

Supporting Information

The Coordination Chemistry of Lanthanide and Actinide Metal ions with Hydroxypyridinone-based Decorporation Agents: Orbital and Density based Analyses

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Table S1: Spin contamination of Metal-HOPO complexes

Metal-HOPO complex		Spin contamination
Sm	f ⁵	0.010 (0.010)
Eu	f ⁶	0.018 (0.027)
Am	f ⁶	0.012 (0.012)
Cm	f ⁷	0.007 (0.007)
Pu	f ⁴	0.027 (0.027)
Th	f ⁰	-

Values in bracket are for L2 ligand

Table S2: Calculated HOMA and Bird Aromaticity Index for bare ligands and Metal-HOPO complexes.^a

	Sm	Eu	Am	Cm	Pu	Th	Ligand
HOMA	0.819 (0.817)	0.811 (0.810)	0.827 (0.825)	0.825 (0.824)	0.891 (0.891)	0.887 (0.886)	0.561 (0.558)
Bird Aromaticity Index	58.620 (58.510)	58.060 (57.950)	59.302 (59.282)	58.967 (58.895)	64.312 (64.422)	63.970 (64.040)	42.595 (42.360)

^aValues in bracket are for L2 ligand

Table S3: Effect of hydrogen bond [between secondary amide and O(-N) atom] on the structure and energetics of Pu⁴⁺-HOPO complexes.

Pu-HOPO complex	3,4,3-Li(1,2-HOPO) (L1)			3,3,3-Li(1,2-HOPO) (L2)		
	M-O(=C)	M-O(-N)	ΔG_{bind} (kcal mol ⁻¹)	M-O(=C)	M-O(-N)	ΔG_{bind} (kcal mol ⁻¹)
With NH...O	2.265-2.383 (2.313)	2.362-2.494 (2.423)	-149.11	2.275-2.380 (2.320)	2.367-2.452 (2.412)	-147.97
Without NH...O bond	2.349-2.378 (2.366)	2.331- 2.350 (2.342)	-143.77	2.296-2.322 (2.337)	2.352-2.467 (2.395)	-141.73

Table S4: Charge Decomposition and Extended Charge Decomposition Analysis of Metal-HOPO complexes.^a

Metal-L complex		CDA			ECDA
		d	b	r	
Sm	f ⁵	0.623 (0.593)	-0.057 (-0.056)	-0.628 (-0.617)	1.2042 (1.1885)
Eu	f ⁶	0.656 (0.662)	-0.047 (-0.047)	-0.548 (-0.556)	1.2172 (1.2625)
Am	f ⁶	0.670 (0.652)	-0.060 (-0.061)	-0.700 (-0.707)	1.474 (1.164)
Cm	f ⁷	0.710 (0.682)	-0.056 (-0.057)	-0.672 (-0.676)	1.345 (1.235)
Pu	f ⁴	0.747 (0.729)	-0.076 (-0.075)	-0.838 (-0.840)	2.162 (2.313)
Th	f ⁰	0.743 (0.732)	-0.083 (-0.081)	-1.025 (-1.025)	2.261 (2.498)

^aValues in bracket are for L2 ligand.

Table S5: Average values of QTAIM parameters for M-O bond critical points (BCP) in Metal-L1 and Metal-L2 complexes.^a

	Type of Bond	Density of all electrons $\rho(r)$	Lagrangian kinetic energy G(r)	Hamiltonian kinetic energy K(r)	Potential energy density V(r)	Energy density H(r)	Laplacian of electron density $\nabla^2\rho$	Ellipticity of electron density, ϵ	-V(r)/G(r)
Sm	M-O (-N)	0.044 (0.045)	0.044 (0.045)	0.004 (0.004)	-0.048 (-0.049)	-0.004 (-0.004)	0.162 (0.164)	0.088 (0.089)	1.090 (1.089)
	M-O (=C)	0.046 (0.045)	0.047 (0.046)	0.004 (0.004)	-0.051 (-0.050)	-0.004 (-0.004)	0.171 (0.169)	0.041 (0.037)	1.085 (1.087)
Eu	M-O (-N)	0.042 (0.043)	0.042 (0.044)	0.003 (0.004)	-0.045 (-0.047)	-0.003 (-0.004)	0.152 (0.159)	0.102 (0.088)	1.071 (1.068)
	M-O (=C)	0.046 (0.044)	0.047 (0.045)	0.005 (0.004)	-0.052 (-0.049)	-0.005 (-0.004)	0.169 (0.166)	0.058 (0.036)	1.106 (1.088)
Am	M-O (-N)	0.051 (0.053)	0.054 (0.056)	0.007 (0.007)	-0.061 (-0.063)	-0.007 (-0.007)	0.190 (0.194)	0.094 (0.096)	1.130 (1.125)
	M-O (=C)	0.052 (0.051)	0.055 (0.054)	0.006 (0.006)	-0.061 (-0.060)	-0.006 (-0.006)	0.193 (0.190)	0.053 (0.049)	1.109 (1.111)
Cm	M-O (-N)	0.049 (0.050)	0.051 (0.052)	0.006 (0.006)	-0.057 (-0.058)	-0.006 (-0.006)	0.182 (0.185)	0.099 (0.102)	1.118 (1.115)
	M-O (=C)	0.052 (0.052)	0.056 (0.055)	0.007 (0.006)	-0.062 (-0.061)	-0.007 (-0.006)	0.197 (0.195)	0.068 (0.080)	1.107 (1.109)
Pu	M-O (-N)	0.059 (0.051)	0.059 (0.054)	0.010 (0.007)	-0.069 (-0.061)	-0.010 (-0.007)	0.193 (0.190)	0.133 (0.094)	1.169 (1.129)
	M-O (=C)	0.073 (0.052)	0.079 (0.055)	0.018 (0.007)	-0.096 (-0.061)	-0.018 (-0.007)	0.245 (0.193)	0.106 (0.053)	1.215 (1.109)
Th	M-O (-N)	0.057 (0.058)	0.055 (0.056)	0.010 (0.011)	-0.065 (-0.066)	-0.010 (-0.011)	0.180 (0.183)	0.120 (0.122)	1.182 (1.178)
	M-O (=C)	0.062 (0.061)	0.061 (0.060)	0.012 (0.012)	-0.073 (-0.072)	-0.012 (-0.012)	0.194 (0.192)	0.086 (0.082)	1.197 (1.200)

^aValues in bracket are for L2 ligand.

Figure S1: DFT optimized structures of Metal-3,3,3-LI(1,2-HOPO) complexes

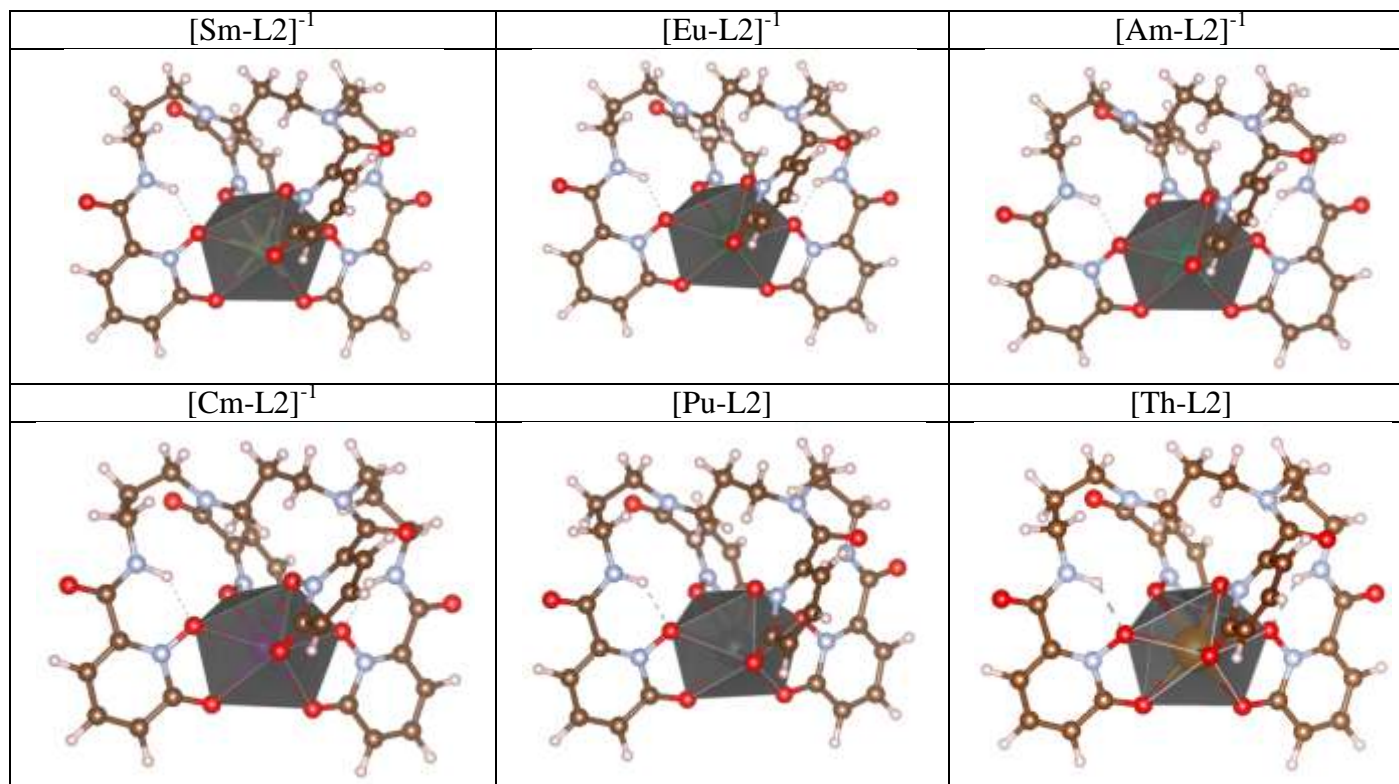


Figure S2: Molecular orbitals of L1 and L2 ligands. The iso-surface values for the contour plots were set to 0.035 e.bohr⁻³ in all cases.

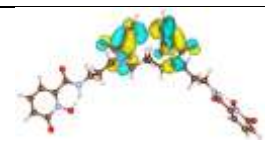

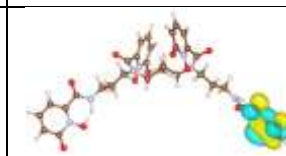
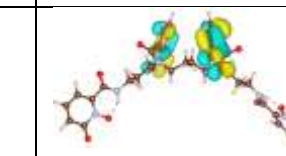
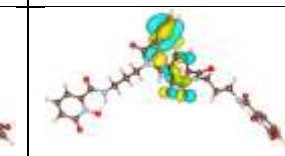
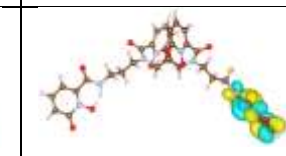
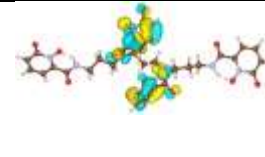
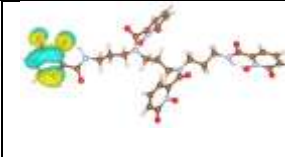
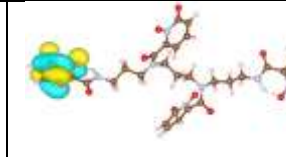
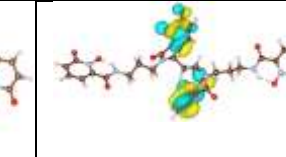
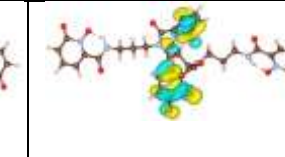
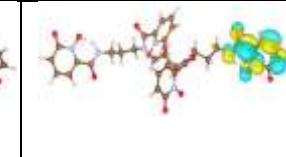
Metal	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO
3,4,3-LI(1,2-HOPO) (L1)						
3,3,3-LI(1,2-HOPO) (L2)						

Figure S3: (a) Molecular orbital energy level diagrams of Metal-L2 complexes (double-headed arrow in the figure represent the gap of HOMO and LUMO). (b) Molecular orbitals with > 20 % metal f/d character (double-headed arrow in the figure represent border between f and d-based orbital).

