

# Competing routes in the extraction of lanthanide nitrates by 1,10-phenanthroline-2,9-dicarboxylic acid diamides: an impact of structure of complexes on the extraction

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## 1. NMR and IR spectra drawings

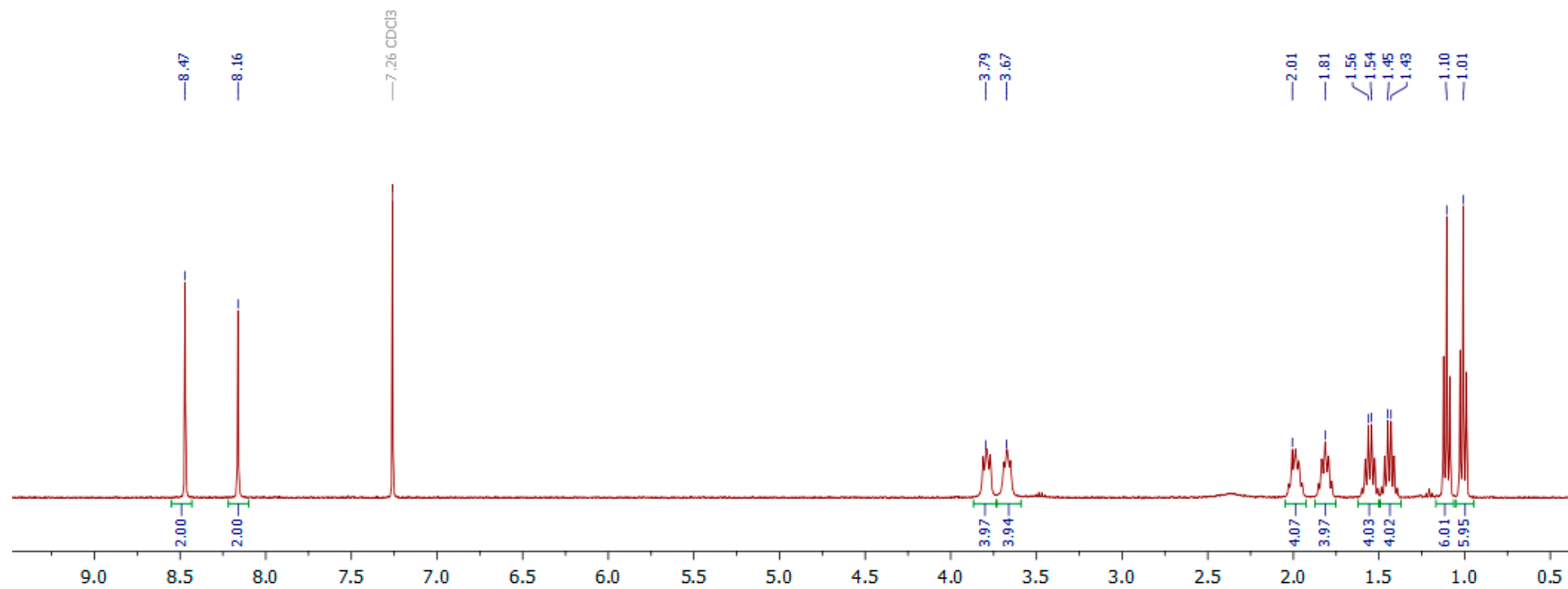
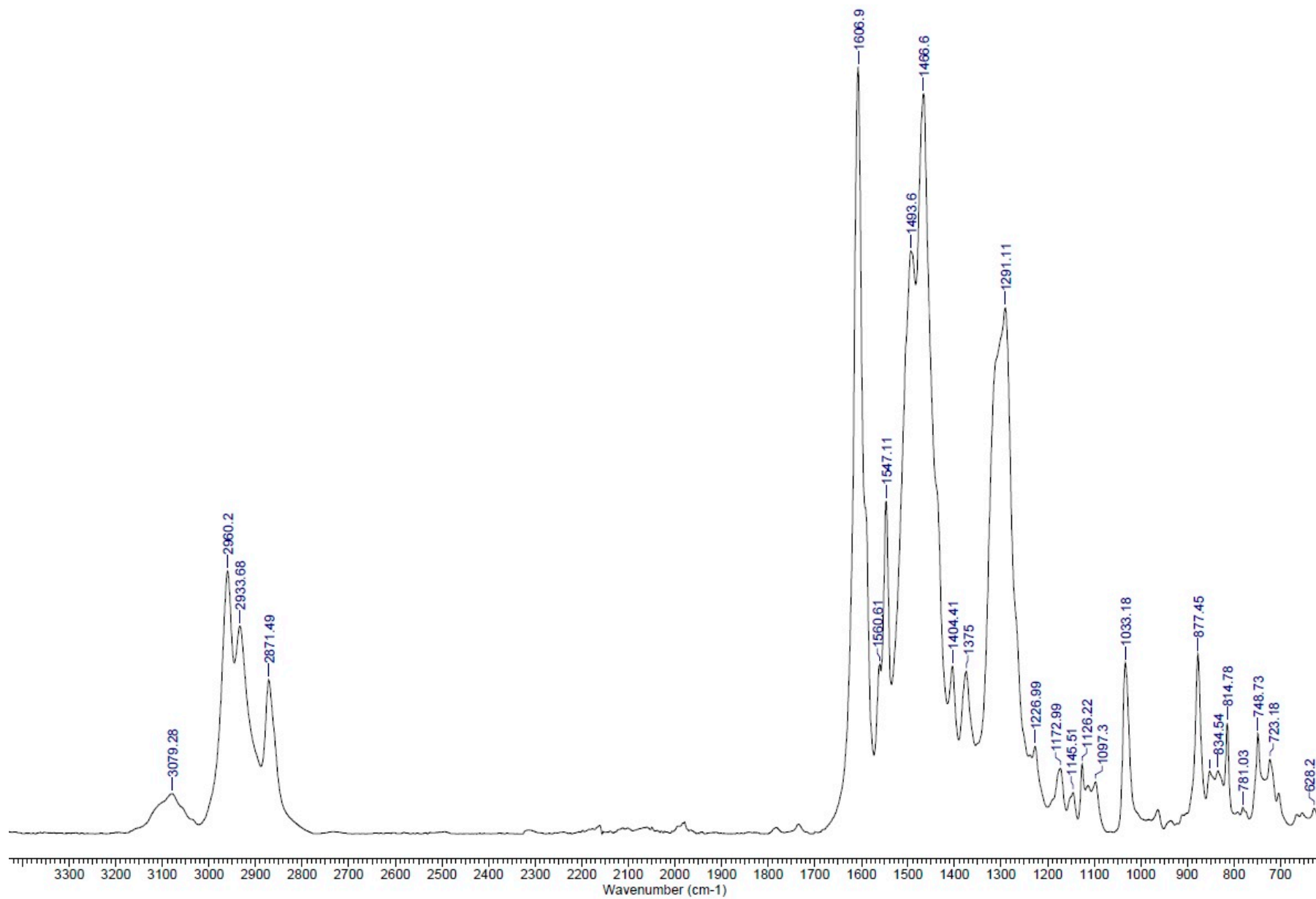


Figure S1.  $^1\text{H}$  NMR spectra of  $\text{L3Lu}(\text{NO}_3)_3$  in  $\text{CDCl}_3$  at  $25^\circ\text{C}$



**Figure S2.** Solid-state IR spectra of L3Lu(NO<sub>3</sub>)<sub>3</sub>

## 2. X-ray diffraction data

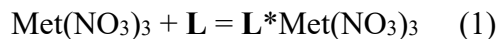
**Table S1** Crystal data and structure refinement parameters for **L3•Lu(NO<sub>3</sub>)<sub>2</sub>•H<sub>2</sub>O]<sup>+</sup>•NO<sub>3</sub><sup>-</sup>**

<b>L3•Lu(NO<sub>3</sub>)<sub>2</sub>•H<sub>2</sub>O]<sup>+</sup>•NO<sub>3</sub><sup>-</sup></b>	
Empirical formula	C <sub>30</sub> H <sub>42</sub> Cl <sub>2</sub> LuN <sub>7</sub> O <sub>12</sub>
Formula weight	938.57
T, K	295
Diffractionmeter	Stoe STADI VARI
Radiation	CuK $\alpha$ , 1.54186 Å
Crystal system	Triclinic
Space group	P-1
Z	2
a, Å	9.3262(3)
b, Å	14.0448(5)
c, Å	15.8316(5)
$\alpha$ /°	66.734(3)
$\beta$ /°	87.821(3)
$\gamma$ /°	85.175(3)
V, Å <sup>3</sup>	1898.29(12)
$D_{\text{calc}}$ (g cm <sup>-3</sup> )	1.642
Linear absorption, $\mu$ (mm <sup>-1</sup> )	6.855
F(000)	944
$2\theta_{\text{max}}$ , °	70.890
Reflections measured	19264
Independent reflections	6642
Observed reflections $[I > 2\sigma(I)]$	5591
Parameters	480
R1 ( $I > 2\sigma(I)$ )	0.0322
wR2 (all reflections)	0.0758
GOF	0.947
$\Delta\rho_{\text{max}}/\Delta\rho_{\text{min}}$ (e Å <sup>-3</sup> )	0.664 / -0.731

### 3. Theoretical computations

All molecular geometries have been fully optimized (tolerance on gradient:  $10^{-7}$  au) at PBE/L1 level.

All stationary points on the potential energy surface (PES) were checked by vibrational analysis and none of them had imaginary frequencies. We used eq. (1) as a model reaction of complex formation.

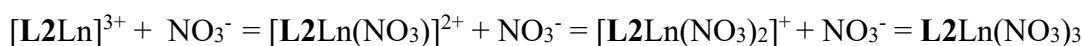


The energy of complex formation in gas phase was calculated according to eq. (2)

$$\Delta E = E_{\text{LMet}(\text{NO}_3)_3} - E_{\text{Met}(\text{NO}_3)_3} - E_{\text{L}} \quad (2)$$

where  $E_{\text{LMet}(\text{NO}_3)_3}$ ,  $E_{\text{Met}(\text{NO}_3)_3}$ ,  $E_{\text{L}}$  are energies for optimized geometrical structures of  $[\text{Met}(\text{NO}_3)_3]\text{L}$ ,  $\text{Met}(\text{NO}_3)_3$ , and  $\text{L}$  respectively.

**Table S2.** Energies of consecutive attachment of  $\text{NO}_3^-$  anions to cations  $[\text{L}_2\text{Ln}]^{3+}$  (gas phase approximation) in kcal/mol.



	$\text{NO}_3^-$		$2\text{NO}_3^-$		$3\text{NO}_3^-$	
Ln	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
La	-288.9	-276.0	-197.5	-186.4	-117.0	-104.0
Ce	-286.9	-274.3	-202.6	-191.1	-118.5	-104.2
Pr	-286.0	-273.4	-199.5	-187.7	-115.5	-102.8
Nd	-287.5	-273.5	-199.1	-188.0	-114.4	-101.8
Pm	-287.8	-271.2	-200.1	-187.6	-113.3	-100.1
Sm	-283.6	-266.6	-200.5	-188.1	-111.5	-99.0
Eu	-279.4	-260.8	-200.6	-187.9	-111.4	-98.1
Gd	-295.5	-281.8	-201.5	-189.6	-111.1	-97.2
Tb	-295.5	-280.2	-201.9	-189.8	-110.6	-97.0
Dy	-293.1	-276.7	-202.5	-190.0	-109.3	-95.4
Ho	-295.3	-279.0	-201.7	-189.5	109.0	94.9
Er	-295.0	-275.7	-202.8	-190.9	-107.5	-92.7
Tm	-291.0	-273.1	-202.9	-189.9	-106.3	-92.7
Yb	-287.4	-267.8	-202.8	-189.7	-105.9	-92.2
Lu	-303.8	-289.9	-205.0	-192.1	-102.9	-89.2

**Table S3**  $\Delta E$  and  $\Delta G$  for  $[\text{L3Ln}(\text{NO}_3)]^{2+}$  ( $\text{kcal}\cdot\text{mol}^{-1}$ ) and subsequent addition of  $\text{NO}_3^-$  (eq 1).

	$[\text{LLn}(\text{NO}_3)]^{2+}$		$[\text{LLn}(\text{NO}_3)_2]^+$		$\text{LLn}(\text{NO}_3)_3$	
Ln	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
La	-244.2	-226.5	-129.9	-112.8	-54.1	-36.2
Ce	-531.8	-229.4	-132.9	-116.0	-59.9	-38.6
Pr	-248.2	-229.9	-130.4;	-112.9	-52.3	-33.9
Nd	-250.8	-233.0	-130.3	-112.1	-49.5	-30.3
Pm	-252.7	-232.6	-131.8	-113.6	-49.5	-29.8
Sm	-251.4	-232.7	-130.9	-112.3	-48.0	-29.6
Eu	-243.9	-225.2	-128.9	-110.4	-47.5	-28.3
Gd	-266.7	-248.1	-141.0	-123.0	-50.5	-30.1
Tb	-268.6	-249.9	-141.7	-123.3	-50.0	-30.0
Dy	-269.3	-250.6	-142.2	-123.5	-48.4	-28.3
Ho	-272.9	-254.1	-143.0	-125.8	-47.2	-27.3
Er	-274.9	-255.6	-144.5	-125.1	-46.9	-26.2
Tm	-274.0	-254.5	-143.3	-123.9	-44.8	-24.9
Yb	-268.5	-249.1	-141.7	-122.4	-44.4	-24.7
Lu	-292.0	-273.3	-155.3	-135.8	-46.0	-25.1

**Table S4.** Energies of consecutive attachment of  $\text{NO}_3^-$  anions to cations  $[(\text{L4})\text{Ln}]^{3+}$  (gas phase approximation) in kcal/mol.

	$\text{NO}_3^-$		$2\text{NO}_3^-$		$3\text{NO}_3^-$	
Ln	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$	$\Delta E$	$\Delta G$
La	-292.8	-280.4	-198.8	-188.1	-117.1	-104.8
Ce	-291.7	-279.5	-203.3	-192.0	-119.7	-105.6
Pr	-290.9	-277.9	-201.3	-289.8	-115.5	-102.9
Nd	-292.4	-279.9	-200.6	-188.2	-114.3	-101.7
Pm	-293.9	-280.8	-201.6	-189.5	-113.1	-99.7
Sm	-291.5	-278.1	-202.3	-202.3	-111.1	-99.2
Eu	-288.3	-274.8	-202.8	-202.8	-110.8	-97.7
Gd	-300.5	-287.3	-203.1	-203.1	-110.8	-97.3
Tb	-301.0	-287.6	-203.6	-203.6	-110.3	-96.8
Dy	-299.5	-285.8	-204.2	-204.2	-109.0	-95.6
Ho	-301.8	-288.3	-203.5	-203.5	-108.6	-94.7
Er	-302.4	-288.2	-204.6	-204.6	-107.6	-94.4
Tm	-299.5	-285.4	-204.8	-204.8	-105.8	-93.0
Yb	-297.1	-282.7	-205.1	-205.1	-106.0	-92.8
Lu	-308.7	-295.4	-206.9	-206.9	-102.9	-89.6

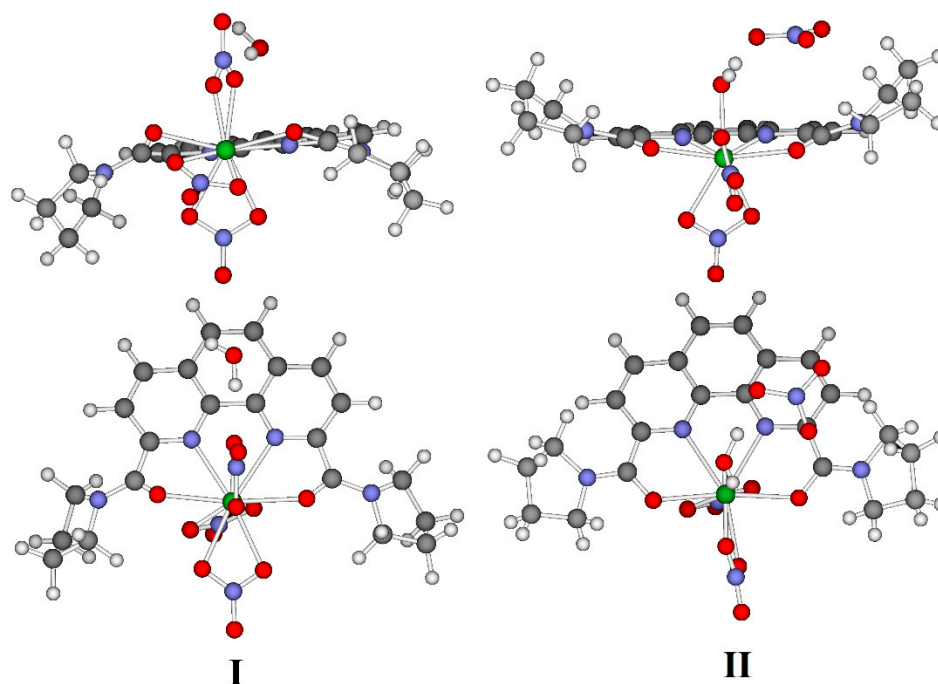
**Table S5.** Energies of successive addition of nitrate anions  $\Delta E$  and ( $\Delta G$ ) in kcal/mol to the cation  $[Ln]^{3+}$  calculated according to  $[LLn]^{3+} + NO_3^- = [LLn(NO_3)]^{2+} + NO_3^- = [LLn(NO_3)_2]^+ + NO_3^- = LLn(NO_3)_3$  reaction

Ln	$NO_3^-$	$2 NO_3^-$	$3 NO_3^-$
La	-305.8 (-292.9)	-211.6 (-199.1)	-127.1 (-115.0)
Nd	-305.9 (-288.8)	-213.8 (-202.5)	-126.4 (-112.3)
Eu	-293.9 (-274.7)	-215.0 (-202.8)	-124.5 (-110.3)
Dy	-311.8 (-293.3)	-218.8 (-206.4)	-124.3 (-109.9)
Yb	-303.7 (-284.5)	-219.4 (-204.6)	-123.0 (-110.5)
Lu	-327.6 (313.7)	-223.2 (-210.9)	-122.7 (-107.8)

**Table S6** The formation energies calculated with PBE and B3LYP

	$NO_3^-$		$2NO_3^-$		$3NO_3^-$	
Ln	$\Delta E$ (pbe)	$\Delta E$ (b3lyp)	$\Delta E$ (pbe)	$\Delta E$ (b3lyp)	$\Delta E$	$\Delta E$ b3lyp
La	-244.2	-243.9	-129.9	-133.1	-54.1	-54.9
Ce	-246.7	-246.5	-132.9	-132.4	-59.9	-52.6
Pr	-248.2	-249.8	-130.4	-134.0	-52.3	-51.4
Nd	-250.8	-254.0	-130.3	-135.6	-49.5	-51.5
Pm	-252.7	-257.1	-131.8	-137.7	-49.5	-51.4
Sm	-251.4	-258.7	-130.9	-138.4	-48.0	-50.5
Eu	-243.9	-252.2	-128.9	-137.8	-47.5	-50.0
Gd	-266.7	-269.4	-141.0	-145.8	-50.5	-51.2
Tb	-268.6	-272.8	-141.7	-147.1	-50.0	-50.1
Dy	-269.3	-276.4	-142.2	-148.5	-48.4	-48.9
Ho	-272.9	-280.2	-143.0	-150.2	-47.2	-48.4
Er	-274.9	-283.1	-144.5	-151.7	-46.9	-47.5
Tm	-274.0	-285.5	-143.3	-152.6	-44.8	-45.9
Yb	-268.5	-285.0	-141.7	-153.5	-44.4	-45.2
Lu	-292.0	-293.5	-155.3	-157.9	-46.0	-45.1

To compare two types of complexes (water molecules in outer coordination sphere – I, and water molecule in inner coordination sphere – II, Figure S3) we optimized molecular geometries of complexes for ligands **L2-L4** with lanthanides (from La to Lu) at PBE/L1 level of theory (tolerance on gradient:  $10^{-7}$  au) using a PRIODA-19 program developed by Laikov [Laikov, D.N. Atomic basis functions for molecular electronic structure calculations. *Theor. Chem. Acc.* **2019**, *138*, 40. <https://doi.org/10.1007/s00214-019-2432-3>].



**Figure S3.** Structures of two types of complexes - **I** (H<sub>2</sub>O in outer coordination sphere) and **II** (H<sub>2</sub>O in inner coordination sphere)

#### xyz data

##### Ligand L2

E= -2458.982234, E0 = -2458.342421, G= 351.5475 at T=298.150 K

Cl -4.53443527 4.40782070 -3.30053735

Cl -5.20993662 -3.14527750 -3.72041559

N -1.58535874 1.57410634 -1.30706620

N 0.96606773 2.99341249 -0.67157280

N -1.96913099 -1.11286223 -1.25714874

N -0.84170198 -3.00824738 0.75871980

O -0.56885952 4.25740814 0.46990582

O -0.44765243 -4.12524939 -1.20433164

C -1.43717253 2.89075065 -1.25154722

C -2.35162997 3.80709767 -1.81764197

H -2.20297217 4.87944508 -1.68790185

C -3.41632152 3.30162501 -2.53062534

C -3.61005259 1.89812601 -2.64236975

C -4.67225695 1.29334116 -3.37782502



H -5.38231325 1.94188643 -3.89373946  
 C -4.79865408 -0.06619585 -3.44670129  
 H -5.60693121 -0.51818967 -4.02406454  
 C -3.88919783 -0.92622989 -2.76246381  
 C -3.96260095 -2.34531999 -2.78722715  
 C -3.05696177 -3.10590053 -2.08098865  
 H -3.07142639 -4.19566965 -2.11343741  
 C -2.09451294 -2.43249488 -1.29575145  
 C -2.82537818 -0.36878082 -1.98864388  
 C -2.65613294 1.07947350 -1.96334422  
 C -0.29725426 3.44706345 -0.41638678  
 C -1.06037009 -3.27035451 -0.56429797  
 C -1.70463181 -2.15802717 1.58808339  
 C 0.23426451 -3.76782417 1.41046417  
 C 1.34055781 2.20614219 -1.85286653  
 C 2.03013325 3.47519851 0.22013471  
 C 1.62998557 -3.16302752 1.20893681  
 H -0.00834809 -3.82895160 2.48452663  
 H 0.22206604 -4.78754520 0.98940086  
 C -1.12626934 -0.78447652 1.94855750  
 H -2.66160440 -2.02196336 1.06232202  
 H -1.92896783 -2.72383618 2.51184750  
 C 1.62091506 0.72113293 -1.59324086  
 H 0.53570330 2.29863524 -2.59744716  
 H 2.23542213 2.68474150 -2.29323483  
 C 2.16048789 2.67094588 1.52033222  
 H 2.97518253 3.44673061 -0.34755954  
 H 1.80247271 4.52535582 0.47030666  
 C 3.26494503 3.22325730 2.42810750  
 H 1.19304430 2.70602965 2.04886317  
 H 2.36468482 1.61193776 1.28418291

C	2.02803922	-0.00002292	-2.88443780
H	2.42687702	0.61724430	-0.84474093
H	0.70812231	0.26499325	-1.17504060
C	2.72007632	-3.99781919	1.88993597
H	1.82959163	-3.10392523	0.12579536
H	1.64876735	-2.13102961	1.60090816
C	-2.09456635	0.00827873	2.83558178
H	-0.16361018	-0.90987897	2.47600698
H	-0.93166536	-0.23468895	1.01260710
C	4.12180185	-3.41199923	1.68955493
H	2.50317740	-4.07657433	2.97146010
H	2.68930459	-5.02819872	1.49131024
C	-1.55695331	1.38939714	3.22525668
H	-3.05628777	0.12640262	2.30291581
H	-2.31657791	-0.57392162	3.74963379
C	2.32253218	-1.48881066	-2.67208004
H	1.21854603	0.11076291	-3.62945199
H	2.91731095	0.49516228	-3.31770873
C	3.40155411	2.43509221	3.73514533
H	4.22890186	3.21095324	1.88628721
H	3.05033231	4.28323317	2.65592408
H	4.19660521	2.85094142	4.37433958
H	2.46034217	2.45833111	4.30896235
H	3.64668345	1.37837982	3.53653741
H	2.63812494	-1.97017121	-3.61147046
H	3.13130260	-1.62948549	-1.93511772
H	1.43302679	-2.02478313	-2.30385494
H	4.88971519	-4.02866936	2.18315411
H	4.37408400	-3.35267925	0.61787719
H	4.18844986	-2.39311194	2.10620070
H	-2.26293159	1.92003047	3.88388872

H -0.59786135 1.30170643 3.76326346

H -1.38971162 2.01961970 2.33704352

**L2\*La(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E=-11871.787674, E0 = -11871.076771, G= 378.7348 at T=298.150 K

Cl -5.52118683 3.59837317 -0.2400401504

Cl -4.38623381 -3.19738984 -3.48092198

N -1.69283342 1.23818433 0.26213586

N -0.28642842 4.05627060 1.93433750

N -1.30030036 -1.16488612 -0.86667764

N 1.05000436 -3.66783786 -1.70320821

O -0.14073125 1.83043957 2.34949422

O 0.47518417 -2.79157329 0.31123731

C -1.84679866 2.42922735 0.83684456

C -3.02722931 3.18242908 0.70002151

H -3.16264749 4.12369585 1.23089075

C -4.04665565 2.68231130 -0.08873926

C -3.90203261 1.44048798 -0.75178862

C -4.89546633 0.84421414 -1.58462596

H -5.83060169 1.38308001 -1.74390006

C -4.69530916 -0.37813923 -2.16199136

H -5.46665573 -0.82594907 -2.79024363

C -3.48345780 -1.10290587 -1.95097494

C -3.20584965 -2.38504481 -2.48773479

C -2.00227666 -3.01612091 -2.22525167

H -1.80567050 -4.01272917 -2.62082672

C -1.06370854 -2.35790467 -1.40922642

C -2.46233416 -0.54132229 -1.13065004

C -2.67516470 0.75805753 -0.51914692

C -0.69064093 2.78104997 1.75505984

C 0.22485520 -2.97264719 -0.89792532

C	-0.65421605	5.19099426	1.07624745
C	-1.48526990	6.26927900	1.78149235
H	-1.18050897	4.80873203	0.18921770
C	0.83327162	4.27372122	2.87819672
H	0.69303340	3.57358527	3.71508789
H	0.73461306	5.30092669	3.26618242
C	2.29183006	-4.18392086	-1.08006573
H	2.69113755	-3.39154005	-0.42373064
H	3.01042366	-4.34939528	-1.89830792
C	0.97217679	-3.67206335	-3.16986108
H	0.17602775	-2.98035526	-3.48210168
C	0.75203305	-5.06074381	-3.77712798
La	0.52532554	-0.33016407	1.12207365
N	-1.16401744	-1.32574427	3.41740680
O	0.10716507	-1.21217322	3.51882935
O	-1.65627444	-1.09990525	2.21650243
O	-1.89204764	-1.61406648	4.34921169
N	3.32002831	-0.50873744	2.16504765
O	2.61901855	0.58735543	2.21699691
O	2.70825720	-1.53133619	1.65417182
O	4.46740055	-0.56312203	2.56487679
N	1.66057611	0.86460227	-1.41033554
O	2.07067084	1.33865988	-2.45466447
O	1.67609537	-0.41467583	-1.17989731
O	1.17555130	1.59906828	-0.45959499
H	0.28735605	5.63254833	0.70394754
C	2.21249080	4.05425978	2.24726582
C	-1.83816373	7.42449617	0.83680278
H	-2.41054344	5.82494307	2.19241667
H	-0.92633003	6.66178751	2.64913559
C	-2.65392041	8.52238655	1.52635920

H	-0.90643018	7.85543394	0.42758515
H	-2.40174556	7.03043604	-0.02873448
H	-2.89497113	9.33754063	0.82639349
H	-3.60367799	8.12432098	1.92015207
H	-2.09714532	8.95809841	2.37220860
C	3.33389282	4.22418261	3.27883816
H	2.25808954	3.03486896	1.83176661
H	2.36417317	4.75796747	1.40798879
C	4.71430779	3.92046738	2.68848133
H	3.31338668	5.25012112	3.69341159
H	3.14491701	3.53657341	4.12333822
H	5.50749493	4.06097078	3.43984270
H	4.75921345	2.87649322	2.33798957
H	4.93724346	4.57912302	1.83193922
C	2.08455968	-5.46927023	-0.27366072
H	1.91634023	-3.23864079	-3.54672623
C	0.69763070	-5.01149321	-5.30874491
H	1.56493974	-5.73708725	-3.45814157
H	-0.18445583	-5.49581289	-3.38114619
C	0.48896462	-6.39290428	-5.93681860
H	-0.11549123	-4.33247280	-5.62473249
H	1.63507223	-4.56775284	-5.69023228
H	0.45274404	-6.32897329	-7.03552198
H	1.30822134	-7.07910728	-5.66619682
H	-0.45543024	-6.84723186	-5.59425783
C	3.38866401	-5.92495823	0.39186180
H	1.32561123	-5.27840471	0.50372154
H	1.69439518	-6.26850605	-0.93022513
C	3.21227241	-7.20634842	1.21206057
H	4.16461992	-6.08067942	-0.38090113
H	3.75600076	-5.11373758	1.04577553

H 4.16115999 -7.51276445 1.67991567  
H 2.47343063 -7.05905008 2.01712108  
H 2.86125565 -8.04042435 0.58118731  
O -4.20741940 0.12163923 2.19404197  
H -3.38024902 -0.40931782 2.27442670  
H -4.55460644 0.10392769 3.10203767

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11871.774736, E0 = -11871.063432, G= 380.8389 at T=298.150 K

La -0.90557778 -0.53899211 0.01477725  
Cl 3.70405483 2.05276918 4.92820263  
Cl 2.53523493 5.61195564 -1.65928566  
O -1.17187881 0.48950687 -2.19344378  
O -0.91260630 -1.28505540 2.49133277  
O -3.38669705 -0.90585071 0.22898123  
O -4.38261271 -2.87217236 0.15231645  
O -2.21448231 -2.71067953 -0.21090414  
O 0.87810749 -2.36670685 0.41152176  
O 0.65099835 -1.67686772 -1.66008866  
O 2.09690571 -3.27093482 -1.18425202  
O -1.98220778 1.56760597 0.83224189  
H -1.80795026 2.57499647 0.53841579  
H -2.95173597 1.46102524 0.87919813  
N 1.02540529 0.38882813 1.69111860  
N 0.60068011 -2.56193995 3.60543251  
N 0.69848949 1.59142613 -0.72227836  
N -0.73378199 1.64996779 -4.06485653  
N -3.37630558 -2.19962430 0.05909375  
N 1.24737215 -2.47609258 -0.82957286  
C 1.16364586 -0.24081823 2.85840631  
C 1.98785567 0.25250623 3.88407755  
H 2.04941487 -0.24853213 4.85002232

C	2.69512248	1.42014396	3.65620470
C	2.59299231	2.10291576	2.41829491
C	3.26793718	3.32259965	2.11498189
H	3.93592787	3.75023103	2.86367893
C	3.06292129	3.95565796	0.92259926
H	3.56061077	4.90174723	0.70481586
C	2.18162298	3.41509056	-0.06068257
C	1.52350950	2.17533803	0.17089124
C	1.71975112	1.51751041	1.45313787
C	1.85734117	4.05787563	-1.27775002
C	0.97842526	3.47742534	-2.17200947
H	0.67411959	4.05204344	-3.03900218
C	0.43212906	2.21021557	-1.88222003
C	-0.54912430	1.42482102	-2.74836969
C	-0.10703258	2.68534255	-4.89651203
H	-0.01798707	2.26061988	-5.91051769
H	0.92609680	2.85101795	-4.55589676
C	-0.91849494	3.99041128	-4.92966127
H	-1.87649906	3.79989767	-5.44569445
H	-1.19468141	4.28542519	-3.89980054
C	-0.17012870	5.12444782	-5.63890934
H	0.07592789	4.82357073	-6.67413950
H	0.79866999	5.30024147	-5.13283157
C	-0.97818482	6.42646980	-5.64852190
H	-1.93053472	6.29577446	-6.18828726
H	-0.42038512	7.23951578	-6.13934374
H	-1.21554923	6.74201107	-4.61987019
C	-1.73700118	0.80172646	-4.74390984
H	-2.13875961	1.39224577	-5.58307314
H	-2.55601859	0.61227828	-4.03478384
C	-1.14358759	-0.52018702	-5.24356556

