

Theoretical Investigations into the Bonding and Separation Properties of Non-rigid, Partially Rigid, and Rigid Ligands Derived from Et-Tol-PTA with Trivalent Lanthanides and Actinides

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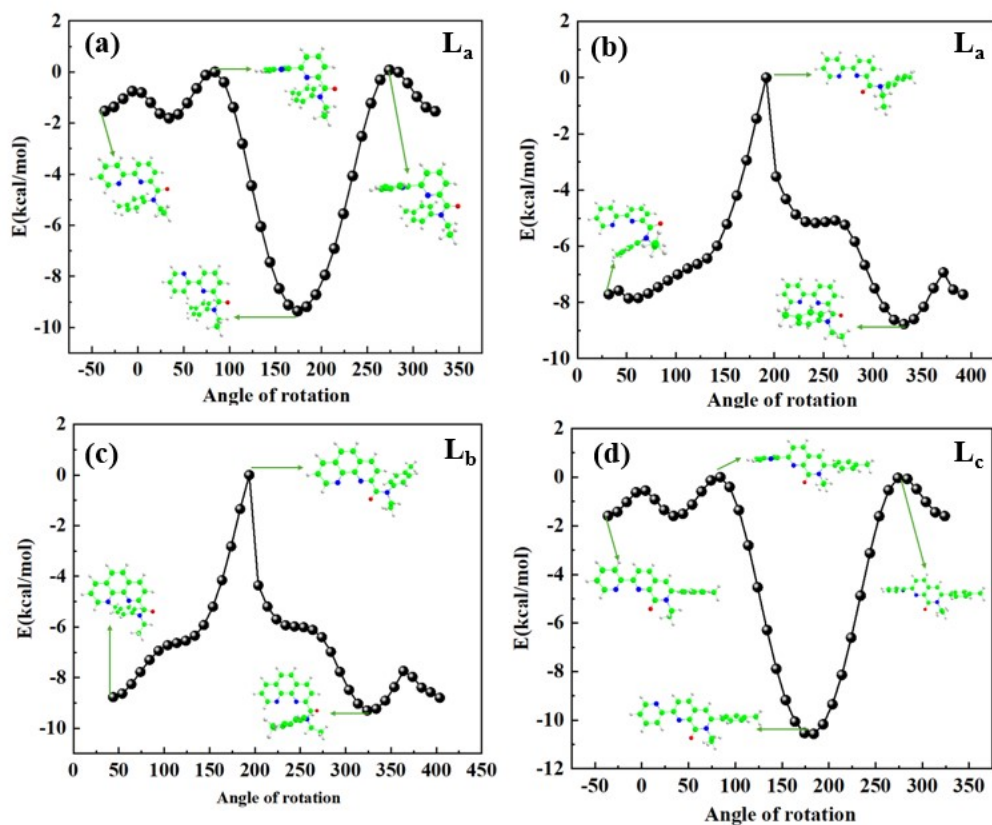


Figure S1 The potential energy curve of the L_a - L_c rotating around the selected C-C single bonds with PBE0/6-311G* levels (The L_a ligand possesses two C-C single bonds whose rotation changes the relative conformation of the N_1 , N_2 and O donor atoms, we conducted potential energy curve scans for each of these two bonds, (a) and (b))

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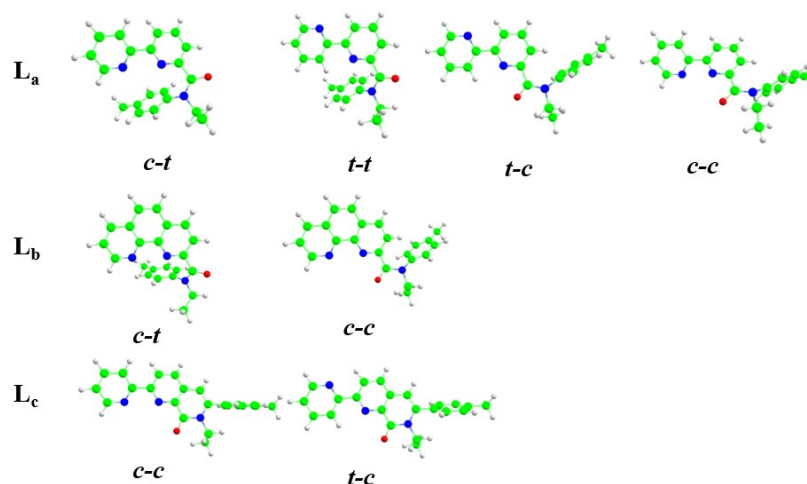


Figure S2 The cis-conformation (c) and trans-conformation (t) of the L_a - L_c ligand.

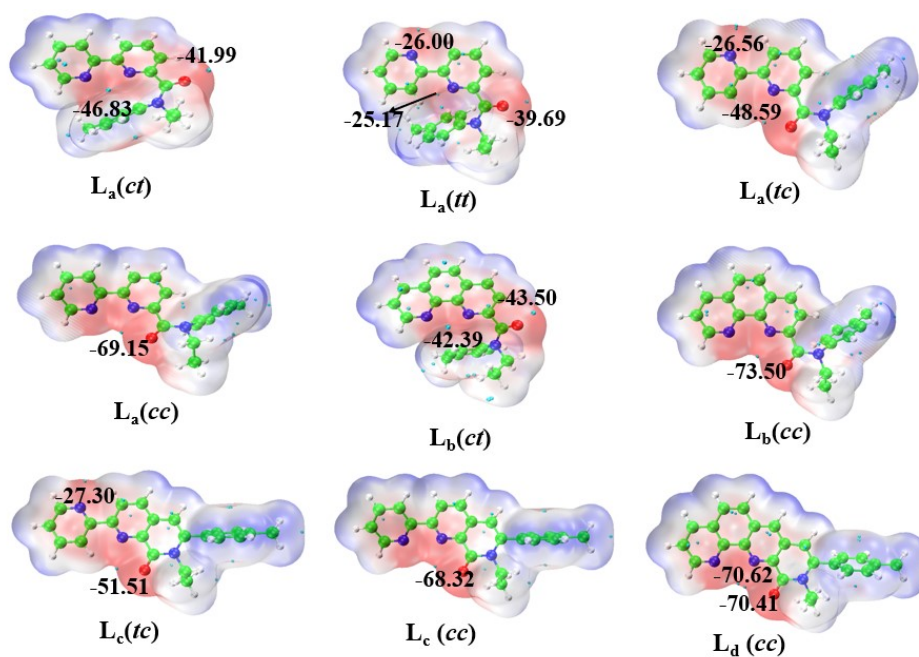


Figure S3 The electrostatic potential (ESP) diagrams for the cis-conformation (c) and trans-conformation (t) of the L_a - L_d ligand.

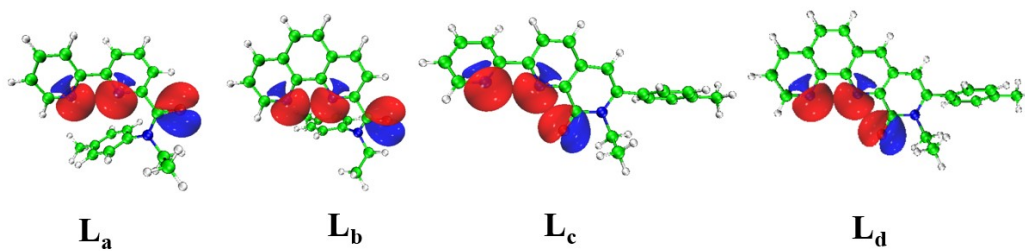


Figure S4 The LMO (Localized Molecular Orbital) orbitals of ligands.

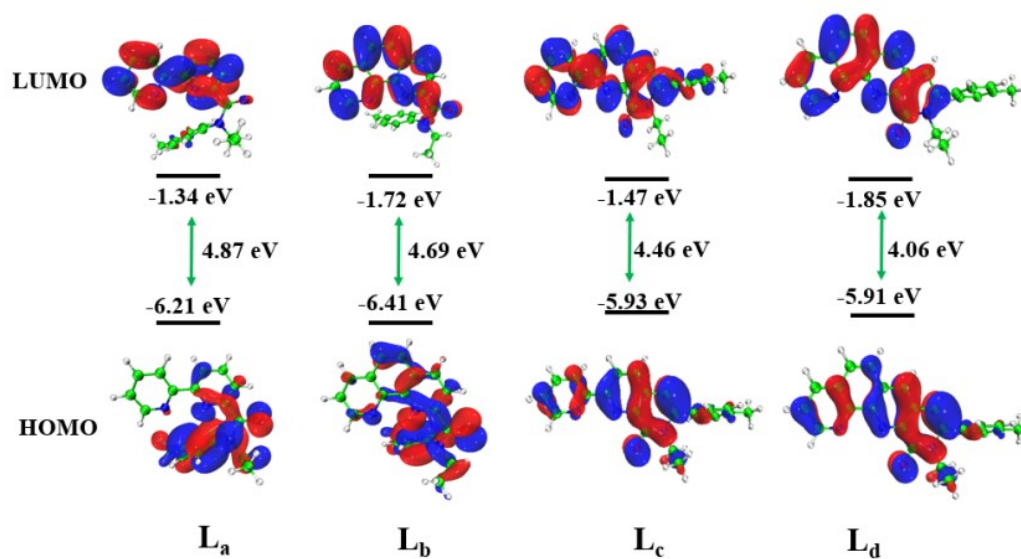


Figure S5 HOMO-LUMO orbital energy level diagram of ligands

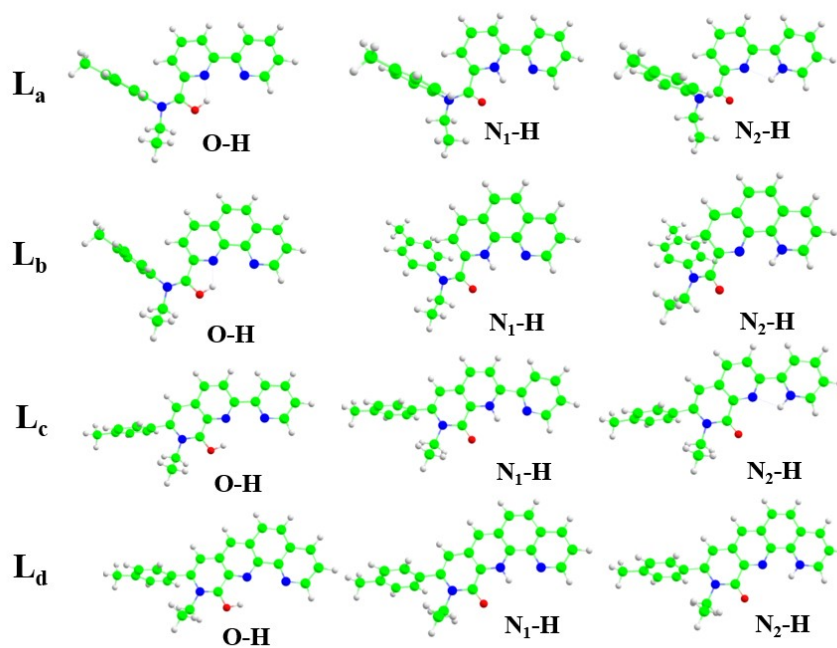


Figure S6 The protonation structural of ligands

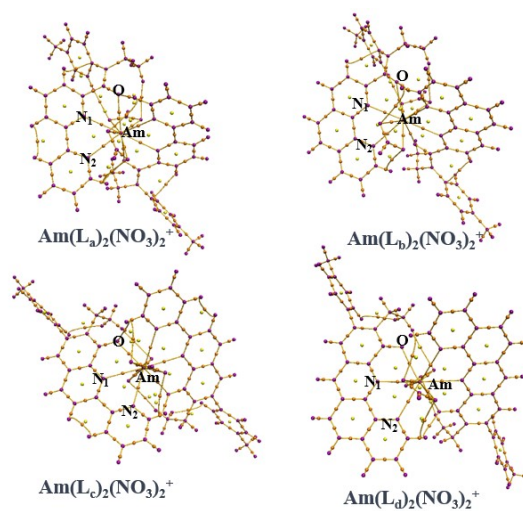


Figure S7 molecular graphs of $Am(L)_2(NO_3)_2^+$ complexes (Yellow represents the ring critical point, while yellow-brown represents the bond critical point)

Table S1 Natural atomic charges and Mulliken charges of N₁,N₂,O in ligands

Ligands	Natural atomic charges			Mulliken charges		
	N ₁	N ₂	O	N ₁	N ₂	O
L _a	-0.4315	-0.4320	-0.6334	-0.3122	-0.3343	-0.3813
L _b	-0.4297	-0.4338	-0.6292	-0.3438	-0.3746	-0.3804
L _c	-0.3873	-0.4283	-0.5950	-0.3115	-0.3291	-0.3484
L _d	-0.3750	-0.4166	-0.5888	-0.3218	-0.3393	-0.3432

Table S2 Bond lengths of O-M,N_{1,2}-M and average N_{ave}-M with several functionals method

BP86	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.5054	2.6407	2.6634	2.6520
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4975	2.6830	2.6868	2.6849
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.5086	2.6858	2.6980	2.6919
TPSSH	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.4857	2.6300	2.6483	2.6392
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4750	2.6650	2.6720	2.6685
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.4625	2.6348	2.6605	2.6477
b3lyp	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.5144	2.6828	2.6970	2.6899
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4996	2.7118	2.7082	2.7100
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.4681	2.6687	2.6915	2.6801
PBE0	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.4909	2.6403	2.6565	2.6484
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4776	2.6708	2.6672	2.6690
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.4448	2.6298	2.6524	2.6411
M06-2X	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.5112	2.6450	2.6680	2.6565
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4736	2.6570	2.6504	2.6537
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.4227	2.6163	2.6377	2.6270

Table S3 Bond lengths of O-M,N_{1,2}-M and average N_{ave}-M with PBE0/6-311G*-RECP level.

Complexes	O-M	N ₁ -M	N ₂ -M	N _{ave} -M
Am(L _a) ₂ (NO ₃) ₂ ⁺	2.4759	2.6549	2.6489	2.6519
Cm(L _a) ₂ (NO ₃) ₂ ⁺	2.4636	2.6855	2.6579	2.6717
Eu(L _a) ₂ (NO ₃) ₂ ⁺	2.4279	2.6513	2.6415	2.6464
Am(L _b) ₂ (NO ₃) ₂ ⁺	2.4909	2.6403	2.6565	2.6484
Cm(L _b) ₂ (NO ₃) ₂ ⁺	2.4776	2.6708	2.6672	2.6690
Eu(L _b) ₂ (NO ₃) ₂ ⁺	2.4448	2.6298	2.6524	2.6411
Am(L _c) ₂ (NO ₃) ₂ ⁺	2.4982	2.6314	2.6688	2.6501
Cm(L _c) ₂ (NO ₃) ₂ ⁺	2.4889	2.6640	2.6803	2.6722
Eu(L _c) ₂ (NO ₃) ₂ ⁺	2.4587	2.6216	2.6661	2.6438

Am(L _d) ₂ (NO ₃) ₂ ⁺	2.5190	2.6216	2.6818	2.6517
Cm(L _d) ₂ (NO ₃) ₂ ⁺	2.5094	2.6527	2.6958	2.6743
Eu(L _d) ₂ (NO ₃) ₂ ⁺	2.4813	2.6316	2.6760	2.6538

Table S4 $\angle N_1MN_2$ and $\angle N_1MO$ bond angles in Am(L)₂(NO₃)₂⁺ complexes with PBE0/6-311G*-RECP level.

	$\angle N_1MN_2$	$\angle N_1MO$
Am(L _a) ₂ (NO ₃) ₂ ⁺	61.25	122.25
Cm(L _a) ₂ (NO ₃) ₂ ⁺	60.64	121.22
Eu(L _a) ₂ (NO ₃) ₂ ⁺	61.19	122.33
Am(L _b) ₂ (NO ₃) ₂ ⁺	61.78	122.29
Cm(L _b) ₂ (NO ₃) ₂ ⁺	61.15	121.35
Eu(L _b) ₂ (NO ₃) ₂ ⁺	61.71	122.69
Am(L _c) ₂ (NO ₃) ₂ ⁺	60.50	123.12
Cm(L _c) ₂ (NO ₃) ₂ ⁺	59.89	122.02
Eu(L _c) ₂ (NO ₃) ₂ ⁺	60.40	123.37
Am(L _d) ₂ (NO ₃) ₂ ⁺	61.16	123.32
Cm(L _d) ₂ (NO ₃) ₂ ⁺	60.48	122.16
Eu(L _d) ₂ (NO ₃) ₂ ⁺	60.71	122.76

Table S5 The averaged electron density (ρ), Laplacian ($\nabla^2\rho$), local electron energy density (H(r)) and the ratio between the absolute value of potential energy density(V) and Lagrangian kinetic energy(G) at the N₁-M, N₂-M and O-M at BCPs, for the M(L)₂(NO₃)₂⁺ complexes calculated by the def-TZVP method

Am(L _a) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Am	0.0490	0.1900	-0.4969	1.0947	0.2543
N ₁ -Am	0.0392	0.1181	-0.3558	1.1075	0.2160
N ₂ -Am	0.0409	0.1229	-0.4240	1.1212	0.2313
Cm(L _a) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Cm	0.0495	0.1912	-0.4862	1.0923	0.2487
N ₁ -Cm	0.0368	0.1123	-0.2998	1.0965	0.1863
N ₂ -Cm	0.0396	0.1172	-0.3784	1.1143	0.2172
Eu(L _a) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Eu	0.0475	0.1905	-0.2869	1.0568	0.2228
N ₁ -Eu	0.0346	0.1110	-0.1223	1.0422	0.1734
N ₂ -Eu	0.0361	0.1134	-0.1601	1.0534	0.1881
Am(L _b) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Am	0.0474	0.1838	-0.4482	1.0889	0.2469
N ₁ -Am	0.0407	0.1217	-0.3946	1.1148	0.2236
N ₂ -Am	0.0402	0.1214	-0.4043	1.1176	0.2276

Cm(L _b) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Cm	0.0479	0.1851	-0.4392	1.0867	0.2416
N ₁ -Cm	0.0381	0.1159	-0.3367	1.1041	0.1928
N ₂ -Cm	0.0388	0.1152	-0.3562	1.1101	0.2134
Eu(L _b) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Eu	0.0456	0.1832	-0.2354	1.0489	0.2152
N ₁ -Eu	0.0365	0.1156	-0.1671	1.0547	0.1823
N ₂ -Eu	0.0353	0.1112	-0.1414	1.0484	0.1838
Am(L _c) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Am	0.0472	0.1806	-0.4583	1.0922	0.2491
N ₁ -Am	0.0412	0.1239	-0.3993	1.1142	0.2390
N ₂ -Am	0.0391	0.1183	-0.3697	1.1111	0.2221
Cm(L _c) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Cm	0.0474	0.1798	-0.4409	1.0893	0.2420
N ₁ -Cm	0.0385	0.1176	-0.3428	1.1044	0.1938
N ₂ -Cm	0.0376	0.1121	-0.3202	1.1026	0.2073
Eu(L _c) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Eu	0.0449	0.1772	-0.2322	1.0498	0.2147
N ₁ -Eu	0.0370	0.1176	-0.1752	1.0562	0.1845
N ₂ -Eu	0.0341	0.1081	-0.1097	1.0390	0.1786
Am(L _d) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Am	0.0450	0.1724	-0.3887	1.0827	0.2379
N ₁ -Am	0.0421	0.1265	-0.4284	1.1193	0.2304
N ₂ -Am	0.0380	0.1154	-0.3388	1.1051	0.2172
Cm(L _d) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Cm	0.0451	0.1715	-0.3732	1.0801	0.2315
N ₁ -Cm	0.0396	0.1204	-0.3718	1.1100	0.1993
N ₂ -Cm	0.0363	0.1086	-0.2866	1.0954	0.2016
Eu(L _d) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Eu	0.0424	0.1668	-0.1643	1.0379	0.2052
N ₁ -Eu	0.0364	0.1197	-0.1509	1.0480	0.1720
N ₂ -Eu	0.0334	0.1052	-0.0984	1.0360	0.1742

Table S6 The averaged electron density (ρ), Laplacian ($\nabla^2\rho$), local electron energy density (H(r)) and the ratio between the absolute value of potential energy density(V) and Lagrangian kinetic energy(G) at the N₁-M, N₂-M and O-M at BCPs, for the M(L)₂(NO₃)₂⁺ complexes calculated by the ZORA method

Am(L _a) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Am	0.0485	0.2026	-0.2101	1.0398	0.2566
N ₁ -Am	0.0385	0.1252	-0.1586	1.0482	0.2193
N ₂ -Am	0.0404	0.1298	-0.2186	1.0631	0.2342
Cm(L _a) ₂ (NO ₃) ₂ ⁺	ρ	$\nabla^2\rho$	H(r)*10 ²	V /G	δ
O-Cm	0.0489	0.2055	-0.1867	1.0351	0.2515
N ₁ -Cm	0.0362	0.1181	-0.1263	1.0410	0.1895

N ₂ -Cm	0.0390	0.1240	-0.1892	1.0575	0.2210
Eu(L _a) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Eu	0.0469	0.2011	-0.0236	1.0047	0.2253
N ₁ -Eu	0.0341	0.1185	0.0291	0.9901	0.1676
N ₂ -Eu	0.0357	0.1165	-0.0315	1.0107	0.1890
Am(L _b) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Am	0.0468	0.1956	-0.1764	1.0348	0.2492
N ₁ -Am	0.0399	0.1293	-0.1864	1.0545	0.2272
N ₂ -Am	0.0397	0.1281	-0.2052	1.0602	0.2307
Cm(L _b) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Cm	0.0473	0.1986	-0.1538	1.0300	0.2444
N ₁ -Cm	0.0375	0.1224	-0.1492	1.0465	0.1960
N ₂ -Cm	0.0383	0.1217	-0.1748	1.0543	0.2169
Eu(L _b) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Eu	0.0449	0.1935	0.0168	0.9965	0.2167
N ₁ -Eu	0.0359	0.1205	-0.0201	1.0066	0.1842
N ₂ -Eu	0.0348	0.1146	-0.0161	1.0056	0.1858
Am(L _c) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Am	0.0467	0.1920	-0.1892	1.0379	0.2513
N ₁ -Am	0.0404	0.1318	-0.1842	1.0530	0.2298
N ₂ -Am	0.0385	0.1243	-0.1830	1.0556	0.2252
Cm(L _c) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Cm	0.0468	0.1927	-0.1630	1.0327	0.2446
N ₁ -Cm	0.0379	0.1245	-0.1483	1.0676	0.1971
N ₂ -Cm	0.0370	0.1179	-0.1523	1.0492	0.2107
Eu(L _c) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Eu	0.0442	0.0938	0.0142	0.9970	0.2157
N ₁ -Eu	0.0364	0.1227	-0.0238	1.0077	0.1869
N ₂ -Eu	0.0336	0.1109	0.0056	0.9980	0.1809
Am(L _d) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Am	0.0444	0.1828	-0.1392	1.0296	0.2400
N ₁ -Am	0.0414	0.1348	-0.2063	1.0577	0.2342
N ₂ -Am	0.0375	0.1210	-0.1629	1.0511	0.2203
Cm(L _d) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Cm	0.0446	0.1832	-0.1159	1.0247	0.2341
N ₁ -Cm	0.0390	0.1278	-0.1669	1.0496	0.2027
N ₂ -Cm	0.0358	0.1139	-0.1318	1.0442	0.2050
Eu(L _d) ₂ (NO ₃) ₂ ⁺	ρ	∇ ² ρ	H(r)*10 ²	V /G	δ
O-Eu	0.0417	0.1761	0.0579	0.9867	0.2061
N ₁ -Eu	0.0356	0.1200	-0.0128	1.0043	0.1843
N ₂ -Eu	0.0329	0.1086	0.0148	0.9945	0.1778

Table S7 Charge decomposition analysis of α , β -spin orbitals and $(\alpha+\beta)$ -spin orbitals for $M(L_a)_2(NO_3)_2^+$, $M(L_c)_2(NO_3)_2^+$ and $M(L_d)_2(NO_3)_2^+$ complexes with PBE0/def-TZVP level.