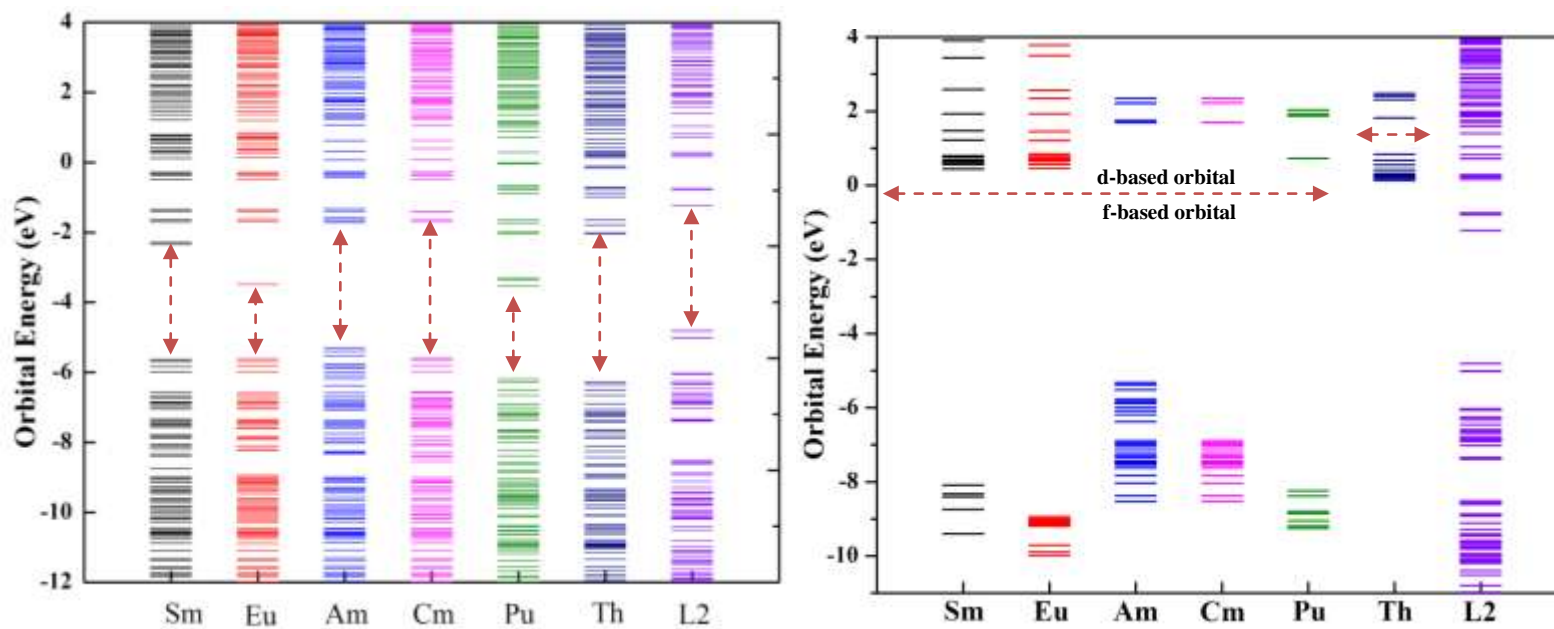
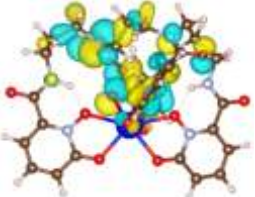
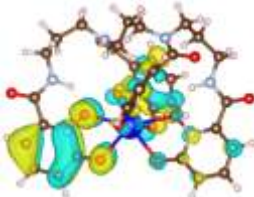
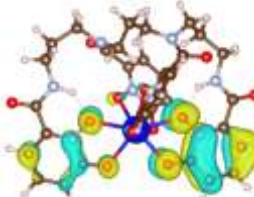
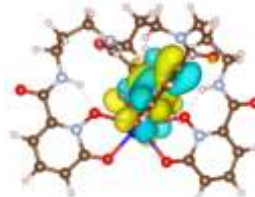
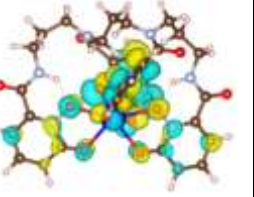
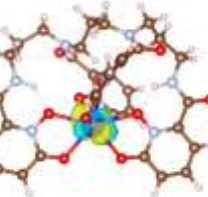
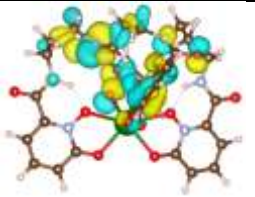
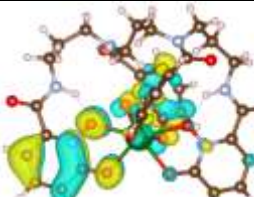
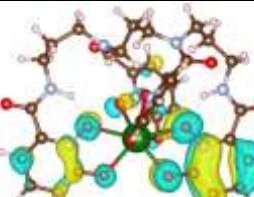
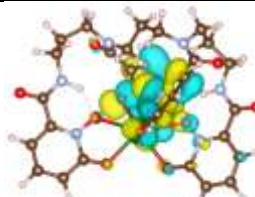
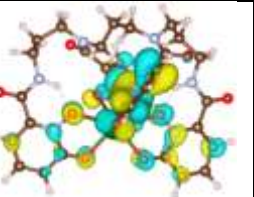
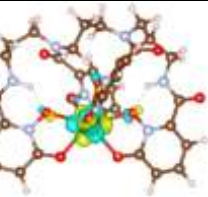
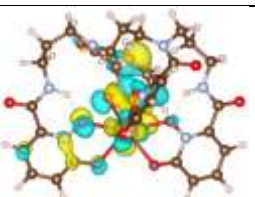
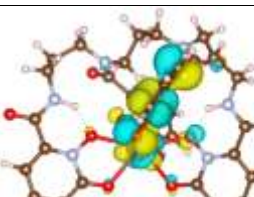
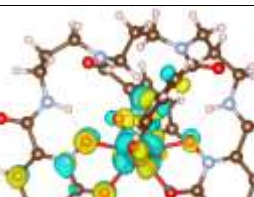
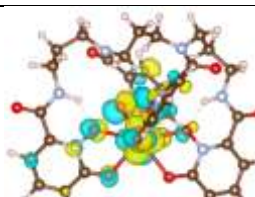
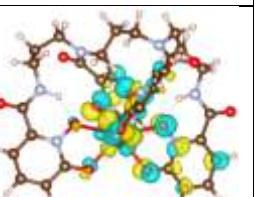
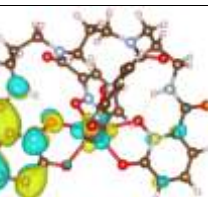


Figure S4: α Spin molecular orbitals of Metal-L2 complexes. The iso-surface values for the contour plots were set to 0.035 e.bohr⁻³ in all cases.

Metal	HOMO-4	HOMO-3	HOMO-2	HOMO-1	HOMO	LUMO
Sm						
d/f	0.2/0.2	3.6/0.7	1.0/2.1	0.8/1.5	0.5/96.8	0.3/94.8
Energy (eV)	-6.576	-5.994	-5.836	-5.682	-5.637	-2.344
Eu						
d/f	0.2/0.2	3.3/0.9	0.9/2.7	0.8/1.9	0.5/1.3	0.2/92.7
Energy (eV)	-6.584	-5.979	-5.822	-5.686	-5.621	-3.484
Am						
d/f	0.3/44.1	1.0/43.2	1.1/63.5	0.1/57.1	0.4/54.9	0.4/19.3
Energy (eV)	-5.833	-5.765	-5.516	-5.386	-5.320	-1.711

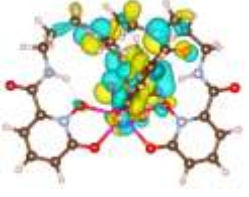
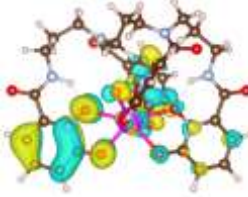
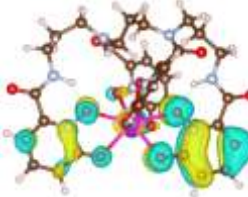
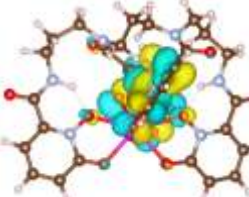
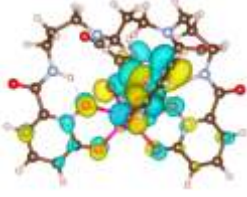
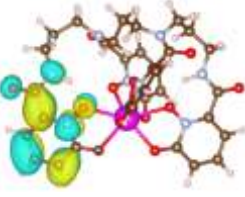
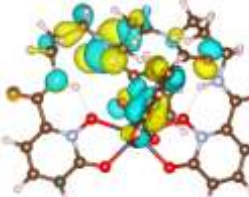
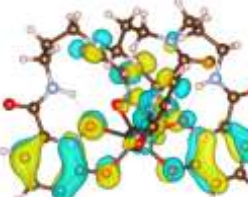
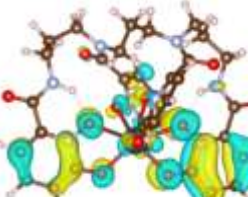
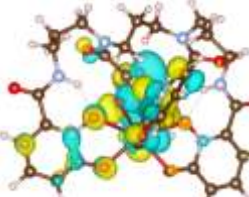
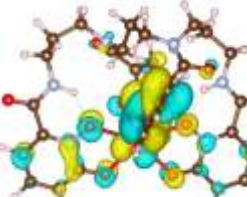
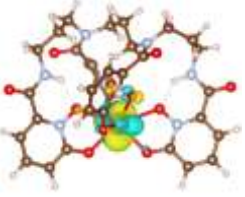
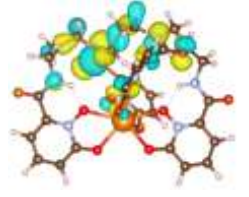

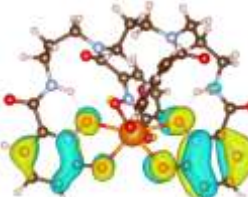
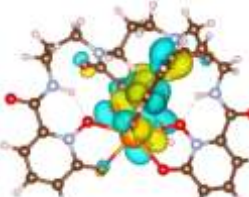
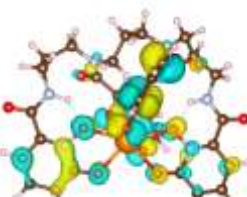
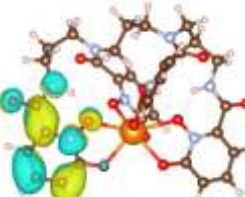
Cm						
d/f	0.5/14.1	0.3/3.3	0.5/6.5	0.6/4.2	0.5/2.9	0.1/0.1
Energy (eV)	-6.557	-5.970	-5.795	-5.652	-5.597	-1.704
Pu						
d/f	0.4/0.4	3.7/2.1	0.7/4.8	0.4/4.8	0.3/2.5	1.3/90.7
Energy (eV)	-6.918	-6.655	-6.522	-6.291	-6.188	-3.530
Th						
d/f	0.3/0	3.6/0.9	0.7/1.7	0.5/1.5	0.4/0.9	0.4/0.9
Energy (eV)	-6.888	-6.655	-6.518	-6.353	-6.276	-2.029

Figure S5: α Spin molecular orbitals of Metal-L2 complexes with maximum f orbital contribution. The iso-surface values for the contour plots were set to 0.035 e.bohr⁻³ in all cases.

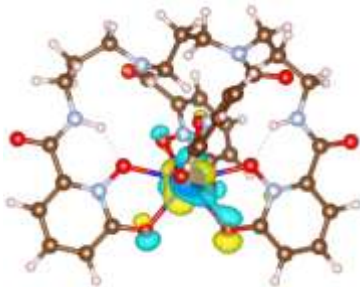
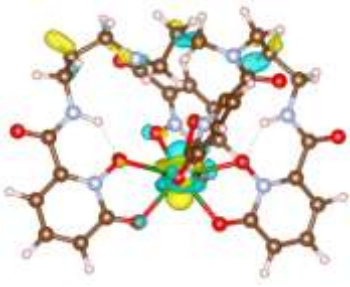
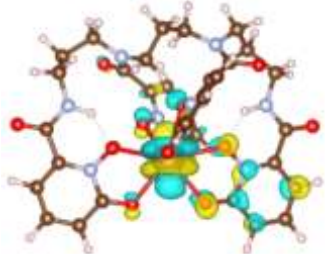
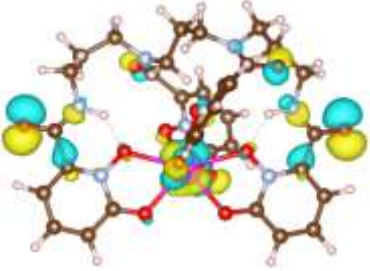
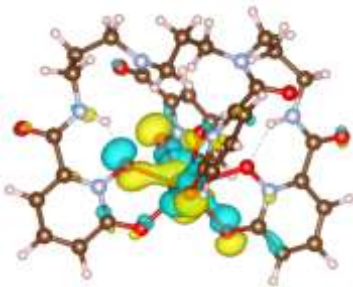
M-L2			
Sm (HOMO-26)		Eu (HOMO-38)	
d/f	0.2/85.9	d/f	0.0/78.3
Energy	-8.748	Energy	-9.705
Am (HOMO-7)		Cm (HOMO-19)	
d/f	0.5/76.4	d/f	0.1/45.8
Energy	-6.085	Energy	-7.457
Pu (HOMO-19)			
d/f	0.8/60.1		
Energy	-8.383		

Figure S6: Number of occupied orbitals with respect to contribution of *f*-character.