H -0.70573640 -1.05975318 -4.38607597  
 H -0.31868348 -0.31203210 -5.95044231  
 C -2.19966102 -1.39700365 -5.92581749  
 H -3.01440597 -1.60255909 -5.20764256  
 H -2.65711498 -0.84163755 -6.76603794  
 C -1.62187994 -2.72137499 -6.43423033  
 H -0.81905240 -2.54904509 -7.17063332  
 H -2.39810324 -3.33565354 -6.91742420  
 H -1.19506848 -3.30809975 -5.60402346  
 C 0.22379448 -1.42423105 2.99256229  
 C 1.99055982 -2.91476679 3.92825103  
 H 2.65329289 -2.12481117 3.54632950  
 H 2.23609781 -3.82237768 3.34775209  
 C 2.23794508 -3.15871620 5.41954422  
 H 1.97193849 -2.25219655 5.99457264  
 H 1.56752741 -3.95927048 5.77995872  
 C 3.69496369 -3.54562330 5.70024443  
 H 4.36340618 -2.74355531 5.33703423  
 H 3.94938993 -4.44738340 5.11435032  
 C 3.96088219 -3.80488563 7.18626595  
 H 3.74181175 -2.91002011 7.79193497  
 H 5.01301861 -4.07941151 7.35970259  
 H 3.33156991 -4.62741709 7.56401110  
 C -0.39793333 -3.65673971 3.62120819  
 H 0.16079836 -4.59200382 3.78379297  
 H -0.85151875 -3.69982290 2.61814022  
 C -1.47589254 -3.48551536 4.69683218  
 H -1.96606469 -2.50736117 4.55533934  
 H -0.99602926 -3.47374272 5.69140911  
 C -2.53629351 -4.59858704 4.64217663  
 H -2.03860784 -5.58470631 4.70799732



H -3.16465712 -4.51286507 5.54579878  
 C -3.43373227 -4.54869413 3.39970875  
 H -3.94013882 -3.57267952 3.31637073  
 H -4.21235418 -5.32648420 3.44798470  
 H -2.87297702 -4.70698833 2.46468496  
 O -1.42130482 3.96580911 0.25120541  
 O -1.18899536 5.35874510 -1.42993319  
 O -2.19500279 3.43431735 -1.75108588  
 N -1.61725271 4.26839685 -1.00152552

**L2\*La(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11514.812210, E0 = -11514.139526, G= 361.0390 at T=298.150 K

Cl -5.47865820 3.60568333 -0.25474846  
 Cl -4.19033432 -3.14690876 -3.49129748  
 N -1.63633609 1.30424452 0.32509458  
 N -0.29275426 4.12395287 2.05832100  
 N -1.17663717 -1.09121096 -0.82738602  
 N 1.16823232 -3.64805102 -1.68192685  
 O -0.06287735 1.88896334 2.35606217  
 O 0.75646001 -2.54885483 0.26143229  
 C -1.81836879 2.49624062 0.90478343  
 C -3.00665498 3.22823739 0.74305034  
 H -3.17423081 4.16334438 1.27494264  
 C -4.00386810 2.71709967 -0.07346840  
 C -3.82234430 1.47856045 -0.74217075  
 C -4.78719091 0.87996185 -1.60755026  
 H -5.72219658 1.41061783 -1.79281914  
 C -4.55444527 -0.33410576 -2.19035816  
 H -5.30189276 -0.78344876 -2.84584117  
 C -3.33874130 -1.04449046 -1.95411527  
 C -3.04010487 -2.32375455 -2.49256015  
 C -1.82753122 -2.93545413 -2.21669078

H -1.62237787 -3.93050098 -2.60967469  
 C -0.90356147 -2.27197194 -1.39070511  
 C -2.34585881 -0.47947487 -1.10620761  
 C -2.59306645 0.80880469 -0.48642531  
 C -0.66928947 2.85898304 1.82704532  
 C 0.41242865 -2.85270357 -0.91127950  
 C -0.77887309 5.31948996 1.34436953  
 C -1.67892241 6.22712278 2.19027781  
 H -1.28582919 5.00371742 0.42070532  
 C 0.85636950 4.33418608 2.97461057  
 H 0.76597464 3.60908747 3.79655218  
 H 0.74551135 5.34646988 3.39361429  
 C 2.38811231 -4.22813749 -1.06446075  
 H 2.89105797 -3.42985678 -0.49496266  
 H 3.04853797 -4.52326918 -1.89410150  
 C 1.01258528 -3.82245994 -3.13901019  
 H 0.26404494 -3.10443330 -3.50345063  
 C 0.66288638 -5.24977636 -3.56888604  
 La 0.27277678 -0.33412692 1.30328000  
 N -1.36689448 -1.73374999 3.31182599  
 O -0.06727159 -1.59461725 3.40301633  
 O -1.90191317 -1.19813228 2.24655128  
 O -2.01591158 -2.31156898 4.14701557  
 N 2.75212026 0.62889576 -0.00764709  
 O 3.76656461 1.03142190 -0.52571267  
 O 2.66902876 0.38702667 1.27515852  
 O 1.65662229 0.40799236 -0.68257791  
 H 0.11802733 5.87839699 1.02598286  
 C 2.21081018 4.18182421 2.27294159  
 C -2.14782333 7.45523357 1.39909041  
 H -2.55314374 5.65975237 2.56044173

H	-1.13243401	6.55605316	3.09133887
C	-3.03729081	8.38350105	2.23153138
H	-1.26451099	8.01209736	1.03802514
H	-2.69471049	7.12488937	0.49670231
H	-3.36035967	9.25320053	1.63962054
H	-3.94167876	7.86115837	2.58404374
H	-2.49991035	8.76028347	3.11670709
C	3.37933803	4.44746971	3.23040485
H	2.29618526	3.15699601	1.87243426
H	2.26903510	4.87577295	1.41415286
C	4.73769283	4.27842236	2.54324389
H	3.29264450	5.46737385	3.64819455
H	3.30940127	3.75061083	4.08546019
H	5.56161547	4.46597052	3.24874449
H	4.85588169	3.25569725	2.14870071
H	4.84878445	4.98045015	1.70041502
C	2.09982824	-5.42500591	-0.15192775
H	1.97227001	-3.51857114	-3.59403419
C	0.51871127	-5.36062527	-5.09242249
H	1.44771004	-5.94438171	-3.22190642
H	-0.27253020	-5.57511568	-3.07633638
C	0.18410525	-6.78434896	-5.54714680
H	-0.26669189	-4.66398764	-5.43912697
H	1.45837581	-5.02918768	-5.56991196
H	0.08516907	-6.83458996	-6.64205694
H	0.97371167	-7.49258471	-5.24838543
H	-0.76464999	-7.13224983	-5.10688019
C	3.39034867	-5.97742701	0.46695367
H	1.41114259	-5.11030006	0.65031314
H	1.59170377	-6.21775484	-0.72913802
C	3.12986588	-7.17623472	1.38384211

H 4.09059811 -6.26853991 -0.33748502  
H 3.88923740 -5.17467451 1.03986764  
H 4.06967592 -7.55356932 1.81521404  
H 2.46406317 -6.90025139 2.21797585  
H 2.65542483 -8.00479889 0.83274043

**L2\*Ce(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12239.208698 , E0 = -12238.498179, G= 379.3895 at T=298.150 K

Cl -5.38830900 3.68461299 -0.47863379  
Cl -4.13156796 -3.01257038 -3.89721632  
N -1.57952487 1.30878425 0.06828741  
N -0.27020249 4.05604219 1.97267938  
N -1.13508022 -1.05593002 -1.10732663  
N 1.11563969 -3.76320195 -1.77267396  
O 0.07227688 1.82056355 2.01922321  
O 0.62034023 -2.58067083 0.09793225  
C -1.74547279 2.48372889 0.68201721  
C -2.92976570 3.23455930 0.53342962  
H -3.10230398 4.14385414 1.10499108  
C -3.91511583 2.76618004 -0.31052810  
C -3.75085568 1.54988134 -1.02195477  
C -4.70132160 0.99020070 -1.91277564  
H -5.62866163 1.53353608 -2.09841919  
C -4.47024155 -0.22129570 -2.52158165  
H -5.21329594 -0.64800137 -3.19697380  
C -3.27779484 -0.95516610 -2.28157377  
C -2.98360920 -2.23294783 -2.83812070  
C -1.80363274 -2.88301563 -2.52851009  
H -1.61830997 -3.88204694 -2.92172813  
C -0.88649243 -2.26191401 -1.66344821  
C -2.28690958 -0.42444131 -1.40324080

C -2.52972674 0.85381311 -0.76309192  
 C -0.59551597 2.79903054 1.59927571  
 C 0.33890465 -2.89565372 -1.08984375  
 C -0.75474203 5.29259443 1.34448814  
 C -1.68810534 6.12443495 2.23271036  
 H -1.23581636 5.04310274 0.38741261  
 C 0.86624587 4.20361662 2.90890908  
 H 0.81638336 3.36672044 3.62088656  
 H 0.70483810 5.14177370 3.46541452  
 C 2.27568698 -4.32761335 -1.04523289  
 H 2.75313783 -3.50746512 -0.48240319  
 H 2.98480606 -4.68198490 -1.81010330  
 C 1.07785046 -3.94647765 -3.22889161  
 H 0.39593640 -3.19815731 -3.65833211  
 C 0.68880904 -5.36011791 -3.67377782  
 Ce 0.59128433 -0.20915997 0.71961832  
 N -0.87836933 -1.19097483 3.08725810  
 O 0.39894247 -1.03545868 3.06846309  
 O -1.47298777 -0.97561318 1.94056702  
 O -1.49967659 -1.50795531 4.08142567  
 N 3.41051388 -0.25812978 1.57015789  
 O 2.71922159 0.83987337 1.43636930  
 O 2.75258040 -1.33871877 1.30962574  
 O 4.57577467 -0.25408569 1.90916455  
 N 1.75157523 0.89068395 -1.76196909  
 O 2.24890351 1.34462714 -2.77142525  
 O 1.87559426 -0.35886976 -1.42217398  
 O 1.05128813 1.60928857 -0.94158620  
 H 0.13794683 5.89086676 1.08934331  
 C 2.22999644 4.20882797 2.20927238  
 C -2.13253021 7.41640711 1.53648126

H	-2.57219505	5.52613258	2.51962209
H	-1.17312479	6.37434483	3.17716765
C	-3.06544590	8.26566696	2.40516806
H	-1.23794591	8.00583172	1.26465333
H	-2.63721180	7.16652060	0.58515871
H	-3.34668374	9.19726181	1.88943577
H	-3.99460602	7.72073364	2.64004898
H	-2.58351040	8.54017925	3.35778785
C	3.37979364	4.31600332	3.21780443
H	2.33991051	3.27367353	1.63666928
H	2.28475451	5.04724312	1.49020946
C	4.75234461	4.25029278	2.54066873
H	3.28667808	5.25376844	3.79777551
H	3.29406118	3.48610330	3.94288301
H	5.56474781	4.33365583	3.27987647
H	4.87396002	3.29282379	2.00842285
H	4.87579250	5.06555557	1.80778885
C	1.90546632	-5.46684074	-0.09047297
H	2.08440590	-3.69871187	-3.61297917
C	0.66890037	-5.49170017	-5.20138121
H	1.40112185	-6.08983231	-3.24902892
H	-0.30286545	-5.62272692	-3.26084018
C	0.29774034	-6.90267420	-5.66791058
H	-0.04615611	-4.76106215	-5.62197304
H	1.66160846	-5.21693707	-5.60201645
H	0.28972638	-6.96893454	-6.76709366
H	1.01782215	-7.64743662	-5.29076815
H	-0.70297348	-7.19081450	-5.30577326
C	3.13811040	-5.99795628	0.65035605
H	1.17209089	-5.08928871	0.64182758
H	1.42082274	-6.28564072	-0.65313965

C 2.79705191 -7.13333464 1.62019706  
 H 3.88787556 -6.34892654 -0.08342401  
 H 3.60972691 -5.16584587 1.20390558  
 H 3.69746971 -7.49629974 2.14053392  
 H 2.07976890 -6.79458904 2.38598585  
 H 2.34472656 -7.98853827 1.09034729  
 O -3.93708754 0.44724032 2.29033947  
 H -3.16999841 -0.16336331 2.21282411  
 H -4.20521307 0.32845590 3.21747613

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12239.196494, E0 = -12238.487842, G= 378.4462 at T=298.150 K

Ce -0.62523645 -0.55376226 -0.03314401  
 Cl 3.94993663 1.87506688 4.83344412  
 Cl 2.63411188 5.58727551 -1.67951775  
 O -0.97555101 0.38601041 -2.19498944  
 O -0.70983666 -1.39045393 2.27455592  
 O -3.04005909 -1.12597537 0.03526488  
 O -3.86225224 -3.09091377 -0.53788334  
 O -1.70407665 -2.68001270 -0.72633463  
 O 1.03768349 -2.44126940 0.32599366  
 O 1.14448130 -1.38802719 -1.58584023  
 O 2.48443675 -3.09583497 -1.19996202  
 O -1.76827526 1.26810539 0.72646701  
 H -1.67760623 2.57110667 0.45238915  
 H -2.70377040 1.07799911 0.93689758  
 N 1.20402145 0.29316759 1.60012889  
 N 0.64825559 -2.61341190 3.62203622  
 N 0.82568026 1.55322123 -0.75317156  
 N -0.78235346 1.68279099 -4.01761866  
 N -2.91909766 -2.33943963 -0.41806275  
 N 1.59989655 -2.34786844 -0.83677566

C	1.34393084	-0.36729190	2.76982832
C	2.19142437	0.11281154	3.78476858
H	2.25534344	-0.38899770	4.74975348
C	2.91225028	1.27086425	3.56687570
C	2.79462934	1.98932195	2.33984709
C	3.46355081	3.20375872	2.04445195
H	4.14754057	3.61530066	2.78796268
C	3.23843241	3.87232447	0.86122900
H	3.73825669	4.82035589	0.65851623
C	2.33809423	3.36101151	-0.10486032
C	1.67392433	2.11658406	0.12416274
C	1.89499485	1.42548251	1.38471854
C	1.97562373	4.01719332	-1.31106782
C	1.08031058	3.44935060	-2.19313645
H	0.77434009	4.02975512	-3.05649900
C	0.53695750	2.17568421	-1.91158986
C	-0.44424382	1.38984990	-2.74436808
C	-0.22475494	2.73612714	-4.87437344
H	-0.21457639	2.32986617	-5.90020227
H	0.83073461	2.89975405	-4.61191273
C	-1.03739476	4.03965378	-4.83821583
H	-2.05049634	3.83717465	-5.22903585
H	-1.18792999	4.37001610	-3.79420996
C	-0.37983760	5.15113735	-5.66371632
H	-0.23721479	4.80582714	-6.70440054
H	0.63264519	5.35553503	-5.26644707
C	-1.20135689	6.44450474	-5.65311289
H	-2.20091414	6.28051138	-6.08817673
H	-0.70514590	7.23692799	-6.23511076
H	-1.34112442	6.81149244	-4.62360477
C	-1.83195496	0.84463900	-4.63635683



H -2.33457613 1.47175324 -5.39065790  
 H -2.56609702 0.59313899 -3.85685682  
 C -1.27117968 -0.43042797 -5.27482462  
 H -0.73787266 -1.00814354 -4.50058365  
 H -0.52839845 -0.16421063 -6.05005550  
 C -2.37853432 -1.29094505 -5.89420176  
 H -3.11011100 -1.55410695 -5.10860634  
 H -2.92935658 -0.69887519 -6.64890957  
 C -1.83573413 -2.57143450 -6.53581715  
 H -1.11549878 -2.34058261 -7.33863592  
 H -2.64816809 -3.17303038 -6.97316504  
 H -1.31788635 -3.19607687 -5.78936005  
 C 0.38510007 -1.50812018 2.89250207  
 C 1.98805106 -3.01096129 4.07571220  
 H 2.72171760 -2.30696774 3.65739202  
 H 2.20852590 -3.99116230 3.61491013  
 C 2.12906098 -3.10792804 5.59797621  
 H 1.87942278 -2.13413000 6.05865860  
 H 1.39306688 -3.83150244 5.99223423  
 C 3.54188418 -3.53479862 6.01387882  
 H 4.27463293 -2.80745387 5.61894751  
 H 3.78233361 -4.50336218 5.53899574  
 C 3.70037436 -3.65261292 7.53285551  
 H 3.49424481 -2.69035339 8.02999878  
 H 4.72294855 -3.95887995 7.80326796  
 H 3.00407434 -4.40000486 7.94760942  
 C -0.41026223 -3.64686036 3.66329837  
 H 0.07786512 -4.58827066 3.96218157  
 H -0.79257601 -3.77152205 2.63786292  
 C -1.55154896 -3.31302953 4.63053703  
 H -1.98348951 -2.33864617 4.34584236

H -1.13953841 -3.20527887 5.64941978  
 C -2.65654325 -4.38256598 4.62773705  
 H -2.21482325 -5.36961269 4.86235714  
 H -3.35127115 -4.15485191 5.45492125  
 C -3.44762182 -4.46551132 3.31645703  
 H -3.88107109 -3.48607874 3.05270362  
 H -4.27576590 -5.18664455 3.40351319  
 H -2.82285881 -4.78773785 2.46791601  
 O -1.46819985 3.67219424 0.30492765  
 O -1.57330227 5.13740444 -1.33099973  
 O -2.57873321 3.20208144 -1.57577384  
 N -1.90871215 4.02180958 -0.94176048

**L2\*Ce(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11882.232517, E0 = -11881.560848, G= 361.1090 at T=298.150 K

Cl -5.37176180 3.69900680 -0.42174765  
 Cl -4.12010527 -3.06592035 -3.69888377  
 N -1.57435906 1.31503391 0.19515544  
 N -0.24921601 4.08212948 2.06011415  
 N -1.12668526 -1.04497063 -0.97278678  
 N 1.20335293 -3.65389204 -1.77674294  
 O 0.03733343 1.83831060 2.15759802  
 O 0.84455293 -2.39075756 0.07019125  
 C -1.74472821 2.51593924 0.77995223  
 C -2.91562796 3.26557374 0.60402292  
 H -3.07979107 4.19858932 1.13907838  
 C -3.91691947 2.77663231 -0.22915383  
 C -3.75164390 1.53929985 -0.89868563  
 C -4.71432543 0.95591152 -1.77827358  
 H -5.64094973 1.49920523 -1.96981692  
 C -4.48943520 -0.25698864 -2.36817718  
 H -5.23480844 -0.69289857 -3.03515053

C -3.28209949 -0.98139185 -2.12789989  
 C -2.98117828 -2.25211406 -2.67678571  
 C -1.76812088 -2.87147713 -2.39419365  
 H -1.57106054 -3.86460018 -2.79385114  
 C -0.84980536 -2.22428298 -1.55539858  
 C -2.29950261 -0.42629093 -1.26221907  
 C -2.53833389 0.84528905 -0.63742107  
 C -0.60551989 2.83897948 1.71231592  
 C 0.46126199 -2.78928065 -1.07198119  
 C -0.75104028 5.32997751 1.45479739  
 C -1.70027912 6.12430382 2.35945368  
 H -1.22014582 5.09325171 0.48864743  
 C 0.87956965 4.23216629 3.01174450  
 H 0.80249387 3.42483974 3.75433755  
 H 0.72866333 5.19232893 3.52974677  
 C 2.41766787 -4.20261192 -1.11949694  
 H 2.94066381 -3.36922312 -0.62325644  
 H 3.06393695 -4.58095980 -1.92611229  
 C 1.02363956 -3.96681976 -3.20785260  
 H 0.31842116 -3.24313521 -3.64055991  
 C 0.58483082 -5.40726280 -3.48863792  
 Ce 0.25847045 -0.26903543 1.04033720  
 N -1.33193338 -1.61066687 3.04951525  
 O -0.03670777 -1.40521550 3.13699627  
 O -1.86966145 -1.15085793 1.95458436  
 O -1.95804513 -2.17408037 3.90756607  
 N 2.61328292 0.78084582 -0.29241836  
 O 3.60555053 1.21334219 -0.82179904  
 O 2.61418366 0.31255138 0.93177485  
 O 1.45071471 0.74054140 -0.88195556  
 H 0.13830672 5.94133663 1.22405994

C	2.24953318	4.19850397	2.32476211
C	-2.18806362	7.40883112	1.67663741
H	-2.56443930	5.49862432	2.65013051
H	-1.18552589	6.38079309	3.30192542
C	-3.12436485	8.22769547	2.57023025
H	-1.31418574	8.02237892	1.39257824
H	-2.70393538	7.15104389	0.73327988
H	-3.45858145	9.14137840	2.05574083
H	-4.02114344	7.64932013	2.84637451
H	-2.61991811	8.53167915	3.50164032
C	3.38969564	4.41122341	3.32863092
H	2.37767410	3.22265792	1.82530618
H	2.29602695	4.97560549	1.53982341
C	4.76707315	4.36733007	2.66049123
H	3.25284648	5.38028669	3.84281373
H	3.33302021	3.63116479	4.10955286
H	5.56782770	4.51943827	3.40041065
H	4.93938828	3.39389801	2.17218041
H	4.86378098	5.15225697	1.89238167
C	2.11602783	-5.31257296	-0.10645812
H	1.99756312	-3.77418160	-3.69130325
C	0.40432814	-5.65779161	-4.99162102
H	1.33659458	-6.10811806	-3.08552790
H	-0.35693198	-5.62789965	-2.95239830
C	-0.01937350	-7.09732342	-5.29816151
H	-0.34738353	-4.95388126	-5.39391518
H	1.35121906	-5.42970943	-5.51337624
H	-0.14211828	-7.24877501	-6.38131666
H	0.73423231	-7.81772804	-4.94116306
H	-0.97786266	-7.34390688	-4.81292295
C	3.40276980	-5.83502626	0.54550809

H 1.44131219 -4.91854095 0.67229199  
H 1.58771789 -6.14136934 -0.61000025  
C 3.13020229 -6.94809389 1.56158948  
H 4.08928061 -6.20555592 -0.23782155  
H 3.92171144 -4.99656773 1.04472804  
H 4.06748152 -7.30554628 2.01485682  
H 2.47786808 -6.59136581 2.37554359  
H 2.63554621 -7.81080770 1.08584547

**L2\*Pr(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12616.278499, E0 = -12615.567862, G= 379.2671 at T=298.150 K

Cl -5.45373631 3.64594746 -0.36233506  
Cl -4.23733473 -3.08298326 -3.72143936  
N -1.63138175 1.28029072 0.15902267  
N -0.26997915 4.05509996 1.95617723  
N -1.20925748 -1.09520602 -0.99140257  
N 1.08793366 -3.71354103 -1.71837425  
O -0.02753886 1.81279469 2.17026925  
O 0.52533245 -2.67822123 0.22099334  
C -1.79550397 2.45916438 0.75773787  
C -2.97744823 3.21069050 0.61885798  
H -3.13305807 4.13351345 1.17470980  
C -3.97920084 2.72921753 -0.20344464  
C -3.82012486 1.50646293 -0.89708978  
C -4.78959084 0.93066472 -1.76754725  
H -5.72065496 1.47195911 -1.94125640  
C -4.57052994 -0.28137580 -2.36471725  
H -5.32423878 -0.71665490 -3.02266550  
C -3.36732316 -1.01271439 -2.13580513  
C -3.08159351 -2.28978729 -2.68305635  
C -1.89084482 -2.93255472 -2.38718271

H -1.69707179 -3.93027329 -2.78053951  
 C -0.97006112 -2.29426193 -1.53999639  
 C -2.36617064 -0.46677396 -1.28114128  
 C -2.59689546 0.81711155 -0.65358639  
 C -0.63707024 2.78630519 1.67482960  
 C 0.27992368 -2.92570424 -0.98144770  
 C -0.71129769 5.25470448 1.23177004  
 C -1.59175587 6.19845009 2.05983782  
 H -1.22405851 4.94561386 0.30919319  
 C 0.87282026 4.22867346 2.88071132  
 H 0.79464436 3.44338751 3.64688253  
 H 0.74590647 5.20750475 3.37211370  
 C 2.27973080 -4.25972939 -1.02789545  
 H 2.70736027 -3.45246553 -0.40882787  
 H 3.00815988 -4.51886272 -1.81249297  
 C 1.05004513 -3.80689526 -3.18338323  
 H 0.31538877 -3.08144188 -3.56228828  
 C 0.74936247 -5.21275997 -3.71233797  
 Pr 0.53391773 -0.26000503 0.88574195  
 N -1.01802433 -1.20904231 3.20602965  
 O 0.25414073 -1.04836047 3.24795437  
 O -1.56055796 -1.02586329 2.02438378  
 O -1.69154227 -1.50255930 4.17499304  
 N 3.30701852 -0.39096686 1.83523548  
 O 2.63402700 0.72034639 1.77182174  
 O 2.64923072 -1.44161689 1.46166337  
 O 4.46104193 -0.43382856 2.21246839  
 N 1.69852149 0.85941505 -1.58343518  
 O 2.17695856 1.32337189 -2.60032272  
 O 1.76419449 -0.40565860 -1.29642010  
 O 1.07891762 1.58876848 -0.70886314

H	0.20039651	5.78824949	0.90922594
C	2.23379660	4.13573647	2.18208432
C	-2.02176833	7.43011236	1.25400293
H	-2.48419929	5.65872192	2.42674184
H	-1.04232812	6.52159929	2.96162963
C	-2.88734436	8.39588070	2.06906319
H	-1.12145138	7.95641041	0.88812971
H	-2.57508612	7.10401726	0.35416910
H	-3.18275332	9.26941872	1.46720028
H	-3.80814624	7.90314913	2.42242575
H	-2.34399772	8.76474380	2.95453238
C	3.38856649	4.24591398	3.18448496
H	2.30101824	3.16670632	1.66171551
H	2.32436395	4.92958546	1.41756260
C	4.75553989	4.07819891	2.51394367
H	3.33979940	5.21784019	3.71139073
H	3.26531148	3.46157169	3.95331788
H	5.57206869	4.16831207	3.24783897
H	4.83175135	3.08549237	2.04122758
H	4.91484690	4.84150600	1.73349774
C	1.97432947	-5.47870111	-0.15217362
H	2.03384399	-3.46759844	-3.55569243
C	0.73427176	-5.25414085	-5.24504423
H	1.50660396	-5.92078590	-3.33096647
H	-0.22330332	-5.56006098	-3.31692457
C	0.44786143	-6.65457201	-5.79557037
H	-0.02389486	-4.54385042	-5.62284756
H	1.70805597	-4.89707184	-5.62662458
H	0.44216105	-6.65547323	-6.89675617
H	1.21214628	-7.37570524	-5.46207619
H	-0.53304005	-7.02369976	-5.45319176

C 3.23094702 -5.97231865 0.57461488  
 H 1.21027589 -5.19514942 0.59121317  
 H 1.55075133 -6.29105234 -0.77076411  
 C 2.95513916 -7.18918276 1.46295202  
 H 4.01407719 -6.22123051 -0.16586767  
 H 3.63261175 -5.14747190 1.19019961  
 H 3.87124658 -7.52438784 1.97445095  
 H 2.20706725 -6.94957256 2.23665833  
 H 2.56852698 -8.03653717 0.87187904  
 O -4.11285162 0.22764041 2.15792370  
 H -3.29721355 -0.32432437 2.17030644  
 H -4.40072966 0.19272828 3.08601308

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12616.265677, E0 = -12615.555044, G= 380.9306 at T=298.150 K

Pr -0.69520229 -0.54104149 -0.04697223  
 Cl 3.77544761 1.97976458 4.88030815  
 Cl 2.64330840 5.53899860 -1.73164701  
 O -1.10553730 0.43634158 -2.18674374  
 O -0.78625804 -1.40101147 2.30643773  
 O -3.11039996 -0.88609236 0.18373486  
 O -4.13167667 -2.82830834 -0.04110397  
 O -1.96359289 -2.65723777 -0.40026802  
 O 1.02433634 -2.34041142 0.28040057  
 O 0.80212116 -1.56011403 -1.75295341  
 O 2.24118686 -3.18175840 -1.35196888  
 O -1.74117851 1.47989440 0.79913855  
 H -1.58787930 2.51683235 0.54162073  
 H -2.70890450 1.34337568 0.81185240  
 N 1.10366154 0.33247852 1.62462080  
 N 0.64210051 -2.60766959 3.59102678  
 N 0.77012837 1.54133463 -0.76427078



N	-0.78626162	1.64386523	-4.05211926
N	-3.11877894	-2.16299891	-0.08688645
N	1.39758873	-2.40059614	-0.96242309
C	1.24249685	-0.31023255	2.79033780
C	2.06035042	0.18465777	3.81944346
H	2.11384988	-0.31101286	4.78819895
C	2.77243257	1.35284185	3.59957242
C	2.67914796	2.03952742	2.36279440
C	3.36157537	3.25392246	2.05745959
H	4.03212929	3.67789435	2.80615187
C	3.16244602	3.88872242	0.86309516
H	3.66798019	4.83058167	0.64512146
C	2.27579427	3.35519552	-0.11833322
C	1.60940588	2.12136149	0.12114875
C	1.80302536	1.46261382	1.39697111
C	1.94983172	3.99461436	-1.33593965
C	1.05138052	3.42281604	-2.21885443
H	0.74896169	3.99901152	-3.08538556
C	0.49072194	2.16508698	-1.92099702
C	-0.52044427	1.39268804	-2.75488949
C	-0.20737053	2.69391370	-4.90019369
H	-0.18795285	2.28962088	-5.92627907
H	0.84728330	2.84441829	-4.62472343
C	-1.00828695	4.00476456	-4.85613251
H	-2.00228453	3.82826114	-5.30467510
H	-1.20749140	4.29032993	-3.80635095
C	-0.30228788	5.14217854	-5.60240602
H	-0.13093682	4.85268831	-6.65585375
H	0.70053834	5.30525923	-5.16265965
C	-1.09953892	6.44943476	-5.54028559
H	-2.08712840	6.33187008	-6.01599693

H -0.57033288 7.26548624 -6.05715036  
 H -1.26487410 6.75215960 -4.49385881  
 C -1.82654285 0.80665773 -4.68723869  
 H -2.28086972 1.41486418 -5.48600149  
 H -2.59958911 0.59724098 -3.93350649  
 C -1.26188552 -0.50087577 -5.25362301  
 H -0.77063304 -1.05782080 -4.43726063  
 H -0.48324701 -0.27334037 -6.00553799  
 C -2.35664749 -1.36555731 -5.88873148  
 H -3.12203455 -1.59444869 -5.12493753  
 H -2.86977172 -0.79087555 -6.68250704  
 C -1.80828643 -2.67268586 -6.46920681  
 H -1.05788338 -2.47623849 -7.25330448  
 H -2.61246729 -3.27917552 -6.91509533  
 H -1.32397449 -3.27814984 -5.68529558  
 C 0.31271341 -1.49701953 2.90030599  
 C 1.99976647 -2.94646740 4.03970528  
 H 2.69921947 -2.19516230 3.64578772  
 H 2.27174640 -3.89989781 3.55158162  
 C 2.14008880 -3.08091354 5.55907249  
 H 1.83904469 -2.13548040 6.04755211  
 H 1.44075930 -3.85252047 5.92766237  
 C 3.57146120 -3.44758844 5.96900892  
 H 4.26804304 -2.67336750 5.59825230  
 H 3.86194849 -4.38876390 5.46785641  
 C 3.73076320 -3.60079503 7.48469925  
 H 3.47506046 -2.66485715 8.00832844  
 H 4.76655197 -3.86308765 7.75083351  
 H 3.07168770 -4.39380026 7.87467241  
 C -0.36403596 -3.69498944 3.59936881  
 H 0.17485061 -4.62290335 3.84879422

