881300	3.79387100
H	-0.44405900	0.64881300	3.79387100

**Np(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

Np	0.00000000	0.00000000	0.59634500
N	0.96957300	1.89130400	-1.29848800
N	-1.88344000	0.97439100	-1.27494800
N	-0.96957300	-1.89130400	-1.29848800
N	1.88344000	-0.97439100	-1.27494800
O	1.93443300	1.43447900	1.18098900
O	-1.47115800	1.84740300	1.28554200
O	-1.93443300	-1.43447900	1.18098900
O	1.47115800	-1.84740300	1.28554200
O	2.85881500	3.49798800	1.28000200
O	-3.53629100	2.76444300	1.35710900
O	-2.85881500	-3.49798800	1.28000200
O	3.53629100	-2.76444300	1.35710900
C	2.10824600	2.64994400	0.79734400
C	-2.67567600	2.03644200	0.86470700
C	-2.10824600	-2.64994400	0.79734400
C	2.67567600	-2.03644200	0.86470700
C	0.00000000	2.22659500	-2.35683000
C	-1.43549500	2.26694400	-1.83989200
C	-2.20122700	0.02203500	-2.35655300
C	-2.24891400	-1.42693800	-1.88111700
C	0.00000000	-2.22659500	-2.35683000
C	1.43549500	-2.26694400	-1.83989200
C	2.20122700	-0.02203500	-2.35655300
C	2.24891400	1.42693800	-1.88111700
C	1.24015600	3.05790100	-0.42040900
C	-3.05573700	1.21532500	-0.39467200
C	-1.24015600	-3.05790100	-0.42040900
C	3.05573700	-1.21532500	-0.39467200
H	0.09059200	1.47839900	-3.15081700
H	0.24149400	3.20119000	-2.81515200
H	-1.51597900	3.01248700	-1.04679300
H	-2.10635600	2.58809300	-2.65531700
H	-1.44053600	0.13016500	-3.13614900
H	-3.16863200	0.27374800	-2.82475500
H	-3.01399000	-1.53110600	-1.11056900
H	-2.54872600	-2.07205300	-2.72481100
H	-0.09059200	-1.47839900	-3.15081700
H	-0.24149400	-3.20119000	-2.81515200
H	1.51597900	-3.01248700	-1.04679300
H	2.10635600	-2.58809300	-2.65531700
H	1.44053600	-0.13016500	-3.13614900
H	3.16863200	-0.27374800	-2.82475500
H	3.01399000	1.53110600	-1.11056900
H	2.54872600	2.07205300	-2.72481100
H	1.73541200	3.86725800	-0.97668400
H	0.28945200	3.43052000	-0.02795200
H	-3.86132600	1.72845700	-0.93972200
H	-3.42546900	0.25055000	-0.03615100
H	-1.73541200	-3.86725800	-0.97668400
H	-0.28945200	-3.43052000	-0.02795200
H	3.86132600	-1.72845700	-0.93972200
H	3.42546900	-0.25055000	-0.03615100
O	0.00000000	0.00000000	3.17420400
H	0.54548700	-0.56966100	3.72745400
H	-0.54548700	0.56966100	3.72745400