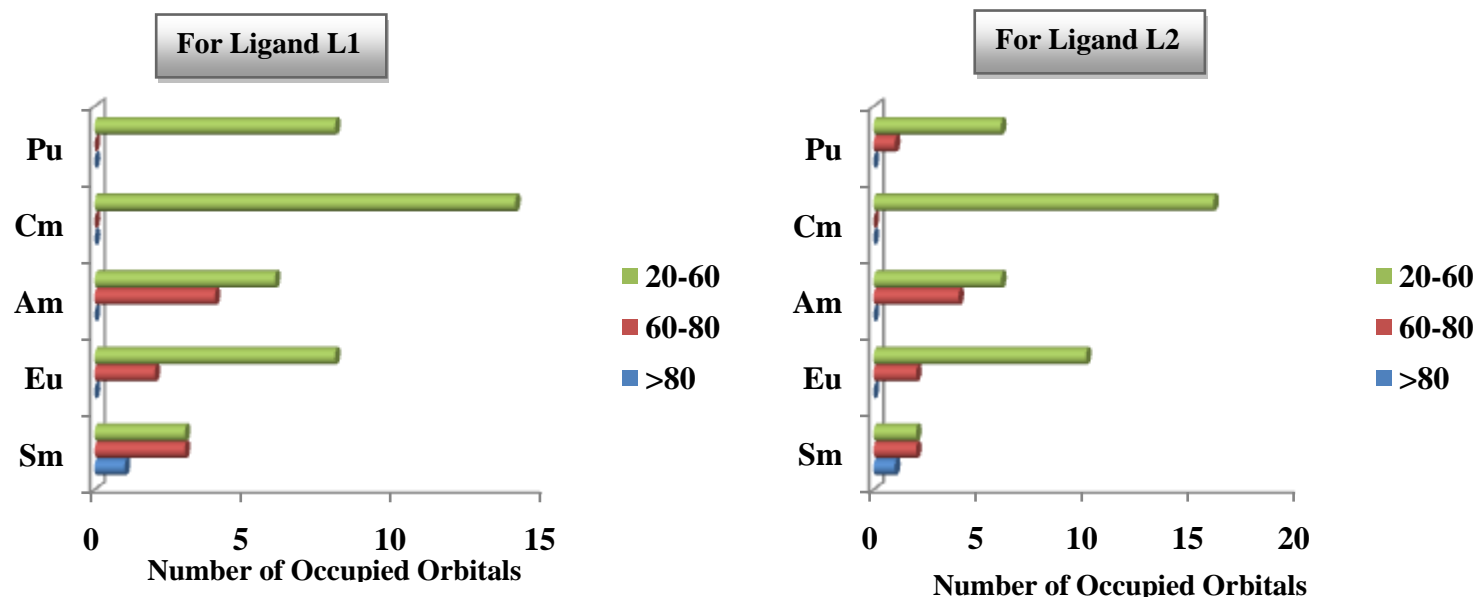
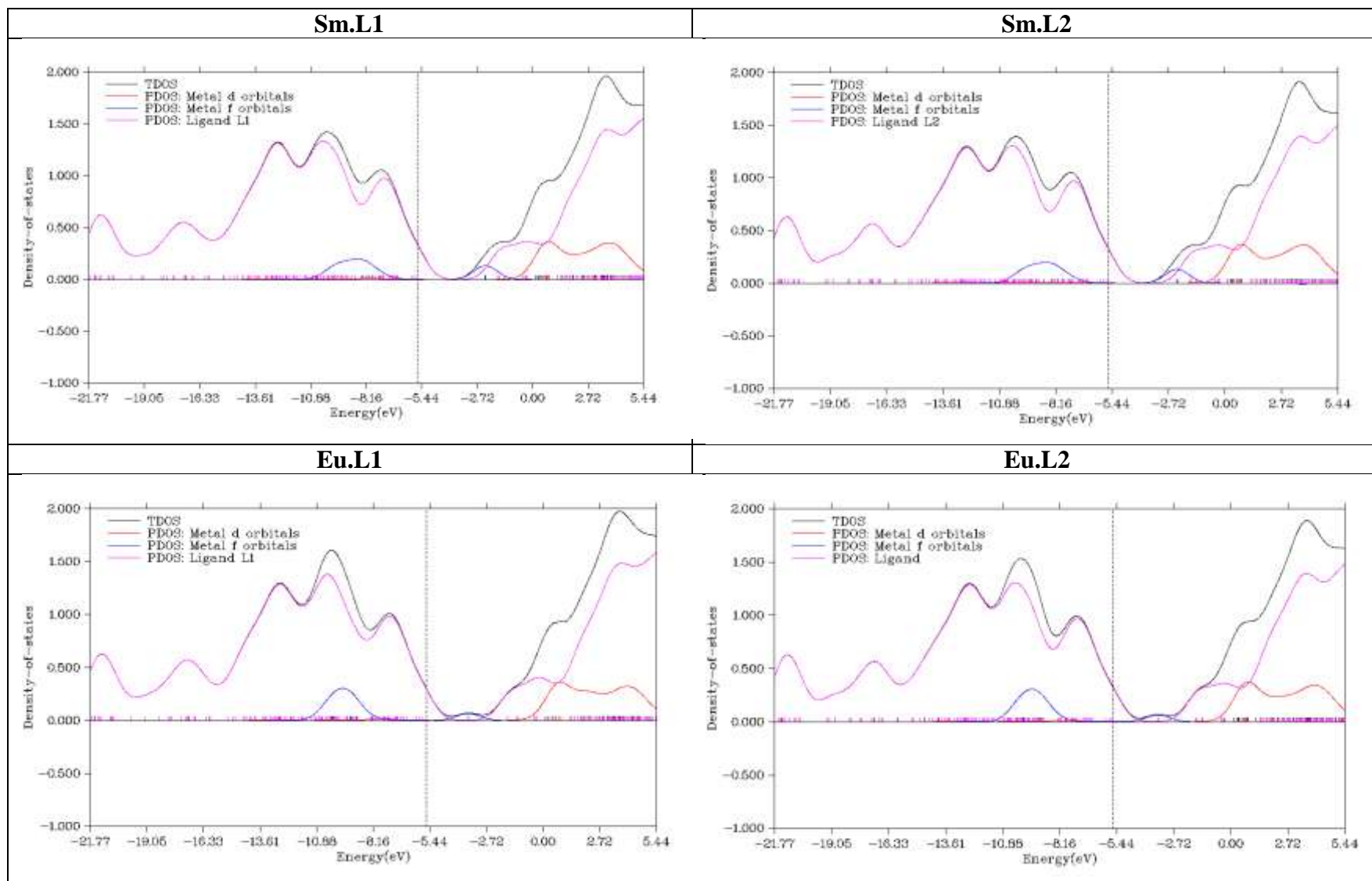
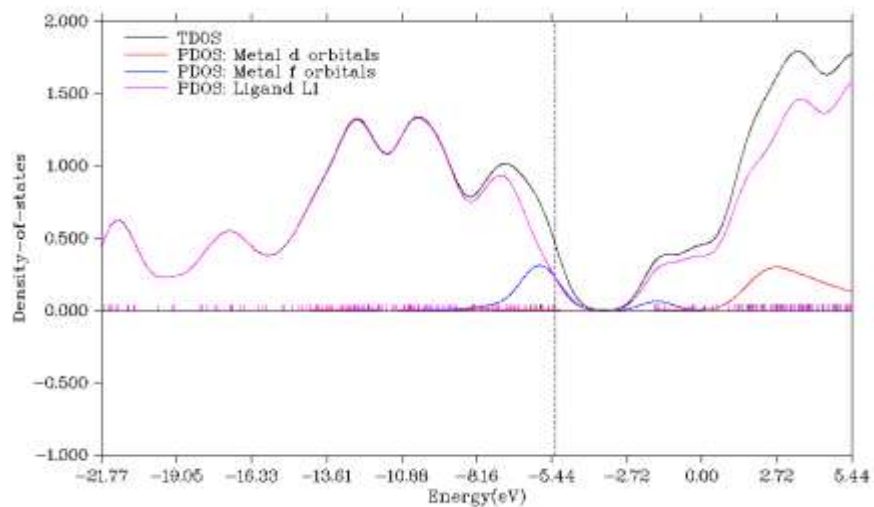
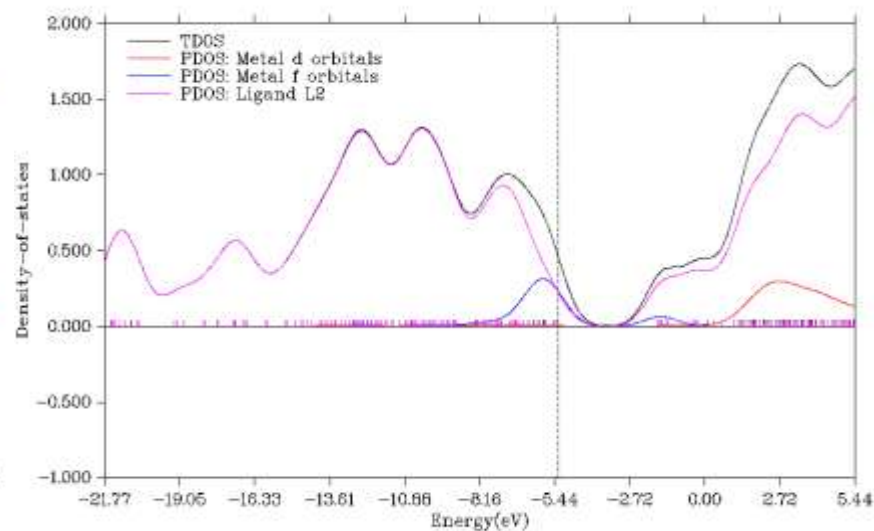
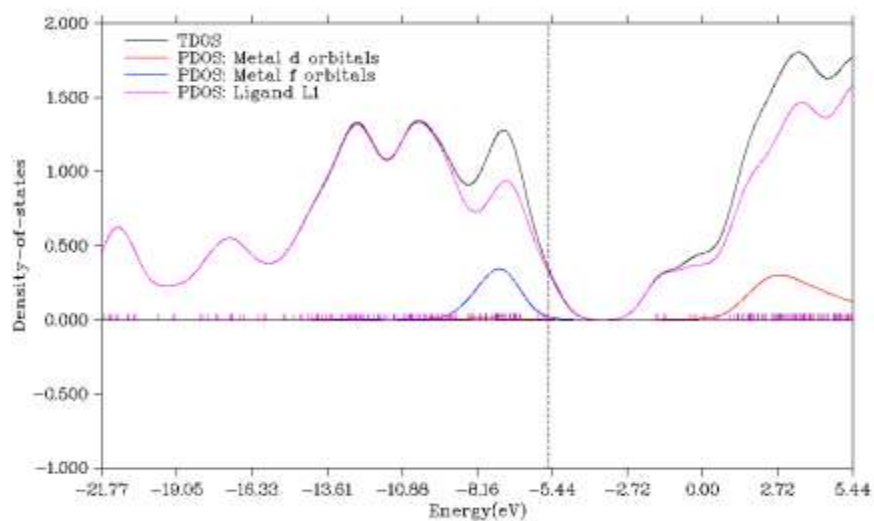
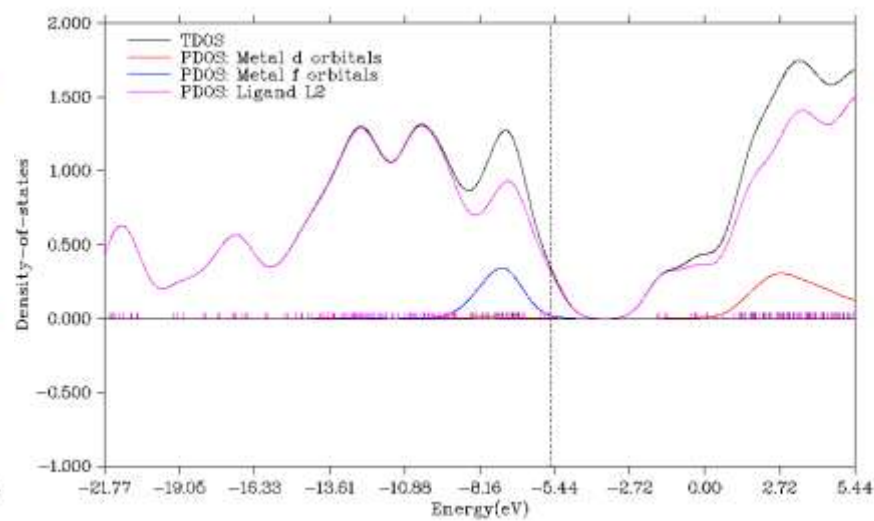


Figure S7: Total density-of-states (TDOS) and Projected density-of-states (PDOS) for interaction between metal (d and f) and ligands in the complexes.