H -0.75446022 -3.78849602 2.57352233  
 C -1.50756109 -3.46081901 4.59296656  
 H -1.98619497 -2.49435425 4.36075258  
 H -1.09044051 -3.38605857 5.61271763  
 C -2.56373620 -4.57791519 4.54306889  
 H -2.07280636 -5.55620956 4.70573092  
 H -3.24922514 -4.43505764 5.39653301  
 C -3.37870026 -4.61270428 3.24451423  
 H -3.87401772 -3.64471531 3.06140018  
 H -4.16181374 -5.38586473 3.29455924  
 H -2.75754094 -4.83434439 2.36195135  
 O -1.25395989 3.88567877 0.28543919  
 O -1.14449942 5.30302715 -1.38812637  
 O -2.18831396 3.39063811 -1.65806293  
 N -1.54719889 4.20889425 -0.94931620

**L2\*Pr(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12259.306664, E0 = -12258.634131, G= 361.9967 at T=298.150 K

Cl -5.39641762 3.67587280 -0.38351601  
 Cl -4.14047480 -3.09310985 -3.62966561  
 N -1.58849895 1.31840777 0.22415876  
 N -0.26305139 4.08742857 2.07211971  
 N -1.13934803 -1.05580342 -0.93505263  
 N 1.19321871 -3.65127921 -1.74041617  
 O 0.00217906 1.84279275 2.22336578  
 O 0.81977284 -2.43771768 0.13793729  
 C -1.76425743 2.50893760 0.81608081  
 C -2.94175577 3.25480461 0.64444602  
 H -3.10993266 4.18452454 1.18464625  
 C -3.93527293 2.76507473 -0.19181851  
 C -3.76166797 1.53038311 -0.86827910  
 C -4.72206974 0.94507802 -1.74854445

H -5.64909697 1.48670554 -1.94261146  
 C -4.49634027 -0.26993024 -2.33352447  
 H -5.24131775 -0.70856482 -2.99909878  
 C -3.29084897 -0.99432069 -2.08609867  
 C -2.99545979 -2.27515984 -2.61922145  
 C -1.78893781 -2.89624929 -2.32921481  
 H -1.59326756 -3.89494514 -2.71660233  
 C -0.86602122 -2.23853230 -1.49844074  
 C -2.30406237 -0.43784016 -1.22625041  
 C -2.54442191 0.84459269 -0.60423243  
 C -0.62367964 2.83631349 1.75393391  
 C 0.44995534 -2.80623317 -1.01172948  
 C -0.75582308 5.32278872 1.43506670  
 C -1.69229770 6.15065098 2.32268357  
 H -1.23385084 5.06547785 0.47848493  
 C 0.86863887 4.25126219 3.01803827  
 H 0.78325707 3.46467113 3.78177977  
 H 0.72967291 5.22665310 3.51024199  
 C 2.41337681 -4.20568037 -1.09943986  
 H 2.93056750 -3.37958884 -0.58509076  
 H 3.06118298 -4.55966234 -1.91588485  
 C 1.01704073 -3.92377043 -3.18004107  
 H 0.29420444 -3.20437932 -3.59036231  
 C 0.61012769 -5.36459446 -3.50275803  
 Pr 0.27168879 -0.27385667 1.09871256  
 N -1.36439455 -1.56270671 3.09270692  
 O -0.05915033 -1.44040000 3.16333246  
 O -1.89224374 -1.04274535 2.02048683  
 O -2.01131368 -2.10762310 3.94904184  
 N 2.59127474 0.69570929 -0.33935228  
 O 3.57876921 1.08819330 -0.90965748

O	2.58719850	0.40033033	0.93870085
O	1.44455111	0.52795243	-0.93299890
H	0.13735200	5.91922569	1.18100762
C	2.23704743	4.18227863	2.33037877
C	-2.16938829	7.42322540	1.61066365
H	-2.56219149	5.54194403	2.63221288
H	-1.17133963	6.42435646	3.25680923
C	-3.09808493	8.27044678	2.48554754
H	-1.29052246	8.02252865	1.31206679
H	-2.68816829	7.14823580	0.67373455
H	-3.42379737	9.17581272	1.95133483
H	-4.00028515	7.70662165	2.77391124
H	-2.59107041	8.58983898	3.41036463
C	3.38096285	4.40433502	3.32795262
H	2.35219264	3.19281483	1.85485065
H	2.29270291	4.94018126	1.52729189
C	4.75694847	4.32668257	2.65996218
H	3.25744724	5.38686275	3.81954885
H	3.31499195	3.64343882	4.12685013
H	5.56046629	4.48585272	3.39543581
H	4.91551447	3.33978558	2.19463229
H	4.86295366	5.09196234	1.87341952
C	2.12276411	-5.34093666	-0.11173600
H	1.98442113	-3.69357157	-3.66049099
C	0.43877697	-5.57845926	-5.01242161
H	1.37535203	-6.06034088	-3.11640286
H	-0.32812181	-5.62032652	-2.97573495
C	0.04899942	-7.01856518	-5.35867643
H	-0.32803389	-4.88153601	-5.39804029
H	1.38138795	-5.31504679	-5.52517271
H	-0.06750580	-7.14431667	-6.44576931

H 0.81801134 -7.73069954 -5.01833630  
 H -0.90469599 -7.30006599 -4.88302851  
 C 3.41503954 -5.87093639 0.52291328  
 H 1.44889688 -4.96917200 0.67853534  
 H 1.59766388 -6.16094112 -0.63287002  
 C 3.15292692 -7.00948858 1.51323175  
 H 4.10091591 -6.21856117 -0.27141842  
 H 3.93090105 -5.04170322 1.04028189  
 H 4.09395838 -7.37181902 1.95473516  
 H 2.50131583 -6.67611980 2.33756232  
 H 2.66189194 -7.86373615 1.01880145

**L2\*Nd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13003.181345, E0 = -13002.470367, G= 379.3146 at T=298.150 K

Cl -5.48306513 3.62480307 -0.29397711  
 Cl -4.32288647 -3.14390564 -3.59373236  
 N -1.66019404 1.25357819 0.20753388  
 N -0.26813528 4.05006313 1.94254708  
 N -1.26416516 -1.13283002 -0.92786747  
 N 1.06807792 -3.68355918 -1.68759596  
 O -0.07035071 1.81109416 2.24438834  
 O 0.46269599 -2.75029564 0.29264635  
 C -1.81336474 2.44039130 0.79231060  
 C -2.99384570 3.19439077 0.65836912  
 H -3.13509893 4.12752962 1.20145106  
 C -4.00971222 2.70570111 -0.14263384  
 C -3.86211610 1.47290266 -0.82086045  
 C -4.84755516 0.88641441 -1.67029309  
 H -5.78023005 1.42832315 -1.83407950  
 C -4.64289141 -0.33076030 -2.25764060  
 H -5.40811443 -0.77122390 -2.89854193

C -3.43511939 -1.06073010 -2.03955126  
 C -3.15453434 -2.34055376 -2.57874918  
 C -1.95822847 -2.97882271 -2.29821301  
 H -1.76315451 -3.97671914 -2.69118404  
 C -1.02864075 -2.32904029 -1.46611607  
 C -2.42210770 -0.50601095 -1.20505762  
 C -2.63859653 0.78605831 -0.58587468  
 C -0.65144658 2.77580237 1.70683420  
 C 0.23804326 -2.95379186 -0.91756630  
 C -0.67531633 5.22211885 1.15623879  
 C -1.53028619 6.23192835 1.93138325  
 H -1.19707477 4.87924051 0.25066924  
 C 0.86938477 4.23987865 2.87014556  
 H 0.76560205 3.49139833 3.66950274  
 H 0.76016629 5.24205732 3.31674337  
 C 2.28327775 -4.21073437 -1.02283216  
 H 2.68045640 -3.41243529 -0.37239906  
 H 3.01844382 -4.40804482 -1.81904697  
 C 1.02161944 -3.72430158 -3.15464568  
 H 0.25091767 -3.02040672 -3.50170398  
 C 0.77839100 -5.12214088 -3.73190379  
 Nd 0.49895307 -0.29528913 0.98471403  
 N -1.11655092 -1.25480592 3.25001812  
 O 0.15872703 -1.13815582 3.31030226  
 O -1.63939512 -1.00990903 2.07107234  
 O -1.81099498 -1.56004918 4.20106983  
 N 3.24560142 -0.46877268 1.95740163  
 O 2.56010675 0.63790548 1.94670117  
 O 2.60135531 -1.50640261 1.53235328  
 O 4.39985371 -0.51527512 2.33579803  
 N 1.65537167 0.87102842 -1.46308458

O 2.12930584 1.33032131 -2.48566771  
O 1.69794309 -0.40175349 -1.19091904  
O 1.07092631 1.60231888 -0.57341218  
H 0.24995054 5.71316624 0.80581915  
C 2.23500967 4.08414173 2.19208288  
C -1.92628276 7.43078518 1.06122923  
H -2.43783402 5.73705816 2.32374287  
H -0.97338891 6.58728933 2.81629252  
C -2.76643205 8.46074486 1.82259738  
H -1.01206732 7.91317177 0.67030865  
H -2.48737097 7.07284641 0.17846540  
H -3.03814578 9.30911541 1.17524970  
H -3.70024872 8.01189041 2.19956589  
H -2.21398807 8.86104202 2.68857789  
C 3.38136768 4.20989180 3.20217586  
H 2.28305149 3.09211206 1.71468616  
H 2.35308552 4.84112740 1.39468920  
C 4.75058222 3.97599244 2.55640817  
H 3.35291696 5.20572901 3.68413687  
H 3.22926354 3.46463680 4.00404119  
H 5.56152201 4.08009863 3.29468751  
H 4.80584812 2.96023846 2.13217044  
H 4.93773127 4.69700146 1.74259782  
C 2.02944851 -5.47465038 -0.19597931  
H 1.98484266 -3.32609248 -3.52213144  
C 0.75293595 -5.10965204 -5.26499414  
H 1.56865668 -5.80950785 -3.38109183  
H -0.17535757 -5.52480984 -3.34286404  
C 0.52579266 -6.50131893 -5.86333418  
H -0.03967197 -4.42171526 -5.61235142  
H 1.70656085 -4.69546270 -5.63965988



H 0.51110888 -6.46360636 -6.96377993  
 H 1.32477260 -7.19807291 -5.56085396  
 H -0.43443191 -6.92688036 -5.52786875  
 C 3.30775189 -5.94557190 0.50781852  
 H 1.25816965 -5.25054932 0.56013751  
 H 1.63600945 -6.27849007 -0.84491885  
 C 3.08548522 -7.20889616 1.34477437  
 H 4.09819937 -6.13072109 -0.24348538  
 H 3.67661715 -5.13084888 1.15642023  
 H 4.01579618 -7.52530718 1.84239972  
 H 2.32884312 -7.03395748 2.12740779  
 H 2.73502564 -8.04681396 0.71873111  
 O -4.21508408 0.18133336 2.15964150  
 H -3.38237858 -0.34427053 2.19742179  
 H -4.51571035 0.15925528 3.08399057

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13003.170460, E0 = -13002.458810, G= 381.7123 at T=298.150 K

Nd -0.71445066 -0.54265755 -0.03806892  
 Cl 3.77309155 2.00870347 4.88240099  
 Cl 2.65678215 5.53405046 -1.74529326  
 O -1.12710333 0.45573783 -2.16159058  
 O -0.80035657 -1.35960197 2.33530307  
 O -3.13239837 -0.89884204 0.15804134  
 O -4.12135172 -2.84696150 -0.14233173  
 O -1.95137239 -2.63389421 -0.46769580  
 O 1.00918341 -2.33145666 0.31257561  
 O 0.83643264 -1.51906681 -1.71283102  
 O 2.28903437 -3.12391043 -1.29561281  
 O -1.76882923 1.47456300 0.83753932  
 H -1.60650229 2.49262476 0.57086080  
 H -2.73661876 1.34219790 0.82419801

N	1.11174846	0.34417188	1.63223422
N	0.64353085	-2.59420896	3.57678938
N	0.76895511	1.54976356	-0.76002955
N	-0.79159254	1.63504875	-4.04293776
N	-3.11903906	-2.16332102	-0.15287037
N	1.41984344	-2.36269689	-0.91881847
C	1.24019277	-0.28634518	2.80089450
C	2.05503368	0.21264388	3.83197975
H	2.10358858	-0.27733102	4.80400038
C	2.77197671	1.37512457	3.60430145
C	2.68533325	2.05261230	2.36237812
C	3.37163377	3.26403689	2.05111527
H	4.04279470	3.69092107	2.79751277
C	3.17365146	3.89154863	0.85370797
H	3.68106842	4.83129930	0.63067967
C	2.28362489	3.35660529	-0.12496827
C	1.61395717	2.12644815	0.11813687
C	1.81074226	1.47032130	1.39823353
C	1.95601714	3.99493217	-1.34355903
C	1.05287910	3.42464948	-2.22111869
H	0.74964964	3.99866438	-3.08895588
C	0.48721987	2.16968226	-1.91585219
C	-0.53247750	1.39608586	-2.74195576
C	-0.20799778	2.67761087	-4.89676237
H	-0.18994799	2.26814175	-5.92076635
H	0.84735197	2.82519197	-4.62212420
C	-1.00368583	3.99194145	-4.85750628
H	-1.99662030	3.81886911	-5.30973339
H	-1.20606422	4.27642441	-3.80790067
C	-0.29115510	5.12696505	-5.60107183
H	-0.12056493	4.83872843	-6.65497541

H 0.71232772 5.28409100 -5.16055059  
 C -1.08146465 6.43834734 -5.53666306  
 H -2.07004714 6.32653141 -6.01170254  
 H -0.54849261 7.25232506 -6.05293083  
 H -1.24426782 6.74051571 -4.48964787  
 C -1.83740962 0.79921269 -4.67081738  
 H -2.28564000 1.40168905 -5.47738838  
 H -2.61326742 0.60447264 -3.91592169  
 C -1.28171456 -0.51924151 -5.22048426  
 H -0.79184544 -1.06785083 -4.39765263  
 H -0.50346559 -0.30666026 -5.97716570  
 C -2.38331604 -1.38624704 -5.84035492  
 H -3.14785147 -1.59894586 -5.07101297  
 H -2.89495301 -0.82018590 -6.64125061  
 C -1.84473276 -2.70535922 -6.40257168  
 H -1.09456587 -2.52557421 -7.19090748  
 H -2.65383196 -3.31299853 -6.83788443  
 H -1.36305523 -3.30228567 -5.61055374  
 C 0.30424860 -1.47340000 2.91051102  
 C 2.00309181 -2.92982531 4.02215195  
 H 2.69839692 -2.16833878 3.64050007  
 H 2.28290296 -3.87414479 3.52140450  
 C 2.13728738 -3.08155084 5.54037476  
 H 1.82727695 -2.14325237 6.03709269  
 H 1.43998218 -3.86095381 5.89608288  
 C 3.56737494 -3.44404769 5.95838356  
 H 4.26342440 -2.66409850 5.59883070  
 H 3.86682510 -4.38076591 5.45435238  
 C 3.71087813 -3.60486770 7.47482586  
 H 3.44100094 -2.67311811 8.00002003  
 H 4.74313688 -3.86268401 7.75478220

H 3.04945064 -4.40308571 7.85157013  
 C -0.35667744 -3.68743992 3.56758690  
 H 0.18811592 -4.61665678 3.79832935  
 H -0.74665833 -3.76441169 2.54014611  
 C -1.50101316 -3.47880554 4.56575537  
 H -1.98298967 -2.50932908 4.35447359  
 H -1.08484960 -3.42559719 5.58725452  
 C -2.55322671 -4.59826040 4.48971939  
 H -2.05923367 -5.57832575 4.63089371  
 H -3.23993015 -4.47668934 5.34548712  
 C -3.36684155 -4.60658026 3.18982625  
 H -3.86374760 -3.63574862 3.02717161  
 H -4.14850187 -5.38207531 3.22250628  
 H -2.74455428 -4.80842781 2.30339050  
 O -1.23806310 3.89142060 0.31028804  
 O -1.08751142 5.32111645 -1.34957349  
 O -2.13550758 3.41609955 -1.65382814  
 N -1.50368273 4.22599173 -0.92240453

**L2\*Nd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12646.211128 , E0 = -12645.538252, G= 362.3006 at T=298.150 K

Cl -5.40932178 3.67242122 -0.38010222  
 Cl -4.14332390 -3.08037496 -3.64773250  
 N -1.58766496 1.33563316 0.19888641  
 N -0.27079800 4.08988667 2.06938624  
 N -1.14694643 -1.05053735 -0.94528294  
 N 1.17601597 -3.66043973 -1.71192229  
 O -0.00372904 1.84451151 2.20993114  
 O 0.77084213 -2.45895410 0.16981509  
 C -1.77030528 2.51517606 0.80528599  
 C -2.95423365 3.25511575 0.64505595  
 H -3.12758088 4.17735243 1.19649947

C -3.94365978 2.76864386 -0.19650868  
 C -3.76462173 1.54033399 -0.88382965  
 C -4.72340393 0.95690840 -1.76687527  
 H -5.65147972 1.49716175 -1.95967042  
 C -4.49514771 -0.25605628 -2.35500813  
 H -5.23917007 -0.69372338 -3.02230930  
 C -3.29109287 -0.98221695 -2.10515857  
 C -2.99891520 -2.26685429 -2.63362193  
 C -1.79890597 -2.89341998 -2.33371520  
 H -1.60488677 -3.89446259 -2.71635771  
 C -0.87785083 -2.23773384 -1.49780321  
 C -2.30412006 -0.42765746 -1.24509978  
 C -2.54354501 0.85897899 -0.62488461  
 C -0.62747639 2.83859515 1.74715459  
 C 0.42619050 -2.81607676 -0.98959094  
 C -0.77329904 5.32705164 1.44380510  
 C -1.70837891 6.14416647 2.34268236  
 H -1.25560737 5.07553196 0.48774678  
 C 0.86859459 4.25169802 3.00682473  
 H 0.79377872 3.45766020 3.76391554  
 H 0.72924829 5.22209692 3.50870109  
 C 2.38358331 -4.22390938 -1.05605328  
 H 2.89640117 -3.40253448 -0.52970219  
 H 3.04249573 -4.57580900 -1.86446142  
 C 1.02370012 -3.91537642 -3.15723133  
 H 0.30708811 -3.19153380 -3.57079768  
 C 0.62400836 -5.35228539 -3.50475478  
 Nd 0.30163482 -0.25344494 1.05552733  
 N -1.19422495 -1.56015015 3.12231970  
 O 0.10750161 -1.40781641 3.13413668  
 O -1.78392243 -1.05825925 2.07298231

O	-1.79030120	-2.11647081	4.00844860
N	2.61765623	0.65524304	-0.41939208
O	3.60016894	1.03996599	-1.00455165
O	2.55786657	0.58983701	0.88813788
O	1.53043032	0.27512273	-1.02653694
H	0.11551759	5.92956352	1.18895113
C	2.22995687	4.19406033	2.30420041
C	-2.18867159	7.42384386	1.64574230
H	-2.57672906	5.53122520	2.64837527
H	-1.18504608	6.40821838	3.27820015
C	-3.11681724	8.26012421	2.53167510
H	-1.31098056	8.02742577	1.35239553
H	-2.70877719	7.15885496	0.70663482
H	-3.44440532	9.17111015	2.00828242
H	-4.01791668	7.69214821	2.81528330
H	-2.60852265	8.56967068	3.45911646
C	3.38377523	4.40135241	3.29360700
H	2.34157419	3.21244144	1.81177795
H	2.27697301	4.96572113	1.51363921
C	4.75212765	4.33939934	2.60846829
H	3.26369548	5.37407589	3.80520654
H	3.32856917	3.62511134	4.07842064
H	5.56426382	4.48404264	3.33742428
H	4.90545511	3.36271238	2.12055945
H	4.84820414	5.12122202	1.83702862
C	2.07385421	-5.36295700	-0.07872106
H	1.99803340	-3.67719674	-3.61951613
C	0.48258445	-5.54759789	-5.02001572
H	1.38198125	-6.05244112	-3.11205769
H	-0.32435355	-5.61471558	-2.99952388
C	0.10011003	-6.98306942	-5.39263153

H -0.27642110 -4.84567928 -5.41201830  
 H 1.43518031 -5.27753592 -5.51036978  
 H 0.00444829 -7.09425879 -6.48335505  
 H 0.86277926 -7.69973040 -5.04752636  
 H -0.86235690 -7.27112961 -4.93908024  
 C 3.35449457 -5.89850473 0.57461149  
 H 1.38808811 -4.99294424 0.70203596  
 H 1.55570984 -6.17931557 -0.61246669  
 C 3.07484794 -7.04157543 1.55486739  
 H 4.05305815 -6.24301958 -0.20998926  
 H 3.86265516 -5.07245827 1.10463572  
 H 4.00843668 -7.40721178 2.00931597  
 H 2.41057038 -6.71130657 2.37025237  
 H 2.59076071 -7.89267111 1.04827654

**L2\*Pm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13400.043888, E0 = -13399.332734, G= 379.4690 at T=298.150 K

Cl -5.47805405 3.61840534 -0.31192183  
 Cl -4.34088802 -3.16435575 -3.58919096  
 N -1.64773500 1.25201511 0.16953260  
 N -0.28521395 4.02737904 1.96376204  
 N -1.26818037 -1.14379692 -0.94989157  
 N 1.07262146 -3.68067575 -1.75478482  
 O -0.11362352 1.78334999 2.26442075  
 O 0.53093022 -2.69785523 0.21724044  
 C -1.80686045 2.43172312 0.76738077  
 C -2.98925519 3.18383312 0.63939273  
 H -3.12903595 4.11432838 1.18762696  
 C -4.00518703 2.69828439 -0.16274418  
 C -3.85974526 1.46483219 -0.84019846  
 C -4.85061073 0.87601167 -1.68175662

H -5.78430700 1.41768003 -1.84048033  
 C -4.65034294 -0.34253535 -2.26770115  
 H -5.41971016 -0.78432643 -2.90269709  
 C -3.44178891 -1.07211256 -2.05414128  
 C -3.16382074 -2.35396910 -2.58992577  
 C -1.96254694 -2.98739147 -2.32101774  
 H -1.77014065 -3.98514915 -2.71526241  
 C -1.02748883 -2.33381343 -1.49705327  
 C -2.42430019 -0.51629692 -1.22594571  
 C -2.63341832 0.78049833 -0.61287898  
 C -0.66464710 2.75512648 1.71097338  
 C 0.26138616 -2.93645883 -0.97670949  
 C -0.64853430 5.19592667 1.15136182  
 C -1.50560927 6.23295403 1.88707614  
 H -1.15208828 4.84929323 0.23684524  
 C 0.81554335 4.21135855 2.93560362  
 H 0.68367696 3.45229101 3.72072005  
 H 0.68468392 5.20727539 3.39052153  
 C 2.31116295 -4.18346548 -1.11415029  
 H 2.72270179 -3.36661601 -0.49677035  
 H 3.02256203 -4.39845848 -1.92718959  
 C 0.97738302 -3.77289963 -3.21725512  
 H 0.20257597 -3.07416558 -3.56518674  
 C 0.70517993 -5.18803930 -3.73704457  
 Pm 0.51450884 -0.27297559 0.94822425  
 N -1.02939558 -1.23404860 3.24300838  
 O 0.24209028 -1.10117185 3.28739262  
 O -1.56971538 -1.00717199 2.06580853  
 O -1.71205568 -1.54028273 4.20254803  
 N 3.22060204 -0.42359716 2.00531626  
 O 2.49945164 0.65194726 2.06984210



O 2.63293600 -1.43471563 1.44662511  
 O 4.35875750 -0.47616142 2.43089557  
 N 1.62223399 1.05234706 -1.42822707  
 O 2.05308533 1.58256507 -2.43562555  
 O 1.57110715 -0.24167506 -1.29517138  
 O 1.18104279 1.72613740 -0.41879544  
 H 0.29446819 5.66489315 0.81818289  
 C 2.20778656 4.06849337 2.31104302  
 C -1.85139596 7.42672873 0.98889756  
 H -2.43440366 5.76202631 2.25868368  
 H -0.96833295 6.59080935 2.78295588  
 C -2.69210362 8.48445702 1.71052909  
 H -0.91612226 7.88457823 0.61879742  
 H -2.39348435 7.06747627 0.09488240  
 H -2.92706656 9.32878780 1.04378808  
 H -3.64569759 8.06012440 2.06581903  
 H -2.15723014 8.88588047 2.58696628  
 C 3.31063747 4.17604828 3.37046099  
 H 2.27578998 3.08552909 1.81801212  
 H 2.35867357 4.83996868 1.53340352  
 C 4.70606852 3.95424938 2.77874470  
 H 3.26139379 5.16285992 3.86909223  
 H 3.12567067 3.41592312 4.15111542  
 H 5.48527908 4.04601955 3.55203676  
 H 4.78053522 2.94594049 2.34000254  
 H 4.92623806 4.68928051 1.98600066  
 C 2.09172750 -5.42576265 -0.24543506  
 H 1.93183291 -3.39819288 -3.62945199  
 C 0.63009602 -5.22891998 -5.26799774  
 H 1.50132298 -5.86919641 -3.38752937  
 H -0.23808274 -5.56933737 -3.30342960

C 0.36976877 -6.63805056 -5.80921268  
 H -0.16630068 -4.54465866 -5.61398792  
 H 1.57511997 -4.83872986 -5.68749905  
 H 0.32016867 -6.63866997 -6.90926933  
 H 1.17090881 -7.33275604 -5.50778913  
 H -0.58347201 -7.04071951 -5.42866421  
 C 3.39375138 -5.86566210 0.43463427  
 H 1.34030151 -5.18672609 0.52584249  
 H 1.68756747 -6.25079727 -0.86019433  
 C 3.20725060 -7.10772038 1.31119847  
 H 4.16486216 -6.06395388 -0.33324507  
 H 3.77198100 -5.03028440 1.05073643  
 H 4.15423107 -7.40203524 1.79054892  
 H 2.47137046 -6.91817856 2.11002731  
 H 2.84749460 -7.96547079 0.71817708  
 O -4.16168785 0.14027429 2.12275457  
 H -3.31895137 -0.36784601 2.17991424  
 H -4.45988894 0.15193707 3.04805541

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13400.033374, E0 = -13399.321796, G= 381.8308 at T=298.150 K

Pm -0.74179590 -0.49398690 -0.03551845  
 Cl 3.71114516 2.03300261 4.91167736  
 Cl 2.63304567 5.57379484 -1.71834087  
 O -1.12365580 0.47990125 -2.16611958  
 O -0.85284269 -1.31729460 2.34999084  
 O -3.13332224 -0.86393976 0.24313971  
 O -4.10401869 -2.84292865 0.16286688  
 O -1.94450247 -2.63757634 -0.22880927  
 O 1.00139725 -2.25111318 0.31835982  
 O 0.60699046 -1.65339613 -1.74721897  
 O 2.05937409 -3.25878119 -1.32935262

O	-1.79142547	1.51803708	0.81951702
H	-1.64480400	2.53689575	0.54975659
H	-2.75621438	1.38143039	0.88366634
N	1.07772338	0.37366372	1.63474381
N	0.60397130	-2.57075763	3.56060243
N	0.76244283	1.57737517	-0.75713712
N	-0.76263553	1.64215779	-4.05363894
N	-3.10951424	-2.15366721	0.06242230
N	1.26040280	-2.42987704	-0.93953317
C	1.19792724	-0.25922012	2.80212831
C	2.00510716	0.23692466	3.84089327
H	2.04901838	-0.26018372	4.80969715
C	2.72065902	1.40216208	3.62412500
C	2.64137220	2.08383608	2.38412690
C	3.32446051	3.29999375	2.08223367
H	3.98685837	3.72758675	2.83606601
C	3.13456798	3.93073153	0.88524854
H	3.63952374	4.87361956	0.67003775
C	2.25720930	3.39326739	-0.10380992
C	1.59342980	2.15872836	0.13041729
C	1.77825975	1.50083137	1.41079223
C	1.93764555	4.03046227	-1.32542837
C	1.04760790	3.45503926	-2.21357322
H	0.74909598	4.02784538	-3.08409572
C	0.48669675	2.19643331	-1.91444421
C	-0.52313936	1.41532183	-2.74709678
C	-0.17000608	2.68188190	-4.90461683
H	-0.13076586	2.26507592	-5.92503977
H	0.87913132	2.83818865	-4.61145353
C	-0.97330886	3.99202871	-4.88843918
H	-1.95544696	3.81211448	-5.36110783

H -1.19915366 4.27860069 -3.84419608  
 C -0.25072783 5.12794495 -5.62088346  
 H -0.05586531 4.83688259 -6.66975307  
 H 0.74238187 5.29150343 -5.15943241  
 C -1.04859698 6.43561888 -5.57818222  
 H -2.02626920 6.31714916 -6.07371283  
 H -0.50872999 7.25033426 -6.08602238  
 H -1.23499787 6.74076843 -4.53596544  
 C -1.79277623 0.79413193 -4.69167852  
 H -2.22677660 1.38437474 -5.51486111  
 H -2.58309960 0.60577387 -3.95033240  
 C -1.22010148 -0.52910298 -5.21190834  
 H -0.74797976 -1.06617808 -4.37119818  
 H -0.42551294 -0.32266831 -5.95317030  
 C -2.30379677 -1.40783799 -5.84677267  
 H -3.08704209 -1.61149502 -5.09393263  
 H -2.79660511 -0.85553914 -6.66880322  
 C -1.74721611 -2.73376966 -6.37453365  
 H -0.97651309 -2.56376839 -7.14504290  
 H -2.54284453 -3.35011888 -6.82226753  
 H -1.28533351 -3.31696892 -5.56084681  
 C 0.25658733 -1.44350302 2.90857148  
 C 1.97355008 -2.91491985 3.96654820  
 H 2.65859461 -2.14178181 3.58966541  
 H 2.24406314 -3.84450960 3.43383288  
 C 2.14670682 -3.10744524 5.47611713  
 H 1.85143900 -2.18303394 6.00648737  
 H 1.45947301 -3.89686823 5.82926369  
 C 3.58826709 -3.48112345 5.84162569  
 H 4.27317190 -2.68983936 5.48537731  
 H 3.87234378 -4.40130472 5.29956388

C	3.78073239	-3.69006991	7.34679317
H	3.53180575	-2.77591062	7.91068268
H	4.82318544	-3.95651960	7.58087635
H	3.13384247	-4.50074148	7.72048426
C	-0.39677420	-3.66331697	3.55573487
H	0.15324552	-4.59667826	3.75597024
H	-0.81342572	-3.72024369	2.53731847
C	-1.51323473	-3.47170734	4.58819675
H	-2.02093291	-2.51325774	4.38592434
H	-1.06578827	-3.40235233	5.59549475
C	-2.54325199	-4.61351204	4.55519772
H	-2.02416945	-5.58025360	4.69850016
H	-3.21036601	-4.49337912	5.42659903
C	-3.38866377	-4.65984631	3.27681684
H	-3.91028166	-3.70296931	3.11040282
H	-4.15236712	-5.45121336	3.34174299
H	-2.78474975	-4.86171532	2.37800360
O	-1.28448212	3.93749785	0.28535268
O	-1.10257828	5.36036825	-1.37673473
O	-2.12570882	3.44500875	-1.69937849
N	-1.52034271	4.26389551	-0.95526940