Complexes	Spin orbital	d	b	b-d
$Am(L_a)_2(NO_3)_2^+$	α -spin	0.2107	-0.0315	0.2422
	β -spin	0.1848	-0.0427	0.2275
	$(\alpha+\beta)$ -spin	0.3955	-0.0742	0.4696
$Cm(L_a)_2(NO_3)_2^+$	α -spin	0.2075	-0.0332	0.2407
	β -spin	0.1880	-0.0402	0.2282
	$(\alpha+\beta)$ -spin	0.3955	-0.0735	0.4690
$Eu(L_a)_2(NO_3)_2^+$	α -spin	0.1597	-0.0652	0.4369
	β -spin	0.1397	-0.0723	0.2120
	$(\alpha+\beta)$ -spin	0.2993	-0.1375	0.4368
$Am(L_c)_2(NO_3)_2^+$	α -spin	0.2077	-0.0380	0.2457
	β -spin	0.1810	-0.0487	0.2297
	$(\alpha+\beta)$ -spin	0.3887	-0.0887	0.4754
$Cm(L_c)_2(NO_3)_2^+$	α -spin	0.2035	-0.0416	0.2451
	β -spin	0.1839	-0.0476	0.2315
	$(\alpha+\beta)$ -spin	0.3875	-0.0891	0.4766
$Eu(L_c)_2(NO_3)_2^+$	α -spin	0.1531	-0.0716	0.2247
	β -spin	0.1340	-0.0786	0.2246
	$(\alpha+\beta)$ -spin	0.2871	-0.1502	0.4373
$Am(L_d)_2(NO_3)_2^+$	α -spin	0.2074	-0.0415	0.2489
	β -spin	0.1804	-0.0520	0.2324
	$(\alpha+\beta)$ -spin	0.3878	-0.0935	0.4813
$Cm(L_d)_2(NO_3)_2^+$	α -spin	0.2003	-0.0453	0.2456
	β -spin	0.1806	-0.0508	0.2314
	$(\alpha+\beta)$ -spin	0.3809	-0.0961	0.4770
$Eu(L_d)_2(NO_3)_2^+$	α -spin	0.1446	-0.0773	0.2219
	β -spin	0.1232	-0.0839	0.2070
	$(\alpha+\beta)$ -spin	0.2678	-0.1611	0.4289

Cartesian coordinates

PBE0/6-311G*-RECP

Am(L_a)₂(NO₃)₂⁺

	X	Y	Z
C	0.73099200	5.79429300	0.26635600
C	-0.43219400	5.27513700	0.81095600
N	0.25087300	3.06057700	0.21801500
C	1.36513300	3.56216800	-0.33298500
C	2.29175700	2.59032600	-0.95501100
N	2.19523200	1.31973500	-0.55920500
C	3.01932800	0.40457300	-1.08159600
C	3.93180600	0.70999400	-2.08375500
C	4.00515600	2.02207500	-2.52839700
C	2.74570200	-0.97941700	-0.56231100
O	1.64650700	-1.18288700	-0.02258100
N	3.61878600	-1.99027100	-0.70385300
C	5.01431700	-1.82484100	-0.95870200
C	3.14701900	-3.34496100	-0.35040500
C	2.18715300	-3.92837100	-1.37134500
C	5.60507100	-2.46838900	-2.04397200
C	7.15696800	-0.92145500	-0.34479300
C	5.79754500	-1.06232600	-0.09926300
H	0.93398700	6.85956200	0.29921300
H	-1.17398600	5.91231600	1.27800300
H	4.55857100	-0.05342500	-2.52294900
H	4.68649600	2.29030500	-3.32851200
H	2.67092400	-3.28958500	0.63151400
H	4.04123800	-3.96094400	-0.25255500
H	1.90009800	-4.93774600	-1.06587200
H	2.64524200	-3.99826400	-2.36102100
H	1.27660400	-3.33251500	-1.44987100
H	4.99610000	-3.06269700	-2.71808900
H	7.75692100	-0.31952600	0.33148700
H	5.34373600	-0.58010200	0.76139500
N	0.47650300	1.70310600	3.14748000
O	-0.71045500	1.57083500	2.71554200
O	0.72509800	2.17414700	4.21909200
O	1.39004700	1.29620700	2.35587700
N	-0.70454400	-0.63987600	-2.14578000
O	-0.01166100	0.40829500	-2.00961500
O	-0.92601700	-1.13703500	-3.21754100
O	-1.16589100	-1.13766700	-1.06789400
C	6.96590500	-2.32869800	-2.27044500
H	7.41504500	-2.83149300	-3.12220000

C	-0.62640100	3.90167400	0.76615500
H	-1.51230500	3.44687900	1.19170400
C	0.27617000	-3.12051000	4.61515700
C	1.40465600	-2.53542500	4.06410400
N	0.04180900	-1.33010200	2.50803200
C	-1.05554000	-1.88087400	3.04881100
C	-2.35571200	-1.47370000	2.46666700
N	-2.31179300	-0.63304600	1.42947500
C	-3.44698100	-0.26027400	0.83264000
C	-4.69632900	-0.66464200	1.28405400
C	-4.75222100	-1.50553200	2.38471500
C	-3.23595300	0.75545600	-0.25555200
O	-2.24538200	1.49765900	-0.14778700
N	-4.11736000	0.89684600	-1.25369300
C	-5.03227600	-0.13189700	-1.64492400
C	-3.95860600	2.03620700	-2.17471800
C	-3.12127100	1.70518400	-3.39585100
C	-6.39403000	0.14755600	-1.73203800
C	-5.45655900	-2.38193200	-2.36701500
C	-4.55840900	-1.39688500	-1.97701600
H	0.35782100	-3.82214500	5.43857400
H	2.39816300	-2.75029900	4.43991900
H	-5.60032300	-0.32877800	0.79423000
H	-5.70922400	-1.83060100	2.77832600
H	-3.51314600	2.85117100	-1.60479700
H	-4.96654200	2.33879700	-2.46746000
H	-3.12845100	2.55523100	-4.08301800
H	-3.51912300	0.84039600	-3.93179600
H	-2.08416700	1.50230800	-3.12463900
H	-6.76433400	1.13475900	-1.47111900
H	-5.07751000	-3.36680800	-2.62425000
H	-3.49299800	-1.60438800	-1.93640500
C	-7.27599900	-0.84496900	-2.13089600
H	-8.33706100	-0.61969300	-2.19036900
C	1.23338500	-1.64804800	3.01221100
H	2.08392900	-1.15358300	2.55935300
C	7.76681100	-1.55080000	-1.42979500
C	-6.82491900	-2.12771000	-2.45396000
C	3.19467400	2.97822200	-1.94784100
H	3.22677600	4.00367700	-2.29439700
C	1.64180400	4.92675500	-0.31749700
H	2.56841400	5.30908500	-0.72815400
C	-0.96781400	-2.78928900	4.10253800
H	-1.85474600	-3.23933000	4.52900500

C	-3.57506600	-1.92780600	2.97386600
H	-3.61359800	-2.58914800	3.82928100
C	-7.78232900	-3.18465800	-2.91760900
H	-8.75228700	-3.09558200	-2.42295200
H	-7.95991500	-3.10109600	-3.99500200
H	-7.39689100	-4.18865400	-2.72897600
C	9.24158300	-1.42955700	-1.67182200
H	9.76841200	-2.31932500	-1.31178000
H	9.46751500	-1.33100000	-2.73632400
H	9.66633900	-0.56705400	-1.15497600
Am	-0.08543400	0.46341200	0.55062300

Cm(L_a)₂(NO₃)₂⁺

C	0.69807400	5.77482300	0.58276700
C	-0.43969400	5.21284000	1.13848000
N	0.26290000	3.03639700	0.43448200
C	1.35330200	3.58049500	-0.12606500
C	2.28184000	2.65280900	-0.81080600
N	2.20957900	1.36847800	-0.46434000
C	3.03028700	0.48312300	-1.03562000
C	3.92102300	0.83801700	-2.04159200
C	3.97096300	2.16793800	-2.43464700
C	2.77349000	-0.92133100	-0.56049100
O	1.69064300	-1.14901200	0.00338900
N	3.64187200	-1.92423700	-0.76646900
C	5.02818300	-1.74770100	-1.06221800
C	3.18298100	-3.29260100	-0.45047500
C	2.19242500	-3.83900200	-1.46260700
C	5.57905200	-2.33695000	-2.19795600
C	7.19302400	-0.87879700	-0.47806200
C	5.84252500	-1.03024600	-0.19302600
H	0.88379000	6.84140800	0.65356300
H	-1.17838700	5.81639000	1.65265900
H	4.54801000	0.10147300	-2.52389400
H	4.63495500	2.47499300	-3.23542300
H	2.73758300	-3.27585700	0.54706600
H	4.08058300	-3.90970300	-0.40369400
H	1.91678000	-4.86012000	-1.18705000
H	2.61964800	-3.87007400	-2.46793900
H	1.27876400	-3.24330800	-1.49000900
H	4.94558000	-2.89634300	-2.87929900
H	7.81753000	-0.31195600	0.20628700
H	5.41955000	-0.59147900	0.70571300
N	0.54291000	1.45746400	3.28106200

O	-0.64755100	1.40703400	2.83214400
O	0.79717100	1.85293100	4.38114000
O	1.44321400	1.05571000	2.47534400
N	-0.66148300	-0.58095700	-2.13315500
O	0.00177000	0.47840300	-1.92809700
O	-0.86402600	-1.01101600	-3.23762800
O	-1.11021400	-1.15773000	-1.09335700
C	6.93165200	-2.18714900	-2.46428700
H	7.34967300	-2.64683600	-3.35532700
C	-0.61159500	3.83931200	1.04196400
H	-1.47711600	3.35287000	1.47407900
C	0.11811900	-3.41052500	4.47748400
C	1.26741400	-2.83287400	3.96363500
N	-0.04495800	-1.52488100	2.44619100
C	-1.16205100	-2.07348400	2.94836700
C	-2.44613200	-1.61707400	2.36499800
N	-2.36804200	-0.71318500	1.38715800
C	-3.48047500	-0.29348800	0.78242900
C	-4.74643400	-0.71176500	1.17079600
C	-4.83926800	-1.62068000	2.21403300
C	-3.21842200	0.77709900	-0.24009300
O	-2.21529500	1.49118900	-0.06271400
N	-4.06189100	0.99001100	-1.25649300
C	-4.98432900	0.00264300	-1.72950400
C	-3.85576300	2.17437100	-2.10917900
C	-3.01483100	1.88630700	-3.33854100
C	-6.33707000	0.31342500	-1.84208800
C	-5.42621000	-2.19740100	-2.58303500
C	-4.52316100	-1.25218800	-2.11454700
H	0.17152000	-4.14710400	5.27222100
H	2.25067100	-3.08945200	4.34025300
H	-5.63399000	-0.33785400	0.67830500
H	-5.80960100	-1.96193400	2.55825300
H	-3.39158300	2.93997500	-1.48831900
H	-4.84997900	2.52617700	-2.39423900
H	-2.97856800	2.77758000	-3.97037600
H	-3.43937300	1.07422700	-3.93323200
H	-1.99064400	1.62399800	-3.06888700
H	-6.69761200	1.29227300	-1.53951700
H	-5.05716700	-3.17459100	-2.88086000
H	-3.46363000	-1.48385800	-2.05328400
C	-7.22405700	-0.63951900	-2.31922600
H	-8.27853700	-0.39069800	-2.39808100
C	1.13171900	-1.89576900	2.95004200

H	1.99950100	-1.40345200	2.52945200
C	7.76321800	-1.45331200	-1.61391000
C	-6.78660100	-1.91188500	-2.69673400
C	3.16050300	3.09235500	-1.80385200
H	3.17535500	4.13071400	-2.11127600
C	1.60612600	4.94816100	-0.06127100
H	2.51402800	5.36318100	-0.48174700
C	-1.11042400	-3.02596200	3.96463200
H	-2.01409700	-3.46789400	4.36357700
C	-3.68298900	-2.09256100	2.80751700
H	-3.75220000	-2.81098600	3.61365500
C	-7.74765100	-2.92411900	-3.24487400
H	-8.73869000	-2.82418900	-2.79646300
H	-7.86745600	-2.79864200	-4.32619100
H	-7.39957600	-3.94477100	-3.07347700
C	9.22914500	-1.32124900	-1.90012900
H	9.76849100	-2.22062200	-1.58522200
H	9.42004200	-1.18888400	-2.96774000
H	9.66950900	-0.47446000	-1.37042200
Cm	-0.08648700	0.42801700	0.61429400

Eu(L_a)₂(NO₃)₂⁺

C	0.62410500	5.85130300	0.27454100
C	-0.53271100	5.31281400	0.81361800
N	0.20731300	3.10518800	0.26029300
C	1.31617600	3.62553000	-0.28484900
C	2.27196600	2.66702300	-0.88342100
N	2.18305600	1.39888400	-0.48446800
C	3.01968500	0.48729500	-0.99052500
C	3.95007800	0.79786900	-1.97501600
C	4.02298800	2.11110500	-2.41803500
C	2.73185200	-0.89341200	-0.46737900
O	1.64195300	-1.07248000	0.10025600
N	3.57253700	-1.92689700	-0.63017800
C	4.96256500	-1.80507800	-0.93607200
C	3.07611600	-3.26760500	-0.25534100
C	2.05678200	-3.82430300	-1.23276200
C	5.48691200	-2.43947300	-2.05979500
C	7.15922400	-0.99912800	-0.38083100
C	5.80559300	-1.09634200	-0.08735100
H	0.80218900	6.92135200	0.29381000
H	-1.29450600	5.93883400	1.26328900
H	4.59093100	0.04052400	-2.40360300

H	4.71998400	2.38357600	-3.20311700
H	2.64534200	-3.19873300	0.74655100
H	3.95597700	-3.90869400	-0.19572900
H	1.76614800	-4.83041600	-0.91982500
H	2.46623700	-3.89621600	-2.24335000
H	1.15479600	-3.21147100	-1.26401800
H	4.83075000	-2.99163400	-2.72534500
H	7.80634800	-0.43814400	0.28715200
H	5.40213600	-0.62044400	0.80137700
N	0.42092300	1.76261300	3.16145800
O	-0.75800300	1.61823800	2.71319300
O	0.65095200	2.24514700	4.23187400
O	1.34760400	1.35462600	2.38690700
N	-0.66116100	-0.58150200	-2.05158200
O	-0.00621900	0.48868700	-1.90587700
O	-0.87984300	-1.06717100	-3.12976300
O	-1.08803300	-1.11388300	-0.97735800
C	6.84276200	-2.34347900	-2.33491900
H	7.24017200	-2.83788700	-3.21673600
C	-0.69429900	3.93462100	0.78636700
H	-1.57324800	3.46591000	1.21098200
C	0.30896200	-3.07365700	4.66868900
C	1.42711100	-2.44507900	4.14503800
N	0.05416100	-1.26498800	2.57775500
C	-1.03343300	-1.85627400	3.09444600
C	-2.33575700	-1.47878300	2.49757600
N	-2.29430100	-0.63110800	1.46820800
C	-3.42620200	-0.27718500	0.85667900
C	-4.67426700	-0.70977800	1.28548800
C	-4.72883700	-1.56018000	2.37937100
C	-3.20819300	0.74687400	-0.22228100
O	-2.22026300	1.49028100	-0.09811700
N	-4.07690900	0.89278700	-1.23047100
C	-4.98341000	-0.13662200	-1.63908800
C	-3.91530600	2.04069000	-2.14056900
C	-3.08762900	1.71835500	-3.37054700
C	-6.34561300	0.13641800	-1.73655100
C	-5.38874300	-2.38283500	-2.38352300
C	-4.49966200	-1.39628700	-1.97724700
H	0.39898100	-3.78295300	5.48466400
H	2.42030900	-2.63188000	4.53646500
H	-5.57812000	-0.38921100	0.78526200
H	-5.68486600	-1.90766300	2.75586500
H	-3.46136500	2.84617900	-1.56413100

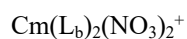
H	-4.92295700	2.35341300	-2.42409900
H	-3.09311700	2.57731500	-4.04659200
H	-3.49555000	0.86363800	-3.91496900
H	-2.05041400	1.50387000	-3.10933200
H	-6.72358500	1.11936100	-1.47072300
H	-5.00215200	-3.36360300	-2.64516200
H	-3.43374300	-1.59924400	-1.92808000
C	-7.21858200	-0.85759000	-2.15144200
H	-8.28027300	-0.63754900	-2.21860700
C	1.24593000	-1.55097200	3.10029700
H	2.08726800	-1.02129900	2.67070900
C	7.70359200	-1.62001500	-1.50505300
C	-6.75768600	-2.13516400	-2.48078200
C	3.19144800	3.06167100	-1.85887500
H	3.22230500	4.08603100	-2.20881900
C	1.56104700	4.99633400	-0.28573100
H	2.48304400	5.39426100	-0.69179400
C	-0.93575500	-2.77509800	4.13822800
H	-1.81601400	-3.25784100	4.54242900
C	-3.55242100	-1.96255200	2.98407900
H	-3.58998600	-2.63018500	3.83480900
C	-7.70497800	-3.19358500	-2.96151600
H	-8.68115200	-3.11127200	-2.47808200
H	-7.86993700	-3.10499000	-4.04051400
H	-7.31751800	-4.19695500	-2.77362100
C	9.17196000	-1.54684100	-1.79958700
H	9.68212400	-2.45231900	-1.45489300
H	9.36310800	-1.45814600	-2.87159400
H	9.64244600	-0.69748400	-1.30078500
Eu	-0.08947300	0.51882600	0.61590700

Am(L_b)₂(NO₃)₂⁺

C	-0.87285400	5.12676900	-2.48563600
C	0.22410600	4.41219900	-2.89939700
N	-0.43849200	2.52800600	-1.57857300
C	-1.53707400	3.20639900	-1.19218000
C	-1.79161100	4.53161400	-1.60313200
C	-2.48220100	2.54781400	-0.32473400
C	-3.59843300	3.27134300	0.15543400
N	-2.26643900	1.26420000	0.00094300
C	-3.11895200	0.64088600	0.80292700
C	-4.21881700	1.29664600	1.37894200
C	-4.45307900	2.60907100	1.04858300