Am.L1**Am.L2****Cm.L1****Cm.L2**

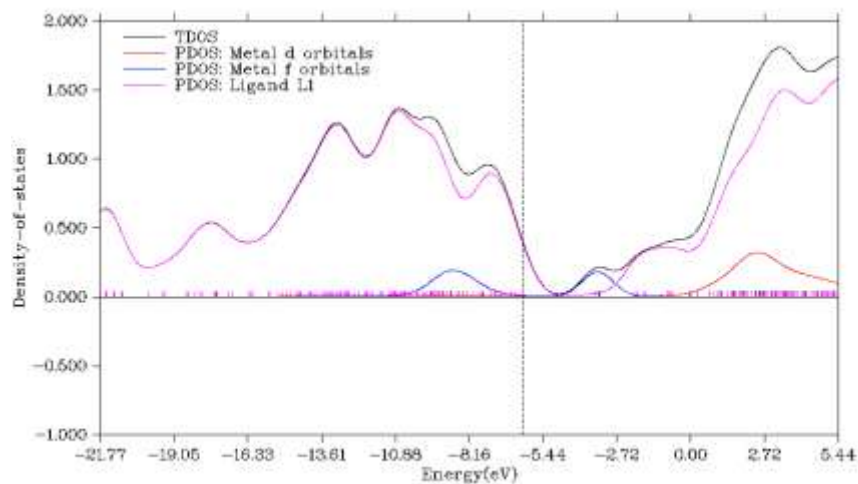
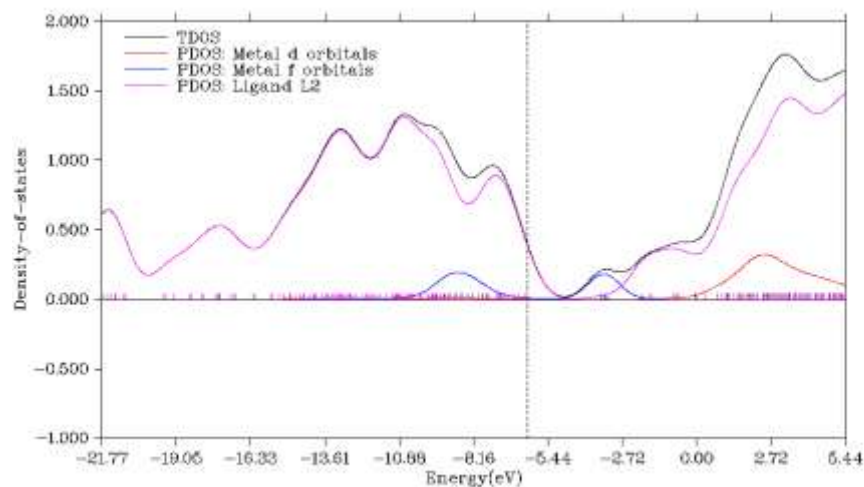
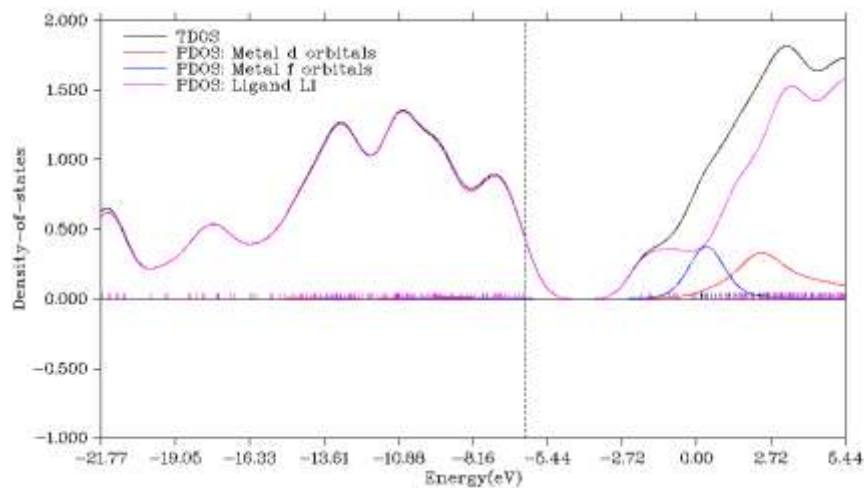
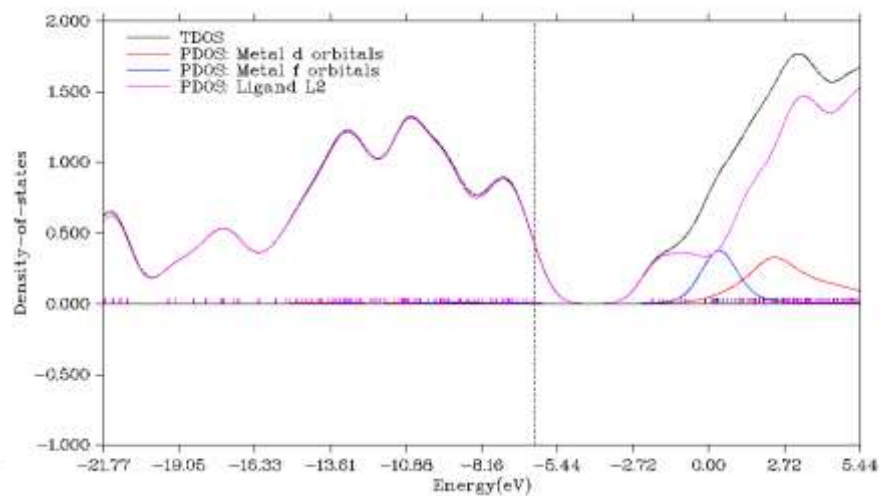
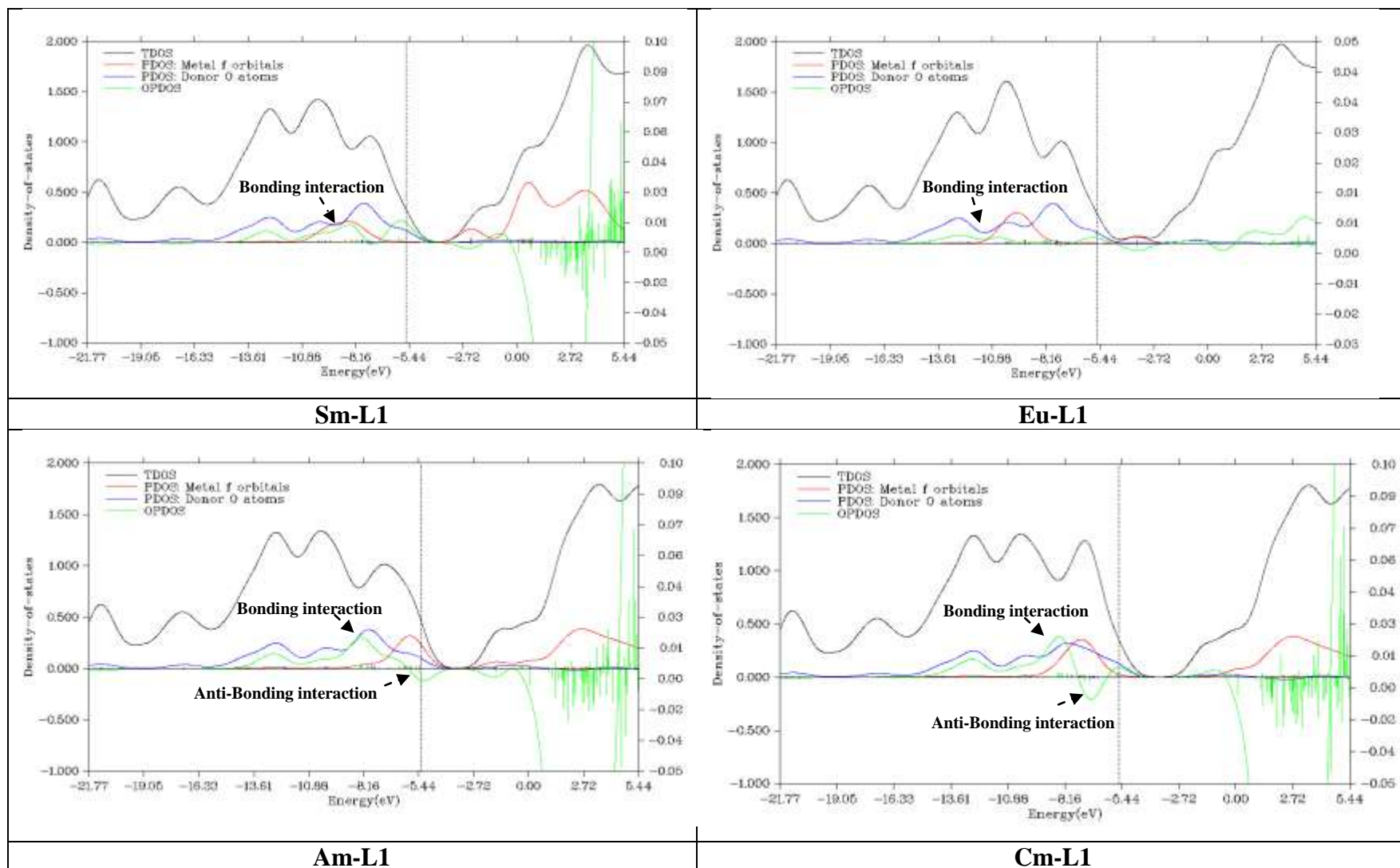
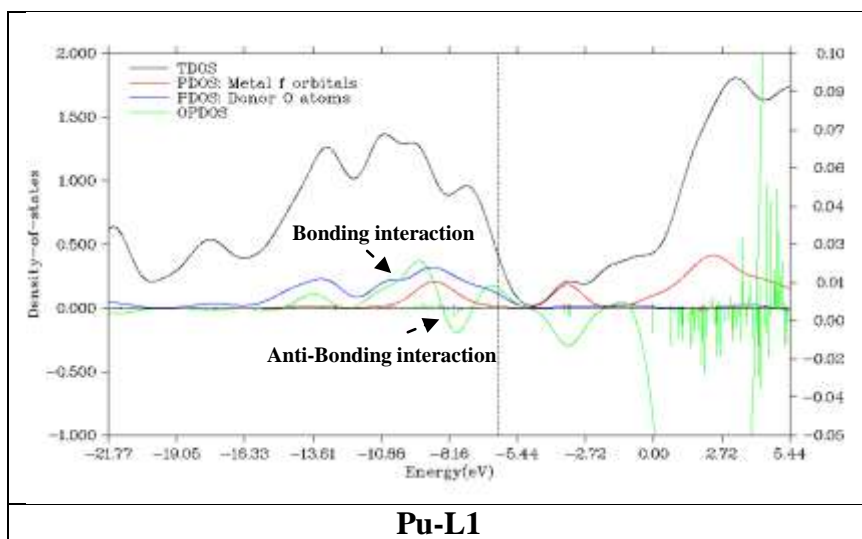
Pu.L1**Pu.L2****Th.L1****Th.L2**

Figure S8: Overlap population density-of-states (OPDOS) between metal f orbital and the donor O atoms. Positive value of OPDOS (Color code: green) indicate bonding interaction, whereas negative value indicates anti-bonding interaction.





Optimized structural coordinates of metal bound HOPO complexes:

[Sm-L1] ⁻¹			[Eu-L1] ⁻¹			[Am-L1] ⁻¹					
C	-1.1970311	1.8146090	-2.8430976	C	-1.1950876	1.7792190	-2.8732126	C	-1.2214606	1.8148725	-2.8182562
C	-0.6359616	2.2715888	-4.0350045	C	-0.6409934	2.2415822	-4.0663400	C	-0.6723802	2.2783923	-4.0129079
C	0.3911841	1.5446651	-4.6431746	C	0.3960238	1.5279315	-4.6733450	C	0.3603960	1.5638926	-4.6271415
C	0.8245574	0.3466823	-4.0918969	C	0.8519897	0.3415700	-4.1150352	C	0.8115131	0.3714702	-4.0781244
C	0.2607543	-0.1558808	-2.8941971	C	0.3003695	-0.1629193	-2.9123504	C	0.2586092	-0.1368258	-2.8780717
N	-0.7387560	0.6535327	-2.2886987	N	-0.7221524	0.6248823	-2.3182482	N	-0.7466400	0.6583012	-2.2691057
H	0.8437896	1.9122392	-5.5656659	H	0.8397504	1.8974976	-5.5994621	H	0.8035846	1.9375368	-5.5518425
H	-1.0473307	3.1754670	-4.4782797	H	-1.0652263	3.1387165	-4.5111770	H	-1.0967339	3.1775499	-4.4537426
H	1.6088776	-0.2520290	-4.5530050	H	1.6867410	-0.2452205	-4.5736201	H	1.6013701	-0.2175884	-4.5422865
O	-1.2523214	0.1806548	-1.1645454	O	-1.2368389	0.1432197	-1.1972118	O	-1.2519393	0.1778046	-1.1409113
O	0.5516170	-1.2356699	-2.3048569	O	0.6190036	-1.2284175	-2.3108544	O	0.5650629	-1.2142458	-2.2893838
C	-2.4335329	2.5115217	-2.3144888	C	-2.4349319	2.4690673	-2.3418556	C	-2.4594177	2.5007519	-2.2782943
O	-3.3302730	2.7568340	-3.1347468	O	-3.3369445	2.7043617	-3.15990128	O	-3.3657438	2.7367994	-3.0904827
N	-2.5388098	2.8994573	-1.0073330	N	-2.5328021	2.8702592	-1.0379534	N	-2.5539879	2.8905344	-0.9710883
C	-1.4726232	2.8329532	-0.0052499	C	-1.4680451	2.8014096	-0.0349742	C	-1.4748405	2.8371023	0.0186036
H	-1.9690825	2.7110870	0.9701327	H	-1.9635483	2.6552262	0.9376792	H	-1.9597255	2.7287807	1.0012904
H	-0.9011230	1.9104738	-0.1563928	H	-0.8864218	1.8899622	-0.1994846	H	-0.9042749	1.9132408	-0.1268185
C	4.3480575	-1.4661783	-1.1920382	C	4.3552951	-1.4532582	-1.1932602	C	4.3511428	-1.4862868	-1.1882974
C	5.1668734	-2.4180092	-1.7933437	C	5.1764150	-2.3929118	-1.8093155	C	5.1741773	-2.4464673	-1.7708310
C	4.7512739	-3.7491808	-1.8873053	C	4.7743611	-3.7285815	-1.9104615	C	4.7666035	-3.7815974	-1.8315188
C	3.5100888	-4.1280999	-1.4011350	C	3.5413407	-4.1237180	-1.4199094	C	3.5282478	-4.1562135	-1.3331544
C	2.6392362	-3.1869322	-0.7974407	C	2.6598953	-3.1929915	-0.8120477	C	2.6524328	-3.2050309	-0.7557164
N	3.1392820	-1.8631403	-0.6774287	N	3.1560566	-1.8648011	-0.6670951	N	3.1464496	-1.8795578	-0.6616714
H	5.4005747	-4.4893676	-2.3587896	H	5.4291611	-4.4580350	-2.3908022	H	5.4192680	-4.5294661	-2.2858934
H	6.1157082	-2.0611961	-2.1875859	H	6.1204739	-2.0244688	-2.2041780	H	6.1212032	-2.0938070	-2.1728006
H	3.1411401	-5.1502525	-1.4781601	H	3.1812926	-5.1485903	-1.5026096	H	3.1660469	-5.1824233	-1.3837173
O	2.3340926	-1.0218803	-0.0370020	O	2.3625267	-1.0448720	0.0065763	O	2.3391327	-1.0286356	-0.0312363
O	1.4778664	-3.4164207	-0.3530319	O	1.4948762	-3.4306531	-0.3922311	O	1.4842064	-3.4284734	-0.3190121
C	4.8336746	-0.0285187	-1.1854684	C	4.8342552	-0.0135010	-1.1754060	C	4.8328503	-0.0474364	-1.2054116
O	5.9357245	0.2380035	-1.6890788	O	5.9327629	0.2615775	-1.6819264	O	5.9311498	0.2148726	-1.7196104
N	4.0127752	0.9103778	-0.6560597	N	4.0104540	0.9170294	-0.6367374	N	4.0153529	0.8970700	-0.6798600
H	3.1557081	0.5506202	-0.2104902	H	3.1604834	0.5502450	-0.1844254	H	3.1609959	0.5411961	-0.2258850
C	4.4105814	2.3107650	-0.6503218	C	4.4014561	2.3195707	-0.6243304	C	4.4192731	2.2958241	-0.6811969
H	5.1449938	2.4901760	0.1528002	H	5.1262127	2.5011529	0.1869730	H	5.1589945	2.4740779	0.1174023
H	4.9337877	2.4883579	-1.6015048	H	4.9337647	2.4999116	-1.5697742	H	4.9392827	2.4677010	-1.6351622
C	2.0047249	0.8920492	3.2059542	C	1.9860905	0.8788035	3.2030582	C	2.0139877	0.9158140	3.1968469
C	2.4195664	0.6318550	4.5092325	C	2.3965678	0.6194228	4.5082642	C	2.4234428	0.6687026	4.5047254
C	1.9074158	-0.4756850	5.1932814	C	1.8915627	-0.4939337	5.1880401	C	1.8970404	-0.4231255	5.2020545
C	1.0638426	-1.3639353	4.5439949	C	1.0629708	-1.3907257	4.5312895	C	1.0438266	-1.3100745	4.5617940
C	0.6843884	-1.1650327	3.1920178	C	0.6991910	-1.1991932	3.1734024	C	0.6752993	-1.1256817	3.2064288
N	1.0872670	0.0694484	2.6082587	N	1.0804739	0.0486400	2.5975961	N	1.0906395	0.0943456	2.6084874
H	2.2073703	-0.6642852	6.2255603	H	2.1854447	-0.6798255	6.2226094	H	2.1918073	-0.6021095	6.2374642
H	3.1771560	1.2799883	4.9447943	H	3.1434048	1.2757154	4.9500636	H	3.1864311	1.3149759	4.9332936
H	0.6963678	-2.2705175	5.0233074	H	0.7027754	-2.3024792	5.0064440	H	0.6649359	-2.2057903	5.0523958
O	0.5809033	0.3455707	1.4144227	O	0.5627547	0.3304719	1.4115964	O	0.5881876	0.3604638	1.4080476
O	0.0276775	-1.9615110	2.4664681	O	0.0782400	-2.0106256	2.4361845	O	0.0193975	-1.9288700	2.4830375
C	2.7495536	1.9231442	2.3882518	C	2.7261172	1.9196407	2.3940626	C	2.7646391	1.9322400	2.3670116

O	3.9829276	1.8320055	2.3625914	O	3.9606373	1.8400897	2.3755990	O	3.9967982	1.8309987	2.3345157
N	2.0690238	2.9076142	1.7237828	N	2.0410527	2.9004155	1.7291737	N	2.0876381	2.9177762	1.6995431
C	2.8892262	3.8105630	0.9051084	C	2.8575078	3.8117433	0.9160099	C	2.9107590	3.8120579	0.8743012
H	2.3404990	4.7537317	0.8058509	H	2.2990677	4.7484802	0.8101548	H	2.3656916	4.7570181	0.7705429
H	3.8222770	4.0228051	1.4523283	H	3.7842757	4.0355563	1.4694824	H	3.8464373	4.0234718	1.4177201
C	-4.6759227	-1.9703761	0.6370326	C	-4.6670539	-1.9319480	0.6883255	C	-4.6805157	-1.9893592	0.5971162
C	-5.5567201	-3.0385159	0.4831320	C	-5.5613174	-2.9887372	0.5320274	C	-5.5659522	-3.0458889	0.3974760
C	-5.0741724	-4.3068944	0.1529340	C	-5.0978001	-4.2559049	0.1729269	C	-5.0866845	-4.3061968	0.0330388
C	-3.7160657	-4.5038386	-0.0523178	C	-3.7453665	-4.4607698	-0.0586174	C	-3.7273787	-4.5046400	-0.1612529
C	-2.7905009	-3.4405230	0.0801327	C	-2.8057954	-3.4106103	0.0800497	C	-2.7969210	-3.4531602	0.0205500
N	-3.3278367	-2.1928094	0.4922726	N	-3.3227633	-2.1616509	0.5202239	N	-3.3321820	-2.2157803	0.4631347
H	-5.7691707	-5.1404932	0.0370244	H	-5.8024738	-5.0809368	0.0544182	H	-5.7845481	-5.1317656	-0.1179266
H	-6.6139256	-2.8209576	0.6167314	H	-6.6140393	-2.7608570	0.6825214	H	-6.6234974	-2.8256489	0.5233468
H	-3.3055424	-5.4716462	-0.3384333	H	-3.3480267	-5.4266158	-0.3691302	H	-3.3187539	-5.4657060	-0.4716028
O	-2.4319684	-1.2426583	0.7034578	O	-2.4171165	-1.2216371	0.7360428	O	-2.4334691	-1.2762944	0.7219803
O	-1.5428689	-3.4963317	-0.1303553	O	-1.5618423	-3.4817757	-0.1412656	O	-1.5452094	-3.5145684	-0.1667487
C	-5.2663352	-0.5993329	0.8958925	C	-5.2442959	-0.5588324	0.9598546	C	-5.2671575	-0.6230396	0.8873040
O	-6.4755273	-0.4983499	1.1490368	O	-6.4505701	-0.4482719	1.2234520	O	-6.4779184	-0.5228216	1.1325923
N	-4.4254881	0.4630384	0.7746018	N	-4.3972622	0.4976493	0.8314241	N	-4.4217065	0.4388787	0.7996977
H	-3.4327069	0.2190882	0.6306979	H	-3.4070341	0.2457431	0.6806734	H	-3.4285802	0.1963757	0.6601651
C	-4.8996591	1.8230371	0.9618036	C	-4.8694140	1.8609749	0.9950765	C	-4.8949191	1.7962111	1.0070459
H	-4.2686214	2.3239896	1.7167928	H	-4.2296246	2.3801272	1.7300086	H	-4.2554935	2.2890496	1.7598737
H	-5.9065626	1.7240132	1.3893107	H	-5.8711796	1.7717095	1.4370063	H	-5.8974329	1.6932277	1.4439866
C	3.2395504	3.3018183	-0.5103612	C	3.2238664	3.3043821	-0.4958012	C	3.2551927	3.2951891	-0.5398549
H	2.3410343	2.8906214	-0.9963875	H	2.3322931	2.8873716	-0.9896667	H	2.3524024	2.8899296	-1.0229869
H	3.5128705	4.2002882	-1.0881930	H	3.4974689	4.2037924	-1.0721048	H	3.5341848	4.1903458	-1.1203159
C	0.7070983	3.2608514	2.1936021	C	0.6747513	3.2411813	2.1952445	C	0.7347835	3.2874524	2.1825300
H	0.1097827	2.3383740	2.1446971	H	0.0853734	2.13137972	2.1396440	H	0.13111013	2.3684434	2.1560391
H	0.7730951	3.5654872	3.2528213	H	0.7340296	3.5416110	3.2560526	H	0.8167066	3.6070846	3.2364064
C	-0.0379344	4.3761287	1.4520648	C	-0.0749204	4.3533047	1.4544968	C	-0.0158439	4.3957750	1.4359671
H	0.5536881	5.3053930	1.4449944	H	0.5052718	5.2898426	1.4623498	H	0.5794726	5.3222804	1.4075476
H	-0.9093435	4.5987332	2.0928109	H	-0.9566937	4.5596305	2.0864634	H	-0.8764011	4.6311169	2.0868096
C	-0.5662093	4.0798460	0.0400205	C	-0.5805471	4.0611315	0.0333785	C	-0.5667555	4.0836802	0.0358978
H	0.2583046	3.9622202	-0.6793966	H	0.2554612	3.9620019	-0.6753564	H	0.2464810	3.9572929	-0.6948219
H	-1.1407099	4.9595824	-0.2931664	H	-1.1629529	4.9353019	-0.3006082	H	-1.1456916	4.9603004	-0.2980076
C	-3.7795526	3.5936456	-0.6346067	C	-3.7647294	3.5802027	-0.6664307	C	-3.7943911	3.5807814	-0.5884150
H	-4.0591312	4.2539900	-1.4683978	H	-4.0521195	4.2171324	-1.5154436	H	-4.0819728	4.2419657	-1.4189984
H	-3.5484064	4.2245782	0.2382231	H	-3.5172249	4.2352087	0.1841955	H	-3.5578270	4.2108894	0.2834455
C	-4.9806054	2.6865050	-0.3196548	C	-4.9668915	2.6918859	-0.3065347	C	-4.9911097	2.6707264	-0.2658103
H	-5.1859470	2.0423196	-1.1856943	H	-5.1933129	2.0262440	-1.1510494	H	-5.2063761	2.0324240	-1.1336839
H	-5.8500799	3.3584478	-0.2195208	H	-5.8290615	3.3736761	-0.2087401	H	-5.8598104	3.3411789	-0.1511513
Sm	-0.0655941	-1.5875047	0.0590249	Eu	-0.0623132	-1.6021060	0.0332292	Am	-0.0651121	-1.5847330	0.0675034
[Cm-L1] ⁻¹				[Pu-L1]				[Th-L1]			
C	-1.2034959	1.7358688	-2.8941192	C	-1.2242573	1.5424509	-2.9536672	C	-1.1872582	1.7239343	-2.8301264
C	-0.6575855	2.1853500	-4.0953841	C	-0.7308712	1.9160688	-4.1990745	C	-0.6398274	2.1650228	-4.0305447
C	0.3598641	1.4525562	-4.7140589	C	0.2452677	1.1374328	-4.8323713	C	0.3604460	1.4170106	-4.6606046
C	0.8011933	0.2588162	-4.1616670	C	0.7036485	-0.0328484	-4.2462060	C	0.7839598	0.2103859	-4.1214823
C	0.2548238	-0.2369565	-2.9521860	C	0.2097671	-0.4350761	-2.9876303	C	0.2346029	-0.2615203	-2.9119262
N	-0.7392461	0.5766456	-2.3424185	N	-0.7322008	0.4053865	-2.3795433	N	-0.7235113	0.5581294	-2.2949539