**L2\*Pm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13043.075840, E0 = -13042.402793, G= 362.5775 at T=298.150 K

Cl	-5.40494204	3.67035246	-0.36559176
Cl	-4.14995766	-3.09151530	-3.63096952
N	-1.60707581	1.30371678	0.24178673
N	-0.26240143	4.05865574	2.08433795
N	-1.15030372	-1.06002474	-0.93406308
N	1.19035065	-3.64475465	-1.74256170
O	-0.02444683	1.81158924	2.25601387
O	0.81781644	-2.42378855	0.13141863

C -1.77891397 2.48868012 0.83766127  
 C -2.95463657 3.23988366 0.66686022  
 H -3.12019396 4.16856050 1.21003163  
 C -3.94599915 2.75639439 -0.17424841  
 C -3.77260423 1.52512598 -0.85766679  
 C -4.73048735 0.94454443 -1.74369621  
 H -5.65637445 1.48783720 -1.93860233  
 C -4.50406647 -0.26891372 -2.33181834  
 H -5.24808168 -0.70470273 -3.00041056  
 C -3.29971361 -0.99569243 -2.08437181  
 C -3.00437331 -2.27648211 -2.61932898  
 C -1.79893720 -2.89804029 -2.32997513  
 H -1.60294139 -3.89599991 -2.71923137  
 C -0.87567008 -2.24050808 -1.49784589  
 C -2.31337070 -0.44378129 -1.22176647  
 C -2.55697823 0.83704382 -0.59189200  
 C -0.63338649 2.80781841 1.77807403  
 C 0.44566518 -2.80085349 -1.01320291  
 C -0.74028355 5.29123545 1.43036807  
 C -1.66361868 6.14497566 2.30690074  
 H -1.22328115 5.02678871 0.47828805  
 C 0.87020016 4.22106409 3.02944350  
 H 0.77646476 3.44224930 3.80018044  
 H 0.74040055 5.20245409 3.51211905  
 C 2.41837859 -4.18624878 -1.10508621  
 H 2.93204570 -3.35272384 -0.59917682  
 H 3.06388021 -4.54119730 -1.92292166  
 C 1.00973094 -3.92384863 -3.18025112  
 H 0.28194016 -3.20989394 -3.59135294  
 C 0.60966992 -5.36814117 -3.49587631  
 Pm 0.24870405 -0.28524241 1.10229540

N	-1.40434241	-1.60918534	3.02989459
O	-0.11500743	-1.41616285	3.15927696
O	-1.90424240	-1.13988698	1.92294025
O	-2.06379461	-2.17299652	3.86555624
N	2.45881510	0.87945753	-0.31707495
O	3.40958929	1.36445487	-0.88057125
O	2.54291868	0.35959482	0.88234574
O	1.26915169	0.83002299	-0.84041637
H	0.16019642	5.87167454	1.16532302
C	2.23818469	4.13215017	2.34351540
C	-2.11756539	7.41683817	1.57863533
H	-2.54434991	5.55507183	2.62221551
H	-1.13961732	6.42113590	3.23855710
C	-3.03349853	8.29067707	2.44071198
H	-1.22772896	7.99714231	1.27507961
H	-2.63880348	7.13955975	0.64376831
H	-3.34193802	9.19480705	1.89422679
H	-3.94612598	7.74630833	2.73358512
H	-2.52323604	8.61273575	3.36280370
C	3.38412166	4.35477018	3.33857465
H	2.34425020	3.13625026	1.87982142
H	2.30140829	4.87956524	1.53139293
C	4.75901937	4.25811720	2.67072535
H	3.26934791	5.34353924	3.81966400
H	3.31173801	3.60307407	4.14557171
H	5.56427908	4.41584730	3.40461516
H	4.90785980	3.26594687	2.21350932
H	4.87186432	5.01553297	1.87761700
C	2.14245248	-5.31666040	-0.10767048
H	1.97377455	-3.69079447	-3.66597533
C	0.43541175	-5.58832169	-5.00430250

H 1.38045943 -6.05761003 -3.10944724  
 H -0.32536930 -5.62722921 -2.96475744  
 C 0.06313675 -7.03420448 -5.34591818  
 H -0.34103164 -4.90165186 -5.38911343  
 H 1.37304497 -5.31461239 -5.52082968  
 H -0.05651453 -7.16339684 -6.43224764  
 H 0.84363377 -7.73507547 -5.00831699  
 H -0.88428688 -7.32880068 -4.86564589  
 C 3.44295001 -5.82752800 0.52600020  
 H 1.46796656 -4.94535112 0.68222547  
 H 1.62402785 -6.14618731 -0.62032449  
 C 3.19810891 -6.96109295 1.52639711  
 H 4.12953091 -6.17363453 -0.26838976  
 H 3.95125270 -4.98818111 1.03451252  
 H 4.14554071 -7.30892801 1.96594679  
 H 2.54658008 -6.62862778 2.35114193  
 H 2.71462989 -7.82477093 1.04097807

**L2\*Sm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13806.980575, E0 = -13806.269714, G= 378.9535 at T=298.150 K

Cl -5.48811531 3.63062072 -0.33216551  
 Cl -4.36545563 -3.19699740 -3.52497315  
 N -1.66171885 1.26337349 0.17219321  
 N -0.29028410 4.04469109 1.94784427  
 N -1.28090835 -1.14052904 -0.92614281  
 N 1.06073654 -3.67442393 -1.72933197  
 O -0.12966439 1.80157506 2.25801730  
 O 0.52023965 -2.69943118 0.24966526  
 C -1.81904459 2.44864726 0.75833422  
 C -2.99894166 3.20299625 0.62142724  
 H -3.13639617 4.14037991 1.15841544



C -4.01700592 2.70933747 -0.17292780  
 C -3.87627387 1.46586180 -0.83336532  
 C -4.87037897 0.86624616 -1.66370440  
 H -5.80473948 1.40564215 -1.82620203  
 C -4.67166901 -0.35977012 -2.23473597  
 H -5.44338131 -0.80974150 -2.86113453  
 C -3.46157193 -1.08622801 -2.01806021  
 C -3.18448353 -2.37390900 -2.54052424  
 C -1.98056972 -3.00154757 -2.27080297  
 H -1.78572083 -4.00256205 -2.65576124  
 C -1.04132962 -2.33650327 -1.46066558  
 C -2.44072318 -0.51949686 -1.20180547  
 C -2.64962721 0.78334159 -0.60176319  
 C -0.67658043 2.77307224 1.70046258  
 C 0.25153738 -2.93478870 -0.94397533  
 C -0.64627123 5.21157837 1.12988377  
 C -1.50101829 6.25504446 1.85917974  
 H -1.14962840 4.86322308 0.21582560  
 C 0.80809152 4.22640944 2.92253232  
 H 0.65661353 3.48780560 3.72366762  
 H 0.69540352 5.23462057 3.35449600  
 C 2.30614805 -4.17117310 -1.09843957  
 H 2.72472143 -3.34884262 -0.49290109  
 H 3.00893903 -4.39123201 -1.91753972  
 C 0.96742916 -3.74277544 -3.19301629  
 H 0.18245094 -3.04967666 -3.52923632  
 C 0.71556818 -5.15289640 -3.73583698  
 Sm 0.49274507 -0.26192358 0.95405149  
 N -1.02215886 -1.53584051 3.10560751  
 O 0.25910753 -1.54565012 3.05813313  
 O -1.60729086 -0.97308385 2.07671309

O	-1.66405892	-2.00245690	4.02763987
N	3.20089221	-0.32617331	2.01220202
O	2.33911514	0.60011464	2.30515814
O	2.75960970	-1.24039078	1.21646988
O	4.33543348	-0.32150328	2.45335937
N	1.61208129	0.90875077	-1.49088383
O	2.03727031	1.42904747	-2.50667119
O	1.52670622	-0.36986548	-1.34402919
O	1.20731175	1.61065483	-0.47375455
H	0.29955116	5.67550230	0.79726720
C	2.20157480	4.04095936	2.31184983
C	-1.83804405	7.44737577	0.95578039
H	-2.43318152	5.78919077	2.22862959
H	-0.96534687	6.61318779	2.75594211
C	-2.67772555	8.51075554	1.67025101
H	-0.89932275	7.90031338	0.58833629
H	-2.37755895	7.08729124	0.06057183
H	-2.90620017	9.35385990	0.99973780
H	-3.63462234	8.09134388	2.02245426
H	-2.14521527	8.91277599	2.54784679
C	3.29960942	4.16642714	3.37442780
H	2.25478840	3.03959441	1.85496914
H	2.36873174	4.78212404	1.50854588
C	4.69405031	3.88616657	2.80549669
H	3.27041698	5.17462301	3.82987285
H	3.09062076	3.44510674	4.18525839
H	5.46950388	4.00197458	3.57930946
H	4.75258303	2.85498762	2.42049026
H	4.93495750	4.57478094	1.97793531
C	2.09669518	-5.40932751	-0.22159705
H	1.91603422	-3.34659886	-3.59888411

C 0.64943403 -5.17196751 -5.26760054  
 H 1.51815307 -5.82955217 -3.39211106  
 H -0.22534719 -5.55217600 -3.31345034  
 C 0.41033190 -6.57600594 -5.83140516  
 H -0.15374503 -4.49285936 -5.60796595  
 H 1.59169102 -4.76345205 -5.67572832  
 H 0.36703849 -6.56085920 -6.93165159  
 H 1.21858585 -7.26487064 -5.53553438  
 H -0.53979868 -6.99649334 -5.46247196  
 C 3.40691495 -5.85220671 0.44043514  
 H 1.35706544 -5.16588402 0.55958527  
 H 1.68134451 -6.23491287 -0.82821345  
 C 3.22806454 -7.08923197 1.32575119  
 H 4.16534901 -6.05753088 -0.33815828  
 H 3.79905939 -5.01613283 1.04687822  
 H 4.18069458 -7.38596869 1.79231393  
 H 2.50484252 -6.89251232 2.13430500  
 H 2.85550761 -7.94792891 0.74208289  
 O -4.12074471 0.31657436 2.27313757  
 H -3.31158304 -0.24522540 2.30160046  
 H -4.35789967 0.39315882 3.21278024

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13806.969757, E0 = -13806.258589, G= 380.4480 at T=298.150 K

Sm -0.72473896 -0.51631635 -0.01198136  
 Cl 3.77511454 2.00777268 4.89407539  
 Cl 2.62359142 5.55577660 -1.72554147  
 O -1.12079799 0.43986368 -2.14511156  
 O -0.79961342 -1.34401929 2.34408474  
 O -3.14729524 -0.81765366 0.20016015  
 O -4.19090414 -2.69915938 -0.27859390  
 O -2.01551175 -2.51599646 -0.57910007

O 0.86503232 -2.41725373 0.32356551  
 O 0.99948728 -1.36632180 -1.58908165  
 O 2.34328175 -3.06394196 -1.17564356  
 O -1.78282690 1.48964274 0.86369562  
 H -1.63970041 2.49359870 0.59691936  
 H -2.74856758 1.34257889 0.85138148  
 N 1.13007116 0.34016189 1.63334620  
 N 0.63945240 -2.59472084 3.57644320  
 N 0.74757403 1.57132471 -0.73189193  
 N -0.79302353 1.62309849 -4.02437592  
 N -3.16936421 -2.04468060 -0.22454704  
 N 1.44443583 -2.31823826 -0.83255249  
 C 1.25449455 -0.29134023 2.80063128  
 C 2.06465912 0.20822740 3.83576345  
 H 2.11614156 -0.28651384 4.80538988  
 C 2.77531743 1.37624705 3.61386395  
 C 2.68141961 2.06241298 2.37719703  
 C 3.35702801 3.28177524 2.07010746  
 H 4.02628517 3.71062303 2.81719470  
 C 3.15514135 3.91210508 0.87466305  
 H 3.65866995 4.85463142 0.65428865  
 C 2.26602507 3.37600803 -0.10512177  
 C 1.60041654 2.14407492 0.13809460  
 C 1.81216824 1.47759116 1.41086221  
 C 1.93424726 4.01121044 -1.32405138  
 C 1.03821528 3.43252492 -2.20447731  
 H 0.74066180 4.00040960 -3.07850742  
 C 0.47325698 2.17796922 -1.89393818  
 C -0.53522921 1.38623214 -2.72198272  
 C -0.20966570 2.66297030 -4.88135719  
 H -0.18312384 2.24617791 -5.90227270

H	0.84329009	2.81793308	-4.60186386
C	-1.01106071	3.97390795	-4.85994101
H	-2.00506997	3.78939128	-5.30515432
H	-1.21004403	4.27683735	-3.81519628
C	-0.30571753	5.09853363	-5.62584496
H	-0.14033736	4.79262590	-6.67544222
H	0.69954091	5.26589870	-5.19337368
C	-1.09948373	6.40856981	-5.58201933
H	-2.08908391	6.28560877	-6.05211544
H	-0.57025105	7.21459723	-6.11432791
H	-1.26036191	6.72962475	-4.54033899
C	-1.82450938	0.77243757	-4.65626335
H	-2.27583170	1.36698329	-5.46706200
H	-2.60179067	0.56910479	-3.90527296
C	-1.24916387	-0.54062456	-5.19857454
H	-0.76065856	-1.08086669	-4.36954260
H	-0.46702990	-0.32094568	-5.94921207
C	-2.33523345	-1.42286301	-5.82442141
H	-3.10506558	-1.63879633	-5.06134653
H	-2.84425569	-0.86722726	-6.63423729
C	-1.77609348	-2.73973179	-6.37165165
H	-1.01843035	-2.55689502	-7.15204716
H	-2.57331491	-3.35886264	-6.81265163
H	-1.29785359	-3.32587290	-5.56973410
C	0.30727175	-1.47203994	2.90954208
C	2.00230718	-2.94569254	3.99858832
H	2.69726920	-2.18315816	3.61815476
H	2.26927066	-3.88440514	3.48035574
C	2.15950418	-3.11991262	5.51209116
H	1.86811328	-2.18573523	6.02744913
H	1.46105766	-3.89783835	5.86885977

C	3.59379125	-3.50263858	5.89640188
H	4.28973150	-2.72269654	5.53656864
H	3.87412357	-4.43252563	5.36918449
C	3.76964784	-3.69350219	7.40598679
H	3.52411509	-2.76965928	7.95537424
H	4.80717134	-3.96669531	7.65372276
H	3.11146259	-4.49301815	7.78394461
C	-0.37007836	-3.67899108	3.57077193
H	0.16720521	-4.61347055	3.79776549
H	-0.76486319	-3.75050807	2.54482222
C	-1.50782907	-3.46068549	4.57425308
H	-1.97430706	-2.48155355	4.37309980
H	-1.08818412	-3.42397547	5.59506893
C	-2.57906222	-4.56138563	4.49017954
H	-2.10105538	-5.55147552	4.61526775
H	-3.25902462	-4.43992996	5.35131121
C	-3.40005851	-4.53847885	3.19493914
H	-3.88166547	-3.55724597	3.04908919
H	-4.19371557	-5.30186892	3.22114706
H	-2.78546739	-4.73746681	2.30238461
O	-1.28864670	3.93858194	0.31376323
O	-1.14641070	5.33690071	-1.36974335
O	-2.18863583	3.42542291	-1.63517368
N	-1.55705309	4.24742746	-0.91913509

**L2\*Sm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13450.014875, E0 = -13449.341979, G= 362.3886 at T=298.150 K

Cl	-5.37558460	3.69190335	-0.41452506
Cl	-4.11575794	-3.05974030	-3.70206261
N	-1.57829750	1.32432818	0.18436578
N	-0.24941191	4.05580807	2.07880855
N	-1.12400532	-1.03690755	-0.99202359

N 1.20445371 -3.64922285 -1.76305568  
 O 0.01963539 1.81007040 2.18318987  
 O 0.84851617 -2.37762499 0.07793574  
 C -1.75217891 2.50249696 0.79142833  
 C -2.92926264 3.25366521 0.62521732  
 H -3.10074592 4.17557764 1.17766130  
 C -3.91644406 2.77747607 -0.22522369  
 C -3.74065471 1.55232382 -0.91862047  
 C -4.69501638 0.97702104 -1.81223118  
 H -5.61960697 1.52181184 -2.00919485  
 C -4.46784830 -0.23453224 -2.40436006  
 H -5.20981073 -0.66629225 -3.07782769  
 C -3.26674151 -0.96546936 -2.15279102  
 C -2.97264957 -2.24777913 -2.68462992  
 C -1.77182186 -2.87466574 -2.38687110  
 H -1.58095455 -3.87496805 -2.77212954  
 C -0.84971684 -2.21873331 -1.55132067  
 C -2.28264809 -0.41747627 -1.28544593  
 C -2.52606249 0.86281443 -0.65296078  
 C -0.60617310 2.81060410 1.73517537  
 C 0.46847755 -2.77842283 -1.05682480  
 C -0.74766976 5.30285692 1.46937799  
 C -1.68648410 6.10784864 2.37518024  
 H -1.22369993 5.06588078 0.50665301  
 C 0.88511938 4.20363665 3.02407002  
 H 0.80531448 3.40054679 3.77105570  
 H 0.74419218 5.16779375 3.53744984  
 C 2.42499495 -4.18874025 -1.10982430  
 H 2.94724178 -3.34887815 -0.62357670  
 H 3.06776857 -4.57143688 -1.91723573  
 C 1.02035499 -3.96668386 -3.19222713

H	0.30989611	-3.24887228	-3.62624264
C	0.58967894	-5.41052580	-3.46724725
Sm	0.27463597	-0.27105156	1.05015969
N	-1.40277708	-1.58705425	2.96590853
O	-0.11405826	-1.40045142	3.09950662
O	-1.89695203	-1.11847544	1.86053801
O	-2.06583452	-2.14751458	3.80225396
N	2.47849631	0.88225025	-0.39002195
O	3.43264365	1.35964191	-0.95617968
O	2.56150746	0.37469792	0.81366384
O	1.29298615	0.83030492	-0.91316819
H	0.14336136	5.90782356	1.22846949
C	2.25087762	4.15480375	2.32970238
C	-2.16453648	7.39603138	1.69246495
H	-2.55563664	5.49071455	2.66981483
H	-1.16659403	6.36048365	3.31582427
C	-3.09094882	8.22452354	2.58751512
H	-1.28583455	8.00123978	1.40553546
H	-2.68510985	7.14220190	0.75056213
H	-3.41832113	9.14059734	2.07287335
H	-3.99216199	7.65471888	2.86708474
H	-2.58113837	8.52500153	3.51711297
C	3.39855671	4.36052799	3.32643509
H	2.36753178	3.17608166	1.83313119
H	2.30017114	4.92920542	1.54224694
C	4.77140760	4.30468178	2.64978123
H	3.27258873	5.33142185	3.84001446
H	3.34048462	3.58208156	4.10884666
H	5.57802725	4.44992161	3.38473725
H	4.93170166	3.32993293	2.16016340
H	4.86989594	5.08878136	1.88107264



C 2.13366532 -5.29099751 -0.08552446  
 H 1.99036109 -3.76886439 -3.68149567  
 C 0.41020930 -5.66919899 -4.96894026  
 H 1.34572768 -6.10499811 -3.06111383  
 H -0.35034549 -5.63490868 -2.92924666  
 C -0.00312594 -7.11301804 -5.26940441  
 H -0.34668759 -4.97259045 -5.37438488  
 H 1.35525751 -5.43660641 -5.49200344  
 H -0.12558623 -7.26998472 -6.35177469  
 H 0.75601131 -7.82649040 -4.91023302  
 H -0.95926857 -7.36495209 -4.78225994  
 C 3.42622781 -5.80284262 0.56337458  
 H 1.46241832 -4.89245796 0.69383276  
 H 1.60568357 -6.12621641 -0.57880658  
 C 3.16394353 -6.90845442 1.59026849  
 H 4.10993814 -6.17703724 -0.22067150  
 H 3.94424152 -4.95805740 1.05269468  
 H 4.10514069 -7.25833178 2.04133177  
 H 2.51459932 -6.54746866 2.40468597  
 H 2.67022204 -7.77714109 1.12450516

**L2\*Eu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14224.178487, E0 = -14223.467573, G= 379.8670 at T=298.150 K

Cl -5.43425083 3.65385890 -0.33941340  
 Cl -4.30498266 -3.12228608 -3.62323332  
 N -1.61732674 1.27836430 0.15889169  
 N -0.25993583 4.04981852 1.97717965  
 N -1.22230959 -1.10758781 -0.99251366  
 N 1.05192685 -3.74138117 -1.67294550  
 O -0.00950104 1.80341041 2.17894721  
 O 0.47180277 -2.72405505 0.27678701

C	-1.77319002	2.45622873	0.75971949
C	-2.95393968	3.21062398	0.62691408
H	-3.10373998	4.13379431	1.18382871
C	-3.96209145	2.73289466	-0.18940873
C	-3.81101418	1.50759637	-0.88072908
C	-4.79510021	0.92875046	-1.73723984
H	-5.72404623	1.47596335	-1.90429735
C	-4.59621906	-0.29065192	-2.32178926
H	-5.36296368	-0.72808707	-2.96296763
C	-3.39469695	-1.02884114	-2.09662342
C	-3.12831068	-2.32014728	-2.61670208
C	-1.94418991	-2.97241759	-2.31892872
H	-1.76451373	-3.98148799	-2.69023871
C	-1.00400376	-2.32002616	-1.49994957
C	-2.37610030	-0.47445288	-1.26955318
C	-2.58934450	0.81735975	-0.64631808
C	-0.61387128	2.77729392	1.68510747
C	0.24708495	-2.95841336	-0.92565858
C	-0.68562186	5.24663830	1.23863459
C	-1.57208014	6.20241737	2.04649806
H	-1.18767023	4.93361855	0.31147343
C	0.86145985	4.22902536	2.92622781
H	0.77443165	3.43750930	3.68506265
H	0.71261126	5.20230103	3.42270064
C	2.24882102	-4.28336382	-0.98967904
H	2.66974592	-3.47676873	-0.36478770
H	2.97958708	-4.52847815	-1.77662504
C	1.02934790	-3.78797436	-3.14028215
H	0.27792305	-3.07160687	-3.50387716
C	0.76859272	-5.18375015	-3.71431136
Eu	0.51047897	-0.23910268	0.83988804

N	-1.01825309	-1.27636814	3.11557007
O	0.26107064	-1.18519497	3.11090398
O	-1.59892356	-0.98605347	1.98230124
O	-1.66122043	-1.60226548	4.09790516
N	3.32743692	-0.19337045	1.59841740
O	2.64300990	0.88146275	1.35620487
O	2.67236376	-1.29357457	1.48158288
O	4.50498009	-0.15371591	1.91170490
N	1.62922895	0.59414595	-1.75012529
O	2.08850312	0.95961499	-2.81939816
O	1.79157424	-0.60536188	-1.29840946
O	0.93390375	1.38203847	-0.99533677
H	0.23208058	5.77423716	0.92314631
C	2.23904252	4.15648508	2.25884318
C	-1.98764145	7.42721176	1.22273910
H	-2.47117233	5.67077303	2.40894079
H	-1.03208840	6.53332233	2.95108604
C	-2.85720110	8.40592003	2.01790357
H	-1.08104026	7.94525099	0.86068141
H	-2.53299713	7.09377098	0.32073388
H	-3.14241958	9.27400589	1.40338373
H	-3.78380132	7.92123032	2.36722517
H	-2.32128668	8.78225040	2.90475059
C	3.37103605	4.28941774	3.28476310
H	2.33555150	3.18666172	1.74448514
H	2.33449006	4.94969606	1.49426055
C	4.75271702	4.12134409	2.64409590
H	3.30456519	5.26745510	3.79793906
H	3.23706722	3.51568532	4.06298494
H	5.55363464	4.22435093	3.39330649
H	4.84401035	3.12527514	2.18124223

H 4.92332983 4.87811947 1.85980439  
 C 1.95425797 -5.51298189 -0.12563512  
 H 2.00516510 -3.40844893 -3.49454308  
 C 0.77584457 -5.18150806 -5.24761486  
 H 1.53630877 -5.88559723 -3.34237385  
 H -0.20159809 -5.56358242 -3.34330153  
 C 0.53105277 -6.57188654 -5.84201288  
 H 0.00604632 -4.47888756 -5.61617184  
 H 1.74590528 -4.79049873 -5.60449266  
 H 0.54064882 -6.54137230 -6.94276524  
 H 1.30792916 -7.28383493 -5.51801014  
 H -0.44520193 -6.97418547 -5.52450323  
 C 3.21648955 -6.00978422 0.58907676  
 H 1.19236398 -5.24117374 0.62428200  
 H 1.53171003 -6.32012033 -0.75180650  
 C 2.95034933 -7.23771667 1.46516037  
 H 3.99654579 -6.24722528 -0.15832597  
 H 3.61875033 -5.19067287 1.21186745  
 H 3.87028360 -7.57468319 1.96859765  
 H 2.20462298 -7.01024723 2.24467874  
 H 2.56492352 -8.08000088 0.86613894  
 O -4.11918402 0.29136381 2.19003558  
 H -3.30824804 -0.26904193 2.19156456  
 H -4.37931633 0.28167996 3.12673187

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14224.169022, E0 = -14223.457659, G= 380.5914 at T=298.150 K

Eu -0.74868727 -0.50300997 0.00678426  
 Cl 3.70211816 2.04364014 4.96113253  
 Cl 2.60398030 5.60055494 -1.66543603  
 O -1.20544827 0.55410135 -2.08579659  
 O -0.84507161 -1.32610404 2.37637067

O -3.16758204 -0.82332003 0.04163977  
 O -4.15013075 -2.79725242 0.04540302  
 O -1.96353412 -2.63614440 -0.16712113  
 O 1.11898744 -2.14890575 0.26825014  
 O 0.51875365 -1.63877904 -1.77221978  
 O 2.05938458 -3.17801118 -1.43694580  
 O -1.87639499 1.51848853 0.90394354  
 H -1.73697054 2.48990250 0.62642723  
 H -2.83205199 1.34483695 0.79861897  
 N 1.05869436 0.39737079 1.68606496  
 N 0.63213682 -2.58428454 3.55594373  
 N 0.73733550 1.59988284 -0.70050460  
 N -0.77818078 1.65596342 -3.99746156  
 N -3.14155436 -2.12179375 -0.02434306  
 N 1.26816547 -2.36191845 -1.00121593  
 C 1.19246483 -0.24759649 2.84427071  
 C 2.00437260 0.24233763 3.88289261  
 H 2.05977798 -0.26457685 4.84612846  
 C 2.70960212 1.41556251 3.67300558  
 C 2.62042522 2.10645437 2.43854237  
 C 3.29671597 3.32738376 2.13871551  
 H 3.95979309 3.75547981 2.89183974  
 C 3.10200548 3.96110845 0.94401217  
 H 3.60372066 4.90620565 0.73075646  
 C 2.22641420 3.42211819 -0.04679435  
 C 1.56630599 2.18462133 0.18637417  
 C 1.75535738 1.52525675 1.46646929  
 C 1.90974402 4.05649662 -1.27017927  
 C 1.02151513 3.47724080 -2.15862012  
 H 0.72816539 4.04423332 -3.03533769  
 C 0.46218646 2.21915221 -1.85649395

C -0.56348681 1.44615078 -2.68142176  
 C -0.13852751 2.65116858 -4.86517000  
 H -0.06752800 2.19532394 -5.86726952  
 H 0.90114480 2.81618333 -4.54372978  
 C -0.92375129 3.97101831 -4.93506813  
 H -1.90312755 3.77864480 -5.40819073  
 H -1.15619731 4.32394505 -3.91315651  
 C -0.17492193 5.05129766 -5.72332907  
 H 0.03300718 4.68973970 -6.74733162  
 H 0.81199211 5.23156071 -5.25551653  
 C -0.95587146 6.36836863 -5.78295898  
 H -1.92723179 6.22852755 -6.28518867  
 H -0.39715880 7.13927174 -6.33662701  
 H -1.15479422 6.74957180 -4.76841593  
 C -1.81213582 0.81293106 -4.63610268  
 H -2.22270298 1.39201641 -5.47913933  
 H -2.61641693 0.65261167 -3.90333414  
 C -1.25268614 -0.53083444 -5.11706543  
 H -0.79881704 -1.05448198 -4.25800467  
 H -0.44612405 -0.35462692 -5.85324669  
 C -2.34203935 -1.40818501 -5.74413729  
 H -3.13618088 -1.58275282 -4.99544859  
 H -2.81760049 -0.86831397 -6.58450317  
 C -1.79886723 -2.75409675 -6.23395777  
 H -1.01719594 -2.61346507 -6.99934101  
 H -2.59831166 -3.36959982 -6.67604399  
 H -1.35444736 -3.32375908 -5.40124416  
 C 0.26645535 -1.44659078 2.93158054  
 C 2.00603867 -2.91676664 3.95628023  
 H 2.68023729 -2.12653732 3.59573817  
 H 2.29080319 -3.83172441 3.40601850

C 2.17963552 -3.13644123 5.46212196  
 H 1.87314379 -2.22567534 6.00965214  
 H 1.50077105 -3.94019175 5.79877329  
 C 3.62466574 -3.50103784 5.82291126  
 H 4.30122805 -2.69519663 5.48380899  
 H 3.91998959 -4.40698528 5.26318645  
 C 3.81682038 -3.73785853 7.32399511  
 H 3.55681348 -2.83794308 7.90552425  
 H 4.86167669 -3.99756289 7.55495977  
 H 3.17815113 -4.56284571 7.68010664  
 C -0.35345727 -3.69019318 3.52310395  
 H 0.20896699 -4.62116432 3.69754601  
 H -0.77156663 -3.72503352 2.50426984  
 C -1.47263706 -3.54200315 4.56007004  
 H -1.96712136 -2.56721735 4.41023827  
 H -1.03043032 -3.53652048 5.57195663  
 C -2.51821160 -4.66535807 4.45281744  
 H -2.00978279 -5.64683628 4.50565720  
 H -3.16900492 -4.61104012 5.34293747  
 C -3.38548565 -4.59311771 3.19029427  
 H -3.91101766 -3.62594461 3.12710929  
 H -4.14720774 -5.38897371 3.19240999  
 H -2.79839802 -4.70418262 2.26497102  
 O -1.33334625 4.03357601 0.29363540  
 O -1.17118502 5.44980717 -1.36905253  
 O -2.26668596 3.57832885 -1.64575291  
 N -1.60239673 4.36432076 -0.91704226

**L2\*Eu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13867.212865, E0 = -13866.540227, G= 362.3709 at T=298.150 K

Cl -5.39401102 3.67122936 -0.37240425

Cl -4.13812637 -3.08682418 -3.64184403

N -1.58289623 1.32154453 0.21060356  
 N -0.26063773 4.06977606 2.08740425  
 N -1.13151562 -1.04744995 -0.96218306  
 N 1.19436705 -3.65622830 -1.74417996  
 O 0.00540664 1.82342899 2.22714138  
 O 0.83594263 -2.41224670 0.11827615  
 C -1.75967622 2.49989605 0.81751209  
 C -2.94086504 3.24501157 0.65546453  
 H -3.11217952 4.16772318 1.20687866  
 C -3.93027329 2.76295137 -0.18884823  
 C -3.75347710 1.53658974 -0.88019431  
 C -4.71189594 0.95600098 -1.76604486  
 H -5.63899899 1.49796295 -1.95887113  
 C -4.48580217 -0.25710249 -2.35521984  
 H -5.23106050 -0.69314080 -3.02228189  
 C -3.28167486 -0.98434043 -2.10796547  
 C -2.98911047 -2.26928186 -2.63498688  
 C -1.78656995 -2.89393854 -2.34037900  
 H -1.59580016 -3.89606023 -2.72148013  
 C -0.86012441 -2.23267055 -1.51354301  
 C -2.29227829 -0.43030635 -1.25049198  
 C -2.53417230 0.85263634 -0.62056649  
 C -0.61394298 2.81616497 1.76311982  
 C 0.45983613 -2.79622364 -1.02113211  
 C -0.75008714 5.30520058 1.44865084  
 C -1.68341982 6.13915586 2.33383536  
 H -1.22928488 5.04892540 0.49237147  
 C 0.86888200 4.23193884 3.03539562  
 H 0.78507084 3.43940473 3.79315042  
 H 0.72664201 5.20367289 3.53400397  
 C 2.41514206 -4.20715427 -1.10267758