**Pu(DOTA)(H<sub>2</sub>O)<sup>-</sup> SAP**

Pu	0.00000000	0.00000000	0.62355700
N	0.00000000	2.14007200	-1.17147400
N	2.14026300	-0.01351700	-1.17344600
N	0.00000000	-2.14007200	-1.17147400
N	-2.14026300	0.01351700	-1.17344600
O	-1.45137200	1.86611900	1.23395900
O	1.86255600	1.52029600	1.13374100
O	1.45137200	-1.86611900	1.23395900
O	-1.86255600	-1.52029600	1.13374100
O	3.98567200	2.26071700	0.90924500
O	2.19441800	-3.98613600	1.00682600
O	-3.98567200	-2.26071700	0.90924500
O	-2.19441800	3.98613600	1.00682600
C	-1.44066200	3.05148300	0.72799800
C	3.05412200	1.49320900	0.65341000
C	1.44066200	-3.05148300	0.72799800
C	-3.05412200	-1.49320900	0.65341000
C	1.34245500	2.30675500	-1.77822900
C	1.95127800	0.98484300	-2.24847900
C	2.32312400	-1.36255100	-1.75687100
C	1.01356200	-1.98483200	-2.23642900
C	-1.34245500	-2.30675500	-1.77822900
C	-1.95127800	-0.98484300	-2.24847900
C	-2.32312400	1.36255100	-1.75687100
C	-1.01356200	1.98483200	-2.23642900
C	-0.31566800	3.30756100	-0.30347200
C	3.31729000	0.33128400	-0.33224000
C	0.31566800	-3.30756100	-0.30347200
C	-3.31729000	-0.33128400	-0.33224000
H	0.58254100	3.51628300	0.28452600
H	-0.56613000	4.18981700	-0.90920600
H	4.19217700	0.56203200	-0.95672500
H	3.53844700	-0.54591600	0.28271800
H	0.56613000	-4.18981700	-0.90920600
H	-0.58254100	-3.51628300	0.28452600
H	-3.53844700	0.54591600	0.28271800
H	-4.19217700	-0.56203200	-0.95672500
H	1.98898500	2.77148200	-1.03520100
H	1.29666900	2.99136600	-2.64282400
H	2.91727200	1.20192200	-2.73614200
H	1.30734500	0.53778100	-3.01219500
H	3.02696400	-1.33071100	-2.60674200
H	2.77315200	-1.99400900	-0.99078300
H	1.23868700	-2.96475500	-2.69106800
H	0.57863500	-1.36527600	-3.02679000
H	-1.29666900	-2.99136600	-2.64282400
H	-1.98898500	-2.77148200	-1.03520100
H	-1.30734500	-0.53778100	-3.01219500
H	-2.91727200	-1.20192200	-2.73614200
H	-2.77315200	1.99400900	-0.99078300
H	-3.02696400	1.33071100	-2.60674200
H	-0.57863500	1.36527600	-3.02679000
H	-1.23868700	2.96475500	-2.69106800
O	0.00000000	0.00000000	3.19363300
H	0.45020500	-0.64580000	3.74885400
H	-0.45020500	0.64580000	3.74885400