H	0.7983473	1.8143010	-5.6457200	H	0.6355805	1.4459582	-5.8026612	H	0.7964837	1.7752687	-5.5936920
H	-1.0731251	3.0873294	-4.5386950	H	-1.1532487	2.8005908	-4.6699343	H	-1.0417646	3.0741248	-4.4717571
H	1.5793451	-0.3427123	-4.6296049	H	1.4465045	-0.6708434	-4.7217656	H	1.5420429	-0.4064959	-4.6008706
O	-1.2412305	0.1127596	-1.2052137	O	-1.1634272	-0.0085145	-1.1861200	O	-1.2143436	0.0886062	-1.1415850
O	0.5554441	-1.3104107	-2.3584207	O	0.5257577	-1.4852115	-2.3321498	O	0.5162004	-1.3490412	-2.3020921
C	-2.4288861	2.4458128	-2.3533960	C	-2.4256538	2.2890221	-2.3954235	C	-2.4231010	2.4196384	-2.2852518
O	-3.3326776	2.6912551	-3.1656595	O	-3.3583725	2.4666643	-3.1875061	O	-3.3356896	2.6073825	-3.0978662
N	-2.5151389	2.8511093	-1.0501251	N	-2.4511197	2.7921121	-1.1265711	N	-2.5019666	2.8533129	-0.9938130
C	-1.4492669	2.7736098	-0.0488859	C	-1.3800005	2.7208916	-0.1313471	C	-1.4235378	2.8174771	-0.0030568
H	-1.9407189	2.6016603	0.9217169	H	-1.8577253	2.4775179	0.8313769	H	-1.9048093	2.6620580	0.9754234
H	-0.8541897	1.8735119	-0.2315963	H	-0.7361244	1.8663689	-0.3522431	H	-0.8114053	1.9268207	-0.1705027
C	4.3627428	-1.4066705	-1.1979129	C	4.3557561	-1.2806955	-1.1992040	C	4.3448219	-1.4244766	-1.2288623
C	5.1960361	-2.3521718	-1.7905742	C	5.2388840	-2.2035264	-1.7478377	C	5.1824755	-2.3685154	-1.8117824
C	4.7956212	-3.6869989	-1.8804746	C	4.8914193	-3.5534665	-1.8501491	C	4.8037847	-3.7120326	-1.8768448
C	3.5555344	-4.0756632	-1.3967167	C	3.6466167	-3.9841720	-1.4190378	C	3.5725018	-4.1147768	-1.3817758
C	2.6742575	-3.1408292	-0.8041568	C	2.7332909	-3.0651505	-0.8684615	C	2.6990503	-3.1749710	-0.8025729
N	3.1525440	-1.8118846	-0.6929584	N	3.1422328	-1.7344503	-0.7468602	N	3.1501254	-1.8535878	-0.7107900
H	5.4543475	-4.4238533	-2.3439129	H	5.5963509	-4.2661637	-2.2793261	H	5.4726255	-4.4434996	-2.3316527
H	6.1451448	-1.9875793	-2.1767995	H	6.1937233	-1.8099101	-2.0897486	H	6.1221452	-1.9969800	-2.2145269
C	3.1986185	-5.1025881	-1.4668887	C	3.3251153	-5.0216503	-1.4934136	H	3.2290835	-5.1466228	-1.2384381
O	2.3320380	-0.9710573	-0.0660354	O	2.2606975	-0.9300282	-0.1344665	O	2.3104721	-1.0213909	-0.0744803
O	1.5110753	-3.3884695	-0.3613001	O	1.5491675	-3.3330876	-0.4529664	O	1.5221483	-3.4121461	-0.3441937
C	4.8406898	0.0335556	-1.1803772	C	4.8012596	0.1725143	-1.1579817	C	4.8020174	0.0276236	-1.2478890
O	5.9455392	0.3092348	-1.6731312	O	5.9116581	0.4593809	-0.8686210	O	5.8765549	0.2961022	-1.7959901
N	4.0122594	0.9636138	-0.6471612	N	3.9494588	1.0898609	-0.6404623	N	3.9933721	0.9600253	-0.6879420
H	3.1524634	0.5919986	-0.2146387	H	3.0926298	0.7301487	-0.2091945	H	3.1723512	0.6095104	-0.1861045
C	4.4077220	2.3640033	-0.6148878	C	4.3611565	2.4865902	-0.5507839	C	4.3993320	2.3606073	-0.6608658
H	5.1366667	2.5313037	0.1960591	H	5.1011396	2.6052441	0.2575819	H	5.1466696	2.5182863	0.1340086
H	4.9371325	2.5596281	-1.5593297	H	4.8824642	2.7188720	-1.4904396	H	4.9089318	2.5514511	-1.6156766
C	1.9950138	0.8539545	3.2119851	C	1.8592819	0.7613053	3.1835043	C	1.9325306	0.8955815	3.2137168
C	2.4322984	0.5835414	4.5070472	C	2.2575013	0.4700300	4.4850372	C	2.3299148	0.6630767	4.5249815
C	1.9544956	-0.5443059	5.1802109	C	1.8313341	-0.7097402	5.1010863	C	1.8624761	-0.4671049	5.2046302
C	1.1252885	-1.4429592	4.5252952	C	1.0980747	-1.6423521	4.3794106	C	1.0817126	-1.4049543	4.5444305
C	0.7240926	-1.2314313	3.1829655	C	0.7422486	-1.3831184	3.0426388	C	0.7159518	-1.2087107	3.1973006
N	1.0833591	0.0240137	2.6165349	N	1.0219438	-0.1069638	2.5384748	N	1.0633885	0.0234441	2.6215326
H	2.2717755	-0.7429022	6.2053709	H	2.1231331	-0.9239753	6.1295312	H	2.1557588	-0.6376651	6.2408430
H	3.1839195	1.2399827	4.9403054	H	2.9488834	1.1525156	4.9746545	H	3.0474698	1.3452641	4.9757826
H	0.7880700	-2.3672529	4.9931255	H	0.8162557	-2.6094347	4.7924858	H	0.7616073	-2.3322276	5.0165613
O	0.5503554	0.3111584	1.4346666	O	0.4855878	0.1835996	1.3504202	O	0.5541131	0.2678915	1.4057582
O	0.0810416	-2.0346732	2.4506728	O	0.1937037	-2.2052721	2.2248076	O	0.1016823	-2.0345241	2.4378613
C	2.7250401	1.9030156	2.4035291	C	2.5989949	1.8310533	2.4027723	C	2.6820431	1.8978395	2.3567514
O	3.9598521	1.8312005	2.3840027	O	3.8271082	1.7054524	2.3660721	O	3.9003074	1.7171607	2.2686011
N	2.0361790	2.8853495	1.7427580	N	1.9392212	2.8587034	1.7928750	N	2.0323604	2.9220666	1.7332229
C	2.8558953	3.8179208	0.9562479	C	2.7963131	3.8346664	1.0961915	C	2.8859324	3.8255977	0.9412062
H	2.2956349	4.7558877	0.8708930	H	2.2538547	4.7860033	1.0746815	H	2.3606806	4.7839946	0.8686549
H	3.7787366	4.0293380	1.5209519	H	3.7064294	3.9840895	1.6981394	H	3.8186092	3.9992528	1.5013036
C	-4.6935647	-1.9049568	0.6795608	C	-4.5904670	-1.7600690	0.8000035	C	-4.6726051	-1.9400286	0.6459302
C	-5.5908496	-2.9566161	0.5095431	C	-5.5239557	-2.7764930	0.6262487	C	-5.5774595	-2.9730681	0.4299363
C	-5.1289448	-4.2282984	0.1656108	C	-5.1286876	-4.0456994	0.1992424	C	-5.1317706	-4.2354791	0.0297329
C	-3.7732614	-4.4417271	-0.0384705	C	-3.7927111	-4.2906109	-0.0841262	C	-3.7794599	-4.4608285	-0.1840219
C	-2.8343865	-3.3949105	0.1119508	C	-2.8368684	-3.2761288	0.0907543	C	-2.8461245	-3.4286065	0.0239418

N	-3.3471248	-2.1440626	0.5390590	N	-3.2623989	-2.0414245	0.5885958	N	-3.3353221	-2.2037571	0.4921328
H	-5.8359738	-5.0495607	0.0363872	H	-5.8697499	-4.8339976	0.0661794	H	-5.8500894	-5.0390070	-0.1351998
H	-6.6446219	-2.7215904	0.6400463	H	-6.5620457	-2.5150258	0.8202122	H	-6.6292401	-2.7351830	-0.5728568
H	-3.3751550	-5.4113241	-0.3354998	H	-3.4360719	-5.2521167	-0.4496846	H	-3.3923787	-5.4200015	-0.5239571
O	-2.4391616	-1.2089459	0.7726359	O	-2.2993132	-1.1589699	0.8380919	O	-2.3975521	-1.2956400	0.7706487
O	-1.5846843	-3.4762619	-0.0973034	O	-1.5773376	-3.3748504	-0.1617181	O	-1.5771541	-3.4952953	-0.1729832
C	-5.2679100	-0.5276349	0.9382670	C	-5.1155077	-0.3751662	1.1245558	C	-5.2304274	-0.5633735	0.9657710
O	-6.4788856	-0.4102939	1.1749463	O	-6.2997695	-0.2521373	1.4504126	O	-6.4261825	-0.4647020	1.2545449
N	-4.4112185	0.5226375	0.8297147	N	-4.2588221	0.6652422	0.9470310	N	-4.3846613	0.4941353	0.8374706
H	-3.4202187	0.2635344	0.6988804	H	-3.2834751	0.4175083	0.7458263	H	-3.4003574	0.2680167	0.6640796
C	-4.8775331	1.8892295	0.9828660	C	-4.7224951	2.0395375	1.0655623	C	-4.8532963	1.8598688	1.0242133
H	-4.2436472	2.4067655	1.7238959	H	-4.0587254	2.5898548	1.7534749	H	-4.2134335	2.3612705	1.7701975
H	-5.8855836	1.8077859	1.4115200	H	-5.7078232	1.9752700	1.5449035	H	-5.8545978	1.7669089	1.4640963
C	3.2331069	3.3491672	-0.4659731	C	3.2014160	3.4741937	-0.3485046	C	3.2359462	3.3542159	-0.4873868
H	2.3439635	2.9502515	-0.9789441	H	2.3206061	3.1371578	-0.9175475	H	2.3348991	2.9694306	-0.9906882
H	3.5142555	4.2643056	-1.0133826	H	3.5144365	4.4238477	-0.8115439	H	3.5198475	4.2672729	-1.0349008
C	0.6699080	3.2204158	2.2121504	C	0.5716806	3.2012084	2.2518890	C	0.6963569	3.3264096	2.2351257
H	0.0859508	2.2893033	2.1602515	H	-0.0145196	2.2717610	2.2133096	H	0.0805898	2.4161584	2.2611752
H	0.7290508	3.5244504	3.2722729	H	0.6204637	3.5203787	3.3076005	H	0.8028858	3.6833196	3.2742400
C	-0.0867673	4.3273040	1.4703219	C	-0.1713267	4.2993599	1.4833742	C	-0.0540933	4.4172252	1.4629569
H	0.4818532	5.2708036	1.4891483	H	0.3746742	5.2530801	1.5452617	H	0.5307905	5.3495074	1.4434436
H	-0.9767941	4.5187771	2.0954016	H	-1.0971092	4.4645426	2.0614044	H	-0.9306431	4.6465046	2.0934027
C	-0.5758338	4.0415603	0.0420000	C	-0.5671163	4.0216405	0.0253155	C	-0.5630992	4.0957550	0.0493087
H	0.2674703	3.9586209	-0.6599963	H	0.3175138	3.9854331	-0.6271509	H	0.2700494	4.0078147	-0.6642290
H	-1.1644680	4.9126730	-0.2888257	H	-1.1658328	4.8761471	-0.3257858	H	-1.1641161	4.9542539	-0.2893290
C	-3.7344277	3.5822902	-0.6770712	C	-3.6390073	3.5844909	-0.7636039	C	-3.7319590	3.5775957	-0.6266394
H	-4.0081279	4.2298629	-1.5225545	H	-3.9345615	4.1629885	-1.6497750	H	-4.0107889	4.2161389	-1.4768698
H	-3.4754246	4.2273974	0.1775285	H	-3.3231745	4.2950732	0.0158267	H	-3.4769983	4.2327880	0.2204416
C	-4.9540316	2.7168060	-0.3214971	C	-4.8609074	2.7937801	-0.2745852	C	-4.9447564	2.7056117	-0.2660228
H	-5.1901424	2.0536987	-1.1652777	H	-5.1881148	2.0956881	-1.0576077	H	-5.1959122	2.0560222	-1.1157531
H	-5.8036564	3.4146238	-0.2275207	H	-5.6712158	3.5327856	-0.1610387	H	-5.7910910	3.4024992	-0.1508333
Cm	-0.0702230	-1.6170726	0.0423765	Pu	-0.0302216	-1.7261849	-0.0270250	Th	-0.0594432	-1.6695473	0.0600592
[Sm-L2]⁻¹				[Eu-L2]⁻¹				[Am-L2]⁻¹			
Sm	-0.1704702	-1.5926228	0.0314542	C	-0.7596206	2.0015399	-2.7477033	Am	-0.1496607	-1.5875887	0.0190280
C	-0.7450938	1.9995736	-2.7109600	C	-0.0565803	2.4864205	-3.8495163	C	-0.8614533	2.0273271	-2.6772950
C	-0.0490098	2.4566932	-3.8288862	C	0.9075717	1.6826877	-4.4648192	C	-0.2041529	2.5146438	-3.8056620
C	0.8835335	1.6238124	-4.4544519	C	1.1504023	0.3964221	-4.0014952	C	0.7437897	1.7180100	-4.4550687
C	1.0995291	0.3343598	-3.9868932	C	0.4496642	-0.1284779	-2.8883678	C	1.0148659	0.4350487	-3.9989761
C	0.4015491	-0.1660009	-2.8605555	N	-0.5147176	0.7344107	-2.2990096	C	0.3601767	-0.0917947	-2.8594733
N	-0.5225984	0.7302204	-2.2543840	H	1.4705297	2.0668782	-5.3172034	N	-0.5852562	0.7639467	-2.2346446
H	1.4399599	1.9866063	-5.3204348	H	-0.3040074	3.4802388	-4.2158641	H	1.2703091	2.1050264	-5.3291120
H	-0.2804898	3.4519013	-4.2017931	H	1.8956576	-0.2514031	-4.4612896	H	-0.4742272	3.5049120	-4.1656818
H	1.8169424	-0.3373199	-4.4563792	O	-1.1897118	0.2288388	-1.2789635	H	1.7467360	-0.2086723	-4.4851203
O	-1.1896899	0.2491139	-1.2190244	O	0.5923514	-1.2678360	-2.3586050	O	-1.2136487	0.2536354	-1.1846582
O	0.5123804	-1.3103113	-2.3345210	C	-1.9050493	2.8208264	-2.1900028	O	0.5298590	-1.2308039	-2.3346273
C	-1.8717678	2.8436310	-2.1520693	C	-2.7137605	3.2911542	-3.0027995	C	-1.9948253	2.8371732	-2.0820486
O	-2.6683917	3.3332514	-2.9658497	N	-0.2015548	3.0652685	-0.8472470	O	-2.8319200	3.3043734	-2.8674057
N	-1.9894910	3.0775808	-0.8083056	C	-1.0419989	2.6510752	0.1640148	N	-2.0672642	3.0703034	-0.7356733
C	-1.0167793	2.6653301	0.2044442	C	4.2949636	-1.4708559	-1.0479373	C	-1.0423235	2.6945217	0.2382197