H	2.93684959	-3.37722898	-0.59906983
H	3.05891228	-4.57267380	-1.91729259
C	1.01343572	-3.94085884	-3.18055344
H	0.29330054	-3.22198439	-3.59650826
C	0.59942561	-5.38245249	-3.49052811
Eu	0.27445623	-0.26811689	1.06047606
N	-1.34163260	-1.59399855	3.01919317
O	-0.08826111	-1.27097690	3.18493295
O	-1.83429646	-1.24979258	1.86968601
O	-1.98144829	-2.16478872	3.86803150
N	2.50317669	0.81033301	-0.39626065
O	3.47195721	1.24215817	-0.97474283
O	2.53470302	0.48104918	0.86791986
O	1.35323763	0.63674676	-0.96670121
H	0.14418937	5.89907122	1.19207537
C	2.23854446	4.17094994	2.34952307
C	-2.14916897	7.41513634	1.62048531
H	-2.55862927	5.53674364	2.64078188
H	-1.16325784	6.40919113	3.26943374
C	-3.07331538	8.27062798	2.49215031
H	-1.26471829	8.00715923	1.32380641
H	-2.66759253	7.14393234	0.68224061
H	-3.39003611	9.17820549	1.95625043
H	-3.98092961	7.71452951	2.77854562
H	-2.56609845	8.58671570	3.41799092
C	3.38072968	4.38817787	3.35012412
H	2.35546207	3.18506694	1.86729467
H	2.29416704	4.93524933	1.55248046
C	4.75772381	4.32313681	2.68278599
H	3.25269961	5.36542082	3.85099292
H	3.31733418	3.61952734	4.14170408

H 5.56012440 4.47695923 3.42063808  
 H 4.92024899 3.34227991 2.20628452  
 H 4.86154795 5.09766006 1.90506721  
 C 2.12570786 -5.33023071 -0.10079075  
 H 1.98017824 -3.71958041 -3.66656828  
 C 0.42449290 -5.60755301 -4.99811172  
 H 1.36263275 -6.07810974 -3.10008788  
 H -0.33881199 -5.62991619 -2.95950341  
 C 0.02806728 -7.04840994 -5.33354807  
 H -0.33989602 -4.91015530 -5.38776636  
 H 1.36739028 -5.35178423 -5.51422453  
 H -0.09094554 -7.18116665 -6.41954899  
 H 0.79470819 -7.76155996 -4.98996162  
 H -0.92588216 -7.32265091 -4.85419989  
 C 3.41880417 -5.85317564 0.53799343  
 H 1.45341277 -4.94834042 0.68599731  
 H 1.59905028 -6.15613317 -0.61085075  
 C 3.15894699 -6.97961044 1.54267645  
 H 4.10294628 -6.21066427 -0.25342461  
 H 3.93596625 -5.01764345 1.04388356  
 H 4.10105562 -7.33640146 1.98643529  
 H 2.50890899 -6.63650417 2.36422563  
 H 2.66701794 -7.83981276 1.05962348

**L2\*Gd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14651.737895, E0 = -14651.025965, G= 380.9346 at T=298.150 K

Cl -5.44965744 3.67270160 -0.37655744  
 Cl -4.28738117 -3.08894420 -3.70251942  
 N -1.63883138 1.28706849 0.12192142  
 N -0.26120105 4.03263855 1.95560360  
 N -1.23504496 -1.08004749 -1.03017259

N 1.06794131 -3.68996096 -1.70434475  
 O -0.02645199 1.78550231 2.12615848  
 O 0.46850538 -2.65720725 0.22684632  
 C -1.79207182 2.46301317 0.72545868  
 C -2.97084355 3.22115850 0.59358341  
 H -3.12024331 4.14405441 1.15130901  
 C -3.97959042 2.74797344 -0.22619653  
 C -3.82961965 1.52539623 -0.92215574  
 C -4.80855846 0.94820797 -1.78581750  
 H -5.73855925 1.49326789 -1.95450425  
 C -4.60289812 -0.26720646 -2.37723303  
 H -5.36516094 -0.70247376 -3.02524567  
 C -3.39991617 -1.00361311 -2.15208435  
 C -3.12217903 -2.28766370 -2.68268824  
 C -1.93394852 -2.93360949 -2.38541341  
 H -1.74677408 -3.93766665 -2.76606631  
 C -1.00424707 -2.28351974 -1.55292141  
 C -2.38955569 -0.45289552 -1.31303406  
 C -2.60963750 0.83448952 -0.68518275  
 C -0.62786329 2.76958013 1.64819443  
 C 0.24890026 -2.90905666 -0.97504336  
 C -0.69163322 5.24440384 1.24570179  
 C -1.57532024 6.18040800 2.07926130  
 H -1.19768965 4.95162249 0.31403729  
 C 0.87789369 4.18582821 2.88887644  
 H 0.78960109 3.39039469 3.64343047  
 H 0.75400198 5.15855455 3.39321327  
 C 2.26915622 -4.20786476 -1.00673735  
 H 2.67743158 -3.38626099 -0.39289489  
 H 3.00419569 -4.45784521 -1.78807819  
 C 1.03188455 -3.79379201 -3.16838336

H	0.28529587	-3.08385015	-3.55366635
C	0.75424856	-5.20858574	-3.68588805
Gd	0.52517688	-0.24336459	0.84546238
N	-0.95543337	-1.18597174	3.14225984
O	0.31545028	-1.02986169	3.16152048
O	-1.51692045	-0.98079103	1.97094488
O	-1.61558902	-1.49248767	4.11666441
N	3.26443172	-0.37366119	1.72118723
O	2.57322621	0.73008198	1.65652132
O	2.61402869	-1.43201363	1.37146878
O	4.42621183	-0.39199018	2.08008695
N	1.63400114	0.82958025	-1.60499561
O	2.09099650	1.26409149	-2.64529157
O	1.71244037	-0.42895293	-1.28270984
O	1.02870762	1.57578230	-0.73996574
H	0.22464626	5.77871895	0.93795604
C	2.24243927	4.09135294	2.19760513
C	-1.99252808	7.42482042	1.28620195
H	-2.47384691	5.63987350	2.43000174
H	-1.03310657	6.48779869	2.99079633
C	-2.87578011	8.37582397	2.09950352
H	-1.08649242	7.95861912	0.94635171
H	-2.52646875	7.11167717	0.37024528
H	-3.16068220	9.25863838	1.50616634
H	-3.80243683	7.87609053	2.42680383
H	-2.35052347	8.73106956	3.00128984
C	3.39123464	4.17367601	3.20977712
H	2.30466008	3.12873054	1.66508496
H	2.34609294	4.89627886	1.44644022
C	4.75930309	3.98081708	2.54779887
H	3.35795426	5.14292431	3.74277329

H	3.24663281	3.38683772	3.97236085
H	5.57230234	4.05346203	3.28756332
H	4.81821203	2.98772883	2.07365489
H	4.93872786	4.74301577	1.77063096
C	1.98631489	-5.42535734	-0.12170695
H	2.00917029	-3.43963194	-3.54341793
C	0.74001330	-5.26316738	-5.21819544
H	1.52292335	-5.90061188	-3.29831982
H	-0.21273071	-5.56800270	-3.28714919
C	0.47670639	-6.67274523	-5.75679350
H	-0.02952669	-4.56857395	-5.60224915
H	1.70784652	-4.89346075	-5.60274172
H	0.47109628	-6.68315697	-6.85791779
H	1.25282574	-7.37815619	-5.41717863
H	-0.49790296	-7.05526114	-5.41111088
C	3.25141144	-5.88304615	0.61405385
H	1.21427476	-5.15110683	0.61682379
H	1.58312666	-6.25303555	-0.73367614
C	3.00130844	-7.09888554	1.51131487
H	4.04311895	-6.11941242	-0.12134465
H	3.63020205	-5.04334831	1.22376585
H	3.92286181	-7.40608788	2.03058815
H	2.24321270	-6.87179470	2.27892065
H	2.64003849	-7.96096039	0.92553711
O	-4.10777473	0.16411616	2.06766009
H	-3.26576185	-0.34693867	2.10677981
H	-4.40400219	0.14603145	2.99343109

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14651.731090, E0 = -14651.018903, G= 382.3491 at T=298.150 K

Gd -0.60501808 -0.52865732 -0.06172679

Cl 3.79774427 1.99848509 4.86209393

Cl 2.69609261 5.50533867 -1.78964078  
 O -1.10901296 0.43135181 -2.13508964  
 O -0.74037468 -1.39024556 2.24607706  
 O -2.96417499 -0.94422203 0.10147517  
 O -3.91718531 -2.83889651 -0.50734454  
 O -1.74666572 -2.54068089 -0.76455671  
 O 1.05818117 -2.31835413 0.29023191  
 O 1.01724339 -1.36792159 -1.67713034  
 O 2.42067623 -3.02543783 -1.29208159  
 O -1.65848303 1.40101051 0.85969675  
 H -1.50896347 2.42649817 0.61033416  
 H -2.62401557 1.25439453 0.83735001  
 N 1.17099798 0.32075241 1.59446537  
 N 0.64896899 -2.59309769 3.57644987  
 N 0.80388206 1.53435755 -0.77486050  
 N -0.82929015 1.61750340 -4.02031088  
 N -2.92710686 -2.14654922 -0.39901671  
 N 1.54235685 -2.27556086 -0.91370541  
 C 1.28233945 -0.30492482 2.76655054  
 C 2.08424258 0.20206094 3.80435491  
 H 2.11977887 -0.27935633 4.78111410  
 C 2.80761218 1.36155403 3.57764578  
 C 2.73370624 2.03488326 2.33296037  
 C 3.42100787 3.24542975 2.01795292  
 H 4.09138060 3.67509484 2.76352477  
 C 3.22459149 3.86943579 0.81789404  
 H 3.73364782 4.80787134 0.59281170  
 C 2.33091760 3.33524060 -0.15860768  
 C 1.66262269 2.10701656 0.08976050  
 C 1.86587465 1.44908547 1.36649406  
 C 1.99309123 3.97058892 -1.37614238

C 1.07774222 3.40121388 -2.24273443  
 H 0.77183479 3.97289753 -3.11126804  
 C 0.50648409 2.15111089 -1.92689466  
 C -0.53382576 1.37458813 -2.72826791  
 C -0.27153537 2.66527486 -4.88478708  
 H -0.28799015 2.26351881 -5.91178799  
 H 0.79279512 2.80819225 -4.64447689  
 C -1.06242633 3.98082232 -4.80912638  
 H -2.07000470 3.81326866 -5.22989893  
 H -1.22959721 4.25617552 -3.75102687  
 C -0.37227041 5.12067842 -5.56624985  
 H -0.23792022 4.84129667 -6.62770939  
 H 0.64607692 5.27159500 -5.15873957  
 C -1.15627694 6.43344545 -5.46401310  
 H -2.16068769 6.32802486 -5.90612650  
 H -0.63892692 7.25044489 -5.99126768  
 H -1.28272903 6.72726107 -4.40961361  
 C -1.88868058 0.77916968 -4.62213564  
 H -2.35941935 1.38116431 -5.41621590  
 H -2.64348793 0.58042413 -3.84729457  
 C -1.34355152 -0.53745002 -5.18646193  
 H -0.83503580 -1.08565784 -4.37488461  
 H -0.58327615 -0.32283843 -5.96063995  
 C -2.45776653 -1.40629637 -5.78075886  
 H -3.20411229 -1.61949015 -4.99403954  
 H -2.98766232 -0.84161574 -6.57072687  
 C -1.92953241 -2.72543263 -6.35271168  
 H -1.19492459 -2.54594278 -7.15567541  
 H -2.74672246 -3.33375144 -6.77162457  
 H -1.43249488 -3.32129216 -5.56953335  
 C 0.34041145 -1.49046659 2.86535931

C	1.99356496	-2.93067455	4.06395102
H	2.70606613	-2.18545032	3.68221736
H	2.27610922	-3.88886523	3.59180021
C	2.09085250	-3.05079746	5.58774757
H	1.78403258	-2.09800148	6.05811834
H	1.37471366	-3.81262827	5.94418240
C	3.50696802	-3.42508197	6.04146719
H	4.22053051	-2.66072440	5.68270874
H	3.80313587	-4.37379646	5.55829811
C	3.62217498	-3.56392503	7.56253576
H	3.35988021	-2.62063074	8.06944752
H	4.64772367	-3.83215880	7.86039114
H	2.94555211	-4.34735537	7.94159222
C	-0.35805821	-3.68007302	3.56183267
H	0.16902991	-4.60414696	3.84741783
H	-0.70511085	-3.78930998	2.52200150
C	-1.54154122	-3.42912197	4.50290442
H	-2.00175071	-2.46117806	4.24263477
H	-1.16861689	-3.35076737	5.53936768
C	-2.60444307	-4.53741932	4.41391993
H	-2.13216066	-5.51875925	4.60970783
H	-3.32833195	-4.37862778	5.23205948
C	-3.35700011	-4.57798147	3.07814574
H	-3.82372952	-3.60380602	2.85634398
H	-4.15580130	-5.33601046	3.10207772
H	-2.69797468	-4.82583523	2.23066545
O	-1.15309870	3.83020616	0.37589321
O	-1.04146838	5.29880619	-1.25305879
O	-2.08805799	3.39673185	-1.58044147
N	-1.44434249	4.19299889	-0.84362113

**L2\*Gd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**



E= -14294.772616, E0 = -14294.099230, G= 362.6637 at T=298.150 K

Cl	-5.38440180	3.71400166	-0.46554002
Cl	-4.13414526	-3.04007626	-3.75639248
N	-1.58450902	1.34853840	0.11180023
N	-0.26371500	4.06082439	2.04700470
N	-1.13224590	-1.00790298	-1.06692553
N	1.18611884	-3.64182687	-1.80259216
O	0.02326530	1.81566310	2.09767866
O	0.83049446	-2.33923101	0.01630012
C	-1.75767338	2.52305984	0.72810566
C	-2.93603683	3.27269316	0.56649941
H	-3.10795474	4.19141912	1.12395811
C	-3.92545390	2.79985309	-0.28388843
C	-3.75205159	1.57665765	-0.98205882
C	-4.70953035	1.00066531	-1.87203670
H	-5.63555336	1.54442453	-2.06504583
C	-4.48401785	-0.21127817	-2.46445036
H	-5.22875881	-0.64430618	-3.13400435
C	-3.28132486	-0.94135594	-2.21737885
C	-2.98850036	-2.22585559	-2.74560237
C	-1.78767908	-2.85324669	-2.44680882
H	-1.59982312	-3.85611272	-2.82682490
C	-0.86171865	-2.19598579	-1.61723566
C	-2.29365206	-0.39041305	-1.35724664
C	-2.53577399	0.88894659	-0.72370517
C	-0.60982549	2.82094383	1.67533016
C	0.45387933	-2.75623798	-1.11191523
C	-0.77239019	5.31813717	1.46847701
C	-1.72220349	6.08896494	2.39252710
H	-1.24212027	5.10268307	0.49755850
C	0.87118703	4.19393158	2.99477077

H	0.80285263	3.36647487	3.71568727
H	0.72046906	5.14046669	3.53732228
C	2.40317416	-4.17518568	-1.13642335
H	2.92732549	-3.32876945	-0.66398799
H	3.04552937	-4.57586145	-1.93538237
C	1.00129473	-3.98497009	-3.22541523
H	0.29975539	-3.26803660	-3.67542505
C	0.55508447	-5.42931128	-3.47223735
Gd	0.24122663	-0.24015240	0.95070964
N	-1.08721924	-1.57350564	3.03735232
O	0.19295418	-1.32185495	3.04826331
O	-1.71078181	-1.14793146	1.96189249
O	-1.65315676	-2.14622331	3.93183756
N	2.68032026	0.75869852	-0.05132899
O	3.71858954	1.20516574	-0.47340071
O	2.57753515	0.17727780	1.11013925
O	1.55701447	0.82502657	-0.72645104
H	0.11328476	5.93801069	1.24704993
C	2.23452950	4.18015099	2.29446697
C	-2.21278453	7.38970423	1.74337411
H	-2.58516383	5.45486212	2.66904736
H	-1.20696247	6.32181120	3.34074140
C	-3.15016055	8.18329620	2.65841889
H	-1.34019578	8.01197910	1.47502339
H	-2.72854209	7.15585613	0.79360503
H	-3.48697567	9.10934448	2.16839767
H	-4.04534674	7.59600639	2.92066097
H	-2.64541745	8.46400547	3.59689307
C	3.38695431	4.33545685	3.29466224
H	2.34825230	3.22621536	1.75213242
H	2.28123999	4.99022961	1.54366994

C 4.75572395 4.30276299 2.60813832  
 H 3.26806784 5.28246260 3.85251260  
 H 3.32818484 3.52139139 4.03964281  
 H 5.56714725 4.40934610 3.34432554  
 H 4.90703392 3.35036969 2.07386112  
 H 4.85494947 5.12096310 1.87588382  
 C 2.10471916 -5.25611877 -0.09161983  
 H 1.97414494 -3.80760527 -3.71662092  
 C 0.37704706 -5.71717644 -4.96874952  
 H 1.30174136 -6.12350368 -3.04879212  
 H -0.38897336 -5.63194609 -2.93255711  
 C -0.06035202 -7.15968275 -5.24008036  
 H -0.36603710 -5.01638174 -5.39233208  
 H 1.32786405 -5.51224756 -5.49283123  
 H -0.17866667 -7.33832264 -6.31953144  
 H 0.68352258 -7.87841892 -4.86014509  
 H -1.02394485 -7.38352680 -4.75393009  
 C 3.39463639 -5.75788927 0.57049757  
 H 1.43378866 -4.83951616 0.67834759  
 H 1.57550657 -6.09950256 -0.56953430  
 C 3.12707376 -6.84187794 1.61887681  
 H 4.07931805 -6.14940691 -0.20419598  
 H 3.91259170 -4.90443325 1.04426777  
 H 4.06677151 -7.18442869 2.07863045  
 H 2.47735381 -6.46239567 2.42444205  
 H 2.63222146 -7.71873140 1.16984093

**L2\*Tb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15089.681394, E0 = -15088.969479, G= 381.1737 at T=298.150 K

Cl -5.41335154 3.69257998 -0.43099645  
 Cl -4.24714279 -3.07050657 -3.76040697

N -1.60499394 1.29868269 0.07526462  
 N -0.25641274 4.02858400 1.96857285  
 N -1.19890928 -1.05727434 -1.08782935  
 N 1.08408141 -3.70465994 -1.72803903  
 O 0.01634821 1.78119636 2.05539989  
 O 0.52066606 -2.59254026 0.16861753  
 C -1.76082277 2.47561002 0.68480688  
 C -2.93881249 3.23345017 0.54884171  
 H -3.09206557 4.15247440 1.11142397  
 C -3.94416547 2.76611376 -0.27805752  
 C -3.79230762 1.54513383 -0.97851497  
 C -4.76712990 0.97189015 -1.84787762  
 H -5.69576979 1.51880515 -2.01815987  
 C -4.56215334 -0.24374048 -2.44252443  
 H -5.32353783 -0.67610592 -3.09339380  
 C -3.36220121 -0.98108661 -2.21451473  
 C -3.08338785 -2.26682091 -2.74056649  
 C -1.89789653 -2.91448474 -2.43689084  
 H -1.71518004 -3.92182088 -2.81041217  
 C -0.96727020 -2.26315045 -1.60586178  
 C -2.35319638 -0.43076593 -1.37183487  
 C -2.57385874 0.85252547 -0.73845434  
 C -0.60488379 2.77264667 1.61206245  
 C 0.28341603 -2.88344431 -1.02154076  
 C -0.69896525 5.26038933 1.30208147  
 C -1.60712647 6.14776993 2.16229558  
 H -1.18854976 4.99645615 0.35315454  
 C 0.87341189 4.16405869 2.91521025  
 H 0.79433399 3.33860683 3.63784409  
 H 0.72899324 5.11398840 3.45638990  
 C 2.27436662 -4.22922945 -1.01698077

H 2.70949697 -3.39753318 -0.43641591  
 H 2.99716735 -4.53075838 -1.79153645  
 C 1.04015362 -3.85890508 -3.18740988  
 H 0.31236044 -3.14249325 -3.59583139  
 C 0.72389936 -5.28295374 -3.65528059  
 Tb 0.54197568 -0.18736294 0.74093294  
 N -0.87306422 -1.18508756 3.03285599  
 O 0.39783359 -1.01109254 3.01735616  
 O -1.46721423 -0.95794022 1.88533676  
 O -1.49729967 -1.52413571 4.01946497  
 N 3.29161000 -0.28543755 1.55443525  
 O 2.57967663 0.80677694 1.47118223  
 O 2.65107417 -1.35769820 1.24594295  
 O 4.45898199 -0.27196860 1.89378905  
 N 1.62176812 0.88613260 -1.70213437  
 O 2.08709693 1.31065714 -2.74186945  
 O 1.71319675 -0.36907935 -1.36059916  
 O 0.99544758 1.63079047 -0.85467041  
 H 0.21163458 5.82202435 1.02783954  
 C 2.24441218 4.12147617 2.23162556  
 C -2.03847671 7.41597509 1.41610599  
 H -2.49915218 5.57874489 2.48311567  
 H -1.07833445 6.42784214 3.09044838  
 C -2.93177080 8.32543945 2.26539850  
 H -1.13896179 7.97255278 1.09613776  
 H -2.57096887 7.13234329 0.48965341  
 H -3.22831869 9.22639465 1.70600402  
 H -3.85182023 7.80257225 2.57467628  
 H -2.40946722 8.65285301 3.17936993  
 C 3.38472986 4.19833660 3.25385857  
 H 2.33147931 3.17738914 1.67010748

H	2.33499837	4.95194960	1.50705218
C	4.76098061	4.05760479	2.59553719
H	3.32602811	5.14958286	3.81618762
H	3.25361705	3.38578820	3.99163365
H	5.56770897	4.12464857	3.34266710
H	4.84598207	3.08251667	2.08902049
H	4.92768049	4.84868193	1.84488785
C	1.95986581	-5.40410519	-0.08609218
H	2.02577257	-3.54549074	-3.57675767
C	0.70765644	-5.39089727	-5.18472528
H	1.47367096	-5.98152971	-3.24311233
H	-0.25212836	-5.60236835	-3.24475503
C	0.40577304	-6.81082678	-5.67362976
H	-0.04274003	-4.68945313	-5.59342575
H	1.68513477	-5.06151485	-5.58134747
H	0.39978936	-6.85978270	-6.77370310
H	1.16229403	-7.52484989	-5.30871868
H	-0.57893211	-7.15405893	-5.31558514
C	3.21701884	-5.89080524	0.64460802
H	1.21139312	-5.07481527	0.65409487
H	1.51475036	-6.23478842	-0.66380769
C	2.92488337	-7.05538368	1.59607863
H	3.97957683	-6.19701004	-0.09587019
H	3.64921737	-5.04706240	1.21167636
H	3.84012604	-7.38829565	2.11061788
H	2.19508123	-6.75880861	2.36732960
H	2.50835776	-7.92037106	1.05276632
O	-4.06780195	0.17282265	2.03856850
H	-3.22348428	-0.33436617	2.06025958
H	-4.34694338	0.15180314	2.96954536

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15089.675885, E0 = -15088.963990, G= 382.3431 at T=298.150 K

Tb -0.51039428 -0.52922684 -0.08533583

Cl 3.87726283 1.93962169 4.81938887

Cl 2.70349669 5.51202202 -1.79569256

O -1.05808973 0.40355265 -2.13381767

O -0.67813766 -1.41463852 2.17055035

O -2.85774779 -0.98244691 0.06385112

O -3.77027893 -2.87163305 -0.61877114

O -1.60248291 -2.52440929 -0.83719385

O 1.12346733 -2.33922076 0.25577661

O 1.12832510 -1.31045675 -1.66857970

O 2.51385379 -2.99297833 -1.32509494

O -1.59335947 1.34286201 0.84913307

H -1.46164227 2.38114023 0.61122644

H -2.55602908 1.17834795 0.82756221

N 1.22499192 0.29163179 1.55099392

N 0.65723902 -2.60748005 3.56284642

N 0.83871454 1.52799892 -0.79200995

N -0.84139162 1.61771810 -4.00929832

N -2.79578400 -2.16462660 -0.47404128

N 1.63374174 -2.25445700 -0.93144393

C 1.34051549 -0.34415951 2.72294927

C 2.15072966 0.15583958 3.75713301

H 2.18921328 -0.32943031 4.73168325

C 2.87695694 1.31467736 3.53647065

C 2.79360890 2.00110245 2.29732203

C 3.47555566 3.21480751 1.98681593

H 4.15145969 3.63815069 2.73117399

C 3.26914930 3.85288405 0.79379946

H 3.77570367 4.79405403 0.57505083

C 2.36807132 3.32734346 -0.17856233

C 1.70544136 2.09520435 0.06749933  
 C 1.91938102 1.42370021 1.33341360  
 C 2.01351619 3.96954608 -1.38846135  
 C 1.09196401 3.40328121 -2.25065351  
 H 0.77629083 3.97974324 -3.11265898  
 C 0.52859974 2.14836240 -1.93825448  
 C -0.51265651 1.36635089 -2.72814989  
 C -0.31504843 2.68165946 -4.87414455  
 H -0.34962341 2.29030204 -5.90471649  
 H 0.75253814 2.83382463 -4.65529108  
 C -1.11837232 3.98718500 -4.76783466  
 H -2.13496065 3.81097698 -5.16256809  
 H -1.25982964 4.25523901 -3.70430064  
 C -0.46089685 5.13881493 -5.53618336  
 H -0.34908131 4.86588144 -6.60195208  
 H 0.56512386 5.30047655 -5.15277529  
 C -1.25839913 6.44120884 -5.40876770  
 H -2.27140021 6.32551098 -5.82810926  
 H -0.76348829 7.26716948 -5.94353008  
 H -1.36409366 6.72815323 -4.35022926  
 C -1.90196371 0.77078122 -4.59701061  
 H -2.39796805 1.37474990 -5.37400007  
 H -2.63693905 0.55367565 -3.80814147  
 C -1.35120726 -0.53231275 -5.18668509  
 H -0.81803501 -1.08120477 -4.39162445  
 H -0.61116683 -0.29941580 -5.97503471  
 C -2.46573520 -1.41187274 -5.76448250  
 H -3.19434524 -1.63805830 -4.96487617  
 H -3.01718044 -0.85044819 -6.54182911  
 C -1.93080604 -2.72164154 -6.35153723  
 H -1.21447682 -2.52924299 -7.16788054



H -2.74730444 -3.34003305 -6.75678205  
 H -1.41043854 -3.31242943 -5.57986784  
 C 0.38817286 -1.51451266 2.82012439  
 C 1.98337078 -2.96245217 4.08661079  
 H 2.72113085 -2.24790621 3.69440556  
 H 2.24963832 -3.94252777 3.65111804  
 C 2.05066156 -3.03735399 5.61510134  
 H 1.75654256 -2.06432176 6.05078650  
 H 1.31138909 -3.77212811 5.98105192  
 C 3.44976854 -3.42813969 6.10616541  
 H 4.18623447 -2.69027805 5.73834276  
 H 3.73385715 -4.39704370 5.65692997  
 C 3.53442955 -3.52361560 7.63257647  
 H 3.28377628 -2.56007123 8.10616302  
 H 4.54832315 -3.80457449 7.95741129  
 H 2.83405423 -4.28063726 8.02203178  
 C -0.37452620 -3.67056775 3.55789065  
 H 0.12475011 -4.59816790 3.87988448  
 H -0.70513487 -3.80121589 2.51524854  
 C -1.56907248 -3.36562634 4.46879721  
 H -2.00394511 -2.39725304 4.16943932  
 H -1.21247995 -3.26125550 5.50869799  
 C -2.65334892 -4.45415401 4.39709520  
 H -2.20617747 -5.43740606 4.63722420  
 H -3.38978219 -4.25115061 5.19397593  
 C -3.38011980 -4.52720642 3.04844356  
 H -3.81801915 -3.55108953 2.78093410  
 H -4.19756603 -5.26464748 3.08400559  
 H -2.71026707 -4.82256413 2.22501349  
 O -1.13919926 3.77500510 0.39068362  
 O -1.08360910 5.25181723 -1.23383236

O -2.11357641 3.33798313 -1.54591250

N -1.46343195 4.13933372 -0.82287627

**L2\*Tb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15089.681394, E0 = -15088.969479, G= 381.1737 at T=298.150 K

Cl -5.36586714 3.73997188 -0.50237966

Cl -4.12523890 -3.03251433 -3.77973294

N -1.57930803 1.35430419 0.08889898

N -0.25083527 4.05573225 2.04057860

N -1.13055027 -0.99542338 -1.08486140

N 1.18761623 -3.63775516 -1.79588604

O 0.05387235 1.81347227 2.03332591

O 0.83114254 -2.31102562 0.00488343

C -1.74536943 2.53497171 0.69885135

C -2.91912889 3.28960180 0.53191704

H -3.08819771 4.21150732 1.08460557

C -3.91197562 2.81795144 -0.31677532

C -3.74529934 1.59098518 -1.00917184

C -4.70349932 1.01403439 -1.89818847

H -5.62800694 1.55948794 -2.09384537

C -4.48050022 -0.20036353 -2.48732233

H -5.22592402 -0.63293034 -3.15646887

C -3.27905440 -0.93241644 -2.23865008

C -2.98345280 -2.21630192 -2.76574349

C -1.78186405 -2.84277177 -2.46349788

H -1.59355164 -3.84592867 -2.84241295

C -0.85756040 -2.18505168 -1.63327157

C -2.29358482 -0.37986204 -1.37791967

C -2.53318024 0.89826918 -0.74776047

C -0.59359556 2.82399082 1.64051342

C 0.45477179 -2.74165344 -1.12012041

C -0.76976717 5.32467604 1.49802959

C	-1.72744834	6.05940628	2.44319081
H	-1.23526466	5.13343716	0.52006054
C	0.88688260	4.17138004	2.98723888
H	0.82169902	3.33064318	3.69295907
H	0.73609847	5.10734224	3.54786944
C	2.39990425	-4.16695881	-1.11810374
H	2.92577171	-3.31652570	-0.65488684
H	3.04369092	-4.58054256	-1.90926695
C	1.00842607	-3.99690557	-3.21544814
H	0.31104904	-3.28321433	-3.67680097
C	0.56065071	-5.44314528	-3.44765472
Tb	0.23084009	-0.21444194	0.87929791
N	-1.11282253	-1.52102196	2.95241570
O	0.17305923	-1.28985548	2.95305657
O	-1.73355007	-1.08226705	1.88333976
O	-1.67988539	-2.08528590	3.85097742
N	2.62796330	0.71476907	-0.23891862
O	3.65918612	1.12279105	-0.71146429
O	2.54090595	0.23852555	0.97263086
O	1.49594355	0.71499151	-0.89949220
H	0.11097562	5.95852089	1.29744267
C	2.24918675	4.17352486	2.28457928
C	-2.22637391	7.37614155	1.83383274
H	-2.58584571	5.41045046	2.69835401
H	-1.21499348	6.26652145	3.39890027
C	-3.16154552	8.13971138	2.77635694
H	-1.35749364	8.00942421	1.57942164
H	-2.74581385	7.16790295	0.88012111
H	-3.50461888	9.07793140	2.31470108
H	-4.05320883	7.54241610	3.02785611
H	-2.65167737	8.39577866	3.71911621