C	-2.69676000	-0.77236100	1.09797100
O	-1.52915800	-1.09127000	0.82263100
N	-3.51321500	-1.66743700	1.68083400
C	-4.93759700	-1.57209500	1.70129600
C	-2.91202900	-2.94546700	2.11439700
C	-2.05579300	-2.80988000	3.36011000
C	-5.62273700	-1.63326900	2.91262300
C	-7.03508800	-1.39235300	0.53793200
C	-5.64877900	-1.46702800	0.51077800
H	-1.04145000	6.14243200	-2.83111100
H	0.94751500	4.83371100	-3.58760700
H	-4.87165500	0.78498600	2.07171500
H	-5.29868600	3.13854900	1.47662500
H	-2.31668500	-3.33493600	1.28502200
H	-3.74346800	-3.63110800	2.27971200
H	-1.65829000	-3.78943000	3.63753600
H	-2.63399500	-2.43342200	4.20755600
H	-1.20931000	-2.14291600	3.19050100
H	-5.06981900	-1.71258900	3.84337600
H	-7.57853300	-1.30409200	-0.39827000
H	-5.11730100	-1.44109700	-0.43593000
N	-0.62199500	-0.13317300	-3.40676200
O	0.57557100	0.05393100	-3.02798400
O	-0.91982600	-0.27947400	-4.55680400
O	-1.49060500	-0.15729200	-2.47306300
N	0.77386800	0.69284800	2.26191500
O	0.00978700	1.46166100	1.61149500
O	1.03376100	0.86560500	3.42237000
O	1.26502200	-0.27978800	1.60211100
C	-7.00778000	-1.56876800	2.92429800
H	-7.53192000	-1.61169800	3.87482100
C	-3.80811900	4.62068300	-0.26002700
H	-4.67460400	5.15401400	0.11783300
C	-2.94647700	5.22014400	-1.11722100
H	-3.11518100	6.24208400	-1.44260800
C	0.40798900	3.11344900	-2.40869800
H	1.27202400	2.52633400	-2.69666600
C	0.08676100	-5.01869600	-2.36335100
C	-1.09715500	-4.35619800	-2.14967100
N	0.06553800	-2.41000500	-1.37089400
C	1.23360700	-3.04894300	-1.58606600
C	1.30078000	-4.36745800	-2.08404800
C	2.45758900	-2.34587900	-1.30168100
C	3.69633800	-2.98700900	-1.52540300

N	2.37398200	-1.08718300	-0.84411200
C	3.48272800	-0.42477400	-0.55366400
C	4.75905800	-0.97208500	-0.75512300
C	4.85877500	-2.24990900	-1.24878300
C	3.22071300	1.00053700	-0.15030500
O	2.18392500	1.52722900	-0.58605900
N	4.10458800	1.68558700	0.58794500
C	5.07293300	1.05396500	1.43017300
C	3.88670700	3.12970400	0.77933600
C	3.04099600	3.45133100	1.99731200
C	6.41885200	1.39767200	1.32101800
C	5.61642100	-0.47664000	3.19879700
C	4.66688500	0.12415500	2.38190600
H	0.09752100	-6.03273000	-2.75177300
H	-2.05210900	-4.82044800	-2.36698400
H	5.64649400	-0.39531400	-0.53133700
H	5.83295500	-2.69466300	-1.42750700
H	3.42028300	3.50824700	-0.13020400
H	4.87711200	3.58214000	0.86495000
H	3.00112300	4.53468400	2.13758800
H	3.46235400	3.01326600	2.90503900
H	2.01842600	3.09061900	1.87731900
H	6.73648800	2.12133100	0.57595000
H	5.29009300	-1.20152300	3.93890600
H	3.61365600	-0.12052300	2.48605600
C	3.72452600	-4.32331900	-2.02759000
H	4.68658300	-4.79754200	-2.19385600
C	2.57269500	-4.98591200	-2.29461500
H	2.59782000	-6.00096200	-2.67880600
C	-1.05709400	-3.04758800	-1.65291300
H	-1.97313700	-2.48902800	-1.49824400
C	-7.73999100	-1.44353100	1.74032400
C	6.96927400	-0.15423300	3.10230400
C	-9.23860200	-1.40222100	1.76594100
H	-9.65287900	-2.41182100	1.85586400
H	-9.61033200	-0.82519900	2.61595600
H	-9.64664500	-0.96228000	0.85404100
C	7.35193200	0.79512300	2.15008300
H	8.39988600	1.06499500	2.05439600
C	7.98351600	-0.77456000	4.01627100
H	8.92951900	-0.96010800	3.50191800
H	8.20002800	-0.11270500	4.86138600
H	7.63015900	-1.72221400	4.42728300
Am	0.07185600	0.14989800	-0.57341300



C	-0.84802900	5.01287100	-2.68142300
C	0.22139800	4.25857100	-3.09750600
N	-0.46201600	2.42746000	-1.71326200
C	-1.53594800	3.14503400	-1.32586100
C	-1.76470400	4.46501500	-1.76685200
C	-2.48475700	2.53371600	-0.42836500
C	-3.57595700	3.29384100	0.05074600
N	-2.29472400	1.25444400	-0.08078600
C	-3.14853600	0.66372900	0.74076900
C	-4.22535900	1.35542400	1.31999700
C	-4.43263300	2.66758600	0.96850200
C	-2.74997600	-0.75628900	1.04321300
O	-1.59689300	-1.10628100	0.74314800
N	-3.57126400	-1.62549300	1.65597200
C	-4.99197400	-1.49452300	1.71364300
C	-2.99092900	-2.91275200	2.09035700
C	-2.10494400	-2.78464500	3.31591900
C	-5.64485700	-1.51948800	2.94373400
C	-7.11474500	-1.28245900	0.60362200
C	-5.73203300	-1.39152500	0.54060700
H	-0.99663500	6.02333700	-3.05057400
H	0.94130100	4.64232900	-3.81099000
H	-4.88119900	0.87351000	2.03105400
H	-5.25984000	3.22403300	1.39836100
H	-2.42278100	-3.32485400	1.25309900
H	-3.83439000	-3.57693500	2.28047700
H	-1.72612200	-3.77074000	3.59633300
H	-2.65538800	-2.38446800	4.17091700
H	-1.24582800	-2.14111100	3.12090400
H	-5.06901300	-1.59690900	3.86063000
H	-7.68108800	-1.19630800	-0.31910700
H	-5.22520400	-1.39500400	-0.41981300
N	-0.63852700	-0.36282600	-3.40900500
O	0.55018500	-0.09881800	-3.03666100
O	-0.92104300	-0.56633500	-4.55377400
O	-1.50477800	-0.39803900	-2.47675500
N	0.71263100	0.66360600	2.24144900
O	-0.03211400	1.42261500	1.55351700
O	0.95529900	0.87525400	3.39974500
O	1.20022200	-0.33443600	1.62315100
C	-7.02727300	-1.42107200	2.99123600
H	-7.52643600	-1.43581400	3.95592300

C	-3.75728400	4.63828000	-0.39338200
H	-4.60370300	5.20352000	-0.01635000
C	-2.89390000	5.19411200	-1.27836300
H	-3.04212900	6.21186600	-1.62611200
C	0.38191300	2.96898200	-2.57579500
H	1.22399600	2.35219200	-2.86714900
C	0.30660400	-5.16802000	-2.14561200
C	-0.90233000	-4.54314300	-1.96158300
N	0.18151900	-2.52086600	-1.26556400
C	1.37372400	-3.12356300	-1.45230800
C	1.49358200	-4.45904000	-1.89174300
C	2.57082400	-2.36547100	-1.19358200
C	3.83436000	-2.96985200	-1.37789400
N	2.43717000	-1.09456700	-0.79112500
C	3.51496300	-0.38278700	-0.50866600
C	4.81388100	-0.88841400	-0.67286900
C	4.96557000	-2.17931200	-1.11809400
C	3.18482100	1.03941500	-0.14710500
O	2.12777500	1.50709600	-0.60521400
N	4.02394200	1.78250300	0.58545400
C	5.00971700	1.21429500	1.45282900
C	3.73885100	3.21919700	0.74249000
C	2.89615900	3.53166000	1.96485400
C	6.34043400	1.61253400	1.35006000
C	5.59595300	-0.25300400	3.26094900
C	4.63190400	0.28971300	2.42152500
H	0.35756200	-6.19657800	-2.49024100
H	-1.83813300	-5.05282300	-2.15967800
H	5.67729700	-0.27262600	-0.45905200
H	5.95750700	-2.59428700	-1.26860800
H	3.24186000	3.54940900	-0.16950900
H	4.70738400	3.72109500	0.80091100
H	2.80020700	4.61515200	2.07332400
H	3.35550800	3.14528700	2.87764600
H	1.89285800	3.11270200	1.87467200
H	6.63602900	2.33217900	0.59220700
H	5.29195200	-0.97481900	4.01348300
H	3.58878900	0.00305200	2.52115300
C	3.91501000	-4.32405200	-1.82301000
H	4.89442400	-4.77074500	-1.96211200
C	2.78923400	-5.03790900	-2.06921100
H	2.85364600	-6.06675600	-2.40971200
C	-0.91473400	-3.21402300	-1.52046200
H	-1.85173900	-2.68613700	-1.38705200

C	-7.78785500	-1.29718800	1.82528400
C	6.93574900	0.12307700	3.17004700
C	-9.28392800	-1.22031300	1.88915500
H	-9.71995800	-2.22099500	1.97646800
H	-9.62062200	-0.64578700	2.75518800
H	-9.70379600	-0.75933000	0.99308000
C	7.28877000	1.06691000	2.20164300
H	8.32559200	1.37794700	2.11044400
C	7.96291600	-0.43613300	4.10867000
H	8.94323000	-0.51592600	3.63340500
H	8.07957500	0.21032800	4.98490400
H	7.68059000	-1.42648100	4.47163000
Cm	0.06648400	0.09495100	-0.60781600

Eu(L_b)₂(NO₃)₂⁺

C	-0.79891300	5.02812000	-2.71019200
C	0.27741800	4.27644900	-3.11349800
N	-0.41656600	2.44310900	-1.73800200
C	-1.49475900	3.15846600	-1.36277100
C	-1.72415100	4.47746700	-1.80609100
C	-2.44832400	2.54143400	-0.47572600
C	-3.55038900	3.29472900	-0.01059000
N	-2.25289700	1.26284000	-0.12560100
C	-3.11644900	0.66664900	0.68376700
C	-4.20444500	1.35252600	1.24819900
C	-4.41507300	2.66378100	0.89560800
C	-2.71614100	-0.75225400	0.98552200
O	-1.56651600	-1.09920600	0.67307600
N	-3.52895300	-1.62337300	1.60762300
C	-4.94939100	-1.49825600	1.68104300
C	-2.94011700	-2.91036600	2.03195100
C	-2.03336800	-2.78369600	3.24239200
C	-5.58772000	-1.51594000	2.91878000
C	-7.08592900	-1.30426900	0.59419800
C	-5.70369900	-1.40798500	0.51594700
H	-0.94630300	6.03792300	-3.08161000
H	1.00418500	4.66226700	-3.81892900
H	-4.86692200	0.86602500	1.94967200
H	-5.25106900	3.21492300	1.31513100
H	-2.38622200	-3.32234500	1.18502200
H	-3.78016600	-3.57471300	2.23622700
H	-1.65865300	-3.77189400	3.52100800
H	-2.56681200	-2.37524000	4.10423800

H	-1.17173700	-2.14890700	3.03100900
H	-5.00052900	-1.58314400	3.82926700
H	-7.66350900	-1.22774800	-0.32241500
H	-5.20795900	-1.41573800	-0.45020000
N	-0.60388000	-0.28488700	-3.40843900
O	0.58671300	-0.05987800	-3.02120700
O	-0.88029500	-0.46560400	-4.55898100
O	-1.47995800	-0.30758700	-2.48662800
N	0.69854900	0.59500300	2.18566200
O	-0.04767900	1.36863800	1.51803700
O	0.94191200	0.77839700	3.34883900
O	1.18697000	-0.38569300	1.54279200
C	-6.97004900	-1.42326100	2.98172500
H	-7.45782300	-1.43221700	3.95227300
C	-3.73353600	4.63848500	-0.45653000
H	-4.58787900	5.19831000	-0.08944800
C	-2.86261300	5.20033500	-1.33028000
H	-3.01252100	6.21762900	-1.67868100
C	0.43534400	2.98679700	-2.59042000
H	1.28063200	2.37046300	-2.87334000
C	0.26010900	-5.09736700	-2.29497400
C	-0.94606300	-4.47333200	-2.09001300
N	0.14655400	-2.47219700	-1.34941000
C	1.33478600	-3.07331600	-1.55789600
C	1.45022000	-4.39776300	-2.03008700
C	2.53198400	-2.32217400	-1.28541100
C	3.79438500	-2.92393500	-1.48581500
N	2.39976600	-1.06075800	-0.85155400
C	3.48040900	-0.36103200	-0.54724300
C	4.77776200	-0.86570800	-0.72369800
C	4.92739500	-2.14373000	-1.20522600
C	3.15181500	1.04943100	-0.14452200
O	2.09288200	1.52536200	-0.58677600
N	3.99145600	1.77377600	0.60657700
C	4.98237500	1.18469000	1.45361500
C	3.70236700	3.20464400	0.80444400
C	2.86808700	3.48226800	2.04102700
C	6.31155700	1.58920500	1.35570700
C	5.58080700	-0.32850500	3.21938500
C	4.61146500	0.23351400	2.39898700
H	0.30623600	-6.11748300	-2.66445900
H	-1.88420000	-4.97565700	-2.29587800
H	5.64201400	-0.25822600	-0.49040100
H	5.91845900	-2.55659400	-1.36677000

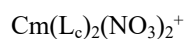
H	3.19728300	3.55711900	-0.09465600
H	4.66952500	3.70858000	0.86881600
H	2.77091700	4.56234200	2.17868100
H	3.33531300	3.07301300	2.93972500
H	1.86482100	3.06388100	1.94812200
H	6.60163900	2.32971600	0.61605200
H	5.28237600	-1.07118200	3.95364400
H	3.56981000	-0.05936500	2.49507300
C	3.87158700	-4.26670400	-1.96547000
H	4.85020200	-4.71078700	-2.11789400
C	2.74454700	-4.97330500	-2.22655400
H	2.80724300	-5.99341700	-2.59270000
C	-0.95255800	-3.15530500	-1.61595200
H	-1.88690300	-2.62701700	-1.46585400
C	-7.74466400	-1.31208800	1.82388400
C	6.91911000	0.05397700	3.13296500
C	-9.24027300	-1.24144900	1.90409600
H	-9.67145800	-2.24451300	1.98830900
H	-9.57013300	-0.67472100	2.77779200
H	-9.67133200	-0.77561900	1.01582900
C	7.26524300	1.02418300	2.18849400
H	8.30075400	1.34062700	2.10107100
C	7.95187300	-0.52670400	4.05221200
H	8.93028200	-0.59140800	3.57077200
H	8.07070800	0.09702500	4.94448000
H	7.67378100	-1.52695300	4.39046100
Eu	0.06957800	0.11385400	-0.63778700

Am(Lc)₂(NO₃)₂⁺

C	-0.94214300	3.70388700	-4.52009000
C	-1.93416400	3.53017700	-3.56946900
N	-0.48883200	2.12103100	-2.28467500
C	0.47038600	2.27488000	-3.21149700
C	1.73789600	1.55817500	-2.95886900
N	1.89614400	1.04063100	-1.75099400
C	3.01131500	0.34892600	-1.48080600
C	4.04023000	0.12420500	-2.40103200
C	3.86655400	0.68456900	-3.68189800
C	3.09984600	-0.18339200	-0.13424000
O	2.22628600	0.05562700	0.71705800
N	4.18999900	-0.94904900	0.17250200
C	4.24270800	-1.47642400	1.54977500

C	3.33264100	-2.67275800	1.76014600
H	-1.10733200	4.33198500	-5.38910900
H	-2.90121100	4.01016300	-3.66363800
H	4.62398200	0.54043100	-4.44587200
H	3.94909100	-0.65724400	2.20738900
H	5.28168100	-1.72524000	1.75703200
H	3.43639800	-3.02525200	2.78936100
H	3.59603000	-3.49967800	1.09784000
H	2.28550200	-2.41341100	1.59955400
N	-0.03675000	3.88050400	0.34174800
O	-1.08737900	3.18167000	0.49140200
O	-0.03410100	5.07188300	0.45757400
O	1.01819100	3.22334300	0.05863800
N	-0.06863200	-1.97686000	-0.32018000
O	0.27586800	-1.18691300	-1.25022300
O	-0.10331600	-3.16836800	-0.46868600
O	-0.37698700	-1.42475400	0.78228500
C	-1.65732900	2.73199600	-2.46746600
H	-2.39484900	2.57843300	-1.68927500
C	1.07571400	2.72355200	5.09558400
C	2.01924700	2.80369200	4.08471900
N	0.53988900	1.67145100	2.58275600
C	-0.37200800	1.57937300	3.56405900
C	-1.63916200	0.90531000	3.21206200
N	-1.84263300	0.66346300	1.92672900
C	-2.97103800	0.04705300	1.55083700
C	-3.96174700	-0.38706800	2.43776300
C	-3.73391000	-0.13098000	3.80428700
C	-3.12353100	-0.15444300	0.12132100
O	-2.29526400	0.29217000	-0.68963200
N	-4.22631000	-0.84156500	-0.30501100
C	-5.19836000	-1.30284700	0.57517800
C	-4.34699500	-1.03144100	-1.76365900
C	-3.43526400	-2.12083200	-2.29871700
H	1.27277100	3.14461100	6.07583900
H	2.97807300	3.28444900	4.23948400
H	-4.45885300	-0.45180000	4.54568200
H	-4.10162200	-0.07309900	-2.22344200
H	-5.39252700	-1.25142500	-1.97027200
H	-3.61093600	-2.23908800	-3.37087800
H	-3.63249600	-3.08280900	-1.82160900
H	-2.38343800	-1.86991300	-2.15833500
C	1.70203300	2.26568000	2.84473900
H	2.39965500	2.32320600	2.01804700

C	5.20472200	-1.19535100	-0.74537400
C	6.35136600	-2.04313500	-0.33755900
C	7.57553300	-1.45628900	-0.02276600
C	6.24246100	-3.43552200	-0.31182300
C	8.66287700	-2.24701600	0.32790400
H	7.67717700	-0.37534600	-0.04668400
C	7.33457800	-4.21480100	0.03522000
H	5.30524400	-3.91128500	-0.58406100
C	8.56317300	-3.63657200	0.36526400
H	9.60782400	-1.77114300	0.57380200
H	7.23373300	-5.29662300	0.04317900
C	-6.36171500	-2.04933500	0.03819800
C	-7.60940000	-1.43201300	-0.04081100
C	-6.24516400	-3.38783900	-0.34139300
C	-8.71215300	-2.13646100	-0.50564500
H	-7.71593300	-0.39271600	0.25552000
C	-7.35388700	-4.08349900	-0.79859200
H	-5.28787300	-3.89352800	-0.26021400
C	-8.60617300	-3.47220000	-0.89187400
H	-9.67464300	-1.63631100	-0.56554700
H	-7.24548900	-5.12635500	-1.08320200
C	-5.08944700	-1.06949900	1.91041600
H	-5.86247600	-1.44544600	2.56902600
C	5.15019700	-0.66320300	-1.99540500
H	5.95456400	-0.87831200	-2.68784800
C	9.73905200	-4.49487400	0.72482700
H	10.10416700	-5.04376600	-0.14896600
H	10.56910200	-3.90136700	1.11201800
H	9.47394700	-5.23706700	1.48256300
C	-9.80434200	-4.24234800	-1.36050500
H	-10.25283400	-4.80261500	-0.53326700
H	-10.57587600	-3.58331400	-1.76348600
H	-9.53946200	-4.96621700	-2.13454500
C	0.27649200	3.06632300	-4.34095600
H	1.06812300	3.20814100	-5.06587300
C	2.72677600	1.39358600	-3.95501200
H	2.57836100	1.80308700	-4.94623200
C	-2.58584600	0.51255500	4.18436700
H	-2.39869700	0.69371700	5.23521600
C	-0.13581100	2.10182900	4.83351100
H	-0.89057900	2.04939800	5.60809100
Am	-0.00349600	0.95941600	0.07059900



C	-1.07093300	3.26293200	-4.78751300
C	-2.01279000	3.22450700	-3.77301200
N	-0.52673300	1.93516700	-2.40941600
C	0.38473800	1.96029000	-3.39578100
C	1.65770700	1.25802200	-3.12530200
N	1.86199600	0.87719900	-1.87632400
C	2.98702800	0.22169800	-1.57025000
C	3.98316500	-0.10601500	-2.49552800
C	3.75757000	0.30228600	-3.82527700
C	3.12565000	-0.14859900	-0.17429800
O	2.28104000	0.18713400	0.67452200
N	4.23035500	-0.87070600	0.18025800
C	4.33797400	-1.23006600	1.60761700
C	3.43699400	-2.38838700	1.99585200
H	-1.27126100	3.79060000	-5.71405100
H	-2.97400100	3.71528800	-3.87122700
H	4.48584900	0.07037000	-4.59597200
H	4.07033000	-0.33686200	2.17371800
H	5.38467800	-1.45572100	1.80209500
H	3.59042500	-2.62280100	3.05217900
H	3.66498000	-3.28733700	1.41974000
H	2.38376200	-2.14128300	1.85757500
N	0.01207100	3.88452400	0.11067600
O	-1.04821300	3.20219200	0.28566700
O	0.01688700	5.08076900	0.14241400
O	1.06743600	3.20417200	-0.10021000
N	0.01280900	-2.00459400	-0.02429400
O	0.28235200	-1.30833900	-1.05095800
O	0.01304200	-3.20559600	-0.04641100
O	-0.25805500	-1.34714100	1.02795800
C	-1.69175500	2.55054400	-2.60226200
H	-2.38920400	2.50899800	-1.77470900
C	1.04923100	3.00348300	4.96507300
C	1.99841100	3.01639800	3.95675400
N	0.52352600	1.79638000	2.51918400
C	-0.39408200	1.76988500	3.49982600
C	-1.66375400	1.07948100	3.18705800
N	-1.86986000	0.77918000	1.91670600
C	-2.99246300	0.13850700	1.57212700
C	-3.98096300	-0.25841000	2.47850200
C	-3.75353800	0.06485100	3.83100200
C	-3.12647600	-0.15385300	0.15680600