C	4.2773101	-1.4659865	-1.0930447	C	5.1487960	-2.4245451	-1.5944967	C	4.3279011	-1.5629505	-1.0246934
C	5.1137147	-2.4217604	-1.6631732	C	4.7529386	-3.7627843	-1.6807570	C	5.1746296	-2.5418354	-1.5381139
C	4.7050545	-3.7556727	-1.7509741	C	3.4950017	-4.1466404	-1.2469696	C	4.7567869	-3.8739637	-1.5975187
C	3.4552029	-4.1344407	-1.2879944	C	2.5814268	-3.2023238	-0.7125068	C	3.4866070	-4.2278275	-1.1682638
C	2.5668482	-3.1910569	-0.7138859	N	3.0686828	-1.8701283	-0.5779206	C	2.5867059	-3.2579382	-0.6626813
N	3.0564601	-1.8606933	-0.6056694	H	5.4333852	-4.5040514	-2.1039254	N	3.0887135	-1.9351019	-0.5678413
H	5.3683908	-4.4985900	-2.1980758	H	6.1130110	-2.0652201	-1.9468527	H	5.4289063	-4.6368803	-1.9950555
H	6.0716573	-2.0677154	-2.0370505	H	3.1415774	-5.1745317	-1.3201491	H	6.1488804	-2.2076086	-1.8872763
H	3.0924927	-5.1591663	-1.3609677	O	2.2416516	-1.0326731	0.0324557	H	3.1195153	-5.2522960	-1.2195453
O	2.2311678	-1.0122954	-0.0024188	O	1.3959152	-3.4325025	-0.3474257	O	2.2554986	-1.0637774	-0.0027785
O	1.4001488	-3.4230854	-0.2857859	C	4.7746986	-0.0316867	-1.0335524	O	1.3933319	-3.4608831	-0.2888896
C	4.7614124	-0.0275560	-1.0798818	O	5.8921689	0.2344144	-1.5019589	C	4.8243946	-0.1289518	-1.0310787
O	5.8718567	0.2392155	-1.5643268	N	3.9373611	0.9093833	-0.5335283	O	5.9489182	0.1173881	-1.4937585
N	3.9338340	0.9114159	-0.5590597	H	3.0673192	0.5520876	-0.1126808	N	3.9933480	0.8279380	-0.5493396
H	3.0689893	0.5506264	-0.1289312	C	4.3456216	2.3066469	-0.5157787	H	3.1121302	0.4840134	-0.1387621
C	4.3388680	2.3092057	-0.5374229	H	5.0487795	2.4817390	0.3166166	C	4.4075595	2.2230947	-0.5450038
H	5.0530374	2.4815117	0.2861955	H	4.9115497	2.4748063	-1.4436920	H	5.0901958	2.4104506	0.3015258
H	4.8907607	2.4862336	-1.4722455	C	1.6840196	0.9001318	3.2542766	H	4.9958875	2.3737205	-1.4618592
C	1.7007568	0.9199876	3.2892776	C	2.0063292	0.6587193	4.5873169	C	1.6943053	1.0106271	3.2572070
C	2.0175496	0.6928184	4.6254933	C	1.4700829	-0.4566950	5.2397186	C	1.9713954	0.8456193	4.6087884
C	1.4678172	-0.4098392	5.2886937	C	0.7002200	-1.3706255	4.5358127	C	1.4013397	-0.2574776	5.2879031
C	0.6895170	-1.3240020	4.5938909	C	0.4258770	-1.1946702	3.1551127	C	0.6410029	-1.1911129	4.5974397
C	0.4094882	-1.1558691	3.2134896	N	0.8291678	0.0552508	2.5981441	C	0.4067611	-1.0646200	3.2057418
N	0.8395519	0.0757620	2.6422257	H	1.6970935	-0.6324846	6.2926511	N	0.8533531	0.1459522	2.6111413
H	1.6875579	-0.5742956	6.3450622	H	2.7150062	1.3258712	5.0735019	H	1.5910620	-0.3917777	6.3541093
H	2.7316641	1.3582484	5.1061385	H	0.3211645	-2.2830893	4.9945681	H	2.6704081	1.5048951	5.0910934
H	0.3001987	-2.2267712	5.0628285	O	0.3892346	0.3267924	1.3833177	H	0.2344503	-2.0776364	5.0826354
O	0.4225581	0.3321456	1.4143759	O	-0.1341158	-2.0166693	2.3816325	O	0.4722583	0.3631310	1.3620388
O	-0.1815156	-1.9697486	2.4521282	C	2.4837716	1.9153531	2.4694656	O	-0.1579354	-1.9037249	2.4470837
C	2.5045278	1.9181466	2.4856428	O	3.7143534	1.8132304	2.5244020	C	2.5215967	1.9768370	2.4388448
O	3.7338201	1.7965847	2.5179229	N	1.8675383	2.8836870	1.7173880	O	3.7477857	1.8326304	2.4787034
N	1.8888099	2.8940717	1.7436390	C	2.7619502	3.7876995	0.9770044	N	1.9258376	2.9451170	1.6709897
C	2.7798574	3.7876159	0.9871202	H	2.2329074	4.7461654	0.8805120	C	2.8335501	3.7895469	0.8779049
H	2.2584100	4.7512800	0.9003327	H	3.6623663	3.9591162	1.5885133	H	2.3180436	4.7486541	0.7291143
H	3.6918197	3.9499225	1.5836996	C	-4.7997595	-1.6865747	0.4056816	H	3.7393096	3.9833021	1.4753149
C	-4.7951107	-1.7058132	0.3386782	C	-5.7509305	-2.6758259	0.1687577	C	-4.7732611	-1.7466166	0.2627242
C	-5.7347279	-2.7010933	0.0816436	C	-5.3507570	-3.9597115	-0.2082126	C	-5.7130648	-2.7087124	-0.0976352
C	-5.3177961	-3.9884531	-0.2647392	C	-4.0042100	-4.2489607	-0.3759694	C	-5.2961036	-3.9668104	-0.5397612
C	-3.9651929	-4.2758975	-0.3834764	C	-3.0062606	-3.2684251	-0.1555945	C	-3.9434421	-4.2548827	-0.6500116
C	-2.9802243	-3.2873656	-0.1448879	N	-3.4674036	-2.0019404	0.2955225	C	-2.9572831	-3.2990987	-0.3047402
N	-3.4599145	-2.0208462	0.2776558	H	-6.1001030	-4.7321141	-0.3903125	N	-3.4393442	-2.0679810	0.2088709
H	-6.0584263	-4.7657717	-0.4608013	H	-6.7934228	-2.3844028	0.2746597	H	-6.0367810	-4.7184284	-0.8187802
H	-6.7814316	-2.4139267	0.1510297	H	-3.6566354	-5.2308072	-0.6955373	H	-6.7591218	-2.4184623	-0.0320552
H	-3.6037276	-5.2601052	-0.6792979	O	-2.5150796	-1.1297848	0.5855774	H	-3.5819325	-5.2146051	-1.0174575
O	-2.5190235	-1.1440758	0.5911337	O	-1.7586740	-3.4119345	-0.3125180	O	-2.4994122	-1.2289326	0.6250186
O	-1.7264413	-3.4245349	-0.2685103	C	-5.2942905	-0.2858653	0.7042585	O	-1.7016753	-3.4388998	-0.4036065
C	-5.2998853	-0.3041936	0.6179939	O	-6.5015007	-0.1001625	0.9147674	C	-5.2753972	-0.3648960	0.6315560
O	-6.5121454	-0.1225221	0.8006713	N	-4.3658167	0.7064845	0.6598487	O	-6.4893840	-0.1860478	0.8038758
N	-4.3747061	0.6923653	0.5931558	H	-3.3917304	0.3793208	0.5483204	N	-4.3434087	0.6233634	0.6903065
H	-3.3967233	0.3714905	0.5047858	C	-4.7282314	2.0960271	0.8663836	H	-3.3662778	0.3030824	0.6018341
C	-4.7461171	2.0774510	0.8168978	H	-4.1719313	2.4944923	1.7343944	C	-4.7076154	1.9961283	0.9877720