**Pu(DOTA)(H<sub>2</sub>O)<sup>-</sup> TSAP**

Pu	0.00000000	0.00000000	0.58043200
N	0.96740400	1.88772700	-1.29565500
N	-1.87983800	0.97295700	-1.27174100
N	-0.96740400	-1.88772700	-1.29565500
N	1.87983800	-0.97295700	-1.27174100
O	1.92593600	1.41301300	1.17827200
O	-1.44787200	1.83865800	1.28380900
O	-1.92593600	-1.41301300	1.17827200
O	1.44787200	-1.83865800	1.28380900
O	2.85431300	3.47357200	1.29464300
O	-3.51146800	2.75654200	1.37650700
O	-2.85431300	-3.47357200	1.29464300
O	3.51146800	-2.75654200	1.37650700
C	2.10192600	2.63133200	0.80473300
C	-2.65621200	2.02922400	0.87410200
C	-2.10192600	-2.63133200	0.80473300
C	2.65621200	-2.02922400	0.87410200
C	0.00000000	2.22703900	-2.35428800
C	-1.43519700	2.26629800	-1.83727500
C	-2.20202600	0.02228700	-2.35325200
C	-2.24795800	-1.42655500	-1.87795800
C	0.00000000	-2.22703900	-2.35428800
C	1.43519700	-2.26629800	-1.83727500
C	2.20202600	-0.02228700	-2.35325200
C	2.24795800	1.42655500	-1.87795800
C	1.23608400	3.04949900	-0.41071800
C	-3.04705700	1.21297100	-0.38471900
C	-1.23608400	-3.04949900	-0.41071800
C	3.04705700	-1.21297100	-0.38471900
H	0.09057400	1.48058700	-3.15000600
H	0.24263200	3.20266100	-2.80977500
H	-1.51610700	3.01190300	-1.04434600
H	-2.10718900	2.58602600	-2.65224000
H	-1.44375800	0.13077700	-3.13524100
H	-3.17093600	0.27472600	-2.81785500
H	-3.01271500	-1.53156800	-1.10727400
H	-2.54671800	-2.07251500	-2.72128900
H	-0.09057400	-1.48058700	-3.15000600
H	-0.24263200	-3.20266100	-2.80977500
H	1.51610700	-3.01190300	-1.04434600
H	2.10718900	-2.58602600	-2.65224000
H	1.44375800	-0.13077700	-3.13524100
H	3.17093600	-0.27472600	-2.81785500
H	3.01271500	1.53156800	-1.10727400
H	2.54671800	2.07251500	-2.72128900
H	1.73284700	3.86189000	-0.96112300
H	0.28498400	3.41935700	-0.01691200
H	-3.85451200	1.72978800	-0.92342900
H	-3.41629700	0.24808700	-0.02635600
H	-1.73284700	-3.86189000	-0.96112300
H	-0.28498400	-3.41935700	-0.01691200
H	3.85451200	-1.72978800	-0.92342900
H	3.41629700	-0.24808700	-0.02635600
O	0.00000000	0.00000000	3.13528400
H	0.53950900	-0.57695600	3.68660300
H	-0.53950900	0.57695600	3.68660300

**U(DOTA)(H<sub>2</sub>O)- SAP**

U	0.00000000	0.00000000	0.66140900
N	0.00000000	2.14854500	-1.17717500
N	2.14754300	-0.01228200	-1.17945000
N	0.00000000	-2.14854500	-1.17717500
N	-2.14754300	0.01228200	-1.17945000
O	-1.46611600	1.91312300	1.22761100
O	1.90569500	1.53221400	1.13330300
O	1.46611600	-1.91312300	1.22761100
O	-1.90569500	-1.53221400	1.13330300
O	4.02764900	2.26481400	0.87094700
O	2.19949900	-4.03270000	0.96171100
O	-4.02764900	2.26481400	0.87094700
O	-2.19949900	4.03270000	0.96171100
C	-1.44735300	3.09069000	0.70406400
C	3.08926100	1.50007900	0.63304000
C	1.44735300	-3.09069000	0.70406400
C	-3.08926100	-1.50007900	0.63304000
C	1.34294800	2.30807100	-1.78524500
C	1.94934800	0.98440400	-2.25449100
C	2.32448500	-1.36275900	-1.76227400
C	1.01401100	-1.98511200	-2.24082600
C	-1.34294800	-2.30807100	-1.78524500
C	-1.94934800	-0.98440400	-2.25449100
C	-2.32448500	1.36275900	-1.76227400
C	-1.01401100	1.98511200	-2.24082600
C	-0.31224300	3.32633000	-0.32202400
C	3.33405300	0.33221800	-0.35147800
C	0.31224300	-3.32633000	-0.32202400
C	-3.33405300	-0.33221800	-0.35147800
H	0.58432000	3.53370600	0.26934900
H	-0.55067400	4.20507200	-0.93780300
H	4.20355600	0.55629500	-0.98595100
H	3.55890600	-0.54375600	0.26421200
H	0.55067400	-4.20507200	-0.93780300
H	-0.58432000	-3.53370600	0.26934900
H	-3.55890600	0.54375600	0.26421200
H	-4.20355600	-0.55629500	-0.98595100
H	1.99108600	2.77256800	-1.04343800
H	1.29899700	2.99110200	-2.65136300
H	2.91181100	1.20140500	-2.74929300
H	1.30113300	0.53515900	-3.01313600
H	3.02648300	-1.33305900	-2.61395100
H	2.77516300	-1.99428700	-0.99670700
H	1.24115900	-2.96248300	-2.70005900
H	0.57742400	-1.36359800	-3.02859400
H	-1.29899700	-2.99110200	-2.65136300
H	-1.99108600	-2.77256800	-1.04343800
H	-1.30113300	-0.53515900	-3.01313600
H	-2.91181100	-1.20140500	-2.74929300
H	-2.77516300	1.99428700	-0.99670700
H	-3.02648300	1.33305900	-2.61395100
H	-0.57742400	1.36359800	-3.02859400
H	-1.24115900	2.96248300	-2.70005900
O	0.00000000	0.00000000	3.28523500
H	0.43651400	-0.65233100	3.84417900
H	-0.43651400	0.65233100	3.84417900