O	-2.26746300	0.20903900	-0.66607500
N	-4.23453400	-0.84852500	-0.23992700
C	-5.21801100	-1.25076500	0.65701400
C	-4.30200800	-1.20703600	-1.66978300
C	-3.47806600	-2.44002200	-1.99282000
H	1.24209400	3.48502800	5.91794700
H	2.95832300	3.50242500	4.08634200
H	-4.47692000	-0.22262000	4.58745600
H	-3.93619900	-0.34364400	-2.22512900
H	-5.35068300	-1.35663500	-1.91772200
H	-3.57593600	-2.67095000	-3.05639100
H	-3.82591900	-3.30901400	-1.42987300
H	-2.41915700	-2.28254500	-1.78217900
C	1.68660000	2.40203100	2.75117700
H	2.38967000	2.40283300	1.92739000
C	5.21409200	-1.21906500	-0.73929300
C	6.38371000	-2.00607000	-0.27925900
C	7.62211700	-1.38425200	-0.12751200
C	6.28403400	-3.37921900	-0.04492100
C	8.73264600	-2.11918400	0.26743700
H	7.71533900	-0.31812200	-0.31179700
C	7.39958300	-4.10395700	0.34418100
H	5.33463500	-3.88626700	-0.18694600
C	8.64291700	-3.48886900	0.51073000
H	9.68775100	-1.61547200	0.38593000
H	7.30471000	-5.17259000	0.51587800
C	-6.39309900	-1.99793100	0.14290400
C	-7.50234300	-1.31816600	-0.36331600
C	-6.42277900	-3.38994200	0.20255800
C	-8.61023500	-2.02305500	-0.80954000
H	-7.49924200	-0.23262200	-0.40368300
C	-7.53727100	-4.08600500	-0.24725200
H	-5.57278400	-3.93160300	0.60666000
C	-8.64863400	-3.41825500	-0.76047900
H	-9.46589400	-1.47796400	-1.19828900
H	-7.54227300	-5.17097000	-0.19400700
C	-5.11005700	-0.96159600	1.98068000
H	-5.89863300	-1.28315300	2.64966700
C	5.11196500	-0.83728400	-2.04067300
H	5.89329300	-1.13012600	-2.73101600
C	9.84636600	-4.28968100	0.90925200
H	10.24506600	-4.84425700	0.05341300
H	10.64771700	-3.65305600	1.28880000
H	9.60214300	-5.02250000	1.68219000

C	-9.86364300	-4.17051800	-1.21481100
H	-10.61244700	-4.21565700	-0.41697900
H	-10.33657200	-3.69019300	-2.07450100
H	-9.62132900	-5.19814000	-1.49271200
C	0.14377800	2.62123300	-4.59775600
H	0.89798600	2.65914100	-5.37369500
C	2.60669900	0.97875400	-4.13489400
H	2.42159000	1.27401600	-5.16007400
C	-2.60645900	0.72866400	4.17979600
H	-2.41757800	0.95679700	5.22131300
C	-0.16298700	2.37030000	4.73495900
H	-0.92355400	2.36915500	5.50573400
Cm	0.00335200	0.95472100	0.02963500

Eu(L_c)₂(NO₃)₂⁺

C	-1.09489700	3.21624400	-4.84397100
C	-2.03821100	3.19450100	-3.83019900
N	-0.54750200	1.94445700	-2.43608300
C	0.36536300	1.95511500	-3.42032600
C	1.63987900	1.26726300	-3.12701300
N	1.83301100	0.90084400	-1.87105500
C	2.96012900	0.25520200	-1.54869500
C	3.96692300	-0.07688600	-2.46036600
C	3.75412500	0.31863500	-3.79588300
C	3.08723400	-0.09873500	-0.14817000
O	2.23552900	0.25049800	0.68650500
N	4.18808500	-0.81781200	0.22492200
C	4.28165900	-1.15989300	1.65749400
C	3.36954900	-2.30677300	2.05406600
H	-1.29713500	3.72157500	-5.78246600
H	-3.00216000	3.67724800	-3.94107600
H	4.49191200	0.08462900	-4.55681500
H	4.01566800	-0.25783000	2.21038100
H	5.32519600	-1.39020700	1.86312500
H	3.51988600	-2.53370700	3.11247400
H	3.58950700	-3.21262300	1.48566900
H	2.31878400	-2.05139400	1.91274600
N	0.00065400	3.89385500	0.00026900
O	-1.05104900	3.21327700	0.22049600
O	0.00095100	5.09086000	0.00023000
O	1.05204300	3.21275200	-0.21989600
N	-0.00057300	-1.90767800	-0.00027700
O	0.28635400	-1.23110500	-1.03434000

O	-0.00106800	-3.10896500	-0.00043200
O	-0.28696700	-1.23113800	1.03396100
C	-1.71540100	2.54812400	-2.64425800
H	-2.41260100	2.52215500	-1.81591000
C	1.09498000	3.21618800	4.84390700
C	2.03851300	3.19388800	3.83035300
N	0.54775400	1.94391100	2.43623900
C	-0.36528900	1.95502800	3.42031300
C	-1.63987600	1.26734300	3.12695000
N	-1.83306900	0.90107000	1.87095800
C	-2.96022400	0.25550800	1.54858200
C	-3.96700600	-0.07662200	2.46025100
C	-3.75414100	0.31874600	3.79580500
C	-3.08737700	-0.09830500	0.14803200
O	-2.23572400	0.25107800	-0.68664100
N	-4.18819900	-0.81740200	-0.22508900
C	-5.18183500	-1.17232000	0.68114400
C	-4.28185500	-1.15924800	-1.65771600
C	-3.36958300	-2.30587200	-2.05464800
H	1.29714100	3.72175400	5.78229200
H	3.00257500	3.67639000	3.94131600
H	-4.49189300	0.08466300	4.55674600
H	-4.01609600	-0.25702800	-2.21046000
H	-5.32537500	-1.38971700	-1.86326900
H	-3.51988200	-2.53245300	-3.11313900
H	-3.58940300	-3.21195800	-1.48657800
H	-2.31885000	-2.05041000	-1.91325400
C	1.71578000	2.54729200	2.64450400
H	2.41317200	2.52087400	1.81632500
C	5.18174700	-1.17265000	-0.68130900
C	6.34744400	-1.95475100	-0.20400300
C	7.58846100	-1.33485900	-0.06592600
C	6.24274200	-3.32232800	0.05922200
C	8.69647400	-2.06567800	0.34328700
H	7.68545100	-0.27301900	-0.27170200
C	7.35585300	-4.04322500	0.46208600
H	5.29133300	-3.82867500	-0.07129800
C	8.60181000	-3.42976800	0.61458700
H	9.65350300	-1.56317800	0.45100200
H	7.25695300	-5.10768000	0.65596400
C	-6.34748800	-1.95452000	0.20392100
C	-7.58876600	-1.33493000	0.06674400
C	-6.24252900	-3.32193900	-0.06000600
C	-8.69676600	-2.06587800	-0.34224500

H	-7.68595000	-0.27320200	0.27300200
C	-7.35563700	-4.04298000	-0.46263100
H	-5.29091500	-3.82808100	0.06980100
C	-8.60185300	-3.42983100	-0.61418500
H	-9.65398300	-1.56359200	-0.44929800
H	-7.25651000	-5.10730900	-0.65707600
C	-5.09287900	-0.80070300	1.98656800
H	-5.88128800	-1.09871700	2.66655100
C	5.09279200	-0.80100200	-1.98671700
H	5.88124600	-1.09891500	-2.66669400
C	9.80289000	-4.22679000	1.02750100
H	10.20691200	-4.78852100	0.17880900
H	10.60188700	-3.58664300	1.40615000
H	9.55428500	-4.95295600	1.80523400
C	-9.80299500	-4.22701200	-1.02660100
H	-10.20837700	-4.78636100	-0.17697300
H	-10.60114200	-3.58722900	-1.40766500
H	-9.55403500	-4.95524200	-1.80226800
C	0.12373400	2.58730900	-4.63770100
H	0.87891100	2.61250500	-5.41322600
C	2.60262200	0.98536600	-4.12267300
H	2.42684200	1.27208600	-5.15184600
C	-2.60258500	0.98537900	4.12262000
H	-2.42669800	1.27193200	5.15182300
C	-0.12376800	2.58749800	4.63756200
H	-0.87912600	2.61312300	5.41290100
Eu	0.00000200	1.00974800	-0.00001700

Am(L_d)₂(NO₃)₂⁺

C	0.81181200	5.34289800	-2.14712100
C	1.81813800	4.41639300	-2.28698400
N	0.41626200	2.67785900	-1.42228600
C	-0.57987700	3.57581400	-1.30067600
C	-0.43137400	4.93508500	-1.63746000
C	-1.84852200	3.11443300	-0.79203500
C	-2.90881000	4.04428300	-0.58514700
N	-1.98025700	1.81912100	-0.52274100
C	-3.12252800	1.38844000	-0.00107100
C	-4.22347900	2.21808200	0.28564100
C	-4.09663900	3.56955200	-0.03766300
C	-3.17465200	-0.03943300	0.27550100
O	-2.23888100	-0.78958800	-0.04657700

N	-4.29250400	-0.52210400	0.89077600
C	-4.30532700	-1.97043700	1.16945200
C	-3.46200800	-2.34752700	2.37377100
H	0.96545000	6.38089000	-2.42679100
H	2.78753700	4.69234400	-2.68550200
H	-4.91995400	4.25382600	0.14713800
H	-3.92608200	-2.46334300	0.27313200
H	-5.34519600	-2.26157600	1.30492300
H	-3.52259000	-3.42715400	2.53180600
H	-3.81854900	-1.85848500	3.28244900
H	-2.41283600	-2.08979100	2.22294800
N	0.10709900	0.45802000	-3.67141000
O	1.14628000	0.20920800	-2.98339800
O	0.14094900	0.59688400	-4.85989300
O	-0.97692400	0.55145000	-3.00785600
N	0.09363200	-0.01954600	2.17621700
O	-0.32696900	1.00884700	1.56716600
O	0.21590200	-0.05512500	3.37080000
O	0.38471000	-1.01362100	1.43871100
C	-2.70893900	5.41902800	-0.93733700
H	-3.52584000	6.11770800	-0.78738200
C	-1.52847300	5.83963700	-1.44760400
H	-1.38846700	6.88228900	-1.71609300
C	1.57598700	3.09155600	-1.90568800
H	2.34638400	2.33539300	-2.00184200
C	-0.98037200	-4.68399700	-3.20657800
C	-1.91534900	-3.67605400	-3.24515100
N	-0.48025700	-2.22008900	-1.99824900
C	0.44861300	-3.19482300	-1.97570500
C	0.24505500	-4.46073500	-2.55858400
C	1.70779200	-2.91293000	-1.33108800
C	2.70667600	-3.92602900	-1.25740700
N	1.89369100	-1.69438200	-0.83156500
C	3.04733700	-1.41709100	-0.23565200
C	4.09244900	-2.34705400	-0.07101500
C	3.89815700	-3.62025000	-0.60743100
C	3.17674500	-0.05368500	0.26333900
O	2.27591600	0.78090000	0.08689100
N	4.32485800	0.26341900	0.93234500
C	5.36040600	-0.65476400	1.10664800
C	4.37530100	1.60276200	1.54830700
C	3.75439900	1.61619600	2.93348100
H	-1.17536200	-5.64430200	-3.67468000
H	-2.86617100	-3.80766400	-3.74848400

H	4.67672500	-4.37284200	-0.51975500
H	3.83828900	2.27189600	0.87771000
H	5.41762300	1.91280300	1.58197600
H	3.79093200	2.63065400	3.33789500
H	4.30030900	0.96399800	3.61890700
H	2.70891200	1.30372000	2.91184800
C	2.44743500	-5.20578600	-1.84837000
H	3.21556100	-5.97028300	-1.78892200
C	1.27460200	-5.45616000	-2.47500500
H	1.09146600	-6.42596200	-2.92753100
C	-1.62231300	-2.45769400	-2.62209600
H	-2.33394600	-1.64013000	-2.63898500
C	-5.37666000	0.29823400	1.20719700
C	-6.55134900	-0.30055600	1.88673500
C	-7.71980600	-0.55402300	1.16991800
C	-6.52819000	-0.56855400	3.25697200
C	-8.83513500	-1.07950500	1.80953400
H	-7.75427600	-0.34397400	0.10501600
C	-7.64832400	-1.08903300	3.88651000
H	-5.63663300	-0.35001500	3.83680900
C	-8.82076700	-1.35650000	3.17596700
H	-9.73517900	-1.27427300	1.23332600
H	-7.61425800	-1.28484300	4.95464000
C	6.58767900	-0.21998100	1.81835000
C	7.55516100	0.55188600	1.17009100
C	6.81801800	-0.62509300	3.13089500
C	8.71736400	0.91640000	1.83091500
H	7.40042500	0.85889400	0.13942300
C	7.98571900	-0.25202600	3.78572800
H	6.07983600	-1.23406900	3.64415000
C	8.95370300	0.52381200	3.15129300
H	9.46115500	1.51233800	1.30914100
H	8.14508300	-0.57422800	4.81073600
C	5.26188800	-1.91722300	0.62032200
H	6.09625200	-2.59369400	0.75833800
C	-5.36231900	1.61963200	0.89876200
H	-6.22191300	2.22302700	1.16316300
C	-10.03506700	-1.89317200	3.87314300
H	-10.58592800	-1.08703600	4.36901500
H	-10.72137800	-2.37593800	3.17477200
H	-9.76751000	-2.62147800	4.64232400
C	10.22529500	0.90760800	3.84723100
H	11.06702800	0.31318900	3.47724500
H	10.47385500	1.95816100	3.67628400

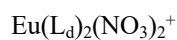
H	10.15942000	0.74829000	4.92500000
Am	-0.00686800	0.10972900	-0.76389000

Cm(L_d)₂(NO₃)₂⁺

C	0.94829300	5.12130600	-2.52859300
C	1.90342600	4.14057900	-2.66017600
N	0.45511800	2.51387000	-1.66301600
C	-0.49230800	3.46494000	-1.55159200
C	-0.29359800	4.79814600	-1.95876800
C	-1.76625800	3.08855400	-0.98857800
C	-2.78236400	4.07095000	-0.80693400
N	-1.94369900	1.81549900	-0.65716100
C	-3.09528300	1.45232400	-0.11046200
C	-4.15951700	2.33608600	0.15253900
C	-3.98027200	3.66852200	-0.22320200
C	-3.20140500	0.03726800	0.21366400
O	-2.29945900	-0.76104100	-0.09097300
N	-4.33265700	-0.37864800	0.85141700
C	-4.40576300	-1.81655300	1.17270400
C	-3.56609700	-2.19710800	2.37861000
H	1.14060300	6.13649100	-2.86286100
H	2.86859500	4.34964500	-3.10680200
H	-4.77201000	4.39326400	-0.05532700
H	-4.05904800	-2.35109700	0.28706800
H	-5.45592300	-2.05716100	1.32662900
H	-3.67984200	-3.26659100	2.57247300
H	-3.88467500	-1.66173000	3.27512600
H	-2.50705800	-1.99896300	2.20825600
N	0.03392000	0.05764200	-3.71168900
O	1.09169500	-0.08276900	-3.01710800
O	0.05248100	0.08327700	-4.90788900
O	-1.04483100	0.16918200	-3.04477300
N	-0.03463600	-0.05886300	2.16111800
O	-0.34300500	0.98229400	1.50357800
O	-0.00381200	-0.07292000	3.36162200
O	0.24195500	-1.08483600	1.46497200
C	-2.52866700	5.41836600	-1.22444200
H	-3.30896400	6.16061300	-1.08943800
C	-1.34326100	5.76023400	-1.78086500
H	-1.16369300	6.78216500	-2.10067300
C	1.61347000	2.84800900	-2.20822800
H	2.34217100	2.05105200	-2.30018200
C	-0.90533900	-5.05437300	-2.70475200

C	-1.86226500	-4.07403100	-2.82546100
N	-0.44198600	-2.47359100	-1.74900200
C	0.50829500	-3.42313100	-1.64884200
C	0.32368000	-4.74386400	-2.10090700
C	1.77050200	-3.05818200	-1.05264700
C	2.78822900	-4.04128800	-0.88462300
N	1.93667600	-1.79470500	-0.68050600
C	3.07996400	-1.44184000	-0.10987100
C	4.14362400	-2.32927600	0.14382300
C	3.97571600	-3.65089900	-0.27214400
C	3.16720000	-0.03973200	0.27351000
O	2.23891100	0.74957300	0.03179800
N	4.30001600	0.36591400	0.91691200
C	5.36041900	-0.50576300	1.17148200
C	4.30222000	1.75102100	1.42469600
C	3.61808600	1.86182100	2.77521400
H	-1.08622000	-6.05963100	-3.07363300
H	-2.81731200	-4.27319700	-3.29764100
H	4.76912200	-4.37634700	-0.11557600
H	3.78703700	2.35640600	0.67995200
H	5.33709700	2.08104800	1.48062700
H	3.63889400	2.90219300	3.10864000
H	4.13047700	1.25958000	3.52899900
H	2.57350800	1.54954900	2.72449800
C	2.54807900	-5.37675200	-1.34590400
H	3.32959000	-6.11928000	-1.21976800
C	1.37420900	-5.70669500	-1.93309200
H	1.20500900	-6.71924200	-2.28662600
C	-1.58772900	-2.79510200	-2.32751500
H	-2.31838100	-1.99871000	-2.40696900
C	-5.37959700	0.49642400	1.14833900
C	-6.57164700	-0.03008400	1.85641500
C	-7.76237700	-0.23569100	1.16114500
C	-6.54159500	-0.27497100	3.23092100
C	-8.89333400	-0.69199200	1.82594200
H	-7.80175200	-0.04387600	0.09298400
C	-7.67719300	-0.72618100	3.88557700
H	-5.63178200	-0.09206600	3.79439800
C	-8.87242400	-0.94557600	3.19678900
H	-9.81051000	-0.85088300	1.26595300
H	-7.63701300	-0.90476100	4.95650700
C	6.57211900	0.02284200	1.84495700
C	7.51616000	0.76985700	1.13559900
C	6.81284400	-0.26810800	3.18554200

C	8.66615300	1.22084700	1.76321800
H	7.35311100	0.98841400	0.08388300
C	7.96807200	0.19173000	3.80671900
H	6.09306400	-0.85640800	3.74679600
C	8.91291800	0.94259900	3.11067500
H	9.39247600	1.79478300	1.19428300
H	8.13612200	-0.04219200	4.85403100
C	5.29839600	-1.80833500	0.79665700
H	6.15062400	-2.44649700	0.99526800
C	-5.31532600	1.80539900	0.79526700
H	-6.14785000	2.45106100	1.04622500
C	-10.10185300	-1.40717100	3.92064700
H	-10.60640400	-0.56455500	4.40510000
H	-10.82009100	-1.87085500	3.24169900
H	-9.85969500	-2.13078900	4.70254200
C	10.17117700	1.42041400	3.77179000
H	11.03717600	0.84943900	3.42169000
H	10.36709000	2.47193600	3.54616400
H	10.12300800	1.31274300	4.85682100
Cm	-0.01285400	0.00343000	-0.78683900



C	-1.04740700	-5.07925200	-2.57917500
C	-1.98135400	-4.07880400	-2.71696000
N	-0.50465600	-2.47875900	-1.71830300
C	0.42251600	-3.44890800	-1.60490700
C	0.19946900	-4.77925900	-2.00779700
C	1.70222600	-3.09274600	-1.04528000
C	2.70206100	-4.09014100	-0.85825600
N	1.89774000	-1.82043000	-0.72328100
C	3.05422700	-1.47361400	-0.17769000
C	4.10497400	-2.37124900	0.09156300
C	3.90650000	-3.70320500	-0.27686500
C	3.17659500	-0.05941600	0.14001800
O	2.28361800	0.74493600	-0.17231000
N	4.31048700	0.34596200	0.77990100
C	4.40053200	1.78458100	1.09356000
C	3.55357200	2.18627300	2.28769800
H	-1.25998700	-6.09120800	-2.91096700
H	-2.94882700	-4.26920200	-3.16701100
H	4.68702800	-4.43896700	-0.10454800
H	4.07143900	2.31885500	0.20091100