C	3.40085268	4.32717371	3.28607845
H	2.36876488	3.22541356	1.73315787
H	2.28930402	4.99241543	1.54285145
C	4.77002048	4.31225348	2.59983301
H	3.27515554	5.26763058	3.85336447
H	3.34835148	3.50553894	4.02314901
H	5.58035278	4.41935873	3.33715606
H	4.92991447	3.36583662	2.05750799
H	4.86246061	5.13762474	1.87478042
C	2.09299088	-5.23300982	-0.06054753
H	1.98424292	-3.82762980	-3.70363450
C	0.39038330	-5.74803209	-4.94171810
H	1.30454886	-6.13329077	-3.01278615
H	-0.38636619	-5.63813782	-2.91048551
C	-0.02958202	-7.19826698	-5.19933319
H	-0.35856211	-5.05959463	-5.37502670
H	1.34087527	-5.53839636	-5.46461964
H	-0.14551650	-7.38859940	-6.27702856
H	0.72353733	-7.90377665	-4.81281662
H	-0.99017841	-7.43062973	-4.71116400
C	3.37796998	-5.73193407	0.61316025
H	1.42088437	-4.80358124	0.70131260
H	1.56199527	-6.08018208	-0.52968800
C	3.10108399	-6.80117321	1.67419183
H	4.06399584	-6.13645649	-0.15361942
H	3.89798594	-4.87482166	1.07800579
H	4.03704643	-7.14215803	2.14260435
H	2.44945645	-6.40852308	2.47186518
H	2.60424995	-7.68145561	1.23417187

**L2\*Dy(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15538.290842, E0 = -15537.578790, G= 381.2858 at T=298.150 K

Cl -5.43009901 3.68634009 -0.39969873  
Cl -4.26394129 -3.07405353 -3.73419547  
N -1.62231791 1.29580939 0.09796743  
N -0.25080734 4.02861977 1.96131504  
N -1.21576476 -1.06395495 -1.05687940  
N 1.07312000 -3.69868731 -1.69510663  
O 0.00860669 1.78106356 2.07501745  
O 0.47218844 -2.63308311 0.21818519  
C -1.77446580 2.47058558 0.70444167  
C -2.95296741 3.22942686 0.57308191  
H -3.10398507 4.14948225 1.13475573  
C -3.96075177 2.76015186 -0.25039402  
C -3.81052375 1.54006457 -0.95047414  
C -4.78738737 0.96500301 -1.81814563  
H -5.71660042 1.51090717 -1.98850298  
C -4.58092022 -0.24989723 -2.41065025  
H -5.34195042 -0.68382722 -3.06103396  
C -3.37917519 -0.98796934 -2.18317199  
C -3.10153508 -2.27299213 -2.71093965  
C -1.91592717 -2.92104554 -2.40656614  
H -1.73052859 -3.92710757 -2.78266740  
C -0.98694181 -2.27101636 -1.57357335  
C -2.37033272 -0.43730554 -1.34266520  
C -2.59180450 0.84767675 -0.71316493  
C -0.60721564 2.76937938 1.62514865  
C 0.25790560 -2.89900041 -0.98142898  
C -0.69537246 5.25341606 1.28354144  
C -1.59058809 6.15640879 2.14107418  
H -1.19669604 4.97972155 0.34355128  
C 0.88983548 4.17036009 2.89436150

H	0.81081676	3.35729027	3.63095403
H	0.75869668	5.13020515	3.42113781
C	2.26411343	-4.21959114	-0.98276645
H	2.67625904	-3.39401484	-0.37696397
H	3.00169158	-4.48778009	-1.75564492
C	1.04717779	-3.81824636	-3.15806246
H	0.31297037	-3.10291696	-3.55701208
C	0.75594449	-5.23498678	-3.66259575
Dy	0.51497823	-0.21724124	0.76746225
N	-0.92847306	-1.16806400	3.04745221
O	0.34395260	-1.01047421	3.04101443
O	-1.51241803	-0.94064939	1.89374089
O	-1.56486678	-1.49391961	4.03083849
N	3.25907707	-0.30678421	1.56937742
O	2.55703497	0.78829628	1.46091175
O	2.60873485	-1.38158143	1.28977954
O	4.42840004	-0.29579550	1.90447438
N	1.59900928	0.80384707	-1.68274283
O	2.06619239	1.21883774	-2.72612023
O	1.70115113	-0.44239658	-1.32044160
O	0.95596737	1.55557811	-0.85206211
H	0.21460363	5.80695820	0.99143243
C	2.25337911	4.10341835	2.19786644
C	-2.02832890	7.41304684	1.37897062
H	-2.47983766	5.59437704	2.48146367
H	-1.05002332	6.44992495	3.05816841
C	-2.91495800	8.33609295	2.22038341
H	-1.13133693	7.96417665	1.04284739
H	-2.56746531	7.11368608	0.46128118
H	-3.21542835	9.22800350	1.64872837
H	-3.83275414	7.81861210	2.54502821

H	-2.38554931	8.67801094	3.12489605
C	3.40445685	4.17356777	3.20859051
H	2.32285380	3.15254402	1.64544177
H	2.34806228	4.92562819	1.46445751
C	4.77145958	3.99794126	2.53935218
H	3.36873460	5.13290644	3.75897479
H	3.26533008	3.37307596	3.95799208
H	5.58647394	4.06164885	3.27774048
H	4.83328772	3.01371431	2.04745793
H	4.94512272	4.77443933	1.77518189
C	1.96249139	-5.42264986	-0.08422456
H	2.03183389	-3.48079991	-3.52921391
C	0.75921929	-5.30772209	-5.19418859
H	1.51012468	-5.93300343	-3.25757504
H	-0.22058953	-5.57655573	-3.27150893
C	0.48140380	-6.71960258	-5.71934938
H	0.00481499	-4.60648966	-5.59580660
H	1.73701942	-4.95697832	-5.57117367
H	0.48903394	-6.74314690	-6.82026052
H	1.24265122	-7.43235254	-5.36184549
H	-0.50297070	-7.08342505	-5.38123178
C	3.21827817	-5.88670206	0.66336954
H	1.19008100	-5.13009357	0.64684170
H	1.55245209	-6.25290394	-0.68809146
C	2.94891071	-7.08793020	1.57467294
H	4.01033163	-6.14224100	-0.06518820
H	3.60488009	-5.04424238	1.26426840
H	3.86403656	-7.39993000	2.10239697
H	2.18980956	-6.84197521	2.33541083
H	2.57992244	-7.95277023	0.99787158
O	-4.10275507	0.20703349	2.06985903

H -3.26296139 -0.30818120 2.08035207

H -4.37556696 0.17680091 3.00244689

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15538.284852, E0 = -15537.572656, G= 382.5816 at T=298.150 K

Dy -0.54037243 -0.52262110 -0.07815127

Cl 3.83082438 1.97670507 4.84258080

Cl 2.70911312 5.50287819 -1.80324221

O -1.07835674 0.41436946 -2.12814665

O -0.70219934 -1.40137935 2.19294071

O -2.89198136 -0.94437665 0.10439493

O -3.81492400 -2.84769702 -0.52336508

O -1.64952636 -2.50614047 -0.77722418

O 1.10273480 -2.30134296 0.26501864

O 1.04486763 -1.34285653 -1.69230258

O 2.45464587 -3.00093341 -1.33004773

O -1.61191130 1.35902798 0.84536314

H -1.47139049 2.39074087 0.61194956

H -2.57578826 1.20226848 0.83218968

N 1.20539808 0.30842677 1.56818640

N 0.65397555 -2.59782386 3.56233382

N 0.83005327 1.52671170 -0.78628516

N -0.83714408 1.61128724 -4.01256561

N -2.83890247 -2.13661385 -0.40677422

N 1.57881558 -2.25475097 -0.93992352

C 1.31469631 -0.32094660 2.73913860

C 2.11630750 0.18415819 3.77846074

H 2.15029287 -0.29806599 4.75477219

C 2.84089351 1.34394348 3.55587387

C 2.76697326 2.02187610 2.31358552

C 3.45179486 3.23434854 1.99993968

H 4.12279463 3.66333985 2.74539709



C	3.25218105	3.86183310	0.80174124
H	3.75965786	4.80166674	0.57885885
C	2.35677600	3.32948256	-0.17434733
C	1.69227171	2.09976339	0.07387216
C	1.89946067	1.43825591	1.34665024
C	2.01168871	3.96575594	-1.38941133
C	1.09275794	3.39579678	-2.25238824
H	0.78148931	3.96827149	-3.11864996
C	0.52471638	2.14442182	-1.93558586
C	-0.51992238	1.36425281	-2.72645378
C	-0.29894885	2.66705537	-4.87960720
H	-0.33060792	2.27138829	-5.90862417
H	0.76870066	2.81336141	-4.65645838
C	-1.09389412	3.97869754	-4.78295183
H	-2.10760856	3.80935550	-5.18795872
H	-1.24460196	4.24677753	-3.72059321
C	-0.42108208	5.12584066	-5.54462624
H	-0.30392739	4.85366678	-6.61000681
H	0.60358590	5.27820635	-5.15375948
C	-1.20814908	6.43492889	-5.42066097
H	-2.21953249	6.32839584	-5.84629250
H	-0.70296460	7.25726128	-5.95142078
H	-1.31775463	6.72152567	-4.36239386
C	-1.90065980	0.76933920	-4.60158443
H	-2.38794613	1.37240565	-5.38485718
H	-2.64146662	0.56183791	-3.81556988
C	-1.35707092	-0.54139042	-5.18090725
H	-0.83492160	-1.09131348	-4.37920284
H	-0.60887355	-0.31893268	-5.96458244
C	-2.47559214	-1.41233218	-5.76397419
H	-3.21003628	-1.63250864	-4.96807575

H -3.01868534 -0.84618133 -6.54385328  
 C -1.94968736 -2.72644258 -6.34952831  
 H -1.22717905 -2.54001164 -7.16182852  
 H -2.77003098 -3.33631706 -6.75993490  
 H -1.43926132 -3.32378626 -5.57619429  
 C 0.36705238 -1.50125670 2.83211350  
 C 1.98694384 -2.94145274 4.07624149  
 H 2.71374393 -2.21146917 3.69196630  
 H 2.26574063 -3.91127062 3.62602210  
 C 2.06016755 -3.03610730 5.60331678  
 H 1.75604331 -2.07238698 6.05270100  
 H 1.33067310 -3.78425956 5.96161795  
 C 3.46521759 -3.41684031 6.08516836  
 H 4.19219732 -2.66648388 5.72377157  
 H 3.75862455 -4.37711811 5.62363195  
 C 3.55585885 -3.52933145 7.61007547  
 H 3.29575944 -2.57434154 8.09575748  
 H 4.57386398 -3.80256486 7.92855358  
 H 2.86532259 -4.29877329 7.99267340  
 C -0.36369833 -3.67479753 3.54695773  
 H 0.14897294 -4.59965801 3.85552812  
 H -0.69509894 -3.79584312 2.50329828  
 C -1.55994058 -3.39754581 4.46431446  
 H -2.01105714 -2.43353128 4.17518759  
 H -1.20195282 -3.29744458 5.50417995  
 C -2.62668729 -4.50279522 4.38501692  
 H -2.16299653 -5.48052216 4.61619949  
 H -3.36478472 -4.31844521 5.18489313  
 C -3.35449553 -4.57644510 3.03698492  
 H -3.81007552 -3.60613561 2.77829242  
 H -4.15881681 -5.32842112 3.06751299

H -2.68131208 -4.85270452 2.20973873  
O -1.12600720 3.79592538 0.39648446  
O -1.03070974 5.28309917 -1.21665859  
O -2.07541299 3.38217235 -1.55711579  
N -1.42770147 4.17188740 -0.81736237

**L2\*Dy(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15538.290842, E0 = -15537.578790, G= 381.2858 at T=298.150 K

Cl -5.36758709 3.74894166 -0.51552254  
Cl -4.12725258 -3.02189350 -3.79348969  
N -1.58097196 1.36686802 0.07094847  
N -0.25369540 4.05466032 2.03829622  
N -1.13306415 -0.98574811 -1.09866834  
N 1.18273425 -3.63233972 -1.80062079  
O 0.04730368 1.81196272 2.02268863  
O 0.82830447 -2.29794502 -0.00550822  
C -1.74910688 2.54165626 0.68802410  
C -2.92378354 3.29660559 0.52317137  
H -3.09475398 4.21601105 1.07951355  
C -3.91351008 2.82790589 -0.33003950  
C -3.74527025 1.60343587 -1.02712786  
C -4.70193815 1.02813411 -1.91877103  
H -5.62614775 1.57361770 -2.11565089  
C -4.47799349 -0.18586186 -2.50843096  
H -5.22256899 -0.61764222 -3.17906594  
C -3.27801013 -0.91959596 -2.25722241  
C -2.98460793 -2.20598578 -2.78044248  
C -1.78553689 -2.83408165 -2.47440839  
H -1.59912694 -3.83879018 -2.85016322  
C -0.86094701 -2.17582369 -1.64374888  
C -2.29243374 -0.36874482 -1.39585197  
C -2.53266954 0.91144633 -0.76568407

C	-0.59683222	2.82479167	1.63353086
C	0.45199025	-2.73197031	-1.12749112
C	-0.77298725	5.32607698	1.50164378
C	-1.73285973	6.05503225	2.44898629
H	-1.23665702	5.14006996	0.52177322
C	0.88503373	4.16590023	2.98438096
H	0.82244217	3.31979418	3.68383241
H	0.73342383	5.09760332	3.55186629
C	2.39668202	-4.15703201	-1.12234938
H	2.92163754	-3.30367255	-0.66347355
H	3.03996539	-4.57329130	-1.91254413
C	1.00058496	-3.99981928	-3.21747494
H	0.30453005	-3.28750467	-3.68288779
C	0.54893076	-5.44650316	-3.43969440
Dy	0.22986785	-0.20782039	0.87054920
N	-1.05762541	-1.54890943	2.94405437
O	0.21497487	-1.27554381	2.95402479
O	-1.68492615	-1.13231444	1.86574817
O	-1.61826372	-2.12964225	3.83669305
N	2.65814900	0.67580223	-0.18973665
O	3.69973564	1.07658851	-0.64646524
O	2.54843330	0.17913343	1.00800347
O	1.53127992	0.70833284	-0.86234444
H	0.10763530	5.96146297	1.30570734
C	2.24621034	4.17513466	2.27960324
C	-2.22576833	7.37797976	1.84825444
H	-2.59414196	5.40609932	2.69441819
H	-1.22448575	6.25205708	3.40898061
C	-3.17777586	8.12805653	2.78464913
H	-1.35467088	8.01602554	1.61432612
H	-2.73035789	7.17985153	0.88444728

H	-3.51406097	9.07176113	2.32913923
H	-4.07264471	7.52585983	3.01171494
H	-2.68531752	8.37227440	3.73969769
C	3.39912915	4.31667566	3.28146505
H	2.36428785	3.23338032	1.71707916
H	2.28601217	5.00215960	1.54696369
C	4.76771069	4.31008720	2.59390950
H	3.27367902	5.25031281	3.86003637
H	3.34730864	3.48620749	4.00856590
H	5.57818604	4.40854549	3.33230019
H	4.92753124	3.37014437	2.04046249
H	4.85970736	5.14414358	1.87880599
C	2.09318924	-5.21848392	-0.05916716
H	1.97591925	-3.83623743	-3.70853019
C	0.37274060	-5.76010752	-4.93125439
H	1.29305267	-6.13540363	-3.00325370
H	-0.39642513	-5.63647175	-2.89777517
C	-0.04622607	-7.21238613	-5.17882729
H	-0.37877190	-5.07499933	-5.36545420
H	1.32082570	-5.55241299	-5.45929527
H	-0.16774566	-7.40882874	-6.25482082
H	0.71041036	-7.91438770	-4.79278708
H	-1.00352931	-7.44411755	-4.68392706
C	3.38040805	-5.71164179	0.61451900
H	1.42186308	-4.78632259	0.70180923
H	1.56281793	-6.06890249	-0.52313828
C	3.10798192	-6.77623653	1.68137062
H	4.06574392	-6.11849403	-0.15165704
H	3.89939904	-4.85117197	1.07422531
H	4.04589128	-7.11289263	2.14910007
H	2.45748472	-6.38091850	2.47862840

H 2.61192012 -7.65969658 1.24685764

**L2\*Ho(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15997.733757, E0 = -15997.021703, G= 381.2149 at T=298.150 K

Cl -5.43554211 3.68190002 -0.40767777

Cl -4.25478649 -3.07395840 -3.74906301

N -1.62530673 1.29563880 0.08996341

N -0.25371474 4.02834463 1.95297956

N -1.21572161 -1.06286108 -1.06132460

N 1.07845342 -3.69495344 -1.70259643

O 0.00430948 1.78089774 2.06546474

O 0.47930837 -2.62224698 0.20680608

C -1.77819955 2.47026849 0.69609040

C -2.95755529 3.22790670 0.56473905

H -3.10920358 4.14831018 1.12572956

C -3.96514153 2.75732660 -0.25833493

C -3.81363368 1.53746808 -0.95841503

C -4.78889084 0.96137685 -1.82716179

H -5.71890068 1.50579667 -1.99799967

C -4.57955551 -0.25246823 -2.42088985

H -5.33897543 -0.68688673 -3.07284427

C -3.37676477 -0.98873228 -2.19298458

C -3.09539652 -2.27184892 -2.72316241

C -1.90814948 -2.91687894 -2.41948891

H -1.71965098 -3.92131972 -2.79827476

C -0.98226398 -2.26679397 -1.58275616

C -2.37027431 -0.43819967 -1.34954751

C -2.59423470 0.84659046 -0.72025752

C -0.61044955 2.76936698 1.61640120

C 0.26375753 -2.89214325 -0.99118733

C -0.70234537 5.25495672 1.28142154

C	-1.59576023	6.15192938	2.14702535
H	-1.20595634	4.98491144	0.34160772
C	0.89172310	4.16841125	2.88028359
H	0.81584507	3.35544658	3.61731958
H	0.76507849	5.12858868	3.40759206
C	2.26780176	-4.21652985	-0.98789245
H	2.68122554	-3.39045620	-0.38380700
H	3.00519323	-4.48905373	-1.75945115
C	1.05082250	-3.82342124	-3.16469264
H	0.31850174	-3.10842204	-3.56760097
C	0.75535929	-5.24239349	-3.66068578
Ho	0.51543206	-0.21847446	0.77683812
N	-0.92657250	-1.16616237	3.04778624
O	0.34359455	-1.00101340	3.05013442
O	-1.50119555	-0.94600272	1.88772368
O	-1.57028627	-1.49182260	4.02663040
N	3.23709750	-0.34402102	1.61404026
O	2.53888249	0.75396812	1.53467488
O	2.58415198	-1.40677822	1.29417503
O	4.40334845	-0.34967107	1.95922089
N	1.61413193	0.86192250	-1.63197148
O	2.09174085	1.29845929	-2.66172695
O	1.69743407	-0.39533460	-1.30293500
O	0.98053759	1.59830928	-0.78204185
H	0.20585823	5.81144619	0.98940927
C	2.25100970	4.09970045	2.17570281
C	-2.02410531	7.42172527	1.40182734
H	-2.48901868	5.59046221	2.47771668
H	-1.05608344	6.42995024	3.06951022
C	-2.90294194	8.33939075	2.25734186
H	-1.12288713	7.97054720	1.07326651

H	-2.56657529	7.14055490	0.48042291
H	-3.19670987	9.24232674	1.69969463
H	-3.82466316	7.82437992	2.57472801
H	-2.37022138	8.66288280	3.16665554
C	3.40801382	4.17708302	3.17890954
H	2.31721640	3.14639235	1.62712467
H	2.33958077	4.91833496	1.43752682
C	4.77194881	4.00781488	2.50196481
H	3.37057662	5.13760567	3.72714520
H	3.27773190	3.37753105	3.93077421
H	5.59082031	4.07572031	3.23569345
H	4.83606148	3.02358222	2.01039457
H	4.93754005	4.78456068	1.73626053
C	1.96255767	-5.41595411	-0.08561295
H	2.03633308	-3.49171901	-3.53879166
C	0.75782037	-5.32431841	-5.19181347
H	1.50787711	-5.93993187	-3.25180984
H	-0.22182854	-5.57913351	-3.26706338
C	0.47662944	-6.73870373	-5.70838118
H	0.00483558	-4.62381935	-5.59736252
H	1.73629177	-4.97810745	-5.57125616
H	0.48393589	-6.76892805	-6.80912828
H	1.23633468	-7.45100737	-5.34673929
H	-0.50848025	-7.09822464	-5.36783314
C	3.21701765	-5.88164806	0.66318184
H	1.19125700	-5.11852789	0.64463800
H	1.54977572	-6.24678373	-0.68680155
C	2.94278550	-7.07671499	1.58117330
H	4.00719547	-6.14455986	-0.06479184
H	3.60783982	-5.03782129	1.25940132
H	3.85733175	-7.39170933	2.10807657



H 2.18717790 -6.82215977 2.34257555  
H 2.56683993 -7.94216347 1.00972855  
O -4.10357380 0.17909481 2.04371977  
H -3.25842476 -0.32708147 2.05971408  
H -4.37998295 0.14868346 2.97523093

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15997.730185, E0 = -15997.017725, G= 382.8520 at T=298.150 K

Ho -0.51321846 -0.52220935 -0.08571949  
Cl 3.84537220 1.96798503 4.83155107  
Cl 2.74077964 5.47812605 -1.82666993  
O -1.08802056 0.41882703 -2.11107898  
O -0.67418879 -1.42630935 2.15821505  
O -2.83727002 -0.94461870 0.08509265  
O -3.77448416 -2.82557511 -0.58760780  
O -1.60618174 -2.49752283 -0.82874650  
O 1.14034665 -2.27746224 0.22955221  
O 1.07096231 -1.29852021 -1.71791363  
O 2.49553204 -2.94788575 -1.37547505  
O -1.54969847 1.35762644 0.86531854  
H -1.40719235 2.38665199 0.62991381  
H -2.51297402 1.20304000 0.81944442  
N 1.21582985 0.30098253 1.56077135  
N 0.66573650 -2.60693407 3.55518413  
N 0.83800960 1.51772451 -0.79204369  
N -0.85654157 1.60777628 -4.00199986  
N -2.79123831 -2.12802935 -0.45367900  
N 1.61395419 -2.21289539 -0.97666037  
C 1.32588303 -0.32859248 2.73102903  
C 2.12737012 0.17742148 3.77010560  
H 2.15918756 -0.30123922 4.74813032  
C 2.85549092 1.33463776 3.54508710

C	2.78582168	2.00882530	2.30081868
C	3.47685504	3.21666884	1.98268998
H	4.15086174	3.64450359	2.72607827
C	3.27910280	3.84135938	0.78269678
H	3.79108858	4.77793407	0.55632967
C	2.37871146	3.31174064	-0.19040209
C	1.70773196	2.08691597	0.06274920
C	1.91441309	1.42716956	1.33620119
C	2.03324676	3.94735980	-1.40573323
C	1.10530519	3.38257146	-2.26249242
H	0.79407620	3.95583391	-3.12829709
C	0.52927482	2.13628244	-1.93975818
C	-0.52837574	1.36252475	-2.71850681
C	-0.32349694	2.66194320	-4.87411594
H	-0.36963269	2.26806426	-5.90323687
H	0.74749273	2.80244470	-4.66369152
C	-1.11104131	3.97708273	-4.76536894
H	-2.13038802	3.81299567	-5.15829277
H	-1.24749088	4.24409819	-3.70082402
C	-0.44291598	5.12314034	-5.53274632
H	-0.33986688	4.85314274	-6.60014677
H	0.58701706	5.27062845	-5.15405416
C	-1.22340274	6.43487835	-5.39567184
H	-2.24023271	6.33320904	-5.80937147
H	-0.72161597	7.25692272	-5.93008471
H	-1.31919205	6.71858311	-4.33528662
C	-1.92787659	0.76809353	-4.57991409
H	-2.41900587	1.37020731	-5.36152220
H	-2.66351390	0.56585342	-3.78767610
C	-1.39297664	-0.54642314	-5.15878057
H	-0.86634529	-1.09502912	-4.35908937

H -0.65007603 -0.32903188 -5.94887638  
 C -2.51847219 -1.41614091 -5.73006868  
 H -3.24724460 -1.63168073 -4.92772293  
 H -3.06609988 -0.85115105 -6.50762606  
 C -2.00057697 -2.73361301 -6.31524563  
 H -1.28405416 -2.55177784 -7.13386774  
 H -2.82566714 -3.34281564 -6.71705008  
 H -1.48551297 -3.32953334 -5.54389906  
 C 0.38451445 -1.51462007 2.81634355  
 C 1.98930800 -2.93925905 4.09995747  
 H 2.72176123 -2.21279907 3.71997333  
 H 2.27914000 -3.91442275 3.66883469  
 C 2.03262544 -3.01343465 5.62937450  
 H 1.71410108 -2.04576135 6.05988884  
 H 1.30008578 -3.76094532 5.98272705  
 C 3.42981219 -3.37980413 6.14411497  
 H 4.15965700 -2.62967515 5.78802824  
 H 3.73799872 -4.34401131 5.70075274  
 C 3.49015689 -3.47265267 7.67184782  
 H 3.21489072 -2.51321292 8.14006424  
 H 4.50301552 -3.73588634 8.01423359  
 H 2.79633474 -4.24129009 8.05007267  
 C -0.34579507 -3.68953729 3.52745652  
 H 0.16639550 -4.60992813 3.84980226  
 H -0.65828061 -3.81765151 2.47886205  
 C -1.55973995 -3.41469932 4.42214870  
 H -2.00793862 -2.45197201 4.12448406  
 H -1.22168088 -3.31378222 5.46855402  
 C -2.62200880 -4.52269936 4.32262802  
 H -2.15968156 -5.49982214 4.55898857  
 H -3.37375450 -4.34229565 5.11058617

C -3.32725000 -4.59446144 2.96252918  
 H -3.78178740 -3.62475753 2.69986606  
 H -4.12930250 -5.34930611 2.97729158  
 H -2.63944101 -4.86572409 2.14567566  
 O -1.06459880 3.79750276 0.40935916  
 O -0.99966121 5.28605795 -1.20403504  
 O -2.05713844 3.38846731 -1.52352977  
 N -1.39110887 4.17559671 -0.79682231

**L2\*Ho(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15640.772405, E0 = -15640.098904, G= 362.8072 at T=298.150 K

Cl -5.36756039 3.75597620 -0.52836746  
 Cl -4.12054253 -3.00795817 -3.82315016  
 N -1.58169329 1.37144184 0.05544505  
 N -0.25953370 4.05167198 2.03860879  
 N -1.14079237 -0.98346847 -1.10440600  
 N 1.17751324 -3.62998796 -1.79001677  
 O 0.04610882 1.81051040 2.00878549  
 O 0.80566263 -2.29390883 0.00173162  
 C -1.75141275 2.54392910 0.67765844  
 C -2.92644215 3.29841495 0.51413590  
 H -3.09837079 4.21538401 1.07421553  
 C -3.91465569 2.83350420 -0.34308246  
 C -3.74568915 1.61116767 -1.04382503  
 C -4.70010471 1.03869426 -1.93981326  
 H -5.62323713 1.58551717 -2.13808060  
 C -4.47522736 -0.17394899 -2.53216219  
 H -5.21781158 -0.60300165 -3.20676923  
 C -3.27752233 -0.91033834 -2.27744889  
 C -2.98285913 -2.19636846 -2.80130792  
 C -1.78663456 -2.82681775 -2.48914146  
 H -1.59854257 -3.83049250 -2.86685681

C -0.86689103 -2.17297649 -1.64941251  
 C -2.29559708 -0.36272946 -1.41035914  
 C -2.53427172 0.91791344 -0.78161180  
 C -0.60008132 2.82349110 1.62582946  
 C 0.44133106 -2.72974229 -1.12306821  
 C -0.78062010 5.32581615 1.51080120  
 C -1.74318087 6.04561996 2.46242380  
 H -1.24295962 5.14656973 0.52896899  
 C 0.87986112 4.15721416 2.98495603  
 H 0.81096494 3.31361008 3.68695855  
 H 0.73444462 5.09186792 3.54917049  
 C 2.38669109 -4.15353966 -1.10272300  
 H 2.91011977 -3.29904318 -0.64399624  
 H 3.03417516 -4.57262754 -1.88792658  
 C 1.00587201 -3.99702811 -3.20824528  
 H 0.31768450 -3.28094530 -3.67971349  
 C 0.54909730 -5.44140244 -3.43457007  
 Ho 0.23256919 -0.18644863 0.83216757  
 N -0.91900867 -1.52296495 2.96185040  
 O 0.34956989 -1.23234820 2.89946151  
 O -1.60921943 -1.12134326 1.91770160  
 O -1.42023563 -2.10546446 3.88763022  
 N 2.64086175 0.65320289 -0.28290820  
 O 3.68452120 1.01630139 -0.76542372  
 O 2.51100969 0.32815632 0.97246903  
 O 1.53392267 0.55419654 -0.97927696  
 H 0.09900480 5.96438932 1.32067502  
 C 2.24140859 4.15365362 2.28068376  
 C -2.23953032 7.37138462 1.87085295  
 H -2.60271144 5.39243841 2.70274115  
 H -1.23588896 6.23749065 3.42402697

C	-3.19477820	8.11135674	2.81196523
H	-1.37015319	8.01383495	1.64266932
H	-2.74251413	7.17898178	0.90503180
H	-3.53333402	9.05779266	2.36391997
H	-4.08813572	7.50477028	3.03322148
H	-2.70409346	8.34926128	3.76951098
C	3.39419746	4.30261517	3.28169966
H	2.35689139	3.20424151	1.73051596
H	2.28395987	4.97282791	1.53932619
C	4.76279306	4.28015375	2.59449959
H	3.27338433	5.24406147	3.84850860
H	3.33804488	3.48141837	4.01891136
H	5.57418442	4.38333225	3.33122540
H	4.91684866	3.33247185	2.05281234
H	4.85921144	5.10471725	1.86900318
C	2.07655668	-5.21149445	-0.03805242
H	1.98613954	-3.83789992	-3.69062018
C	0.38937616	-5.75540400	-4.92788744
H	1.28373551	-6.13408470	-2.98814440
H	-0.40393427	-5.62573195	-2.90418005
C	-0.04921606	-7.20119381	-5.17908669
H	-0.34558603	-5.05991745	-5.37381124
H	1.34778225	-5.56288195	-5.44280767
H	-0.15664051	-7.39815235	-6.25650024
H	0.68864483	-7.91514921	-4.77894974
H	-1.01844633	-7.41435385	-4.69934464
C	3.35957980	-5.70354748	0.64443612
H	1.40130687	-4.77663803	0.71786410
H	1.54818237	-6.06288958	-0.50258422
C	3.08023167	-6.76494932	1.71268511
H	4.04923344	-6.11295462	-0.11649331

H 3.87635541 -4.84209633 1.10480821  
H 4.01507282 -7.10039043 2.18736196  
H 2.42476940 -6.36715412 2.50460744  
H 2.58678293 -7.64958525 1.27759278

**L2\*Er(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16468.111104, E0 = -16467.398768, G= 381.8229 at T=298.150 K