**U(DOTA)(H<sub>2</sub>O)- TSAP**

U	0.00000000	0.00000000	0.61444000
N	-0.97168000	-1.89504600	-1.30194800
N	1.88726100	-0.97594400	-1.27911300
N	0.97168000	1.89504600	-1.30194800
N	-1.88726100	0.97594400	-1.27911300
O	-1.94265100	-1.45794600	1.18384900
O	1.49660500	-1.85619000	1.28598900
O	1.94265100	1.45794600	1.18384900
O	-1.49660500	1.85619000	1.28598900
O	-2.86418000	-3.52379100	1.26293500
O	3.56420300	-2.76979800	1.33719200
O	2.86418000	3.52379100	1.26293500
O	-3.56420300	2.76979800	1.33719200
C	-2.11483900	-2.66995400	0.78873900
C	2.69738500	-2.04286400	0.85418300
C	2.11483900	2.66995400	0.78873900
C	-2.69738500	2.04286400	0.85418300
C	0.00000000	-2.22605600	-2.36001200
C	1.43582500	-2.26759800	-1.84325300
C	2.19994000	-0.02171100	-2.36068700
C	2.24967500	1.42728200	-1.88473700
C	0.00000000	2.22605600	-2.36001200
C	-1.43582500	2.26759800	-1.84325300
C	-2.19994000	0.02171100	-2.36068700
C	-2.24967500	-1.42728200	-1.88473700
C	-1.24433800	-3.06682700	-0.43146600
C	3.06530700	-1.21790200	-0.40677300
C	1.24433800	3.06682700	-0.43146600
C	-3.06530700	1.21790200	-0.40677300
H	-0.09047000	-1.47592200	-3.15208600
H	-0.24024900	-3.19950800	-2.82147600
H	1.51582900	-3.01285500	-1.04979400
H	2.10530400	-2.59047800	-2.65924800
H	1.43644700	-0.12916000	-3.13754500
H	3.16558200	-0.27245100	-2.83313000
H	3.01490300	1.53026300	-1.11412400
H	2.55090000	2.07159800	-2.72863900
H	0.09047000	1.47592200	-3.15208600
H	0.24024900	3.19950800	-2.82147600
H	-1.51582900	3.01285500	-1.04979400
H	-2.10530400	2.59047800	-2.65924800
H	-1.43644700	0.12916000	-3.13754500
H	-3.16558200	0.27245100	-2.83313000
H	-3.01490300	-1.53026300	-1.11412400
H	-2.55090000	-2.07159800	-2.72863900
H	-1.73798900	-3.87282200	-0.99410000
H	-0.29413000	-3.44252000	-0.04042500
H	3.86827700	-1.72783500	-0.95875200
H	3.43655300	-0.25329500	-0.04896100
H	1.73798900	3.87282200	-0.99410000
H	0.29413000	3.44252000	-0.04042500
H	-3.86827700	1.72783500	-0.95875200
H	-3.43655300	0.25329500	-0.04896100
O	0.00000000	0.00000000	3.21814500
H	-0.55322600	0.56056300	3.77321600
H	0.55322600	-0.56056300	3.77321600