H	5.45242200	2.01102400	1.25681700
H	3.69134000	3.25283700	2.48231500
H	3.84599400	1.64421300	3.18912200
H	2.49232800	2.01437300	2.10381600
N	-0.03000600	-0.01728800	-3.73010400
O	-1.08852200	0.12435400	-3.03801800
O	-0.04515600	-0.03606400	-4.92660600
O	1.04624100	-0.13784700	-3.06125000
N	0.07855600	0.10792400	2.05223100
O	0.32842400	-0.95347100	1.40354200
O	0.09399100	0.14373200	3.25282300
O	-0.18930500	1.12894800	1.34799900
C	2.42371700	-5.43500500	-1.26890400
H	3.19037100	-6.19069000	-1.13022300
C	1.23234400	-5.75858600	-1.82427400
H	1.03544100	-6.77882400	-2.13930600
C	-1.66740900	-2.79100400	-2.26705700
H	-2.37833100	-1.97904700	-2.36526500
C	0.97409200	5.06568800	-2.67200400
C	1.91806500	4.07419300	-2.80499800
N	0.47447400	2.47444500	-1.75886300
C	-0.46358500	3.43524000	-1.65048100
C	-0.26152700	4.76075700	-2.07912600
C	-1.73183100	3.07437400	-1.06901500
C	-2.74060400	4.06317800	-0.88462000
N	-1.90818500	1.80562200	-0.72365400
C	-3.05272500	1.45448800	-0.15646900
C	-4.10912100	2.34482900	0.11501000
C	-3.93233200	3.67209000	-0.27981900
C	-3.14124900	0.04937800	0.20920300
O	-2.21235600	-0.73441300	-0.04568200
N	-4.27128300	-0.36261500	0.85245500
C	-5.32766500	0.50997600	1.12271400
C	-4.27221200	-1.75426700	1.34166600
C	-3.54771900	-1.89136100	2.66860900
H	1.17014900	6.07427400	-3.02361800
H	2.87734300	4.26814400	-3.27076800
H	-4.71982500	4.40111600	-0.11062800
H	-3.78655900	-2.35545000	0.57359200
H	-5.30831200	-2.07427800	1.42468600
H	-3.58322300	-2.93347100	2.99541000
H	-4.02075900	-1.28275500	3.44286900
H	-2.49799400	-1.60463800	2.58483600
C	-2.48357700	5.40380100	-1.32168400

H	-3.25687300	6.15313200	-1.18550200
C	-1.30342800	5.73103900	-1.89859100
H	-1.12244600	6.74787100	-2.23353400
C	1.62618300	2.79083500	-2.32842000
H	2.34602300	1.98622600	-2.41879300
C	5.34564300	-0.54160800	1.08216300
C	6.54253800	-0.02834200	1.79138700
C	7.74297200	0.13823300	1.10323100
C	6.50712300	0.24080100	3.16174300
C	8.87905800	0.57999100	1.77001000
H	7.78665700	-0.07245500	0.03881900
C	7.64709700	0.67662500	3.81814600
H	5.58898200	0.08782000	3.72056600
C	8.85298900	0.85727100	3.13563500
H	9.80404000	0.70815200	1.21510400
H	7.60257100	0.87347400	4.88576700
C	-6.53743600	-0.02354100	1.79564900
C	-7.48705600	-0.75953100	1.08188700
C	-6.77045300	0.25123700	3.14082600
C	-8.63502400	-1.21498400	1.70961500
H	-7.32996000	-0.96519800	0.02668000
C	-7.92397900	-0.21313100	3.76218500
H	-6.04646100	0.83094500	3.70558300
C	-8.87417700	-0.95285900	3.06186600
H	-9.36614600	-1.77938800	1.13725000
H	-8.08633000	0.00873300	4.81299300
C	-5.26320400	1.81758500	0.76494400
H	-6.11261100	2.45522900	0.97693200
C	5.26615400	-1.85135800	0.73389900
H	6.08977600	-2.50604000	0.99079300
C	10.08393300	1.30845500	3.86350400
H	10.49888000	0.49545700	4.46814700
H	10.86399200	1.63547700	3.17361600
H	9.86616200	2.13592200	4.54356800
C	-10.12846900	-1.44028000	3.72356000
H	-11.00618000	-0.91472900	3.33433800
H	-10.28637100	-2.50693700	3.54215100
H	-10.10213500	-1.28417600	4.80336300
Eu	0.01121900	0.01060300	-0.85164900

BP86/6-311G*-RECP

Am(L_b)₂(NO₃)₂⁺

C	-0.82493500	5.22584400	-2.40524700
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C	0.28902500	4.51074600	-2.81339600
N	-0.39870600	2.58573400	-1.52113300
C	-1.51542800	3.26611700	-1.13980500
C	-1.76498600	4.61354500	-1.54014900
C	-2.47837700	2.59247300	-0.29104200
C	-3.61187200	3.31943500	0.19142000
N	-2.26561300	1.29000900	0.02269500
C	-3.13915200	0.65387200	0.82288500
C	-4.24995600	1.31670300	1.39888400
C	-4.48257700	2.64286400	1.07689400
C	-2.71831500	-0.76425900	1.11684400
O	-1.53600000	-1.09446100	0.83504800
N	-3.54312500	-1.66491600	1.72453200
C	-4.98065800	-1.58407700	1.72126600
C	-2.92959600	-2.94692900	2.18721700
C	-2.07955600	-2.79066100	3.44957300
C	-5.69315000	-1.67027600	2.92982000
C	-7.07874500	-1.42375800	0.51379300
C	-5.68035700	-1.47473200	0.50942700
H	-0.98891400	6.25462400	-2.74096300
H	1.02943900	4.94712300	-3.48803400
H	-4.91353900	0.79513200	2.08753600
H	-5.33738900	3.17368300	1.50686500
H	-2.31816500	-3.34029500	1.36037800
H	-3.76537100	-3.64116100	2.35077200
H	-1.67418300	-3.77293200	3.74019900
H	-2.67149800	-2.40864200	4.29566700
H	-1.22997300	-2.11480700	3.27947300
H	-5.15240000	-1.74983800	3.87722900
H	-7.61112600	-1.33440100	-0.43860800
H	-5.13024600	-1.43196300	-0.43537700
N	-0.57889500	-0.01502800	-3.43692800
O	0.64044200	0.12192700	-3.02254300
O	-0.87249700	-0.11646200	-4.61364900
O	-1.47998600	-0.03776900	-2.49244500
N	0.79667100	0.73571400	2.27725000
O	0.03140600	1.52987200	1.61032900
O	1.08857000	0.92094900	3.44958100
O	1.25411200	-0.28564200	1.60929500
C	-7.08998600	-1.62891900	2.91744700
H	-7.63303300	-1.69129800	3.86618600
C	-3.81505800	4.68041900	-0.21238800
H	-4.69215800	5.21511800	0.16430400
C	-2.93263600	5.29802000	-1.05844300

H	-3.09896500	6.33279000	-1.37347000
C	0.46902300	3.19575900	-2.33683100
H	1.34595300	2.60974000	-2.61873600
C	-0.07113400	-4.98843100	-2.47842500
C	-1.24593700	-4.28911900	-2.25185900
N	-0.02096500	-2.37462400	-1.41839700
C	1.14083800	-3.05113100	-1.64612400
C	1.16992800	-4.37475000	-2.18070300
C	2.38956900	-2.38516700	-1.34499900
C	3.62436500	-3.05917300	-1.59465600
N	2.33776500	-1.12257300	-0.85180300
C	3.48167300	-0.48511100	-0.55873300
C	4.74986300	-1.06851900	-0.79080700
C	4.81579000	-2.34944900	-1.31281500
C	3.26301900	0.94947200	-0.13861000
O	2.21692500	1.51647300	-0.54756800
N	4.20320000	1.61966800	0.57937600
C	5.17247800	0.95602600	1.41595900
C	4.04225500	3.08948300	0.75789000
C	3.28023100	3.46644200	2.02958000
C	6.53696800	1.27368200	1.30079400
C	5.69682100	-0.60730800	3.18992500
C	4.74901700	0.02147800	2.37421600
H	-0.08944300	-6.00156900	-2.89202700
H	-2.22061300	-4.72477400	-2.48420200
H	5.66097900	-0.51264400	-0.56794900
H	5.78514800	-2.81612600	-1.51289700
H	3.52674700	3.46438300	-0.13623700
H	5.05842900	3.51313400	0.77220000
H	3.26991300	4.56280200	2.13812300
H	3.75717600	3.04445700	2.92714000
H	2.23811200	3.12012500	1.98928500
H	6.87110500	1.99687200	0.55036600
H	5.35556100	-1.33279400	3.93541100
H	3.68274400	-0.19822400	2.48645700
C	3.61329800	-4.39123400	-2.12780000
H	4.56882300	-4.89167300	-2.31129200
C	2.43147000	-5.02489300	-2.40699300
H	2.43051600	-6.04001500	-2.81573300
C	-1.17174200	-2.98403100	-1.72364900
H	-2.07837800	-2.39736600	-1.56092000
C	-7.81065100	-1.50226500	1.71256600
C	7.06764000	-0.31025700	3.08859700
C	-9.32061300	-1.48589400	1.71292500

H	-9.72534500	-2.50710300	1.82178400
H	-9.71999500	-0.89164300	2.54979900
H	-9.72497200	-1.07131200	0.77760100
C	7.46798000	0.64288400	2.12984100
H	8.52914900	0.89304000	2.02815400
C	8.08035200	-0.96005400	4.00128900
H	9.02048300	-1.18366100	3.47284500
H	8.33498400	-0.29397500	4.84408000
H	7.69937400	-1.89863400	4.43078600
Am	0.06397800	0.16650200	-0.56108600

Cm(L_b)₂(NO₃)₂⁺

C	-0.81451100	5.02626900	-2.75224600
C	0.25027500	4.24617200	-3.17344300
N	-0.44702000	2.41958300	-1.75047200
C	-1.51969400	3.16233000	-1.35893200
C	-1.73729000	4.49627500	-1.81712100
C	-2.47556000	2.56727000	-0.44531400
C	-3.56644700	3.35377900	0.03958100
N	-2.29688400	1.27471500	-0.08733800
C	-3.16835300	0.69581800	0.75134900
C	-4.23816700	1.41669200	1.33638100
C	-4.43132800	2.74036000	0.97602400
C	-2.78785500	-0.73328000	1.06639100
O	-1.62742200	-1.11390600	0.76294400
N	-3.63007800	-1.58806700	1.71200700
C	-5.06330400	-1.45009500	1.74276000
C	-3.05657700	-2.88437100	2.18645600
C	-2.17667300	-2.73777900	3.42934900
C	-5.74766300	-1.48374700	2.96989800
C	-7.18243300	-1.23729000	0.58228100
C	-5.78738200	-1.34092500	0.54540400
H	-0.95373500	6.04281700	-3.13350000
H	0.97324100	4.61690800	-3.90391400
H	-4.90037900	0.94449400	2.06119100
H	-5.25329700	3.31587100	1.41262900
H	-2.47593200	-3.31454300	1.35602100
H	-3.91444600	-3.54366300	2.37762000
H	-1.80310600	-3.72945200	3.73049300
H	-2.73712200	-2.31852200	4.27921100
H	-1.30553400	-2.09799800	3.23088000
H	-5.18711600	-1.56396200	3.90567800

H	-7.73439300	-1.14942000	-0.35900900
H	-5.25874000	-1.34251400	-0.41255700
N	-0.65121300	-0.40452000	-3.42139300
O	0.56676000	-0.14951100	-3.03826800
O	-0.94066700	-0.60951600	-4.58511400
O	-1.53498600	-0.42612600	-2.46650100
N	0.72647700	0.68688700	2.24934600
O	-0.01136100	1.46939300	1.52944400
O	0.99064300	0.92577400	3.41944100
O	1.18090600	-0.36650200	1.64047500
C	-7.14187000	-1.38992200	2.98984000
H	-7.66346900	-1.41180000	3.95230500
C	-3.73270600	4.70303000	-0.41820000
H	-4.57523300	5.28848800	-0.03799600
C	-2.85955300	5.24649400	-1.32336400
H	-3.00023000	6.27118300	-1.68101900
C	0.40316100	2.95097800	-2.63657000
H	1.24051900	2.31495000	-2.93105000
C	0.28239200	-5.24041200	-2.12101800
C	-0.93497100	-4.60727700	-1.92963400
N	0.16282900	-2.56349700	-1.23771800
C	1.36511200	-3.17486400	-1.43232500
C	1.48119200	-4.52757300	-1.87418100
C	2.57131600	-2.41257600	-1.18286700
C	3.84739600	-3.02600400	-1.37685200
N	2.43877100	-1.12704800	-0.78100300
C	3.53494500	-0.40856300	-0.50622300
C	4.84074000	-0.92453300	-0.68362000
C	4.98990000	-2.22790200	-1.12873600
C	3.21060200	1.02484000	-0.15334000
O	2.13613700	1.50098000	-0.60668600
N	4.07733800	1.78514300	0.56361500
C	5.07489300	1.21989200	1.43954700
C	3.80563200	3.24429300	0.69302600
C	3.01070900	3.60393500	1.94961600
C	6.41630300	1.62595800	1.33444300
C	5.67104600	-0.24448300	3.27397600
C	4.69781900	0.29195600	2.42304700
H	0.32985900	-6.27801400	-2.46619700
H	-1.87950400	-5.12151000	-2.12276900
H	5.71400900	-0.30379400	-0.48062800
H	5.98830200	-2.64628300	-1.28910300
H	3.26885000	3.54951100	-0.21485400
H	4.78768900	3.74245900	0.69647400

H	2.91289400	4.69931300	2.01731900
H	3.51742300	3.25558200	2.86242900
H	1.99970900	3.17363600	1.92240600
H	6.71418300	2.34496300	0.56497900
H	5.36583700	-0.96599200	4.03865600
H	3.64731600	0.00345400	2.52843000
C	3.92206500	-4.38872900	-1.81947800
H	4.90726300	-4.84183200	-1.96537800
C	2.78228000	-5.11021200	-2.05832300
H	2.84547300	-6.14841100	-2.39853300
C	-0.94602500	-3.26778900	-1.48800300
H	-1.88830500	-2.73415900	-1.34851900
C	-7.88673100	-1.26244400	1.79979800
C	7.02084800	0.13920000	3.18152600
C	-9.39465200	-1.19088100	1.83573800
H	-9.83311500	-2.19509100	1.96957000
H	-9.75184800	-0.57054600	2.67273400
H	-9.80655800	-0.77560800	0.90400700
C	7.37300700	1.08550400	2.19750400
H	8.41684500	1.40248600	2.10315100
C	8.05923300	-0.41354400	4.12870500
H	9.02138200	-0.58737000	3.62162900
H	8.25316900	0.29209500	4.95526900
H	7.73505200	-1.36334600	4.57952700
Cm	0.06015300	0.07899400	-0.60551900

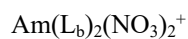
Eu(L_b)₂(NO₃)₂⁺

C	-0.87210800	5.15380900	-2.60869300
C	0.23900500	4.42636200	-3.00258400
N	-0.43797000	2.54415400	-1.64196800
C	-1.55224800	3.23560100	-1.27519000
C	-1.80519900	4.56987800	-1.71659700
C	-2.51442500	2.59021700	-0.39957600
C	-3.64470200	3.33330300	0.06604000
N	-2.30489900	1.29907900	-0.05134900
C	-3.17441600	0.68383000	0.76248900
C	-4.28244800	1.36196100	1.32801100
C	-4.51215500	2.68099900	0.97322900
C	-2.75332100	-0.73599300	1.08031400
O	-1.57484800	-1.07575100	0.80947600
N	-3.58921100	-1.62145200	1.69666700
C	-5.02618900	-1.52898300	1.68860700
C	-2.98999800	-2.90623100	2.16946700
C	-2.14165700	-2.75115100	3.43309900

C	-5.74248000	-1.59187300	2.89629000
C	-7.11988300	-1.37378000	0.47306700
C	-5.72177000	-1.43403100	0.47327900
H	-1.03919100	6.17125100	-2.97617500
H	0.97376400	4.84088200	-3.69698500
H	-4.94586100	0.86086600	2.03206100
H	-5.36438200	3.22435700	1.39281600
H	-2.37927000	-3.31008300	1.34717800
H	-3.83250000	-3.59181000	2.33505900
H	-1.74981300	-3.73610900	3.73310400
H	-2.73054000	-2.35407900	4.27436200
H	-1.28308900	-2.08789700	3.25900600
H	-5.20462700	-1.66094000	3.84620400
H	-7.64919700	-1.29574500	-0.48205500
H	-5.16858300	-1.41001800	-0.47041100
N	-0.61595000	-0.19333700	-3.44533700
O	0.60564200	-0.04324800	-3.06693100
O	-0.92829200	-0.37266300	-4.61264800
O	-1.50565100	-0.14567900	-2.50184500
N	0.76664400	0.76602400	2.24806400
O	-0.01878400	1.52258100	1.56905700
O	1.04025700	0.98418300	3.42193300
O	1.26387600	-0.24528400	1.61056000
C	-7.13899200	-1.54151100	2.87958500
H	-7.68507100	-1.58585300	3.82761800
C	-3.84765300	4.68210900	-0.37763600
H	-4.72174300	5.23046000	-0.01356700
C	-2.96909700	5.27075500	-1.24816300
H	-3.13618000	6.29534600	-1.59474100
C	0.42279500	3.12803700	-2.48245400
H	1.30026700	2.53460400	-2.74923000
C	0.11239600	-5.11799400	-2.33703200
C	-1.08407000	-4.45278200	-2.12371500
N	0.08123600	-2.47152400	-1.36131600
C	1.26314200	-3.11440000	-1.57578100
C	1.33410400	-4.45330800	-2.06811400
C	2.49559200	-2.39947400	-1.30486600
C	3.74943700	-3.04293700	-1.54487300
N	2.41027600	-1.12690900	-0.85015100
C	3.53262600	-0.44617200	-0.58756000
C	4.81905100	-0.99290500	-0.81291500
C	4.92014400	-2.28706400	-1.29568100
C	3.26540600	0.99216200	-0.19799900
O	2.20282300	1.51712400	-0.61538200

N	4.18277700	1.70469600	0.50998700
C	5.17301900	1.08701900	1.35717700
C	3.97241200	3.17074000	0.66490500
C	3.18727900	3.54274900	1.92412200
C	6.52602400	1.44972200	1.24001600
C	5.74834700	-0.43573100	3.15133600
C	4.78116900	0.15041000	2.32670700
H	0.12647000	-6.14394900	-2.71821300
H	-2.04474800	-4.92901900	-2.33412100
H	5.71447700	-0.40267300	-0.61541300
H	5.90200300	-2.72973700	-1.48978000
H	3.45279300	3.51544500	-0.23901700
H	4.97379000	3.62797100	0.68145100
H	3.14521700	4.63965500	2.01843600
H	3.66635900	3.14591800	2.83200000
H	2.15521800	3.16817800	1.87774800
H	6.83670700	2.17406900	0.48068800
H	5.43114500	-1.16380200	3.90490000
H	3.72337200	-0.10628000	2.43948600
C	3.77764600	-4.39083900	-2.03556000
H	4.74716600	-4.86659900	-2.21155000
C	2.61430400	-5.06986300	-2.28411500
H	2.64243800	-6.09707400	-2.66059400
C	-1.04900500	-3.12929200	-1.63674100
H	-1.97418700	-2.56900100	-1.48104300
C	-7.85545400	-1.42892000	1.67084000
C	7.10823300	-0.09292200	3.04797200
C	-9.36533700	-1.40337900	1.66663400
H	-9.77661200	-2.42085300	1.78564000
H	-9.76356000	-0.79736800	2.49558500
H	-9.76449300	-0.99693000	0.72550400
C	7.47677900	0.86161900	2.07808900
H	8.52889100	1.14679500	1.97449700
C	8.14130900	-0.69676400	3.96943800
H	9.08926400	-0.89421700	3.44457400
H	8.37167100	-0.01248800	4.80457400
H	7.79204700	-1.64279900	4.40936300
Eu	0.07181600	0.15041900	-0.59149400

TPSSH/6-311G*-RECP



C	-0.82903500	5.16849500	-2.45002800
C	0.28226900	4.45491400	-2.84461200
N	-0.40585900	2.55201600	-1.54334800
C	-1.51906100	3.23184000	-1.17503900
C	-1.76784700	4.56511300	-1.58663800
C	-2.47930600	2.56605900	-0.32637500
C	-3.60988500	3.28832500	0.14177500
N	-2.26257300	1.27378200	-0.00182000
C	-3.13145600	0.64533700	0.79456700
C	-4.24238800	1.30342900	1.35876500
C	-4.47810100	2.61983900	1.02532300
C	-2.70941900	-0.76762600	1.09372900
O	-1.53639500	-1.09468400	0.80769100
N	-3.52128200	-1.66340000	1.70075800
C	-4.95552100	-1.58189400	1.72414200
C	-2.90300100	-2.94688300	2.14392900
C	-2.03933100	-2.79213400	3.39307900
C	-5.63921100	-1.65611600	2.94130700
C	-7.06427500	-1.43108600	0.56014200
C	-5.67213400	-1.48390100	0.52980400
H	-0.99198400	6.18522700	-2.79394600
H	1.01917200	4.88201000	-3.51468600
H	-4.90037500	0.78981600	2.04480800
H	-5.33041300	3.14590600	1.44334900
H	-2.30764300	-3.32988200	1.31291500
H	-3.73259600	-3.63199300	2.31763600
H	-1.63375500	-3.76848200	3.67156900
H	-2.62132000	-2.41598700	4.23803500
H	-1.20099400	-2.11799400	3.21373000
H	-5.08418500	-1.72869000	3.87085800
H	-7.61011500	-1.34945600	-0.37509600
H	-5.14286400	-1.44891000	-0.41743900
N	-0.57222300	-0.03584500	-3.42333300
O	0.63517000	0.11003700	-3.00639500
O	-0.85173500	-0.13905000	-4.59401700
O	-1.47041000	-0.06581000	-2.49564900
N	0.73745300	0.63496600	2.28575900
O	-0.01944800	1.43266700	1.63211000
O	0.97629000	0.77479700	3.46657800
O	1.24171200	-0.33322900	1.59850800
C	-7.03026200	-1.61387900	2.95484400