Cl -5.39934015 3.71636868 -0.45171857  
Cl -4.23453188 -3.04958940 -3.77446699  
N -1.60164714 1.31804013 0.06289811  
N -0.24051625 4.03068924 1.97010815  
N -1.18592465 -1.03535461 -1.10198343  
N 1.07457113 -3.71440530 -1.68739986  
O 0.04939860 1.78524220 2.00747705  
O 0.48720855 -2.59065437 0.19714071  
C -1.75327647 2.49101853 0.67244577  
C -2.92952657 3.25251508 0.53504199  
H -3.08535981 4.16991758 1.09928536  
C -3.93230438 2.78768659 -0.29713365  
C -3.77976918 1.57022452 -1.00137568  
C -4.75246668 0.99846321 -1.87595749  
H -5.67940855 1.54644871 -2.05177736  
C -4.54565716 -0.21746442 -2.46627951  
H -5.30452394 -0.65039825 -3.11985540  
C -3.34704995 -0.95871627 -2.23186612  
C -3.07281685 -2.24793839 -2.75111556  
C -1.89289880 -2.90069818 -2.43538356  
H -1.71294737 -3.91151428 -2.80107284  
C -0.96197796 -2.24939942 -1.60547185  
C -2.33947825 -0.40784490 -1.39057386  
C -2.56392574 0.87510765 -0.75890785

C	-0.58394104	2.77924061	1.59449959
C	0.27313039	-2.88111830	-0.99626523
C	-0.70491999	5.27405071	1.34083748
C	-1.61806178	6.12460232	2.23241234
H	-1.19730330	5.03105593	0.38781789
C	0.90032554	4.15579653	2.90582752
H	0.82995719	3.32142806	3.61918783
H	0.75966775	5.09876013	3.45995164
C	2.25418305	-4.23663568	-0.95790583
H	2.67797804	-3.40237427	-0.37233013
H	2.98976684	-4.53710890	-1.72075438
C	1.05934954	-3.85808682	-3.14822388
H	0.34040567	-3.13807321	-3.56603885
C	0.75063801	-5.27849817	-3.63145351
Er	0.51368684	-0.17665929	0.67040616
N	-0.89001882	-1.17269075	2.94510245
O	0.38038370	-1.01514590	2.92336607
O	-1.48800635	-0.92780817	1.80353177
O	-1.51470375	-1.51392817	3.93199611
N	3.27090096	-0.18127690	1.37718439
O	2.56050467	0.89638847	1.18658972
O	2.61772037	-1.27727938	1.22265720
O	4.45035028	-0.13598567	1.67429030
N	1.55374348	0.68570828	-1.84643483
O	2.01231217	1.05252683	-2.91218710
O	1.72195697	-0.51815552	-1.39064288
O	0.85150307	1.45651007	-1.08231771
H	0.19645956	5.85494757	1.07667005
C	2.26375914	4.12302303	2.20684171
C	-2.06913018	7.40909481	1.52679002
H	-2.50071287	5.53523207	2.54226732



H	-1.08601069	6.38309336	3.16491365
C	-2.96691537	8.28260612	2.40844274
H	-1.17802393	7.98509312	1.21774590
H	-2.60457397	7.14704084	0.59565461
H	-3.27751064	9.19611740	1.87781894
H	-3.87880611	7.74023533	2.70809317
H	-2.44206667	8.58892632	3.32821226
C	3.41561007	4.18977690	3.21724653
H	2.34715414	3.18439388	1.63542998
H	2.34530711	4.96173000	1.49067926
C	4.78271008	4.03490782	2.54262805
H	3.37253451	5.14092159	3.78098345
H	3.28481960	3.37845850	3.95662069
H	5.59872484	4.09461164	3.28020716
H	4.85177326	3.05929947	2.03473759
H	4.94805908	4.82458305	1.79026389
C	1.92911065	-5.41139126	-0.03063468
H	2.05228472	-3.54206610	-3.51633930
C	0.77021527	-5.37840509	-5.16137791
H	1.48874271	-5.98127604	-3.20551229
H	-0.23563260	-5.59764910	-3.24581528
C	0.47603837	-6.79476547	-5.66511774
H	0.03179924	-4.67256021	-5.58405685
H	1.75772893	-5.04973173	-5.53285313
H	0.49610284	-6.83789444	-6.76528502
H	1.22162652	-7.51297951	-5.28616190
H	-0.51786566	-7.13708639	-5.33244085
C	3.17599797	-5.88625717	0.72497368
H	1.16485453	-5.08526230	0.69472283
H	1.49972439	-6.24609566	-0.61464912
C	2.88079429	-7.05776882	1.66652703

H 3.95961618 -6.17819929 0.00099270  
H 3.58439302 -5.03895283 1.30426478  
H 3.79010224 -7.38026190 2.19798875  
H 2.13163352 -6.77410650 2.42397356  
H 2.48712969 -7.92666578 1.11251664  
O -4.06015825 0.24139284 2.03881907  
H -3.22638535 -0.28391704 2.02858257  
H -4.32835484 0.18481886 2.97147369

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16468.106593, E0 = -16467.394192, G= 382.7415 at T=298.150 K

Er -0.47085753 -0.54065734 -0.09927899  
Cl 3.87687707 1.94427323 4.81430197  
Cl 2.74322605 5.46980095 -1.83235967  
O -1.04823470 0.37897882 -2.13088393  
O -0.64404541 -1.44339466 2.13327122  
O -2.77771854 -1.01165450 -0.05653120  
O -3.68668842 -2.73882771 -1.08708382  
O -1.50432491 -2.42279387 -1.12594664  
O 1.08580756 -2.36056709 0.20803376  
O 1.21836007 -1.23592973 -1.65376401  
O 2.54932928 -2.96435118 -1.32784116  
O -1.56868613 1.29732370 0.82667702  
H -1.41688812 2.33475542 0.62670857  
H -2.52758670 1.14166474 0.72144264  
N 1.25337112 0.27442297 1.54186761  
N 0.66953593 -2.61344886 3.56473947  
N 0.84870464 1.50538540 -0.79693890  
N -0.86088902 1.60395002 -4.00203371  
N -2.70580363 -2.09527111 -0.77670914  
N 1.66286290 -2.22519255 -0.94743800  
C 1.35884821 -0.35351664 2.71354485

C	2.15814567	0.15463613	3.75331664
H	2.18900967	-0.32171917	4.73236895
C	2.88630080	1.31209505	3.52808070
C	2.81383348	1.98906100	2.28557825
C	3.50020504	3.19989014	1.96879137
H	4.17515802	3.62807059	2.71110415
C	3.29692101	3.82654595	0.77070230
H	3.80615401	4.76472807	0.54467744
C	2.39337778	3.29799795	-0.20022373
C	1.72521281	2.07168293	0.05260282
C	1.94334078	1.40644920	1.32092631
C	2.04159403	3.93606281	-1.41230392
C	1.11330485	3.36969042	-2.26756144
H	0.80152953	3.94150686	-3.13403940
C	0.53962904	2.12217116	-1.94537461
C	-0.51158720	1.34175968	-2.72646976
C	-0.34859434	2.67208815	-4.86919689
H	-0.41036630	2.29067516	-5.90224361
H	0.72547603	2.81509471	-4.67658472
C	-1.13956213	3.98248696	-4.73294067
H	-2.16521525	3.81746840	-5.10862780
H	-1.25791311	4.23872852	-3.66372442
C	-0.49006271	5.13840151	-5.50148392
H	-0.40603489	4.87882853	-6.57311535
H	0.54641795	5.28585148	-5.14091349
C	-1.27208817	6.44614363	-5.33777571
H	-2.29595995	6.34492683	-5.73379707
H	-0.78278136	7.27486181	-5.87347364
H	-1.34954643	6.71967554	-4.27321863
C	-1.93439865	0.76271075	-4.57390785
H	-2.43973780	1.36961532	-5.34272814

H -2.65840173 0.54818469 -3.77412081  
 C -1.40242672 -0.54364932 -5.17342377  
 H -0.85888278 -1.09609771 -4.38807535  
 H -0.67681229 -0.31534874 -5.97649717  
 C -2.53446150 -1.41585493 -5.72804546  
 H -3.23409247 -1.65927827 -4.90804958  
 H -3.11253715 -0.84267795 -6.47700739  
 C -2.01740003 -2.71458864 -6.35457373  
 H -1.32678044 -2.50768399 -7.18941069  
 H -2.84648371 -3.32578540 -6.74492741  
 H -1.47396410 -3.31892490 -5.60974169  
 C 0.40776867 -1.53233421 2.80237865  
 C 1.98582423 -2.95387959 4.12225819  
 H 2.72989798 -2.24447370 3.73270464  
 H 2.26424336 -3.94052362 3.71009445  
 C 2.02199721 -3.00185037 5.65298891  
 H 1.71263325 -2.02352524 6.06572628  
 H 1.27981925 -3.73491621 6.01630974  
 C 3.41306591 -3.37483120 6.17949629  
 H 4.15242147 -2.63862276 5.81409025  
 H 3.71244717 -4.34947920 5.75327826  
 C 3.46657515 -3.44316149 7.70877600  
 H 3.20002103 -2.47327161 8.16019154  
 H 4.47527599 -3.71159887 8.05925465  
 H 2.76315546 -4.19801998 8.09686470  
 C -0.35893965 -3.67979503 3.56029582  
 H 0.13853416 -4.60153389 3.90133953  
 H -0.67593461 -3.82442594 2.51536059  
 C -1.56526005 -3.36410999 4.45194435  
 H -2.00682950 -2.40828109 4.12359285  
 H -1.21940768 -3.22941327 5.49194813

C -2.63762736 -4.46527529 4.40020990  
 H -2.18472552 -5.43538904 4.67944288  
 H -3.38772345 -4.24315214 5.17898226  
 C -3.34329081 -4.59060717 3.04427481  
 H -3.78037262 -3.62652063 2.73485875  
 H -4.15774441 -5.33037519 3.09433365  
 H -2.65854168 -4.91245413 2.24325728  
 O -1.06578147 3.74170566 0.44208857  
 O -0.99606836 5.25438643 -1.14875019  
 O -2.05939054 3.36503005 -1.49654007  
 N -1.39076209 4.13926744 -0.75940001

**L2\*Er(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -16111.151042, E0 = -16110.477200, G= 363.6982 at T=298.150 K

Cl -5.28872776 3.79429841 -0.59394646  
 Cl -4.07823849 -2.98460579 -3.87254524  
 N -1.53497565 1.36864948 0.02944658  
 N -0.22183762 4.02839231 2.05584049  
 N -1.09609163 -0.97771293 -1.14408302  
 N 1.20671892 -3.64689016 -1.81512046  
 O 0.09902575 1.79129851 1.97511506  
 O 0.87157285 -2.25779748 -0.05919808  
 C -1.69850624 2.54149222 0.65233672  
 C -2.86467290 3.30757737 0.47543001  
 H -3.03677154 4.22327948 1.03604913  
 C -3.84720922 2.85574579 -0.39466402  
 C -3.68216491 1.63426769 -1.09632170  
 C -4.63247538 1.07222176 -2.00324464  
 H -5.54794264 1.62860656 -2.21039963  
 C -4.41428518 -0.14262551 -2.59336281  
 H -5.15467787 -0.56469947 -3.27472019  
 C -3.22569871 -0.88984472 -2.32808924

C -2.93891335 -2.17880368 -2.84735990  
 C -1.74915540 -2.81834984 -2.52835011  
 H -1.57020783 -3.82480168 -2.90216136  
 C -0.82651240 -2.16878605 -1.68862259  
 C -2.24587560 -0.35027573 -1.45319998  
 C -2.48062539 0.92893910 -0.82153690  
 C -0.55267853 2.80841875 1.61082602  
 C 0.48417658 -2.72285008 -1.16590261  
 C -0.75272638 5.31265402 1.56261873  
 C -1.73983800 5.98528385 2.52314782  
 H -1.19895124 5.16100788 0.56933415  
 C 0.91200036 4.11996794 3.00959730  
 H 0.85479718 3.25196838 3.68209863  
 H 0.74919599 5.03230572 3.60491371  
 C 2.41826200 -4.16189528 -1.12479198  
 H 2.95349765 -3.29987979 -0.69502127  
 H 3.05395126 -4.60939884 -1.90394795  
 C 1.01208520 -4.06217146 -3.21706128  
 H 0.33687434 -3.34751153 -3.70879698  
 C 0.51793885 -5.50268555 -3.38398767  
 Er 0.25691706 -0.18238214 0.78042293  
 N -1.11825848 -1.47893345 2.80462646  
 O 0.16575631 -1.24348450 2.82545257  
 O -1.71867895 -1.04364657 1.72603250  
 O -1.69762754 -2.04522252 3.69498229  
 N 2.48798609 0.88796151 -0.47920540  
 O 3.46561742 1.35594153 -1.00759912  
 O 2.51763272 0.32870299 0.70056748  
 O 1.30428755 0.89769471 -1.03344643  
 H 0.12124097 5.96738243 1.40645027  
 C 2.27568316 4.16462708 2.31066799

C	-2.25932670	7.31592178	1.96341300
H	-2.58676171	5.30642748	2.73452735
H	-1.24716520	6.16041660	3.49555016
C	-3.23264003	8.01275539	2.91890383
H	-1.40206552	7.98104572	1.75515723
H	-2.75494647	7.13801908	0.99093926
H	-3.58998585	8.96235085	2.49266291
H	-4.11346912	7.38222885	3.12281775
H	-2.74953985	8.23782825	3.88339686
C	3.42216969	4.30251455	3.32045960
H	2.41025019	3.23742819	1.72782791
H	2.30541587	5.00859642	1.59715843
C	4.79352713	4.33617926	2.63921738
H	3.27837515	5.22027016	3.91979814
H	3.38202667	3.45504475	4.02846146
H	5.59921169	4.43179369	3.38327861
H	4.97241688	3.41280746	2.06424761
H	4.87351894	5.18819904	1.94421029
C	2.10865259	-5.18682146	-0.02795298
H	1.99106431	-3.94551277	-3.71371150
C	0.32046837	-5.86467266	-4.86185741
H	1.24525535	-6.19646311	-2.92751288
H	-0.42804906	-5.64554739	-2.82885242
C	-0.15886931	-7.30680799	-5.05246353
H	-0.40621239	-5.16695499	-5.31786823
H	1.27248919	-5.71468544	-5.40208912
H	-0.29378644	-7.53866386	-6.11977911
H	0.56929725	-8.02485657	-4.64205217
H	-1.12278652	-7.47812939	-4.54598475
C	3.39396524	-5.67338133	0.65417910
H	1.44598889	-4.72429371	0.72266728

H 1.56675279 -6.04515505 -0.46304289  
 C 3.11543703 -6.70208406 1.75416708  
 H 4.07088375 -6.11082554 -0.10255290  
 H 3.92472148 -4.80512524 1.08491957  
 H 4.05190086 -7.03414631 2.22801161  
 H 2.47251582 -6.27601814 2.54167104  
 H 2.60840487 -7.59311247 1.34880710

**L2\*Tm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16949.610280, E0 = -16948.898417, G= 380.8708 at T=298.150 K

Cl -5.41574669 3.69701004 -0.44276237  
 Cl -4.25915718 -3.07688260 -3.75532436  
 N -1.60530388 1.30902839 0.04729159  
 N -0.25469095 4.02373028 1.95901179  
 N -1.20741487 -1.05771458 -1.08866608  
 N 1.06997359 -3.71164131 -1.70490003  
 O 0.02332109 1.77568734 2.01851439  
 O 0.48168379 -2.60708714 0.19159801  
 C -1.75973165 2.47995114 0.66010982  
 C -2.93958569 3.23744345 0.53120518  
 H -3.09291363 4.15453291 1.09686887  
 C -3.94666791 2.77030563 -0.29383817  
 C -3.79769778 1.54964995 -0.99323702  
 C -4.77584648 0.97257203 -1.85830212  
 H -5.70499277 1.51845884 -2.02923155  
 C -4.57068062 -0.24432114 -2.44738984  
 H -5.33260727 -0.67975014 -3.09578705  
 C -3.36978316 -0.98316628 -2.21752191  
 C -3.09467340 -2.27177906 -2.73757505  
 C -1.91032088 -2.92004895 -2.42934275  
 H -1.72716463 -3.92864490 -2.79962015



C -0.98031771 -2.26778817 -1.59904552  
 C -2.35947585 -0.42999801 -1.38055325  
 C -2.57798243 0.85852438 -0.75780886  
 C -0.59702295 2.76885295 1.58944297  
 C 0.26325753 -2.89312553 -1.00134110  
 C -0.70165420 5.26062632 1.30559289  
 C -1.61016476 6.13746166 2.17632794  
 H -1.19262302 5.00584364 0.35485756  
 C 0.87602186 4.15241766 2.90539336  
 H 0.79752487 3.32133770 3.62166476  
 H 0.73250234 5.09836912 3.45375133  
 C 2.25862050 -4.23044014 -0.98743105  
 H 2.68323445 -3.39716053 -0.40122840  
 H 2.98928571 -4.52319384 -1.75796902  
 C 1.04286313 -3.85000253 -3.16603971  
 H 0.31425792 -3.13449049 -3.57469749  
 C 0.74097580 -5.27108526 -3.65194130  
 Tm 0.52010149 -0.19398677 0.69348127  
 N -0.83710122 -1.20131302 2.97504449  
 O 0.43871003 -1.10855424 2.90388560  
 O -1.46684110 -0.86939400 1.87488103  
 O -1.43548739 -1.55944479 3.97191334  
 N 3.24760270 -0.25834420 1.51365769  
 O 2.49793530 0.80702972 1.49554682  
 O 2.65002966 -1.32862186 1.13613594  
 O 4.41443300 -0.22302122 1.86113429  
 N 1.58871698 0.78187090 -1.76053298  
 O 2.03353453 1.20064723 -2.81294107  
 O 1.69330728 -0.45869017 -1.40019763  
 O 0.96727061 1.53686440 -0.91388893  
 H 0.20668560 5.82765865 1.03464329

C	2.24664736	4.11318684	2.22075129
C	-2.04284477	7.41411924	1.44540536
H	-2.50147581	5.56391859	2.49110007
H	-1.08083189	6.40684223	3.10729575
C	-2.93642998	8.31293201	2.30565572
H	-1.14376462	7.97505665	1.13175344
H	-2.57539535	7.14113903	0.51576346
H	-3.23342514	9.22044182	1.75719762
H	-3.85623026	7.78601503	2.60871482
H	-2.41409826	8.62946701	3.22341657
C	3.38743377	4.18407679	3.24302030
H	2.33196378	3.17053008	1.65673065
H	2.33731532	4.94707394	1.50009155
C	4.76280689	4.03132105	2.58535671
H	3.33569336	5.13695669	3.80311990
H	3.25017214	3.37415457	3.98244834
H	5.56998110	4.09806681	3.33204532
H	4.84202719	3.05258775	2.08510041
H	4.93428993	4.81702375	1.83016527
C	1.94811738	-5.41178179	-0.06344867
H	2.02997446	-3.52529645	-3.54213595
C	0.74572492	-5.36476946	-5.18237734
H	1.48911464	-5.96939087	-3.23631763
H	-0.23865058	-5.59980297	-3.25756311
C	0.45799300	-6.78151560	-5.68877506
H	-0.00281691	-4.66341209	-5.59460831
H	1.72665393	-5.02655315	-5.56267071
H	0.46716076	-6.82016802	-6.78925323
H	1.21322989	-7.49507523	-5.32029152
H	-0.52963006	-7.13325214	-5.34734869
C	3.20281816	-5.87756777	0.68486989

H 1.18439710 -5.09528112 0.66669583  
 H 1.52376115 -6.24823713 -0.64860761  
 C 2.92412925 -7.05749893 1.62090671  
 H 3.98672700 -6.15725279 -0.04364133  
 H 3.60416126 -5.02893686 1.26708770  
 H 3.83854508 -7.37111998 2.14891863  
 H 2.17299676 -6.78719759 2.38125706  
 H 2.54048419 -7.92837667 1.06309152  
 O -4.02888632 0.31540459 2.12388992  
 H -3.19513822 -0.20989102 2.12042642  
 H -4.28290176 0.29587948 3.06192350

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16949.607591, E0 = -16948.895368, G= 382.2292 at T=298.150 K

Tm -0.50220597 -0.50941277 -0.07213591  
 Cl 3.86328220 1.95699048 4.83908510  
 Cl 2.71573949 5.50768423 -1.79941535  
 O -1.07198811 0.41539568 -2.09461856  
 O -0.66319036 -1.41360545 2.15592527  
 O -2.82420135 -0.90998060 0.10630509  
 O -3.79249287 -2.73776245 -0.66029876  
 O -1.61943173 -2.43231058 -0.88024837  
 O 1.08246243 -2.32403564 0.23192306  
 O 1.13278604 -1.25016451 -1.66408181  
 O 2.50381947 -2.94717550 -1.33450449  
 O -1.55724096 1.35305178 0.89227009  
 H -1.44347537 2.36522007 0.65394551  
 H -2.51757216 1.17600965 0.86160541  
 N 1.23628950 0.30045930 1.56044436  
 N 0.66962534 -2.61047935 3.54658651  
 N 0.83326787 1.53802848 -0.77027202  
 N -0.85417140 1.61043751 -3.98325610

N	-2.79683852	-2.06394434	-0.49017102
N	1.61733675	-2.21165848	-0.94333047
C	1.34716046	-0.33469209	2.72716331
C	2.14873409	0.16742007	3.76857305
H	2.18569136	-0.31849197	4.74293375
C	2.87139964	1.32985580	3.55087304
C	2.79301214	2.01521993	2.31315899
C	3.47440171	3.23083901	2.00104642
H	4.14808941	3.65777731	2.74537134
C	3.27107239	3.86239982	0.80543357
H	3.77879357	4.80248308	0.58391613
C	2.37120199	3.33366036	-0.16943473
C	1.70597625	2.10504746	0.08058980
C	1.92382801	1.43465817	1.34690511
C	2.02152491	3.96921587	-1.38335264
C	1.10017049	3.39809084	-2.24424887
H	0.79253060	3.96739554	-3.11418748
C	0.52956837	2.14921904	-1.92156148
C	-0.52105951	1.36343312	-2.70068479
C	-0.31808642	2.65826774	-4.86040974
H	-0.35628834	2.25532365	-5.88645887
H	0.75114530	2.80333304	-4.64436722
C	-1.10788763	3.97338676	-4.77356863
H	-2.12950706	3.79921484	-5.15586662
H	-1.23712850	4.26645803	-3.71533823
C	-0.44560775	5.10251522	-5.57073975
H	-0.34294203	4.80446434	-6.63063097
H	0.58417588	5.26326275	-5.19728899
C	-1.23091686	6.41451597	-5.46898413
H	-2.24711299	6.29823780	-5.88029528
H	-0.73164159	7.22370625	-6.02487230

H -1.32879627 6.72710562 -4.41695213  
 C -1.92028427 0.76349443 -4.56029224  
 H -2.41561747 1.36185431 -5.34227943  
 H -2.65424514 0.55775237 -3.76744962  
 C -1.37823367 -0.54916900 -5.13682699  
 H -0.84706557 -1.09199429 -4.33627224  
 H -0.63847482 -0.32959828 -5.92929554  
 C -2.49974680 -1.42782557 -5.70232964  
 H -3.22467613 -1.64517367 -4.89707232  
 H -3.05295444 -0.86917734 -6.48053885  
 C -1.97496891 -2.74413443 -6.28400612  
 H -1.26145387 -2.56087995 -7.10494566  
 H -2.79727173 -3.35978913 -6.68166828  
 H -1.45466900 -3.33397794 -5.51156759  
 C 0.39660871 -1.51482856 2.80932307  
 C 1.99254477 -2.95521474 4.08435440  
 H 2.72835445 -2.23159623 3.70534897  
 H 2.27420902 -3.93000627 3.64691186  
 C 2.04167533 -3.03757191 5.61318779  
 H 1.73329854 -2.06939721 6.04995108  
 H 1.30422318 -3.78061032 5.96577883  
 C 3.43780470 -3.41865063 6.12003946  
 H 4.17261124 -2.67300367 5.76471472  
 H 3.73567271 -4.38306713 5.67015123  
 C 3.50428081 -3.52027726 7.64696598  
 H 3.23959231 -2.56102347 8.12163544  
 H 4.51635790 -3.79422140 7.98323727  
 H 2.80548525 -4.28485632 8.02426338  
 C -0.35115501 -3.68394732 3.51824903  
 H 0.15381926 -4.61043072 3.83459949  
 H -0.66846865 -3.80406475 2.47013307

C -1.55927050 -3.40131259 4.41840649  
 H -1.99983072 -2.43384719 4.12470293  
 H -1.21653664 -3.30610704 5.46385336  
 C -2.63212895 -4.49910021 4.32026052  
 H -2.17898941 -5.48069334 4.55594683  
 H -3.38109231 -4.31157827 5.10923338  
 C -3.33973718 -4.56418896 2.96097612  
 H -3.78173518 -3.58905292 2.69690681  
 H -4.15129757 -5.30874777 2.97788763  
 H -2.65589619 -4.84567976 2.14426684  
 O -1.12562323 3.83177423 0.40524787  
 O -1.07791686 5.28467321 -1.23648512  
 O -2.14458776 3.38696980 -1.49986529  
 N -1.46591127 4.18220663 -0.79811990

**L2\*Tm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -16592.653060, E0 = -16591.979377, G= 363.6854 at T=298.150 K

Cl -5.31276226 3.77963805 -0.56627053  
 Cl -4.07694292 -2.97838736 -3.89344788  
 N -1.54969597 1.36232519 0.02824079  
 N -0.22502244 4.00827074 2.05605578  
 N -1.10637963 -0.97273088 -1.15263963  
 N 1.20887625 -3.63207984 -1.81924009  
 O 0.08862333 1.77012801 1.96904933  
 O 0.87187225 -2.23034978 -0.07487316  
 C -1.71359313 2.53010774 0.65797490  
 C -2.88258362 3.29477143 0.49200273  
 H -3.05447412 4.20778227 1.05819798  
 C -3.86711621 2.84477258 -0.37752911  
 C -3.70089364 1.62818813 -1.08812916  
 C -4.65019751 1.06707668 -1.99716997  
 H -5.56857586 1.62035489 -2.19989920

C -4.42755270 -0.14329495 -2.59569740  
 H -5.16738653 -0.56347311 -3.27889204  
 C -3.23574424 -0.88813388 -2.33672786  
 C -2.94199276 -2.17292500 -2.86266899  
 C -1.74943161 -2.80914927 -2.54595065  
 H -1.56690741 -3.81291747 -2.92515707  
 C -0.83035195 -2.15917039 -1.70181251  
 C -2.25801086 -0.34967476 -1.45946896  
 C -2.49658513 0.92539430 -0.82098788  
 C -0.56230456 2.79074478 1.61072540  
 C 0.48348427 -2.70478201 -1.17816234  
 C -0.75009960 5.29429626 1.56190526  
 C -1.72432780 5.98025417 2.52658391  
 H -1.20233929 5.14126968 0.57110524  
 C 0.91079038 4.09483337 3.00780129  
 H 0.85127354 3.22673368 3.68002391  
 H 0.75212961 5.00699663 3.60452795  
 C 2.42243314 -4.13741589 -1.12549138  
 H 2.95565677 -3.26995993 -0.70407820  
 H 3.05873823 -4.59009790 -1.90112925  
 C 1.01609600 -4.05803204 -3.21826720  
 H 0.34103352 -3.34745431 -3.71596336  
 C 0.52446306 -5.50028038 -3.37578583  
 Tm 0.24653295 -0.18738450 0.78076261  
 N -1.16885567 -1.49274886 2.77440786  
 O 0.11583429 -1.26339126 2.80774760  
 O -1.75586498 -1.04862356 1.69773579  
 O -1.75582349 -2.06333637 3.65802097  
 N 2.44767737 0.90746838 -0.51381469  
 O 3.41958714 1.38160646 -1.04906702  
 O 2.49186563 0.35100216 0.66674620

O	1.26344597	0.90669614	-1.05592859
H	0.12717496	5.94325686	1.39831495
C	2.27410150	4.13548422	2.30818534
C	-2.22339034	7.32031345	1.97054684
H	-2.58194208	5.31565619	2.74071193
H	-1.22551000	6.14650488	3.49739957
C	-3.18999004	8.02716827	2.92541909
H	-1.35582662	7.97380638	1.76826680
H	-2.71769476	7.15423441	0.99541545
H	-3.53033900	8.98459721	2.50279522
H	-4.08168602	7.40956736	3.12148833
H	-2.70817900	8.23923683	3.89350057
C	3.42102265	4.26942110	3.31806374
H	2.40588284	3.20826411	1.72465920
H	2.30635381	4.97977400	1.59521210
C	4.79250479	4.29999590	2.63697839
H	3.27965474	5.18702412	3.91822958
H	3.37851310	3.42155957	4.02549362
H	5.59858894	4.39166784	3.38106203
H	4.96821833	3.37712598	2.06021070
H	4.87493849	5.15300035	1.94345462
C	2.11704588	-5.15356731	-0.01933708
H	1.99571598	-3.94379783	-3.71424556
C	0.33674794	-5.87513494	-4.85173082
H	1.24998605	-6.18910265	-2.90900612
H	-0.42469645	-5.63947010	-2.82522392
C	-0.13795336	-7.31994772	-5.03339100
H	-0.38858902	-5.18292379	-5.31813288
H	1.29174948	-5.72760868	-5.38740253
H	-0.26496008	-7.56110907	-6.09961605
H	0.58916926	-8.03268528	-4.61198378



H -1.10487735 -7.48940945 -4.53208447  
 C 3.40441585 -5.63204098 0.66450161  
 H 1.45459497 -4.68630743 0.72856343  
 H 1.57611382 -6.01663208 -0.44622880  
 C 3.12986660 -6.65207386 1.77357197  
 H 4.08062744 -6.07471609 -0.08981899  
 H 3.93483138 -4.75957966 1.08704519  
 H 4.06788874 -6.97868681 2.24813747  
 H 2.48792267 -6.22055912 2.55892038  
 H 2.62340498 -7.54722261 1.37668872

**L2\*Yb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -17442.380461, E0 = -17441.668677, G= 381.0711 at T=298.150 K

Cl -5.38248968 3.71172810 -0.46210477  
 Cl -4.24013758 -3.06666422 -3.76432014  
 N -1.57526898 1.32169008 0.02901117  
 N -0.23981678 4.02341175 1.97682178  
 N -1.17322421 -1.04030478 -1.12230897  
 N 1.07261395 -3.73578811 -1.70313466  
 O 0.06615537 1.77792919 1.98590243  
 O 0.51487756 -2.58255696 0.17385004  
 C -1.73072374 2.48959041 0.64796954  
 C -2.91031194 3.24729633 0.51793462  
 H -3.06784630 4.16037083 1.08854187  
 C -3.91377568 2.78461075 -0.31397060  
 C -3.76235056 1.56798148 -1.01982772  
 C -4.73983717 0.99421859 -1.88794529  
 H -5.66743803 1.54227364 -2.06004357  
 C -4.53752041 -0.22387581 -2.47538424  
 H -5.30053377 -0.65840322 -3.12302804  
 C -3.33908916 -0.96590012 -2.24302149