H	-4.2187947	2.4582434	1.7108622	H	-5.7917691	2.0815703	1.1407512	H	-4.1179639	2.3466711	1.8536405
H	-5.8176706	2.0543262	1.0573584	C	3.1863110	3.3157599	-0.4278382	H	-5.7598124	1.9586950	1.3010181
C	3.1760729	3.3131497	-0.4259098	H	2.3135209	2.9416940	-0.9856002	C	3.2449325	3.2347195	-0.5015339
H	2.2932282	2.9320992	-0.9626373	H	3.5188973	4.2232984	-0.9585091	H	2.3663033	2.8253222	-1.0238952
H	3.4900756	4.2211800	-0.9668794	C	0.5296718	3.3845317	2.0624512	H	3.5642731	4.1109900	-1.0893433
C	0.5571919	3.4026722	2.1001001	H	0.0228842	2.6019211	2.6426667	C	0.6142732	3.5018484	2.0293442
H	0.0534896	2.6256371	2.6904126	H	0.6585985	4.2530294	2.7371315	H	0.1124168	2.7691771	2.6764250
H	0.6960497	4.2744233	2.7686228	C	-0.3651816	3.8196387	0.8910954	H	0.7883846	4.4041128	2.6471100
C	-0.3490590	3.8359450	0.9370433	C	-3.2076554	3.8145154	-0.4260492	C	-0.3161894	3.8892095	0.8691832
C	-3.1857516	3.8219442	-0.3893089	H	-3.3423385	4.6398294	-1.1399286	C	-3.2539606	3.7997155	-0.2667093
H	-3.3013646	4.6721699	-1.0770595	H	-2.9938368	4.2536622	0.5593250	H	-3.4147803	4.6458364	-0.9509255
H	-2.9912477	4.2261759	0.6148701	C	-4.5274880	3.0250577	-0.3526618	H	-3.0167284	4.2098715	0.7261879
C	-4.5096464	3.0354758	-0.3723506	H	-4.6745675	2.4613735	-1.2839781	C	-4.5636680	2.9950386	-0.1840590
H	-4.6324963	2.4972113	-1.3219830	H	-5.3270224	3.7845342	-0.3236763	H	-4.7426568	2.4811631	-1.1381727
H	-5.3081969	3.7959999	-0.3457458	H	0.2014201	4.4312640	0.1710897	H	-5.3674793	3.7436945	-0.0820904
H	0.2063013	4.4611527	0.2198437	H	-1.1252886	4.4912784	1.3216411	H	0.2346902	4.4450634	0.0938113
H	-1.1145711	4.4946516	1.3781517	H	-0.2833444	2.0283100	-0.3105602	H	-1.0480858	4.6000897	1.2863877
H	-0.2530544	2.0491925	-0.2709267	H	-1.5308393	1.9938120	0.8985312	H	-0.3189388	2.0348157	-0.2400718
H	-1.5033419	2.0028511	0.9357781	H	-0.1768980	-1.5985688	-0.0285019	H	-1.5016161	2.0834505	1.0296773
				Eu							
[Cm-L2] ⁻¹				[Pu-L2]				[Th-L2]			
Cm	-0.1882126	-1.6057928	-0.0009302	C	-0.6845797	1.7481198	-2.7920429	C	-0.8392417	1.9463764	-2.6664433
C	-0.7513129	1.9634644	-2.7594511	C	-0.0181544	2.1217844	-3.9541070	C	-0.2024846	2.4034523	-3.8156299
C	-0.0558061	2.4257517	-3.8752793	C	0.8676059	1.2326044	-4.5739660	C	0.7150820	1.5831058	-4.4809295
C	0.8778897	1.5961170	-4.5038388	C	1.0628634	-0.0413035	-4.0606293	C	0.9772768	0.2997781	-4.0215952
C	1.0951805	0.3054220	-4.0423916	C	0.3960597	-0.4415418	-2.8845195	C	0.3409841	-0.1867944	-2.8616190
C	0.3990831	-0.2010196	-2.9172074	N	-0.4488162	0.5024291	-2.2829274	N	-0.5530663	0.6874448	-2.2219896
N	-0.5231557	0.6945790	-2.3071880	H	1.3966282	1.5388539	-5.4767759	H	1.2193839	1.9505625	-5.3751462
H	1.4337483	1.9629520	-5.3685046	H	-0.2375444	3.0997802	-4.3761985	H	-0.4690753	3.3896806	-4.1884050
H	-0.2884530	3.4218433	-4.2447682	H	1.7305746	-0.7616608	-4.5298071	H	1.6770609	-0.3654475	-4.5243834
H	1.8130975	-0.3633661	-4.5152586	O	-1.0575570	0.0833824	-1.1743048	O	-1.1527903	0.1902853	-1.1347291
O	-1.1852904	0.2136786	-1.2639105	O	0.4755977	-1.5734874	-2.2953053	O	0.4923077	-1.3322103	-2.3134037
O	0.5118395	-1.3459749	-2.3949490	C	-1.8104831	2.6273741	-2.2722317	C	-1.9776691	2.7609872	-2.0750972
C	-1.8801404	2.8064547	-2.2011675	O	-2.6242715	3.0037526	-3.1233191	O	-2.8252788	3.1707953	-2.8757038
O	-2.6778008	3.2892832	-3.0179343	N	-1.8963327	3.0144372	-0.9624434	N	-2.0408708	3.0482101	-0.7404688
N	-1.9946648	3.0522579	-0.8591893	C	-0.9588874	2.6100851	0.0916014	C	-1.0160544	2.7076509	0.2471157
C	-1.0288748	2.6309852	0.1577985	C	4.2297504	-1.2558184	-1.1735999	C	4.3317600	-1.5181896	-1.0601023
C	4.2970520	-1.4230672	-1.0586423	C	5.1254249	-2.1704302	-1.7158258	C	5.1864994	-2.4828572	-1.5810803
C	5.1555473	-2.3798115	-1.5942330	C	4.8097053	-3.5307298	-1.7734581	C	4.7915331	-3.8218616	-1.6453890
C	4.7564774	-3.7154029	-1.6794055	C	3.5852670	-3.9807400	-1.3044066	C	3.5287382	-4.1997408	-1.2133539
C	3.4945059	-4.0936360	-1.2472201	C	2.6567006	-3.0698354	-0.7657765	C	2.6383284	-3.2389084	-0.6975230
C	2.5874412	-3.1476844	-0.7133565	N	3.0348800	-1.7260622	-0.6904871	N	3.1045880	-1.9228693	-0.6023796
N	3.0617163	-1.8164245	-0.6078371	H	5.5246908	-4.2377065	-2.1954731	H	5.4734694	-4.5701843	-2.0505440
H	5.4351978	-4.4613307	-2.0972662	H	6.0639047	-1.7637885	-2.0865471	H	6.1520838	-2.1315465	-1.9382317
H	6.1234513	-2.0238950	-1.9396051	H	3.2907012	-5.0281372	-1.3432134	H	3.1748072	-5.2278790	-1.2679115
H	3.1400093	-5.1215278	-1.3139741	O	2.1419563	-0.9237308	-0.0923553	O	2.2470964	-1.0691478	-0.0222335
O	2.2145392	-0.9614377	-0.0372162	O	1.4843239	-3.3537508	-0.3272163	O	1.4347583	-3.4496541	-0.2994416
O	1.4062472	-3.3877992	-0.3174822	C	4.6433736	0.2068668	-1.1634670	C	4.8057789	-0.0716189	-1.0790448
C	4.7806840	0.0148233	-1.0339943	O	5.7142028	0.5168125	-1.6969848	O	5.9014576	0.1783809	-1.5928454
O	5.9044227	0.2816758	-1.4869848	N	3.8153417	1.1047226	-0.5749855	N	3.9893394	0.8762354	-0.5559327

N	3.9403593	0.9527030	-0.5330538	H	2.9915777	0.7256618	-0.0981230	H	3.1494386	0.5406096	-0.0757009
H	3.0596985	0.5898204	-0.1368370	C	4.2180501	2.5029369	-0.4830922	C	4.4053665	2.2731610	-0.5366943
C	4.3468811	2.3492870	-0.4932064	H	4.9658752	2.6230538	0.3192329	H	5.1083083	2.4438895	0.2956951
H	5.0452029	2.5141114	0.3454210	H	4.7311296	2.7394452	-1.4257220	H	4.9707077	2.4337760	-1.4645466
H	4.9160747	2.5342363	-1.4162086	C	1.5568991	0.7737233	3.2884511	C	1.6135729	1.0024451	3.2750103
C	1.7108222	0.8745205	3.2775529	C	1.8480236	0.5244144	4.6257179	C	1.8639523	0.8393691	4.6318524
C	2.0710711	0.6168267	4.5987779	C	1.3765523	-0.6430091	5.2348587	C	1.3442038	-0.2740216	5.3033038
C	1.5665325	-0.5140859	5.2468236	C	0.7090134	-1.6015884	4.4827289	C	0.6600527	-1.2590428	4.6044606
C	0.7898416	-1.4269914	4.5474392	C	0.4591850	-1.3820587	3.1144254	C	0.4392409	-1.1286915	3.2178060
C	0.4670449	-1.2269304	3.1824570	N	0.7777896	-0.1177125	2.6056980	N	0.8321064	0.0845038	2.6336150
N	0.8452941	0.0313778	2.6341692	H	1.5822672	-0.8266765	6.2895506	H	1.5211714	-0.3931847	6.3726491
H	1.8233761	-0.7041522	6.2903364	H	2.4918907	1.2241466	5.1545745	H	2.5113346	1.5565883	5.1322735
H	2.7882292	1.2826591	5.0738806	H	0.3978528	-2.5569250	4.9018039	H	0.3046569	-2.1699002	5.0833383
H	0.4356823	-2.3521813	5.0006344	O	0.3404137	0.1475872	1.3755204	O	0.4598139	0.2716031	1.3640910
O	0.3822758	0.3111515	1.4256891	O	-0.0248910	-2.2197249	2.2723836	O	-0.0830908	-1.9896339	2.4289423
O	-0.1242588	-2.0372387	2.4149271	O	2.3567788	1.8028193	2.5100711	C	2.4522641	1.9403853	2.4250763
C	2.4911046	1.9065516	2.4940967	O	3.5792135	1.6327811	2.5082598	O	3.6597078	1.6878954	2.3977171
O	3.7233186	1.8311781	2.5557994	N	1.7587699	2.8359720	1.8464713	N	1.9001856	2.9672657	1.7157860
N	1.8603886	2.8649551	1.7391741	C	2.6632396	3.8003106	1.1940695	C	2.8448458	3.8009203	0.9468869
C	2.7440927	3.7935858	1.0155701	H	2.1539124	4.7737229	1.2226800	H	2.3648053	4.7782138	0.836516
H	2.2014223	4.7456434	0.9312308	H	3.5728613	3.8790584	1.8087683	H	3.7525061	3.9410043	1.5549184
H	3.6391039	3.9687683	1.6337425	C	-4.7039306	-1.5102383	0.4919610	C	-4.7625813	-1.7126204	0.2893549
C	-4.8257327	-1.6585647	0.3872081	C	-5.6939588	-2.4496618	0.2262728	C	-5.7107244	-2.6548997	-0.0910019
C	-5.7745442	-2.6468069	0.1382012	C	-5.3598052	-3.7447122	-0.1759892	C	-5.3140975	-3.9095128	-0.5625472
C	-5.3714407	-3.9379089	-0.2093097	C	-4.0272378	-4.0954840	-0.3398244	C	-3.9661011	-4.2163113	-0.6808461
C	-4.0219139	-4.2341899	-0.3365437	C	-3.0136041	-3.1583065	-0.0760492	C	-2.9883977	-3.2756163	-0.3064747
C	-3.0298782	-3.2525011	-0.1058987	N	-3.3896103	-1.8956510	0.3874657	N	-3.4380675	-2.0610581	0.2238456
N	-3.4919657	-1.9814459	0.3180180	H	-6.1450300	-4.4724870	-0.3816103	H	-6.0658962	-4.6416784	-0.8586383
H	-6.1189777	-4.7097694	-0.4007592	H	-6.7220641	-2.1095821	0.3321034	H	-6.7532561	-2.3537501	-0.0151740
H	-6.8179651	-2.3495992	0.2142961	H	-3.7175666	-5.0828554	-0.6782811	H	-3.6152027	-5.1705100	-1.0705015
H	-3.6687551	-5.2214259	-0.6322192	O	-2.3829795	-1.0884553	0.7238817	O	-2.4707263	-1.2504076	0.6615622
O	-2.5424130	-1.1095759	0.6256153	O	-1.7472887	-3.3513448	-0.2172497	O	-1.7140060	-3.4159182	-0.4006996
O	-1.7767126	-3.4051939	-0.2406036	C	-5.1425685	-0.0911469	0.8042641	C	-5.2490458	-0.3286593	0.6859689
C	-5.3230670	-0.2527687	0.6583266	O	-6.3400959	0.1278078	1.0075186	O	-6.4534386	-0.1643247	0.8976608
O	-6.5350363	-0.0621669	0.8326788	N	-4.1815510	0.8681185	0.7658480	N	-4.3220522	0.6661553	0.7070176
N	-4.3903031	0.7357929	0.6324519	H	-3.2194494	0.5313342	0.6444262	H	-3.3467194	0.3742320	0.5907351
H	-3.4150496	0.4045522	0.5510158	C	-4.5136250	2.2762804	0.9107419	C	-4.6930722	2.0440931	0.9904135
C	-4.7534627	2.1279541	0.8207745	H	-3.8878518	2.7154883	1.7063151	H	-4.1129735	2.4039500	1.8581148
H	-4.2211466	2.5293217	1.7023823	H	-5.5526772	2.2975978	1.2634873	H	-5.7461409	2.0046762	1.2972159
H	-5.8245554	2.1184396	1.0641733	C	3.0626615	3.4914777	-0.2620695	C	3.2459361	3.2842955	-0.4508907
C	3.1817000	3.3507354	-0.3945217	H	2.1816735	3.1839344	-0.8473937	H	2.3629408	2.8973373	-0.9833794
H	2.3152048	2.9808604	-0.9649028	H	3.3900481	4.4525069	-0.6903852	H	3.5672563	4.1761132	-1.0122504
H	3.5112741	4.2702777	-0.9061172	C	0.3982987	3.2880597	2.1595308	C	0.5963276	3.5516228	2.0578382
C	0.5147988	3.3430845	2.0863959	H	-0.1166120	2.4667958	2.6764467	H	0.0800850	2.8438480	2.7223603
H	0.0127015	2.5423467	2.6449781	H	0.4725435	4.1253140	2.8777326	H	0.7810583	4.4654800	2.6511801
H	0.6280637	4.1994470	2.7793251	C	-0.4455834	3.7591418	0.9660665	C	-0.3165062	3.9193034	0.8772322
C	-0.3768452	3.7923770	0.9180644	C	-3.0701322	3.8431164	-0.6302653	C	-3.2261494	3.8071911	-0.3016071
C	-3.1807892	3.8174570	-0.4482830	H	-3.2140352	4.5341513	-1.4715879	H	-3.3735163	4.6289691	-1.0169204
H	-3.2931497	4.6480925	-1.1598857	H	-2.8202864	4.4437475	0.2536065	H	-2.9864412	4.2519719	0.6745337
H	-2.9728585	4.2484827	0.5416002	C	-4.3964496	3.1062521	-0.3865637	C	-4.5452678	3.0239808	-0.1939928
C	-4.5150234	3.0503571	-0.3957276	H	-4.6411403	2.4776681	-1.2539916	H	-4.7491158	2.5042546	-1.1398419

H	-4.6585217	2.4894061	-1.3292659	H	-5.1684565	3.8923137	-0.3501590	H	-5.3336034	3.7873386	-0.0896598
H	-5.3011885	3.8240576	-0.3789148	H	0.1091299	4.4898574	0.3566977	H	0.2443332	4.4736416	0.1085237
H	0.1849228	4.4320880	0.2189438	H	-1.2879334	4.3122446	1.4072955	H	-1.0622456	4.6254502	1.2741907
H	-1.1504426	4.4398865	1.3607456	H	-0.1086654	2.1095929	-0.3807275	H	-0.2733574	2.0606223	-0.2215061
H	-0.2539056	2.0316327	-0.3215053	H	-1.4196958	1.8475335	0.7365085	H	-1.4719496	2.0974429	1.0424808
H	-1.5156707	1.9516669	0.8730507	Pu	-0.1384734	-1.7573045	-0.0027615	Th	-0.1329105	-1.6718065	0.0308271