H	-7.55107000	-1.66675900	3.90644000
C	-3.81553000	4.64185300	-0.27435500
H	-4.68912900	5.17204900	0.09075400
C	-2.93652300	5.24986400	-1.11765500
H	-3.10220500	6.27259300	-1.44131200
C	0.46088900	3.14999100	-2.35672600
H	1.33086800	2.56575200	-2.62825400
C	0.02150600	-4.94878600	-2.52494300
C	-1.15911800	-4.27662700	-2.28983800
N	0.02769000	-2.36359500	-1.43450200
C	1.19455600	-3.01419100	-1.67032400
C	1.24661900	-4.32070500	-2.21796900
C	2.42658900	-2.33414500	-1.35698700
C	3.66550700	-2.98160100	-1.60243500
N	2.35130500	-1.08425700	-0.85262600
C	3.47515500	-0.44016600	-0.53765900
C	4.74945900	-0.99716400	-0.76002500
C	4.83876700	-2.26283500	-1.29878500
C	3.22642300	0.97687000	-0.09407200
O	2.17908200	1.52566100	-0.50263800
N	4.13474800	1.64912800	0.64179100
C	5.11321700	0.99401000	1.46877600
C	3.93344300	3.10730800	0.85020700
C	3.12611200	3.42815200	2.10507900
C	6.46195100	1.35018200	1.37053100
C	5.66313500	-0.58804900	3.20105700
C	4.70837500	0.03173800	2.39644600
H	0.02061400	-5.94795900	-2.94933800
H	-2.11865500	-4.72176400	-2.52568600
H	5.64201500	-0.43543000	-0.51996700
H	5.80892200	-2.70899000	-1.49321300
H	3.43857200	3.48778100	-0.04231300
H	4.93150300	3.54611500	0.90814400
H	3.09422900	4.51234100	2.24370200
H	3.58219100	2.98790200	2.99469200
H	2.10135500	3.06594900	2.01737900
H	6.77772100	2.09495300	0.64633800
H	5.33937300	-1.33511400	3.91969800
H	3.65656500	-0.21926600	2.49225500
C	3.67952000	-4.30271100	-2.15343500
H	4.63644900	-4.78115500	-2.33512300
C	2.51611200	-4.94612300	-2.44758000
H	2.53195500	-5.94682900	-2.86758500
C	-1.10724400	-2.98328600	-1.74497500

H	-2.01575300	-2.41992100	-1.57154500
C	-7.76872400	-1.49739900	1.76808800
C	7.01909100	-0.25277700	3.11681300
C	-9.27636700	-1.48051300	1.79520700
H	-9.67269800	-2.49808000	1.87945400
H	-9.65394000	-0.91364100	2.64973100
H	-9.68881100	-1.04116200	0.88472600
C	7.39954900	0.72832800	2.18883600
H	8.44574600	1.00705900	2.10197100
C	8.04045100	-0.89587400	4.02103200
H	8.98521400	-1.06774800	3.49913900
H	8.25606100	-0.25174700	4.88031600
H	7.68546700	-1.85287000	4.40891300
Am	0.06753500	0.16032200	-0.56523600

Cm(L_b)₂(NO₃)₂⁺

C	-0.80937200	5.00184300	-2.74018000
C	0.27048700	4.23904800	-3.13073800
N	-0.43547600	2.41597900	-1.72795200
C	-1.52028500	3.14388200	-1.36470300
C	-1.74242100	4.46426300	-1.82863300
C	-2.48239000	2.54259800	-0.47077100
C	-3.58405900	3.31204000	-0.01132900
N	-2.29426800	1.25966200	-0.10604200
C	-3.16520200	0.67783700	0.71866300
C	-4.24818700	1.38357200	1.28119800
C	-4.45276800	2.69588000	0.90991600
C	-2.77458000	-0.74220700	1.03709100
O	-1.61953300	-1.11102400	0.72817700
N	-3.59613200	-1.60161000	1.68010800
C	-5.02600600	-1.47301800	1.74440300
C	-3.00769900	-2.89641700	2.13094000
C	-2.11301700	-2.74890900	3.35899600
C	-5.67416200	-1.49822800	2.98264100
C	-7.16242300	-1.28304000	0.63921600
C	-5.77422800	-1.38019500	0.56918100
H	-0.95214200	6.00689900	-3.12505500
H	1.00091900	4.61412800	-3.83796200
H	-4.90870800	0.91200500	1.99444800
H	-5.28316200	3.25764200	1.32570700
H	-2.44184900	-3.31006800	1.29428800
H	-3.85371100	-3.55320600	2.33245800
H	-1.73296300	-3.73318300	3.64553400

H	-2.66467700	-2.34064200	4.20932600
H	-1.25760000	-2.10513200	3.15101800
H	-5.09397000	-1.56686300	3.89698200
H	-7.73334400	-1.20609900	-0.28131700
H	-5.27197700	-1.38478500	-0.39322300
N	-0.59518700	-0.34485200	-3.42413500
O	0.60558900	-0.10510800	-3.01950700
O	-0.86174900	-0.53130000	-4.58727300
O	-1.48899700	-0.37361600	-2.49626500
N	0.65684700	0.59961300	2.27064000
O	-0.07754100	1.38545600	1.57269000
O	0.86782500	0.78155500	3.45170600
O	1.16549400	-0.39439700	1.63042700
C	-7.06231500	-1.41219000	3.03586600
H	-7.55586100	-1.42706600	4.00319100
C	-3.75953100	4.65369500	-0.47741600
H	-4.61002400	5.22416200	-0.11843400
C	-2.88131700	5.20063000	-1.36298400
H	-3.02569000	6.21346400	-1.72566400
C	0.42574200	2.95247900	-2.58916200
H	1.27115600	2.33195200	-2.85837400
C	0.30480900	-5.14746400	-2.24465100
C	-0.90909700	-4.52688000	-2.04050900
N	0.17533700	-2.51070900	-1.29175400
C	1.37440700	-3.11095300	-1.49778700
C	1.49528000	-4.44075000	-1.97402700
C	2.57187800	-2.35579200	-1.22062500
C	3.84305900	-2.95424100	-1.42242200
N	2.43216800	-1.08877300	-0.78373700
C	3.51699100	-0.37920600	-0.48177100
C	4.82055800	-0.88140900	-0.66218600
C	4.97647100	-2.16443200	-1.14280300
C	3.18268100	1.03549200	-0.08949500
O	2.10996300	1.51073500	-0.52796600
N	4.03484200	1.78070600	0.64096000
C	5.03757700	1.20585300	1.49889000
C	3.74536300	3.22959100	0.80844600
C	2.93022900	3.53616500	2.06179800
C	6.36520900	1.63382400	1.40778400
C	5.64887100	-0.29786400	3.27977200
C	4.67324700	0.24768400	2.44770200
H	0.35627700	-6.16641100	-2.61564400
H	-1.84413600	-5.03376600	-2.24859700
H	5.68253900	-0.26812500	-0.43656000

H	5.96931800	-2.57142800	-1.30625800
H	3.22064100	3.55110900	-0.09004600
H	4.71497500	3.73062200	0.84353700
H	2.82623200	4.61976000	2.16528100
H	3.42465600	3.15823500	2.95962500
H	1.93172700	3.10231800	1.99918300
H	6.64978800	2.37555200	0.66777300
H	5.35660000	-1.04282000	4.01393300
H	3.63583100	-0.05895500	2.53828100
C	3.92539700	-4.29957600	-1.90423900
H	4.90521000	-4.74060700	-2.05637000
C	2.79575100	-5.01268400	-2.16861300
H	2.86232800	-6.03197900	-2.53564600
C	-0.92548100	-3.20581400	-1.56353900
H	-1.86179900	-2.68385900	-1.41153100
C	-7.83192200	-1.29988600	1.86874300
C	6.98609600	0.10841600	3.20171900
C	-9.33693900	-1.23654500	1.93899400
H	-9.76156100	-2.24145500	2.03678500
H	-9.67242000	-0.65701500	2.80246000
H	-9.76179800	-0.78658500	1.03941200
C	7.32447700	1.08481100	2.25339000
H	8.35504000	1.41779800	2.17152700
C	8.02727800	-0.45594000	4.13541800
H	9.00831000	-0.50784500	3.65722500
H	8.13076500	0.17488800	5.02496000
H	7.75865600	-1.45859100	4.47490900
Cm	0.06229600	0.08793400	-0.59961300

Eu(L_b)₂(NO₃)₂⁺

C	-0.78937900	5.00821800	-2.78130900
C	0.29638000	4.24938600	-3.16330400
N	-0.40925000	2.42697300	-1.75999500
C	-1.49697800	3.15138900	-1.40320600
C	-1.72446700	4.46913300	-1.87265700
C	-2.45730500	2.54656700	-0.50998700
C	-3.56775300	3.31055100	-0.06135200
N	-2.26240700	1.26593000	-0.13594500
C	-3.13901800	0.68173800	0.68289400
C	-4.23006400	1.38434300	1.23315900
C	-4.43926500	2.69401000	0.85637100
C	-2.74968500	-0.73689600	1.00903400
O	-1.59545800	-1.10549900	0.70566700

N	-3.57592200	-1.59332600	1.65327600
C	-5.00642100	-1.46917400	1.70505700
C	-2.98893300	-2.88742500	2.10770500
C	-2.09493900	-2.73922200	3.33613400
C	-5.66468900	-1.49234900	2.93810500
C	-7.13519100	-1.29014100	0.58263100
C	-5.74608100	-1.38282900	0.52388300
H	-0.93520800	6.01117700	-3.17050200
H	1.02883000	4.62611400	-3.86765600
H	-4.89354400	0.91063400	1.94218500
H	-5.27568400	3.25282300	1.26397900
H	-2.42264300	-3.30386500	1.27260200
H	-3.83562200	-3.54306300	2.31025700
H	-1.72150200	-3.72439600	3.62829700
H	-2.64491900	-2.32273600	4.18357700
H	-1.23506500	-2.10236500	3.12581900
H	-5.09132400	-1.55620400	3.85712100
H	-7.69914800	-1.21817100	-0.34261000
H	-5.23649600	-1.38842200	-0.43467900
N	-0.58327600	-0.29789300	-3.41984200
O	0.61981800	-0.09846000	-3.01257000
O	-0.85135300	-0.47024800	-4.58637900
O	-1.48070100	-0.30384500	-2.49998500
N	0.66039500	0.54661500	2.23755600
O	-0.09596700	1.33019000	1.56685100
O	0.87576300	0.70540700	3.42174300
O	1.18622000	-0.41801400	1.57309900
C	-7.05349700	-1.41114500	2.98024600
H	-7.55455600	-1.42467500	3.94374900
C	-3.74943500	4.64933600	-0.53364000
H	-4.60632100	5.21445400	-0.18143000
C	-2.87006700	5.20001200	-1.41558300
H	-3.01938500	6.21080200	-1.78200500
C	0.45381000	2.96453900	-2.61717900
H	1.30259000	2.34563800	-2.88041000
C	0.27966300	-5.09908000	-2.34943900
C	-0.93382800	-4.48769300	-2.11684400
N	0.15285200	-2.48137200	-1.34608400
C	1.35052000	-3.07183800	-1.58027600
C	1.47095600	-4.39203200	-2.08292300
C	2.54669300	-2.31477400	-1.30429000
C	3.81803600	-2.90404200	-1.53312100
N	2.40845700	-1.05621100	-0.84009800
C	3.49569100	-0.35112800	-0.53355300

C	4.79809500	-0.84619400	-0.73944500
C	4.95248700	-2.11736500	-1.25038900
C	3.16511400	1.05338100	-0.10355900
O	2.09011500	1.53730900	-0.52017900
N	4.02553300	1.78001800	0.63840700
C	5.03644600	1.18551600	1.47233600
C	3.73380400	3.22313100	0.84504800
C	2.91860100	3.49514600	2.10646500
C	6.36189100	1.62079800	1.38259600
C	5.66801400	-0.36223200	3.20827800
C	4.68384700	0.20082700	2.39820600
H	0.33018800	-6.11086600	-2.73968300
H	-1.86951100	-4.99522900	-2.32068200
H	5.66036300	-0.23532000	-0.50829100
H	5.94440900	-2.51789300	-1.43416800
H	3.20766000	3.56781200	-0.04404400
H	4.70223000	3.72529900	0.89300800
H	2.81379200	4.57540900	2.23968900
H	3.41303100	3.09289400	2.99365900
H	1.92011300	3.06306200	2.03205000
H	6.63776800	2.38295700	0.66025700
H	5.38460100	-1.12783300	3.92448300
H	3.64873900	-0.11359800	2.48760200
C	3.90017900	-4.23924100	-2.04278300
H	4.88036500	-4.67164300	-2.21593100
C	2.77117000	-4.95349500	-2.30626900
H	2.83835100	-5.96519500	-2.69368600
C	-0.94823300	-3.17549200	-1.61491000
H	-1.88425200	-2.65965200	-1.43988900
C	-7.81435600	-1.30531700	1.80678600
C	7.00280700	0.05222100	3.13159200
C	-9.32009300	-1.24661800	1.86528000
H	-9.74192500	-2.25150100	1.97459400
H	-9.66384500	-0.65594600	2.71793700
H	-9.74002700	-0.81101600	0.95638200
C	7.32985700	1.05443300	2.20656700
H	8.35833800	1.39408000	2.12571900
C	8.05326500	-0.53126200	4.04288000
H	9.03047000	-0.56850300	3.55554700
H	8.16225400	0.07823800	4.94652600
H	7.79049500	-1.54269100	4.36021600
Eu	0.06521100	0.10291000	-0.61504600

B3LYP/6-311G*-RECP

Am(L_b)₂(NO₃)₂⁺

C	-0.86188200	5.16086700	-2.51258600
C	0.23763600	4.44088800	-2.92034600
N	-0.43969300	2.55414800	-1.59730100
C	-1.54371100	3.23802900	-1.21469200
C	-1.79016400	4.56921200	-1.63154500
C	-2.50086800	2.58482700	-0.34691600
C	-3.61825800	3.32105900	0.12850500
N	-2.29901500	1.29531200	-0.01342500
C	-3.16147600	0.67864700	0.79221200
C	-4.25995600	1.35085000	1.36111400
C	-4.48341700	2.66628400	1.02263000
C	-2.75374000	-0.74458200	1.09793600
O	-1.58635700	-1.07932600	0.81696400
N	-3.57839900	-1.63137200	1.69812600
C	-5.01393300	-1.53867400	1.71110200
C	-2.98006300	-2.92176400	2.14680300
C	-2.12298500	-2.78615100	3.40223500
C	-5.70638100	-1.56636800	2.92375300
C	-7.11511700	-1.42351000	0.53174400
C	-5.72411800	-1.48141400	0.51260500
H	-1.02442500	6.17606600	-2.86025700
H	0.96580100	4.85960300	-3.60457300
H	-4.91955300	0.85096200	2.05330400
H	-5.32677000	3.20285800	1.44469700
H	-2.38551100	-3.31963400	1.32313100
H	-3.81575500	-3.59953700	2.31470300
H	-1.73492100	-3.76847300	3.68353100
H	-2.70162900	-2.40324700	4.24599700
H	-1.27100000	-2.12696100	3.23467700
H	-5.15859500	-1.60834300	3.85895000
H	-7.65410500	-1.37318600	-0.40910800
H	-5.19166700	-1.48166700	-0.43280300
N	-0.61462200	-0.16753200	-3.44589600
O	0.59141800	0.02899600	-3.05971700
O	-0.91292600	-0.31722300	-4.60352300
O	-1.49160300	-0.19600500	-2.50208500
N	0.76872000	0.71658500	2.28615400
O	0.01414400	1.49748800	1.61715400
O	1.03737600	0.90355200	3.45104400
O	1.24115700	-0.28638400	1.63340000

C	-7.09575100	-1.51854800	2.92829500
H	-7.62184500	-1.53577000	3.87783400
C	-3.81757400	4.67398500	-0.29404100
H	-4.68168900	5.21403500	0.07804600
C	-2.94691100	5.26689400	-1.15098100
H	-3.10845800	6.28835800	-1.47946300
C	0.41582700	3.13896300	-2.42653700
H	1.27994900	2.55171900	-2.70926300
C	0.11199300	-5.10717100	-2.29408100
C	-1.07737900	-4.44471100	-2.09136500
N	0.07986400	-2.47607300	-1.33946900
C	1.25717100	-3.11446100	-1.54428100
C	1.32720100	-4.44568700	-2.02460400
C	2.48489500	-2.40125100	-1.27340100
C	3.72887700	-3.04494400	-1.49836600
N	2.40478000	-1.13137200	-0.82976500
C	3.51889700	-0.45798600	-0.56080900
C	4.79630800	-1.00869200	-0.77231700
C	4.89442400	-2.29754300	-1.24549800
C	3.26227100	0.97930300	-0.16989900
O	2.21754000	1.50228500	-0.60473600
N	4.15399700	1.67832100	0.55845200
C	5.13320300	1.06174800	1.41731700
C	3.94401900	3.14142400	0.71687600
C	3.11715800	3.51218900	1.94456300
C	6.48443800	1.39031100	1.28360600
C	5.68407300	-0.40371600	3.24780300
C	4.72965900	0.17102700	2.41181200
H	0.12622900	-6.12652400	-2.66631600
H	-2.02974500	-4.91631400	-2.30201400
H	5.68508200	-0.42800400	-0.57271500
H	5.86772400	-2.74150600	-1.42717400
H	3.46527000	3.49609000	-0.19412800
H	4.93752700	3.58897900	0.77349400
H	3.07787500	4.60077600	2.03741200
H	3.55804800	3.11631100	2.86153300
H	2.09419300	3.14475300	1.86251400
H	6.80197800	2.08106300	0.50906500
H	5.35769500	-1.09500300	4.01842400
H	3.67798200	-0.06353100	2.53722800
C	3.75748000	-4.39310800	-1.97975700
H	4.71939400	-4.86700200	-2.14402800
C	2.60415200	-5.06507900	-2.22996200
H	2.63105000	-6.08567300	-2.59728200

C	-1.04368300	-3.12522600	-1.61402700
H	-1.96178900	-2.57014100	-1.46883100
C	-7.82676300	-1.44336200	1.73512700
C	7.04172400	-0.09424800	3.12784400
C	-9.33412200	-1.41928700	1.75361800
H	-9.73867600	-2.42835500	1.88397400
H	-9.71635300	-0.81136100	2.57690700
H	-9.74326000	-1.02205200	0.82301900
C	7.42308700	0.81428900	2.13113000
H	8.47105100	1.07333500	2.01483500
C	8.06489900	-0.68771300	4.06300000
H	9.00443500	-0.90245500	3.54836900
H	8.29542700	0.00499200	4.87912200
H	7.70821000	-1.61508700	4.51491000
Am	0.06735300	0.13677000	-0.57755300

Cm(L₆)₂(NO₃)₂⁺

C	-0.81779300	5.01916600	-2.74189800
C	0.24248000	4.24589500	-3.15705900
N	-0.46018400	2.42915500	-1.75119300
C	-1.52912800	3.16524500	-1.36367800
C	-1.74133000	4.48988800	-1.81740100
C	-2.48856700	2.57294500	-0.45631100
C	-3.57212600	3.35661700	0.01928400
N	-2.31998900	1.28886000	-0.09491600
C	-3.18609700	0.71526700	0.73459200
C	-4.25369000	1.43377600	1.30721000
C	-4.44051500	2.74902100	0.94408500
C	-2.81313200	-0.71562700	1.05392300
O	-1.66162600	-1.08945600	0.75608900
N	-3.65243700	-1.56766300	1.68210600
C	-5.08414600	-1.42994800	1.71654500
C	-3.08724800	-2.86868700	2.14225500
C	-2.20683300	-2.73986500	3.38216400
C	-5.75762300	-1.41825500	2.93995000
C	-7.19868700	-1.26820300	0.56756600
C	-5.81066100	-1.36912700	0.52802500
H	-0.95357900	6.02795900	-3.11856300
H	0.96393700	4.61482400	-3.87614300
H	-4.91736000	0.97075100	2.02099300
H	-5.25889000	3.32081700	1.36914900
H	-2.51808300	-3.29792900	1.31661800
H	-3.94056200	-3.51771200	2.33333900

H	-1.84619000	-3.72936300	3.67460800
H	-2.75991000	-2.32432000	4.22760500
H	-1.33672800	-2.11149700	3.19073600
H	-5.19685000	-1.46294000	3.86730800
H	-7.75054200	-1.21598800	-0.36569100
H	-5.29288000	-1.40185800	-0.42491100
N	-0.65771400	-0.44440700	-3.42286900
O	0.54171500	-0.16488400	-3.05278500
O	-0.94608200	-0.66047300	-4.57201000
O	-1.52564500	-0.47889900	-2.47523900
N	0.71537900	0.67880500	2.26625700
O	-0.01658500	1.44948400	1.55513900
O	0.97133600	0.91299600	3.42597700
O	1.17489000	-0.35597300	1.66249600
C	-7.14476000	-1.32799000	2.96484000
H	-7.65619400	-1.31494800	3.92241000
C	-3.73372000	4.70355900	-0.43757100
H	-4.57048000	5.28445700	-0.06442500
C	-2.86219500	5.24071000	-1.33035000
H	-2.99680600	6.25714300	-1.68553100
C	0.38950900	2.95523000	-2.62503100
H	1.22205700	2.32741100	-2.91560200
C	0.33350800	-5.27826100	-2.01218000
C	-0.88097300	-4.65602700	-1.83349300
N	0.19659200	-2.60409900	-1.19175200
C	1.39795800	-3.20390200	-1.37342000
C	1.52130300	-4.55426100	-1.78428200
C	2.59817800	-2.43089100	-1.14435300
C	3.86736500	-3.03636300	-1.33246100
N	2.46705200	-1.14626200	-0.76723800
C	3.55009900	-0.41993200	-0.51771300
C	4.85046200	-0.92790400	-0.69461900
C	5.00115900	-2.23210100	-1.10983900
C	3.22232600	1.01520800	-0.17673000
O	2.15241600	1.47095400	-0.63023700
N	4.06870600	1.78117200	0.53601800
C	5.07835700	1.24132700	1.41168300
C	3.78159400	3.23517200	0.65592100
C	2.95797100	3.59667600	1.88857500
C	6.41182300	1.62878300	1.26205600
C	5.70093700	-0.13556900	3.28728300
C	4.71895900	0.36653500	2.43675200
H	0.38816300	-6.31370800	-2.33269700
H	-1.81413500	-5.17674800	-2.01209200

H	5.71511100	-0.30577100	-0.51463900
H	5.99225300	-2.64542700	-1.26583500
H	3.26827200	3.53530800	-0.25562800
H	4.75031400	3.73712300	0.68048800
H	2.85459300	4.68353200	1.94580400
H	3.44114800	3.26056500	2.80814500
H	1.95785900	3.16539100	1.84254100
H	6.69442500	2.30788400	0.46406300
H	5.40916100	-0.81603200	4.08104400
H	3.67975900	0.08700100	2.57474300
C	3.94904800	-4.40468900	-1.74576800
H	4.92842100	-4.84980300	-1.88576900
C	2.82219800	-5.13171200	-1.96144900
H	2.88883100	-6.16765900	-2.27718800
C	-0.90025100	-3.31370300	-1.42307500
H	-1.83970000	-2.79186300	-1.29453900
C	-7.89167700	-1.24855000	1.78191300
C	7.04267200	0.23174500	3.15055400
C	-9.39721600	-1.17938600	1.82248500
H	-9.82979000	-2.17645900	1.95542200
H	-9.74914200	-0.56316700	2.65301400
H	-9.80777800	-0.76715000	0.89901300
C	7.37858300	1.12419800	2.12351800
H	8.41313300	1.42723100	1.99436500
C	8.09486900	-0.28492700	4.09896600
H	9.04627900	-0.45685300	3.59024200
H	8.28392300	0.43542700	4.90172600
H	7.78915700	-1.22173300	4.56846900
Cm	0.05880900	0.06813200	-0.60241400

Eu(L_b)₂(NO₃)₂⁺

C	-0.77610600	5.03042400	-2.77506600
C	0.29113900	4.26099600	-3.17988500
N	-0.41894200	2.44041100	-1.78342700
C	-1.49194300	3.17313100	-1.40524100
C	-1.70641000	4.49704100	-1.85980700
C	-2.45383100	2.57408900	-0.50628000
C	-3.54755400	3.35024900	-0.04142300
N	-2.27862300	1.29049700	-0.14302700
C	-3.15164100	0.71067200	0.67693300
C	-4.22935300	1.42288700	1.23769200
C	-4.42119900	2.73719400	0.87402200
C	-2.77517200	-0.71922000	0.99436800

O	-1.62786000	-1.08961800	0.68136000
N	-3.60438100	-1.57371000	1.63372300
C	-5.03580100	-1.44120900	1.68950300
C	-3.02961300	-2.87561300	2.07997700
C	-2.12284400	-2.75135600	3.30123400
C	-5.69014000	-1.42411800	2.92325400
C	-7.16878400	-1.29370500	0.57286500
C	-5.78118700	-1.39035600	0.51229000
H	-0.91202700	6.03875900	-3.15290400
H	1.01814700	4.63319000	-3.89172600
H	-4.89767300	0.95502200	1.94366700
H	-5.24764400	3.30321800	1.29109500
H	-2.47854500	-3.30420200	1.24165800
H	-3.87931200	-3.52420400	2.28807500
H	-1.76858900	-3.74406100	3.59074100
H	-2.65397200	-2.32562300	4.15566300
H	-1.24893700	-2.13497300	3.08979000
H	-5.11443600	-1.46100300	3.84178000
H	-7.73544800	-1.24908400	-0.35187000
H	-5.27818400	-1.42614000	-0.44841900
N	-0.61634200	-0.36426200	-3.43470700
O	0.58409200	-0.12507100	-3.04646500
O	-0.89591900	-0.55678100	-4.59094100
O	-1.49685000	-0.38603800	-2.50062800
N	0.69651900	0.61239500	2.20968400
O	-0.04282000	1.39292300	1.52028200
O	0.95174800	0.81936500	3.37506800
O	1.16467500	-0.40130700	1.58008100
C	-7.07704300	-1.33852800	2.96936400
H	-7.57350700	-1.32125100	3.93472400
C	-3.71291400	4.69663400	-0.49917100
H	-4.55717200	5.27149300	-0.13364900
C	-2.83610800	5.24071900	-1.38255800
H	-2.97375800	6.25683100	-1.73754100
C	0.43725100	2.96988600	-2.64789800
H	1.27287400	2.34313900	-2.93214000
C	0.29384200	-5.20818900	-2.17334000
C	-0.91904200	-4.58720800	-1.97881700
N	0.16344100	-2.55436900	-1.28837900
C	1.36198300	-3.15223100	-1.48644000
C	1.48344600	-4.49228400	-1.92974500
C	2.56087900	-2.38496900	-1.23846500
C	3.83002500	-2.98668100	-1.43876600
N	2.42924900	-1.10945800	-0.82902000

C	3.51375100	-0.39342100	-0.55335000
C	4.81347300	-0.89896700	-0.73950500
C	4.96428100	-2.19084800	-1.19143900
C	3.18611500	1.02998700	-0.16933700
O	2.11593700	1.49507200	-0.60920000
N	4.03151800	1.77617300	0.56623700
C	5.04251600	1.21289300	1.42503800
C	3.74005900	3.22514700	0.72852700
C	2.91702500	3.54976600	1.97197600
C	6.37464600	1.61011700	1.28869900
C	5.67015100	-0.22119400	3.25560300
C	4.68638700	0.30401800	2.42118700
H	0.34562200	-6.23592400	-2.51824500
H	-1.85345300	-5.10165900	-2.16892600
H	5.67798600	-0.28359400	-0.53694100
H	5.95530600	-2.60112300	-1.35562500
H	3.22451600	3.54962800	-0.17338300
H	4.70720600	3.72941000	0.76603200
H	2.81434200	4.63452400	2.06150000
H	3.40061700	3.18614700	2.88078800
H	1.91651000	3.12085100	1.91427400
H	6.65489900	2.31552800	0.51302800
H	5.38091000	-0.92795200	4.02701200
H	3.64852900	0.01501400	2.54893100
C	3.91081400	-4.34436400	-1.88665900
H	4.89022800	-4.78612200	-2.03663500
C	2.78403000	-5.06572900	-2.12114400
H	2.85078200	-6.09363300	-2.46215900
C	-0.93491500	-3.25493100	-1.53582100
H	-1.87251000	-2.73264200	-1.39507700
C	-7.84267500	-1.26877200	1.79780300
C	7.01034400	0.15601100	3.13188400
C	-9.34759900	-1.20347700	1.86204300
H	-9.77449500	-2.19853900	2.02486900
H	-9.68764400	-0.56969200	2.68434400
H	-9.77502400	-0.81334700	0.93666400
C	7.34306300	1.08239900	2.13426500
H	8.37640900	1.39373700	2.01552500
C	8.06445000	-0.38612700	4.06384900
H	9.01233700	-0.55246300	3.54663200
H	8.26170200	0.31627500	4.88039400
H	7.75606700	-1.33093800	4.51513600
Eu	0.06205500	0.08696300	-0.63848300

M06-2X/6-311G*-RECP

C	-0.78115200	5.14869800	-2.32943600
C	0.22626600	4.37041900	-2.84321100
N	-0.42896500	2.51882500	-1.47193200
C	-1.44576600	3.26581400	-0.98744500
C	-1.65830800	4.60093700	-1.37307300
C	-2.36086000	2.65632400	-0.04714500
C	-3.41586300	3.41462600	0.49643000
N	-2.17368500	1.36532500	0.26899900
C	-3.01197700	0.76633200	1.09055500
C	-4.07800200	1.44139400	1.71155100
C	-4.26552400	2.77003800	1.41470000
C	-2.61367500	-0.66562500	1.36487300
O	-1.41346500	-0.95920800	1.26287200
N	-3.52591600	-1.58092400	1.72530900
C	-4.92794100	-1.42278200	1.47669900
C	-3.03223500	-2.89742200	2.18705200
C	-2.42908600	-2.82471100	3.58220400
C	-5.84422300	-1.65227500	2.50072100
C	-6.73359200	-0.90162300	-0.02119500
C	-5.37204700	-1.06437700	0.20891800
H	-0.91611000	6.17503500	-2.65463900
H	0.90924000	4.75186400	-3.59131000
H	-4.72900500	0.92849800	2.40700900
H	-5.07124700	3.32707600	1.88083500
H	-2.28952100	-3.24981800	1.46859500
H	-3.88530300	-3.57397100	2.15550700
H	-2.09685500	-3.81618200	3.89358400
H	-3.15953800	-2.46790200	4.31058500
H	-1.56589900	-2.15901900	3.59589100
H	-5.49279600	-1.93478300	3.48753200
H	-7.07178800	-0.61476400	-1.01104900
H	-4.65554900	-0.90510200	-0.59203000
N	-1.00178600	-0.38651600	-3.08896300
O	0.23277000	-0.16016900	-2.91880700
O	-1.45850100	-0.76150800	-4.12516300
O	-1.73699600	-0.19762500	-2.05534300
N	1.20560900	1.10076100	2.13681900
O	0.29857300	1.74735600	1.54180800
O	1.69839500	1.46238400	3.16554100
O	1.58412900	0.02849300	1.55220300

C	-7.19982100	-1.50047600	2.25188000
H	-7.91141500	-1.67685700	3.05222400
C	-3.57975200	4.78506100	0.10535900
H	-4.39298000	5.35558100	0.53998700
C	-2.74215600	5.34794300	-0.79627200
H	-2.87438400	6.38011400	-1.10200200
C	0.37110100	3.05322700	-2.37802700
H	1.16398000	2.41400100	-2.74785400
C	-0.46712400	-5.18588800	-1.59941400
C	-1.57597300	-4.39433200	-1.42569800
N	-0.20463600	-2.47171900	-1.00706600
C	0.89037200	-3.24236900	-1.18565200
C	0.81423300	-4.61524200	-1.48391200
C	2.19285400	-2.62044500	-1.07590700
C	3.35314500	-3.39156700	-1.28028600
N	2.24463700	-1.30712300	-0.80321400
C	3.41573500	-0.70309900	-0.70717000
C	4.62997300	-1.38211500	-0.90899700
C	4.58864700	-2.72603100	-1.19609100
C	3.28084400	0.79491600	-0.52100300
O	2.23563400	1.32461300	-0.93332100
N	4.27222600	1.52067700	0.00272900
C	5.29342700	0.96409200	0.84462500
C	4.12924100	2.99259800	0.00254700
C	3.28469000	3.49109900	1.16609500
C	6.63343300	1.18329000	0.53469400
C	5.94153300	-0.30176300	2.77541900
C	4.93937100	0.23393400	1.97359900
H	-0.56460200	-6.24095000	-1.83312300
H	-2.57736000	-4.79396000	-1.52239000
H	5.57403600	-0.85879600	-0.84755300
H	5.50694200	-3.27775200	-1.36657600
H	3.68993100	3.27748900	-0.95306900
H	5.14053000	3.39671800	0.05191700
H	3.32998000	4.58064200	1.21231500
H	3.65232000	3.09817500	2.11604600
H	2.23979900	3.20293700	1.04374900
H	6.89692200	1.75253600	-0.35101800
H	5.66428400	-0.87313700	3.65517800
H	3.89088700	0.09237800	2.21844500
C	3.23561600	-4.79100900	-1.57711200
H	4.14197800	-5.36667900	-1.72802500
C	2.01952700	-5.37561200	-1.67186800
H	1.93099800	-6.43217700	-1.89995900

C	-1.39416700	-3.03410000	-1.13203800
H	-2.24905700	-2.37583100	-1.01234500
C	-7.66750700	-1.11636900	0.99090100
C	7.29002600	-0.10483700	2.48140100
C	-9.14418900	-0.96331300	0.74334500
H	-9.65428700	-1.92460500	0.84004100
H	-9.59411200	-0.28064200	1.46731700
H	-9.34391100	-0.57664800	-0.25591000
C	7.61931200	0.64835100	1.34979200
H	8.66321600	0.81552700	1.10482300
C	8.36928800	-0.65074200	3.37722300
H	9.24722200	-0.95235000	2.80382000
H	8.69110300	0.10913200	4.09438500
H	8.01904800	-1.51328600	3.94497700
Am	0.07200500	0.15380900	-0.42811400

Cm(L₆)₂(NO₃)₂⁺

C	-0.86180600	5.01078100	-2.65373900
C	0.20328000	4.25982800	-3.08621100
N	-0.46745200	2.41945100	-1.70843400
C	-1.53932200	3.13664100	-1.30658400
C	-1.77186100	4.45544200	-1.73358800
C	-2.48179800	2.51650800	-0.39886400
C	-3.56397100	3.26790600	0.10015100
N	-2.28491900	1.23313900	-0.06409600
C	-3.12046900	0.63463400	0.76597100
C	-4.19316000	1.31763700	1.36910000
C	-4.40689500	2.63241100	1.02723500
C	-2.69963800	-0.79327900	1.05124700
O	-1.53439700	-1.11510800	0.76932700
N	-3.52090500	-1.68877400	1.61596100
C	-4.94454900	-1.54745500	1.68361500
C	-2.93103100	-2.98561000	2.02462000
C	-2.03428400	-2.85406000	3.24746700
C	-5.58518500	-1.61925400	2.91781600
C	-7.06219000	-1.20712900	0.60235600
C	-5.68288400	-1.36032700	0.52157200
H	-1.01387500	6.02322600	-3.01319400
H	0.91561000	4.64894300	-3.80226400
H	-4.83551000	0.83259900	2.08958600
H	-5.22700600	3.18490200	1.47327200
H	-2.36574700	-3.37878900	1.17728100
H	-3.76906900	-3.65432000	2.21604700

H	-1.64209400	-3.83505600	3.52047400
H	-2.58772900	-2.46303900	4.10309400
H	-1.18901600	-2.19663200	3.04341000
H	-5.00204700	-1.76379700	3.82107100
H	-7.63191100	-1.05169100	-0.30763000
H	-5.17803600	-1.32497800	-0.43855500
N	-0.66504800	-0.41706800	-3.39325000
O	0.52592800	-0.12495200	-3.04755900
O	-0.95315100	-0.69718900	-4.51695500
O	-1.52723700	-0.39744200	-2.45474200
N	0.80146400	0.77628400	2.20153200
O	-0.03486700	1.45751000	1.53829700
O	1.11870800	1.05870000	3.32299400
O	1.30170700	-0.22356600	1.59363800
C	-6.96346700	-1.47723300	2.98207700
H	-7.45950000	-1.52852600	3.94598900
C	-3.75270900	4.62221100	-0.33469400
H	-4.59509600	5.18108500	0.05736200
C	-2.90188200	5.18343200	-1.22436100
H	-3.05203100	6.20220100	-1.56480700
C	0.37036700	2.96327800	-2.57486700
H	1.21093700	2.34866400	-2.87489800
C	0.25325600	-5.15881500	-2.09211000
C	-0.94979100	-4.52189900	-1.90910600
N	0.15530400	-2.50173700	-1.24041800
C	1.34204800	-3.11935900	-1.42874300
C	1.44914400	-4.45708300	-1.84947400
C	2.55123900	-2.36565000	-1.18129700
C	3.80684600	-2.98047500	-1.34848500
N	2.42529800	-1.08539400	-0.80191400
C	3.50427400	-0.37608400	-0.52897800
C	4.80314400	-0.89461300	-0.66999700
C	4.94494800	-2.19589800	-1.09028600
C	3.17649000	1.06340200	-0.19536800
O	2.12841200	1.53087000	-0.67385000
N	4.01078200	1.80617500	0.53634500
C	4.97309800	1.23183000	1.43483500
C	3.71164000	3.24456300	0.70062900
C	2.73258600	3.49891800	1.83684300
C	6.31107100	1.60788500	1.34688500
C	5.50144500	-0.24744500	3.24688900
C	4.55784000	0.31674100	2.39532500
H	0.29468600	-6.19052700	-2.42554900
H	-1.88986700	-5.02432800	-2.09723500

H	5.66903300	-0.28234900	-0.45853200
H	5.93245800	-2.62484500	-1.22349600
H	3.31751100	3.60558800	-0.24851600
H	4.66760200	3.73500700	0.88701800
H	2.65004000	4.57192200	2.01844900
H	3.06993800	3.02479400	2.76072700
H	1.74061800	3.12090000	1.58780500
H	6.62473600	2.32112500	0.59140100
H	5.17513100	-0.96311100	3.99421200
H	3.50735200	0.05132500	2.47284000
C	3.87629900	-4.34819700	-1.77750000
H	4.85213200	-4.80319600	-1.90654400
C	2.74652500	-5.05244000	-2.01906100
H	2.79921300	-6.08479500	-2.34730900
C	-0.95005400	-3.18549600	-1.47958900
H	-1.88178800	-2.64840400	-1.34198700
C	-7.72404900	-1.26290200	1.82853900
C	6.84887100	0.10097100	3.16959000
C	-9.22106100	-1.13468300	1.91463600
H	-9.68192400	-2.11747300	2.04343700
H	-9.51730600	-0.52065500	2.76674800
H	-9.63725200	-0.68909800	1.01103500
C	7.23714900	1.04057200	2.20960900
H	8.28091900	1.32847100	2.13582000
C	7.85963700	-0.48367800	4.11945900
H	8.81613300	-0.65881300	3.62439800
H	8.04174200	0.20077700	4.95217200
H	7.51283400	-1.42899000	4.53773800
Cm	0.07480000	0.10716200	-0.61178700

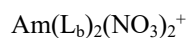
Eu(L_b)₂(NO₃)₂⁺

C	-0.71254200	4.93242800	-2.82510600
C	0.34275000	4.14881600	-3.22305100
N	-0.37580800	2.36324300	-1.79835300
C	-1.43654400	3.11264200	-1.43032300
C	-1.64177800	4.42159300	-1.89903600
C	-2.39732100	2.53566400	-0.51478900
C	-3.47263300	3.31851400	-0.05070900
N	-2.22317100	1.25982200	-0.14218200
C	-3.07813100	0.69800800	0.69441700
C	-4.14436600	1.41633600	1.26733100
C	-4.33430400	2.72400900	0.88587500
C	-2.68435700	-0.73025100	1.01434500
O	-1.53361300	-1.08505600	0.71909100

N	-3.51380100	-1.59156900	1.62146900
C	-4.93321700	-1.42268200	1.70680300
C	-2.94377000	-2.88830400	2.05688600
C	-2.00694700	-2.74115700	3.24756600
C	-5.55506000	-1.44171900	2.95225300
C	-7.06199900	-1.08180600	0.64761800
C	-5.68719700	-1.26159200	0.55077000
H	-0.84184300	5.93603500	-3.21677200
H	1.06932600	4.50384900	-3.94250700
H	-4.80144000	0.96433800	1.99565000
H	-5.14984400	3.30192100	1.30736700
H	-2.41606100	-3.32680900	1.20734600
H	-3.79270100	-3.52684800	2.29707900
H	-1.65565800	-3.72579100	3.56026800
H	-2.51720500	-2.28061300	4.09540500
H	-1.13690800	-2.13753000	2.98958300
H	-4.95936800	-1.56431600	3.85061600
H	-7.64385200	-0.94670900	-0.25799200
H	-5.19657900	-1.26536300	-0.41729900
N	-0.68613700	-0.50966900	-3.34800200
O	0.51641600	-0.23650100	-3.03967000
O	-1.00520000	-0.85377200	-4.44631100
O	-1.53007700	-0.40723400	-2.39788300
N	0.82148800	0.75421200	2.11019900
O	-0.01051600	1.43887900	1.44498700
O	1.18307400	1.07003500	3.20930200
O	1.26491000	-0.28592400	1.52888100
C	-6.92984400	-1.27452800	3.03320200
H	-7.41094100	-1.28380100	4.00588800
C	-3.63483000	4.66187200	-0.52868200
H	-4.47269800	5.24573400	-0.16440200
C	-2.76520900	5.18255600	-1.42481000
H	-2.89527100	6.19276300	-1.79752800
C	0.48040600	2.86495100	-2.67174200
H	1.31105700	2.22527700	-2.94524100
C	0.06609100	-5.17278100	-2.13263600
C	-1.11695700	-4.49582800	-1.93879900
N	0.06828700	-2.52207500	-1.25348600
C	1.21536100	-3.15924600	-1.44834200
C	1.29175000	-4.51158900	-1.88228300
C	2.46302200	-2.39996000	-1.18818800
C	3.73796500	-3.07689100	-1.33559900
N	2.35384200	-1.15912700	-0.83643400
C	3.48767700	-0.42752100	-0.52464500

C	4.77014600	-0.98832700	-0.63420200
C	4.91052900	-2.28774300	-1.04081600
C	3.17064500	0.98743900	-0.23717700
O	2.09744500	1.44529400	-0.68999300
N	4.02333000	1.77185500	0.44227900
C	4.98946400	1.23990800	1.35868600
C	3.71922100	3.21278100	0.54756700
C	2.76564200	3.51537900	1.69460200
C	6.32605000	1.61531400	1.25137000
C	5.53191800	-0.16445500	3.22740900
C	4.58338300	0.36119700	2.35814900
H	0.07345000	-6.20125100	-2.47713500
H	-2.07168700	-4.96860000	-2.13065400
H	5.64389800	-0.39186700	-0.40787000
H	5.89127700	-2.73551300	-1.14995800
H	3.29990400	3.52940900	-0.40669700
H	4.67513200	3.71874600	0.68869300
H	2.67740100	4.59544600	1.82647100
H	3.13131900	3.08875000	2.63097100
H	1.77162400	3.11532300	1.49221300
H	6.63368700	2.29682400	0.46493900
H	5.21199000	-0.85021300	4.00500500
H	3.53492100	0.09311700	2.45010500
C	3.76883100	-4.37554400	-1.75055100
H	4.72165700	-4.87841200	-1.87437900
C	2.54468400	-5.11955300	-2.04207900
H	2.61257600	-6.14554600	-2.37999500
C	-1.07786300	-3.17224000	-1.49421000
H	-1.98479900	-2.59957600	-1.34712000
C	-7.70511000	-1.08628200	1.88517900
C	6.87848700	0.18541800	3.13068300
C	-9.19860000	-0.93219700	1.98858100
H	-9.67459900	-1.90761300	2.11887900
H	-9.47532300	-0.31622700	2.84568900
H	-9.61707400	-0.47684000	1.09085500
C	7.25870100	1.08661600	2.13249100
H	8.30110400	1.37458100	2.04168600
C	7.89408600	-0.35798400	4.09992200
H	8.85855400	-0.52103600	3.61636900
H	8.05347000	0.34582500	4.92113100
H	7.56483800	-1.30282600	4.53347100
Eu	0.08685000	0.08992400	-0.64126000

PBE0/ZORA



C	-0.90830316255950	5.07529038509562	-2.55616406663476
C	0.16693247930101	4.34433073743844	-2.98747261115015
N	-0.47089502092837	2.49387137217836	-1.61613402394087
C	-1.55134553024930	3.18714293686545	-1.21425143770705
C	-1.80543457190304	4.50455081676785	-1.64074836026013
C	-2.48164151884684	2.55191304950885	-0.31909379622554
C	-3.58158525319243	3.28884068303885	0.16929830794349
N	-2.27089459220698	1.27376820800430	0.02120427300481
C	-3.11958755963067	0.66885767666748	0.83343981523927
C	-4.20491259120296	1.33673027600749	1.41533281590958
C	-4.42901622412692	2.64596303737275	1.08007619805559
C	-2.71383221368235	-0.74093854200593	1.14992024575548
O	-1.53398412100614	-1.05839298394081	0.94489767286644
N	-3.57068227011483	-1.62464059279434	1.68509627257982
C	-4.98763960922332	-1.52986956659030	1.57433518883740
C	-3.00979273288620	-2.88899890086328	2.19242426761348
C	-2.28255471634968	-2.72875035780003	3.51235102860463
C	-5.78633657394164	-1.65686247628646	2.70499254579155
C	-6.96131406735185	-1.29206928830095	0.22728040493805
C	-5.58155409126747	-1.36345827376709	0.33068894159836
H	-1.07872112659728	6.08505882638383	-2.91338475641660
H	0.87308571337865	4.74529234864773	-3.70301702438108
H	-4.85251169696563	0.83127712851562	2.11610058362996
H	-5.26091302613368	3.18944243027125	1.51382525876437
H	-2.33077559568226	-3.28435999124194	1.43436147166987
H	-3.84812525055779	-3.57814061913383	2.28688953813709
H	-1.89847806024747	-3.69836341826463	3.83515309676034
H	-2.94735780330735	-2.35406245927877	4.29279862939949
H	-1.43665116788065	-2.04765316277425	3.41690123167420
H	-5.32924078566095	-1.78725796217272	3.67916266786865
H	-7.41170859310969	-1.15571025840836	-0.74992083964699
H	-4.96435140754048	-1.28857374944876	-0.55791765054098
N	-0.68104530817301	-0.27172543638088	-3.33057442904345
O	0.52071359998854	-0.06607916511698	-2.99205148267564
O	-1.00801296305223	-0.45842191731830	-4.46768057759807
O	-1.52512188709787	-0.26836231565267	-2.37899486486518
N	0.81060586182664	0.83074428937124	2.26030958297990
O	0.04631073122768	1.56885042084179	1.58107205288620

O	1.09396006583584	1.07087501353425	3.40282723582265
O	1.27638251974644	-0.18438019204147	1.65542459192395
C	-7.16344369442517	-1.59714464015407	2.58587346796932
H	-7.77586205337777	-1.69170328263423	3.47619830250187
C	-3.78658546336364	4.63226289777004	-0.25803827798957
H	-4.63967306100257	5.17654937204159	0.13028618081707
C	-2.94006103803659	5.21012042312647	-1.14004021438604
H	-3.10491961064962	6.22728392471350	-1.47737621171381
C	0.35358274797503	3.05567733866028	-2.47862111306929
H	1.20513747385931	2.45927635086029	-2.78256680163509
C	0.10627400680510	-5.13379538876003	-2.02547244304052
C	-1.07737013327219	-4.47322177696304	-1.82615657561907
N	0.07679972977784	-2.47886176564943	-1.18258764748042
C	1.24517053417315	-3.11508084749786	-1.38626110777930
C	1.31542959666926	-4.45642584044864	-1.81003567593073
C	2.4659523351635	-2.38649502343768	-1.17291822510155
C	3.70238695440012	-3.02717754506329	-1.39419357652692
N	2.38288934182208	-1.10707563576842	-0.78456894610559
C	3.49062089786122	-0.42191135221959	-0.56609851690043
C	4.76347570966260	-0.96695549903776	-0.77614560397043
C	4.86252181321877	-2.26700333522884	-1.19683417540064
C	3.23296315615401	1.01959736871843	-0.23000224485436
O	2.17946192277443	1.51555869243403	-0.65594025883506
N	4.13558967384206	1.74707312631992	0.43674734714605
C	5.14062888147151	1.17502842502199	1.27345741295866
C	3.92760831257690	3.19807094573784	0.54226009784175
C	3.16202927214461	3.60734682617587	1.78407137516748
C	6.47290399776900	1.53354260606422	1.10302481137998
C	5.76841795183617	-0.24629607150282	3.09910208081209
C	4.78511112392738	0.29299139023386	2.28428729142809
H	0.12245506859403	-6.16658877116750	-2.35596746979884
H	-2.03053187611155	-4.95707410278742	-1.99601867736298
H	5.64873176070444	-0.36920788709176	-0.61509291563951
H	5.83351349175093	-2.71327329450467	-1.38048293546124
H	3.40424479236477	3.51480546912691	-0.35875143768390
H	4.91998394583044	3.65201009162635	0.53827950238399
H	3.12465612081800	4.69705270250869	1.84204671770826
H	3.64840001877995	3.24058457009417	2.68970666590479
H	2.13806179991702	3.23408620201853	1.76118277357227
H	6.75402001024537	2.22112292298095	0.31291936529521
H	5.48069002217864	-0.93541749217544	3.88569145408409
H	3.74187552843122	0.03626202637133	2.43646309655949
C	3.73339949808711	-4.38771428589485	-1.81714033882795
H	4.69584375223811	-4.85897987046135	-1.97994773545174

C	2.58540796500318	-5.07401999121306	-2.01509380821978
H	2.60973357732351	-6.10801111079094	-2.34022713307128
C	-1.04107177758338	-3.14115708511045	-1.40494887963129
H	-1.96149533695246	-2.58847398016393	-1.26099182184803
C	-7.77779457031273	-1.41024543870333	1.34801228140800
C	7.10839523500515	0.09322807927500	2.94198581816124
C	-9.26924598170590	-1.37341203157697	1.22851111035204
H	-9.67891522295880	-2.38742127575721	1.19690680055686
H	-9.72473456736679	-0.86729457859676	2.08137553927587
H	-9.58460396927854	-0.86364034182166	0.31755787483131
C	7.44117685593113	0.99340737754510	1.92966485559521
H	8.47907357922766	1.27351759960652	1.78444708843035
C	8.16015477091748	-0.45930274442995	3.85249708147885
H	9.09730917125728	-0.63259765518760	3.32063678416376
H	8.37331727493769	0.24153484034738	4.66522994473346
H	7.84247275063827	-1.39910695491495	4.30546429503640
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Cm(L_b)₂(NO₃)₂⁺

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N	-0.46690424074632	2.43536815888817	-1.69907539586396
C	-1.52060427402651	3.16063885587298	-1.28092923622002
C	-1.73467892004943	4.49008362813163	-1.69104273307787
C	-2.46446000734993	2.54832478207889	-0.38384817683333
C	-3.53271259711939	3.31519981976705	0.12660179481427
N	-2.29249047726075	1.26132802843337	-0.06587823472427
C	-3.14513183491906	0.67073902467951	0.75038281815322
C	-4.19964005870124	1.36623933170705	1.35802045519501
C	-4.38707143721999	2.68644796971035	1.04100158069979
C	-2.77209940598267	-0.75781467534216	1.03009614154925
O	-1.61778590937391	-1.11501588483485	0.75386363751283
N	-3.62248407386691	-1.61900181549548	1.60828164394652
C	-5.03993943205032	-1.47638704844435	1.59614068448403
C	-3.07494559862469	-2.90725083744652	2.06876247403045
C	-2.25272768064553	-2.78544978971932	3.33611100063927
C	-5.76003234491399	-1.56054075710878	2.78210589647442
C	-7.09373652690422	-1.18703291764835	0.38715659293548
C	-5.71331075173702	-1.30584117906928	0.39452912256086
H	-0.96773079065182	6.05862103882586	-2.95504502781170
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H	-3.93041693306741	-3.56500870293507	2.21759095972027
H	-1.88976075765042	-3.77270171738309	3.62853710039202
H	-2.84650777547803	-2.38815681195162	4.16135713452449
H	-1.38664399135201	-2.14060834773137	3.18605637799018
H	-5.23929187792331	-1.69373637786826	3.72339307622463
H	-7.60742317150082	-1.04790164971802	-0.55789301672655
H	-5.15684189101206	-1.26513241821560	-0.53536712146303
N	-0.68817204293072	-0.37951533123585	-3.39759189373871
O	0.50378822043414	-0.11928828512125	-3.04744251985433
O	-0.99087607982135	-0.57600491387403	-4.53933500589125
O	-1.53715888864836	-0.41938898113266	-2.45526892305842
N	0.72247591718377	0.63699540215474	2.23095469876758
O	0.00651770599727	1.41551053050986	1.53888402735388
O	0.96590134935249	0.84891702578007	3.38897305379510
O	1.17870347088216	-0.37719283060014	1.62391341836523
C	-7.13921253341247	-1.45286217726827	2.75909245355274
H	-7.69022245760421	-1.51333321840725	3.69151454756116
C	-3.69668417857392	4.66948667468238	-0.28423504007613
H	-4.52610055811279	5.23904542832828	0.11892655906065
C	-2.84030502629925	5.22731444325410	-1.17000037076078
H	-2.97434115934769	6.25303371427169	-1.49489842758682
C	0.36707997250281	2.97906243060708	-2.56471534948449
H	1.19519051355627	2.35845874231199	-2.88467105111359
C	0.28391835094730	-5.20213166801893	-2.10022629653316
C	-0.91949650187754	-4.58155503072619	-1.89189245270792
N	0.17091679376804	-2.55606544494862	-1.23251203244420
C	1.35821119108721	-3.15388058736743	-1.44446307479473
C	1.47106836983758	-4.48827848810296	-1.87985566582040
C	2.55725734787714	-2.39190954650476	-1.22246937880274
C	3.81421789521828	-2.99250900718712	-1.44056275417541
N	2.43276371469624	-1.12156943505198	-0.82340810737004
C	3.51436515186204	-0.40770024781040	-0.57836000983874
C	4.80652041151458	-0.90957308642616	-0.77964276989382
C	4.94851964119896	-2.19930174795478	-1.22116669088748
C	3.19657083067956	1.01379952346316	-0.21114958546624
O	2.12878534704605	1.47967450485824	-0.64016934834368
N	4.05423963055778	1.75658252879243	0.49443764362054
C	5.07044786272594	1.19796377032130	1.32723953128694
C	3.78430663364075	3.19339961418307	0.64673903188964
C	3.00250197925445	3.52748244304959	1.90078556678383
C	6.38983665793569	1.61149598760137	1.18588136853942
C	5.72787205658491	-0.25264629466328	3.11903727114906

C	4.73559299773065	0.27356121974537	2.30676716119441
H	0.33232851682548	-6.23088844189826	-2.44007160029818
H	-1.85713890803279	-5.09423044956782	-2.06359986760741
H	5.67207719013112	-0.28942441728172	-0.59686947762725
H	5.93452592061618	-2.61297750889293	-1.40118406550026
H	3.24703449191377	3.51591354584235	-0.24385756860775
H	4.75641704075124	3.68939298650678	0.65822666991197
H	2.91421956094467	4.61194164856113	1.99220258942210
H	3.50763634155353	3.15678223221983	2.79448484841332
H	1.99735683177352	3.10664729246064	1.86684197159525
H	6.65446960303310	2.33261607817356	0.42039398512405
H	5.45645758353995	-0.97546977563866	3.88074405769179
H	3.70132088435700	-0.02788326526814	2.43711681694759
C	3.88756733560194	-4.34639817378550	-1.87895912038185
H	4.86377954614880	-4.78817486338677	-2.04254858961057
C	2.76046506753301	-5.06367201949186	-2.08874197390165
H	2.81683967114466	-6.09299220360295	-2.42465920059427
C	-0.92557036971676	-3.25282361040894	-1.45806308303921
H	-1.86238004855599	-2.73180859917043	-1.30433189181615
C	-7.83237808240236	-1.26061178206427	1.56435799540847
C	7.05598547841553	0.14135088929648	2.99014457516790
C	-9.32636415536638	-1.17152880198566	1.54950943845391
H	-9.77243741459254	-2.17044418915492	1.56389198252780
H	-9.70213906623527	-0.63718514951456	2.42375461734805
H	-9.68754429559347	-0.66375792340498	0.65460193359170
C	7.36729145769161	1.08329814538414	2.00954880150876
H	8.39562432900155	1.40620933379881	1.88704399502868
C	8.11644401748952	-0.39920908708537	3.89769302849189
H	9.06563282980733	-0.52209774043789	3.37320728122093
H	8.29376399859588	0.28437458302562	4.73339624639875
H	7.82834845133497	-1.36313607086535	4.31858042700944
Cm	0.05948947503818	0.07863466006805	-0.60774142670866

Eu(L_b)₂(NO₃)₂⁺

C	-0.85730359507198	5.08191856660574	-2.55148809486470
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C	-1.52257164413609	3.19379959881186	-1.22151722379405
C	-1.76504236115181	4.51420724214126	-1.64495416858196
C	-2.46418591983680	2.56252511729100	-0.33629100911876
C	-3.56462803670698	3.30185459152303	0.14638347668675
N	-2.26070609956508	1.28382941919351	-0.00170303934923
C	-3.11465522308206	0.67693396428633	0.80124443917461

C	-4.20337705668631	1.34448400123119	1.37820243514038
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N	-3.54748694117398	-1.62173635065569	1.65307673801343
C	-4.96659253363087	-1.52891184956844	1.56885288380228
C	-2.97588043480084	-2.88674637721294	2.14709265192025
C	-2.22625251460725	-2.72867618061007	3.45469805144392
C	-5.74429000960620	-1.64994993943423	2.71449631152472
C	-6.96419813209357	-1.30124716414376	0.25594919459435
C	-5.58281787317533	-1.37063730829240	0.33503729922095
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H	0.92951213654299	4.74146663889325	-3.68678608540845
H	-4.85839250292446	0.83864938492490	2.07170128748715
H	-5.25561526315625	3.19937317953505	1.47639552274343
H	-2.30972286550085	-3.27927511126879	1.37637635933438
H	-3.81168551744153	-3.57711700428724	2.25433766302878
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H	-1.38172969063548	-2.04781660529703	3.34612335335975
H	-5.26942428679950	-1.77379145991231	3.68096493490354
H	-7.43232485065936	-1.17088727398636	-0.71371368822025
H	-4.98135184748623	-1.29953848973214	-0.56458724778833
N	-0.67179161463749	-0.25781598708372	-3.29839997925626
O	0.52724566932227	-0.04658309104298	-2.95244461407633
O	-0.99280893121756	-0.43889335454303	-4.43760653515859
O	-1.51677327067739	-0.26556938454699	-2.34897027246802
N	0.77318191209451	0.77976412329484	2.22691127071442
O	0.03627473160242	1.53746272474776	1.53908520665897
O	1.03832097101838	1.00509064564560	3.37705891396871
O	1.23065584764417	-0.23723812583653	1.62116444784280
C	-7.12349786804671	-1.59199977397792	2.61977531839056
H	-7.71975152128093	-1.68142784819857	3.52151325590317
C	-3.75806940596187	4.64816083274422	-0.27758954434728
H	-4.61114206872686	5.19664719472750	0.10485434151352
C	-2.90003313095923	5.22404745349816	-1.15007866188851
H	-3.05612396928683	6.24352335557184	-1.48467363613246
C	0.38877333520380	3.05190443608351	-2.47180954207798
H	1.23777781562184	2.45074239488359	-2.77296752295467
C	0.08806303475844	-5.13547052640874	-2.03284140546836
C	-1.09365525682949	-4.46873152750204	-1.84227950830816
N	0.06422317212566	-2.47731630742729	-1.19384698307147
C	1.22992094574260	-3.12029398454513	-1.39033626892035
C	1.29840158710170	-4.46258836822106	-1.81081113186794

C	2.45206225952275	-2.39640339869468	-1.17140955435804
C	3.68867675080466	-3.04004339336184	-1.38195286505511
N	2.36707154542358	-1.11787431524095	-0.78702158465604
C	3.47217514057187	-0.43374954876753	-0.55932934825092
C	4.74688534995133	-0.97931766501783	-0.75813448642507
C	4.84792214107269	-2.28035703327512	-1.17664725437143
C	3.20151816653272	1.00438068683501	-0.22057715377918
O	2.13941640528110	1.48786000328309	-0.64075694973388
N	4.09635156450240	1.74171131451003	0.44495533492535
C	5.10893256026904	1.17914986732454	1.27922074729555
C	3.87231537982657	3.18998203433199	0.55602202459195
C	3.12048749273125	3.58809378367214	1.80973838788932
C	6.43743782849042	1.54984231428380	1.10687261806291
C	5.75165301108186	-0.23486248092468	3.10552989841860
C	4.76281693700039	0.29475152484884	2.29129510356720
H	0.10151376818671	-6.16901145188137	-2.36116591542765
H	-2.04794051439682	-4.94851850037696	-2.01743187590281
H	5.63178903628300	-0.38287090093712	-0.59026699703756
H	5.82010553542680	-2.72755782520616	-1.35159313769520
H	3.33166688908975	3.50139516025092	-0.33649114716151
H	4.85904079919776	3.65595705124582	0.53787017627035
H	3.06927163930336	4.67716691651955	1.86892837841609
H	3.62600794942271	3.22785059446434	2.70748139292187
H	2.10148152797410	3.20083026454753	1.80231904008523
H	6.71127063882966	2.23931700266015	0.31588426839834
H	5.47117135659283	-0.92622273296203	3.89277050791530
H	3.72232424601982	0.02784601137765	2.44450422479876
C	3.71781828852980	-4.40174128363263	-1.80153465697354
H	4.67936719742390	-4.87742088411415	-1.95672945506859
C	2.56836703553131	-5.08421197260985	-2.00579922897483
H	2.59164146237865	-6.11902328959078	-2.32848721353896
C	-1.05449261979316	-3.13607180273881	-1.42245076921953
H	-1.97367965801711	-2.57997119929837	-1.28470822607177
C	-7.76016080512983	-1.41322804701111	1.39205946068684
C	7.08831733830584	0.11697409587280	2.94649737542729
C	-9.25353301022195	-1.37845130486541	1.29878525122351
H	-9.66195895887690	-2.39308846975441	1.27106693367258
H	-9.69494922070264	-0.87564472390977	2.16089810672413
H	-9.58551186387958	-0.86659762505670	0.39489870407874
C	7.41159252302250	1.01917873058699	1.93296281546979
H	8.44670307773625	1.30868350057295	1.78638286327650
C	8.14585840930645	-0.42489380589960	3.85670258126764
H	9.08592700534453	-0.58439580306257	3.32574595054643
H	8.34863734974818	0.27600190544611	4.67205049315649

H	7.83962233689489	-1.37013645018962	4.30625659373537
Eu	0.06538823871447	0.13661342815131	-0.53874395237134