C -3.07081008 -2.26011729 -2.75307989  
 C -1.89158952 -2.91402435 -2.43718600  
 H -1.71696424 -3.92848730 -2.79527831  
 C -0.95467836 -2.25870275 -1.61690629  
 C -2.32558990 -0.41159683 -1.41122913  
 C -2.54350281 0.87532187 -0.78490025  
 C -0.56819510 2.77285004 1.58016145  
 C 0.28466251 -2.88754535 -1.01178348  
 C -0.70022178 5.27017498 1.35172200  
 C -1.62506974 6.11297607 2.23884511  
 H -1.18168795 5.03297329 0.39173195  
 C 0.88472831 4.14599848 2.93129086  
 H 0.81607538 3.29610372 3.62619901  
 H 0.72254413 5.07504082 3.50286436  
 C 2.25232291 -4.26339865 -0.97894776  
 H 2.69156981 -3.42859435 -0.40591303  
 H 2.97795129 -4.58077383 -1.74449444  
 C 1.04837537 -3.88690972 -3.16305518  
 H 0.33148432 -3.16480875 -3.58065915  
 C 0.72796214 -5.30796146 -3.63688302  
 Yb 0.52135533 -0.16401288 0.62829608  
 N -0.85013324 -1.15948331 2.91296983  
 O 0.42300791 -1.02393532 2.85733581  
 O -1.47494614 -0.89821321 1.79446363  
 O -1.44870949 -1.49722266 3.91854525  
 N 3.28505063 -0.10834240 1.33798599  
 O 2.56542134 0.95188379 1.13576579  
 O 2.65616941 -1.21533334 1.18487990  
 O 4.46338463 -0.04445247 1.64651656  
 N 1.57378626 0.68107170 -1.89160681  
 O 2.02175927 1.05020571 -2.96304512

O 1.73615110 -0.52195048 -1.44384420  
 O 0.88969195 1.45902562 -1.11899137  
 H 0.20190620 5.85587358 1.10081232  
 C 2.25917125 4.14821196 2.25341034  
 C -2.07464314 7.39909172 1.53520513  
 H -2.50822139 5.51889610 2.53789735  
 H -1.10288000 6.36945105 3.17740440  
 C -2.98358893 8.26517296 2.41282058  
 H -1.18303585 7.97985888 1.23677397  
 H -2.60078907 7.13930893 0.59817028  
 H -3.29293180 9.17998409 1.88374436  
 H -3.89596224 7.71787357 2.70175958  
 H -2.46808982 8.56906509 3.33864665  
 C 3.39413738 4.22118521 3.28227472  
 H 2.36689448 3.22069073 1.66817200  
 H 2.33680367 4.99932480 1.55163491  
 C 4.77498007 4.11152172 2.62706685  
 H 3.32024813 5.16040373 3.86240768  
 H 3.27088928 3.39390922 4.00506115  
 H 5.57759142 4.17265987 3.37905860  
 H 4.87500429 3.14968491 2.09852624  
 H 4.93478012 4.92132187 1.89529335  
 C 1.92092347 -5.42467022 -0.03695615  
 H 2.04094410 -3.57924342 -3.53936076  
 C 0.73857582 -5.41709471 -5.16627407  
 H 1.46358955 -6.01328230 -3.21079373  
 H -0.25824311 -5.61853647 -3.24425673  
 C 0.43273404 -6.83472490 -5.65948248  
 H 0.00215796 -4.70932055 -5.58913422  
 H 1.72599900 -5.09682798 -5.54521751  
 H 0.44591889 -6.88503408 -6.75941849

H 1.17607284 -7.55512762 -5.28031254  
 H -0.56123978 -7.16863775 -5.31864595  
 C 3.16661668 -5.90768290 0.71530235  
 H 1.16511083 -5.08251381 0.68976408  
 H 1.47797132 -6.25967789 -0.61012185  
 C 2.86260509 -7.06643772 1.66991460  
 H 3.94167590 -6.21661758 -0.01081526  
 H 3.58968139 -5.06043673 1.28404248  
 H 3.77083755 -7.39502382 2.19939685  
 H 2.12110949 -6.76623487 2.42849517  
 H 2.45515752 -7.93549490 1.12630796  
 O -4.02128172 0.30945313 2.08382964  
 H -3.19688272 -0.22982129 2.05466461  
 H -4.25693607 0.27412954 3.02621913

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -17442.378963, E0 = -17441.666663, G= 382.0452 at T=298.150 K

Yb -0.49752152 -0.51364905 -0.07193659  
 Cl 3.64965248 2.14770293 4.92722273  
 Cl 2.50160646 5.63102388 -1.74830723  
 O -1.13369441 0.44576195 -2.07125449  
 O -0.65706825 -1.43973649 2.15016508  
 O -2.81349969 -0.96931642 0.00158776  
 O -3.65493250 -2.98121715 -0.33212000  
 O -1.49190271 -2.61057091 -0.55054557  
 O 1.33304715 -2.08993483 0.21029221  
 O 0.93284035 -1.32457304 -1.79110503  
 O 2.52008080 -2.82808948 -1.49480331  
 O -1.64623809 1.30762839 0.93288517  
 H -1.58690476 2.29955196 0.67153382  
 H -2.59043026 1.06841516 0.85059792  
 N 1.15226388 0.38412246 1.60155451

N	0.72180861	-2.57111692	3.55114269
N	0.77411914	1.58079827	-0.75206995
N	-0.86420846	1.58920169	-3.98789334
N	-2.70116448	-2.22844815	-0.29756305
N	1.63929451	-2.11832476	-1.04626346
C	1.27648020	-0.25073013	2.76672649
C	2.03863955	0.28297514	3.82226229
H	2.08086538	-0.20451719	4.79567719
C	2.71262145	1.47670376	3.61960816
C	2.63140011	2.15586591	2.37853312
C	3.26962900	3.39736772	2.07624292
H	3.90982866	3.85303187	2.83309197
C	3.06592965	4.01802492	0.87511992
H	3.53863692	4.97807932	0.66209441
C	2.21178007	3.44877028	-0.11834628
C	1.59624374	2.19161677	0.12004913
C	1.80563176	1.53910077	1.39720619
C	1.86343694	4.06603193	-1.34165609
C	0.98141271	3.45662045	-2.21804595
H	0.66503978	4.01128197	-3.09465480
C	0.46025351	2.18477488	-1.90498245
C	-0.56659603	1.37246490	-2.69025803
C	-0.30510926	2.61709237	-4.87264490
H	-0.28612205	2.18241143	-5.88624334
H	0.74896091	2.79241610	-4.60976839
C	-1.12325656	3.91795206	-4.86891842
H	-2.12728071	3.70688391	-5.27799129
H	-1.29495192	4.25392580	-3.82961082
C	-0.45524740	5.02569818	-5.69113636
H	-0.30234078	4.67869377	-6.72972393
H	0.55412382	5.22928715	-5.28494644

C -1.27405167 6.32094812 -5.68884706  
 H -2.26992106 6.15837717 -6.13269424  
 H -0.77146292 7.11215734 -6.26707745  
 H -1.42159617 6.68740320 -4.66024971  
 C -1.89694059 0.71229446 -4.58014011  
 H -2.37878942 1.28469837 -5.38949537  
 H -2.65021777 0.50821328 -3.80525208  
 C -1.31052697 -0.60044932 -5.11202717  
 H -0.78617507 -1.11265314 -4.28696108  
 H -0.55608213 -0.38158590 -5.89071989  
 C -2.39663076 -1.51696348 -5.68645906  
 H -3.13541508 -1.73641622 -4.89442348  
 H -2.94485712 -0.98713291 -6.48803043  
 C -1.82603550 -2.83071923 -6.22957325  
 H -1.09932506 -2.64519310 -7.03827763  
 H -2.62332749 -3.47519088 -6.63240814  
 H -1.30768299 -3.39114833 -5.43429470  
 C 0.39355755 -1.48357034 2.82267284  
 C 2.05443573 -2.84280777 4.10622263  
 H 2.75259542 -2.07421970 3.74502039  
 H 2.39961886 -3.79522943 3.66507888  
 C 2.08597016 -2.93737459 5.63495159  
 H 1.71352684 -1.99387419 6.07576752  
 H 1.38940632 -3.72675824 5.96937275  
 C 3.49476576 -3.23895741 6.15990019  
 H 4.18850374 -2.44684196 5.82309532  
 H 3.85694885 -4.17899656 5.70565367  
 C 3.54418802 -3.35224485 7.68669367  
 H 3.21405768 -2.41589904 8.16606998  
 H 4.56579828 -3.56753016 8.03651619  
 H 2.88759422 -4.16179085 8.04548550

C -0.23207703 -3.70354772 3.49462676  
 H 0.32534108 -4.60307789 3.80065846  
 H -0.53411829 -3.82448673 2.44201660  
 C -1.46157622 -3.51015162 4.38954973  
 H -1.96758664 -2.57473803 4.09699631  
 H -1.13111115 -3.39432311 5.43687248  
 C -2.45304418 -4.68132401 4.28330851  
 H -1.92979705 -5.62845707 4.51479721  
 H -3.21457791 -4.55297375 5.07215977  
 C -3.15178084 -4.79010677 2.92250443  
 H -3.67246342 -3.85269499 2.66671872  
 H -3.89996052 -5.59860229 2.93093038  
 H -2.44788742 -5.00499439 2.10300040  
 O -1.32408679 3.83784127 0.36739483  
 O -1.30108845 5.27897930 -1.27932191  
 O -2.35671830 3.37673783 -1.52041137  
 N -1.67655420 4.17432213 -0.82817471

**L2\*Yb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -17085.422767, E0 = -17084.749394, G= 363.3538 at T=298.150 K

Cl -5.32929707 3.76598859 -0.53570992  
 Cl -4.08405256 -2.98492312 -3.87137675  
 N -1.55460119 1.36347187 0.04432033  
 N -0.23162405 4.01879263 2.06070518  
 N -1.11103320 -0.97333884 -1.13905740  
 N 1.20369995 -3.63194704 -1.80298066  
 O 0.07941451 1.77833772 1.99680197  
 O 0.85540915 -2.24922919 -0.04335627  
 C -1.72170365 2.52976322 0.67687356  
 C -2.89439821 3.28931379 0.51506191  
 H -3.06811190 4.20051670 1.08382857  
 C -3.87920499 2.83695841 -0.35298467

C -3.71000171 1.62239516 -1.06665254  
 C -4.66030741 1.05960119 -1.97377467  
 H -5.58062077 1.61080325 -2.17325735  
 C -4.43671846 -0.14990105 -2.57370806  
 H -5.17770767 -0.57140315 -3.25482631  
 C -3.24277401 -0.89235866 -2.31774640  
 C -2.94828129 -2.17775869 -2.84253907  
 C -1.75556254 -2.81340265 -2.52531338  
 H -1.57202244 -3.81767488 -2.90266061  
 C -0.83603877 -2.16185522 -1.68263638  
 C -2.26333785 -0.35133991 -1.44409955  
 C -2.50240827 0.92347783 -0.80405170  
 C -0.56866097 2.79461622 1.62937319  
 C 0.47575763 -2.71175694 -1.15317953  
 C -0.75686842 5.29893589 1.55272400  
 C -1.72387147 5.99966049 2.51418781  
 H -1.21653843 5.13393927 0.56726825  
 C 0.90838748 4.11501217 3.00595975  
 H 0.85095561 3.25463319 3.68817902  
 H 0.75512105 5.03459406 3.59257650  
 C 2.41363382 -4.14632034 -1.11054707  
 H 2.94475245 -3.28498745 -0.67428851  
 H 3.05446434 -4.58792448 -1.88886666  
 C 1.01973248 -4.03662157 -3.20937681  
 H 0.34090844 -3.32360435 -3.69843531  
 C 0.53858596 -5.47948265 -3.39180875  
 Yb 0.23017333 -0.18653125 0.78997082  
 N -1.14511633 -1.50698054 2.79519773  
 O 0.11343934 -1.17763209 2.85970259  
 O -1.73073268 -1.14134312 1.69012225  
 O -1.71458924 -2.09697795 3.67885137



N	2.47782969	0.83140874	-0.47458819
O	3.47737169	1.25298464	-1.00447476
O	2.46399593	0.38730809	0.75133985
O	1.32264495	0.78198618	-1.07013762
H	0.11989534	5.94469786	1.37415993
C	2.26794457	4.14407825	2.29835391
C	-2.22918057	7.33022261	1.94132376
H	-2.57901335	5.33768177	2.74570918
H	-1.21735787	6.18155289	3.47814536
C	-3.18295336	8.05435371	2.89622498
H	-1.36402035	7.97954512	1.71661842
H	-2.73607850	7.14707422	0.97577631
H	-3.53102493	9.00290298	2.46012473
H	-4.07056665	7.43947744	3.11774397
H	-2.68707371	8.28592968	3.85264778
C	3.42184281	4.29063368	3.29840279
H	2.39445233	3.20800352	1.72797775
H	2.29691935	4.97831535	1.57342160
C	4.78830814	4.31006670	2.60687065
H	3.28598499	5.21665478	3.88673735
H	3.38339496	3.45266581	4.01765871
H	5.60059643	4.41103983	3.34287310
H	4.95847464	3.37907791	2.04163814
H	4.86638165	5.15322208	1.90089476
C	2.10354733	-5.17794609	-0.02026437
H	2.00010586	-3.90766406	-3.70040441
C	0.36237276	-5.83322334	-4.87433958
H	1.26556730	-6.17088938	-2.93114805
H	-0.41306299	-5.63306952	-2.84946895
C	-0.09999227	-7.27870512	-5.08090019
H	-0.36556965	-5.13956738	-5.33434010

H 1.31936646 -5.67006922 -5.40183735  
 H -0.22019953 -7.50412464 -6.15132952  
 H 0.63085926 -7.99216604 -4.66726208  
 H -1.06781840 -7.46351099 -4.58681822  
 C 3.38740301 -5.66348553 0.66524482  
 H 1.43548739 -4.72196293 0.72957993  
 H 1.56668544 -6.03595591 -0.46210790  
 C 3.10763836 -6.69777775 1.75966179  
 H 4.06866074 -6.09568548 -0.09053395  
 H 3.91408706 -4.79558277 1.10166764  
 H 4.04286528 -7.02935076 2.23619819  
 H 2.46001196 -6.27721453 2.54625511  
 H 2.60496640 -7.58844852 1.34823442

**L2\*Lu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -17946.583685, E0 = -17945.886268, G= 370.6310 at T=298.150 K

Cl -5.40096951 3.72568989 -0.48241910  
 Cl -4.21313429 -3.02566624 -3.84313369  
 N -1.60058439 1.32812321 0.01478831  
 N -0.24152119 4.01332521 1.96000946  
 N -1.18311334 -1.01448476 -1.14600492  
 N 1.08156979 -3.69777298 -1.70859396  
 O 0.05485684 1.77018344 1.95000577  
 O 0.49306321 -2.53891587 0.15193282  
 C -1.75353181 2.49453211 0.63508642  
 C -2.93147969 3.25532985 0.50439984  
 H -3.08943391 4.16865206 1.07458258  
 C -3.93347096 2.79647064 -0.33281717  
 C -3.77994084 1.58439147 -1.04592550  
 C -4.74910545 1.01484120 -1.92608464  
 H -5.67722988 1.56107605 -2.10147643

C -4.53754330 -0.19741207 -2.52311778  
 H -5.29380131 -0.62795419 -3.18130541  
 C -3.33833599 -0.93818569 -2.28903222  
 C -3.05834007 -2.22439861 -2.81186366  
 C -1.87798142 -2.87527752 -2.49250507  
 H -1.69576585 -3.88475442 -2.86048365  
 C -0.95348930 -2.22514248 -1.65432680  
 C -2.33517504 -0.38975218 -1.44119465  
 C -2.56328011 0.89066428 -0.80626070  
 C -0.58240068 2.76972055 1.55855095  
 C 0.27942115 -2.85096025 -1.03699768  
 C -0.71529585 5.26826477 1.36256373  
 C -1.63382053 6.08908367 2.27631545  
 H -1.20578659 5.04640436 0.40344921  
 C 0.90690070 4.12161779 2.88856936  
 H 0.84496230 3.27209640 3.58452559  
 H 0.76923633 5.05268240 3.46317625  
 C 2.25558949 -4.21394491 -0.96410370  
 H 2.68240213 -3.37188506 -0.39188299  
 H 2.99127936 -4.53373814 -1.71887767  
 C 1.06316602 -3.88153744 -3.16490483  
 H 0.35613352 -3.16155553 -3.60249519  
 C 0.73299521 -5.30995989 -3.60918140  
 Lu 0.54525089 -0.16991778 0.64647847  
 N -0.79883605 -1.11891019 2.93146324  
 O 0.46840605 -0.93652225 2.89502573  
 O -1.40817833 -0.89344919 1.78879201  
 O -1.40943527 -1.46430206 3.92397571  
 N 3.26310706 -0.24375494 1.40458751  
 O 2.53861570 0.83887988 1.31136441  
 O 2.62404060 -1.32500374 1.12664342

O	4.43619442	-0.21444438	1.72504330
N	1.57757401	0.83629882	-1.77969563
O	2.03227735	1.25151706	-2.82752848
O	1.69213235	-0.40723449	-1.40992105
O	0.93488473	1.58235610	-0.94294322
H	0.18181451	5.86203718	1.11320043
C	2.26342201	4.10548449	2.17563176
C	-2.09392357	7.38885689	1.60535359
H	-2.51214170	5.48567820	2.57100081
H	-1.10258782	6.32613659	3.21493125
C	-2.99661493	8.23289394	2.51047778
H	-1.20683753	7.97858858	1.31107974
H	-2.62842488	7.14812851	0.66792268
H	-3.31344962	9.15821362	2.00462270
H	-3.90470576	7.67684507	2.79621029
H	-2.47285628	8.51781464	3.43768096
C	3.42452002	4.15727758	3.17609119
H	2.34273291	3.17672372	1.58795798
H	2.33528972	4.95679712	1.47347379
C	4.78565168	4.01671886	2.48668456
H	3.38443661	5.09878254	3.75605845
H	3.30251908	3.33264756	3.90184736
H	5.60835600	4.07004595	3.21730733
H	4.85319614	3.04715037	1.96728289
H	4.94127655	4.81607246	1.74244726
C	1.91873622	-5.36849642	-0.01571996
H	2.06127405	-3.59227848	-3.54047346
C	0.74769348	-5.45124102	-5.13593626
H	1.46198034	-6.01125145	-3.16563821
H	-0.25667053	-5.60476971	-3.21310067
C	0.43244562	-6.87655354	-5.60022402

H 0.01819678 -4.74684286 -5.57615232  
 H 1.73884690 -5.14674187 -5.51811314  
 H 0.44871122 -6.94987965 -6.69880390  
 H 1.16909575 -7.59442234 -5.20367527  
 H -0.56509596 -7.19570112 -5.25574827  
 C 3.15908408 -5.83384705 0.75656199  
 H 1.15271282 -5.02363920 0.69896662  
 H 1.48792493 -6.21280622 -0.58460176  
 C 2.85199499 -6.98339653 1.72112668  
 H 3.94467211 -6.14563322 0.04308714  
 H 3.56873488 -4.97639275 1.31959748  
 H 3.75647855 -7.29942703 2.26444364  
 H 2.10033321 -6.67923355 2.46805739  
 H 2.45631957 -7.86165857 1.18358481  
 O -4.02363634 0.18865563 1.97094250  
 H -3.16809916 -0.30011269 1.98326015  
 H -4.31648493 0.11741020 2.89504337

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -17946.584694, E0 = -17945.871519, G= 383.7764 at T=298.150 K

Lu -0.38925478 -0.54040021 -0.13133764  
 Cl 3.91386080 1.92051959 4.78502083  
 Cl 2.76781487 5.45857191 -1.86208224  
 O -1.03491378 0.37200183 -2.10894871  
 O -0.58690661 -1.47546387 2.05081415  
 O -2.66951990 -1.01504111 0.00669881  
 O -3.56261253 -2.85569096 -0.82415658  
 O -1.39434981 -2.47358608 -0.98944205  
 O 1.24503446 -2.27551174 0.17953081  
 O 1.22517967 -1.22047210 -1.72556877  
 O 2.64717126 -2.88022757 -1.41371202  
 O -1.44383252 1.25703216 0.85772145

H	-1.31648588	2.29535818	0.64831203
H	-2.40468216	1.08667028	0.81192130
N	1.29085469	0.26145408	1.50690472
N	0.67919451	-2.62114906	3.54018879
N	0.88487405	1.49377370	-0.81875825
N	-0.88623154	1.59608054	-3.98496509
N	-2.59459686	-2.15512705	-0.61657232
N	1.75306642	-2.16447520	-1.00905371
C	1.39339721	-0.37031639	2.67691803
C	2.19168591	0.13684888	3.71823955
H	2.21838856	-0.33780551	4.69802046
C	2.92472506	1.29215956	3.49593759
C	2.85718536	1.97022414	2.25400305
C	3.54480815	3.18046331	1.93607903
H	4.22222519	3.60680056	2.67726398
C	3.33904099	3.81045723	0.73956448
H	3.84867287	4.74877071	0.51501250
C	2.43114495	3.28563142	-0.22956550
C	1.76655269	2.05878425	0.02438002
C	1.98577189	1.39059448	1.28966415
C	2.06811523	3.92530489	-1.43789458
C	1.12878442	3.36243916	-2.28453684
H	0.80804598	3.93771029	-3.14560056
C	0.55685622	2.11491847	-1.95893621
C	-0.51133031	1.33530927	-2.71801066
C	-0.39210349	2.66787648	-4.85852575
H	-0.47431651	2.29017997	-5.89138889
H	0.68539047	2.81062937	-4.68627787
C	-1.18119586	3.97676086	-4.69940758
H	-2.21334529	3.81378984	-5.05784893
H	-1.28012407	4.22473574	-3.62632298

C -0.54642808 5.13862801 -5.47129917  
 H -0.48170406 4.88722944 -6.54618931  
 H 0.49630147 5.28448153 -5.12856340  
 C -1.32637012 6.44438601 -5.28326702  
 H -2.35706115 6.34545183 -5.66170073  
 H -0.84730989 7.27768850 -5.82104778  
 H -1.38482261 6.70921040 -4.21533680  
 C -1.96741462 0.75242740 -4.53840828  
 H -2.49147058 1.36014616 -5.29388571  
 H -2.67304468 0.53067446 -3.72439003  
 C -1.43991661 -0.54849255 -5.15363789  
 H -0.87889892 -1.10120165 -4.38069677  
 H -0.72965777 -0.31317821 -5.96819496  
 C -2.57725167 -1.42371798 -5.69236088  
 H -3.26999760 -1.65981174 -4.86441660  
 H -3.16251826 -0.85422176 -6.43857908  
 C -2.06794024 -2.72618079 -6.31731319  
 H -1.38760066 -2.52387571 -7.16158915  
 H -2.90152526 -3.33972716 -6.69411707  
 H -1.51518917 -3.32641292 -5.57607555  
 C 0.44326159 -1.55090559 2.75411654  
 C 1.97610068 -2.95755005 4.14317799  
 H 2.73725843 -2.26448750 3.75747037  
 H 2.25760674 -3.95602798 3.76306701  
 C 1.96790528 -2.96940804 5.67509127  
 H 1.65442502 -1.97940266 6.05559587  
 H 1.20922089 -3.68788934 6.03332138  
 C 3.33994460 -3.34027362 6.25073814  
 H 4.09605885 -2.62005949 5.88772917  
 H 3.64241576 -4.32813501 5.85854673  
 C 3.34909701 -3.36894655 7.78220129

H	3.07886744	-2.38519502	8.20012188
H	4.34468126	-3.63684320	8.16865826
H	2.62754560	-4.10695982	8.16930771
C	-0.35201794	-3.68521595	3.51676726
H	0.12929334	-4.60176659	3.89295149
H	-0.63059247	-3.84800124	2.46352005
C	-1.59045124	-3.35056615	4.35609055
H	-2.00738239	-2.39220858	4.00406885
H	-1.28650010	-3.21348453	5.40878534
C	-2.67293811	-4.43936586	4.26413107
H	-2.24307895	-5.41439199	4.56214428
H	-3.44997549	-4.20681000	5.01285839
C	-3.32648396	-4.55747795	2.88160896
H	-3.73960257	-3.58881235	2.55409360
H	-4.15145540	-5.28700399	2.89976072
H	-2.61556292	-4.88829231	2.10778356
O	-0.99026686	3.71045876	0.46529081
O	-0.96853375	5.24184370	-1.10906363
O	-2.01794100	3.34468722	-1.45775330
N	-1.34311843	4.11840343	-0.72439331

**L2\*Lu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -17589.630064, E0 = -17588.955848, G= 364.1108 at T=298.150 K

Cl	-5.31990147	3.79573941	-0.59598070
Cl	-4.08503866	-2.95736623	-3.93930101
N	-1.55847538	1.37596738	-0.01325433
N	-0.23429707	4.00838614	2.03612804
N	-1.11661065	-0.95412999	-1.19654679
N	1.19269443	-3.62621975	-1.83872163
O	0.09048594	1.77369308	1.91599882
O	0.85410166	-2.20764351	-0.10926218
C	-1.72036278	2.54179597	0.62226433



C	-2.88964224	3.30616760	0.45882672
H	-3.06145191	4.21678591	1.02882826
C	-3.87533760	2.86009145	-0.41196299
C	-3.71069813	1.64576674	-1.12736535
C	-4.66022062	1.08668220	-2.03755856
H	-5.57864761	1.64032149	-2.23900938
C	-4.43781853	-0.12271463	-2.63856196
H	-5.17799807	-0.54141903	-3.32226276
C	-3.24614692	-0.86849558	-2.38102984
C	-2.95178008	-2.15341854	-2.90718102
C	-1.76007915	-2.79077411	-2.58790517
H	-1.57828045	-3.79507279	-2.96611404
C	-0.84103286	-2.14311409	-1.74250901
C	-2.26874423	-0.33088166	-1.50407135
C	-2.50694275	0.94238079	-0.86338490
C	-0.56594008	2.79531431	1.57506716
C	0.46928614	-2.69035006	-1.20870960
C	-0.76811314	5.29861593	1.56354332
C	-1.74726558	5.96097136	2.53976750
H	-1.21842408	5.16006565	0.56972319
C	0.90629435	4.08621740	2.98334718
H	0.85992551	3.20230627	3.63551593
H	0.74250054	4.98360395	3.60071445
C	2.40177894	-4.12836599	-1.13404214
H	2.93621850	-3.25790143	-0.72062117
H	3.03901362	-4.59293127	-1.90184200
C	1.00403571	-4.06515074	-3.23394465
H	0.33654320	-3.35552692	-3.74323750
C	0.50393081	-5.50588799	-3.37861991
Lu	0.21365815	-0.16912778	0.71880490
N	-0.93587261	-1.47989357	2.81490564

O 0.33415630 -1.19624460 2.75775003  
 O -1.61895239 -1.07159483 1.76397955  
 O -1.44704294 -2.06075788 3.73541331  
 N 2.56892943 0.80799794 -0.26651236  
 O 3.59887791 1.25911832 -0.70006639  
 O 2.47831893 0.20317081 0.88225335  
 O 1.42823100 0.89015198 -0.91848797  
 H 0.10456937 5.95623446 1.41121423  
 C 2.26363444 4.15423298 2.27443433  
 C -2.26169848 7.30327463 2.00345659  
 H -2.59726238 5.28439331 2.74683285  
 H -1.24761391 6.11866570 3.51151633  
 C -3.22733974 7.99013853 2.97380972  
 H -1.40134430 7.96672392 1.80297267  
 H -2.76143456 7.14436007 1.02984929  
 H -3.58178043 8.94786263 2.56369042  
 H -4.11037207 7.36095095 3.17222595  
 H -2.73874569 8.19806194 3.93934870  
 C 3.42030096 4.25090599 3.27730131  
 H 2.39045429 3.24890041 1.65686607  
 H 2.28950834 5.02302122 1.59147692  
 C 4.78443766 4.29972649 2.58255267  
 H 3.28790665 5.14782095 3.90983129  
 H 3.38205886 3.37890196 3.95481896  
 H 5.59892988 4.36419678 3.32018113  
 H 4.95018721 3.39535260 1.97447693  
 H 4.86249495 5.17476940 1.91651607  
 C 2.08857870 -5.12919712 -0.01619195  
 H 1.98679686 -3.96255565 -3.72614694  
 C 0.32395080 -5.89595985 -4.85157871  
 H 1.22191179 -6.19381714 -2.89915252

H -0.44968712 -5.63295031 -2.83280802  
 C -0.15700723 -7.34025145 -5.02052116  
 H -0.39455920 -5.20521402 -5.33059502  
 H 1.28331220 -5.75916815 -5.38222933  
 H -0.27940825 -7.59203863 -6.08479643  
 H 0.56437021 -8.05190659 -4.58766079  
 H -1.12740707 -7.49962234 -4.52265501  
 C 3.37315416 -5.60281134 0.67656142  
 H 1.42737520 -4.64923382 0.72464573  
 H 1.54494464 -5.99546909 -0.43311587  
 C 3.09244633 -6.60345650 1.80159593  
 H 4.04820919 -6.06037140 -0.06982511  
 H 3.90606499 -4.72571421 1.08592141  
 H 4.02821207 -6.92720318 2.28242779  
 H 2.45228791 -6.15555239 2.57907128  
 H 2.58169913 -7.50233173 1.41891623

### Ligand L3

E= -1220.515792, E0 = -1220.117374, G= 215.1705 at T=298.150 K

C 0.50669205 0.02459001 3.43878412  
 C 1.65194976 -0.15478058 2.45634866  
 C 2.94941902 -0.22254448 3.01915288  
 C 4.02924776 -0.34749103 2.17403865  
 C 3.82200646 -0.36818823 0.77446008  
 C 2.47820854 -0.25195736 0.30834275  
 N 1.42391551 -0.16117065 1.14918780  
 C -0.68469733 0.00051874 -3.41051316  
 O -0.94687265 -0.54335201 -4.48569393  
 N -1.62547255 0.67241019 -2.68815398  
 C -2.98840904 0.77429807 -3.24336934  
 C -1.44992077 1.54152274 -1.50394046  
 N -0.73509741 -0.42177150 3.09669256

H 5.04816818 -0.42520496 2.56525731  
 C 4.89857864 -0.49543497 -0.15820450  
 O 0.73250860 0.57666463 4.51799297  
 C -1.82659876 -0.26538542 4.07663679  
 C -1.13993752 -1.27355349 1.95685780  
 H 3.04688096 -0.16337749 4.10412169  
 C -3.62119865 1.93100297 -2.45962405  
 C -2.89870000 -1.25131309 3.59593415  
 H -2.19443703 0.77664077 4.06664944  
 H -2.93743372 0.94305414 -4.33017063  
 C 2.23036814 -0.23849554 -1.12788475  
 N 0.96082073 -0.08456746 -1.56525326  
 C 3.33590221 -0.38020167 -2.01918149  
 C 0.73348153 -0.09074555 -2.87252092  
 C 4.66387749 -0.50653398 -1.50386131  
 H 5.91745186 -0.58595049 0.23012935  
 C 3.05575061 -0.39294878 -3.40611219  
 H 3.87853026 -0.50942796 -4.11788321  
 C 1.75433242 -0.26687273 -3.83769584  
 H 5.49091721 -0.61078346 -2.21254206  
 H 1.47054589 -0.30576456 -4.89037704  
 H -3.53143024 -0.17471781 -3.08313370  
 H -1.45009196 -0.47031078 5.09075403  
 C -2.89220858 1.87693322 -1.10746789  
 H -0.87621468 1.02255476 -0.72698718  
 H -0.90009797 2.46109080 -1.78134537  
 C -2.66784883 -1.30512011 2.07721400  
 H -0.76934236 -0.85583246 1.01328051  
 H -0.72056228 -2.29136992 2.07093000  
 H -2.95513272 2.81654596 -0.53849608  
 H -3.30747581 1.06634068 -0.48479947

H -4.71237135 1.82304430 -2.37133956  
H -3.41066813 2.88933539 -2.96303487  
H -3.10026789 -2.19737029 1.60025954  
H -3.09985852 -0.41123211 1.59600663  
H -3.91300201 -0.92677683 3.87157226  
H -2.72420502 -2.24599981 4.03898191

**L3\*La(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -10633.323658, E0 = -10632.853809, G= 243.2600 at T=298.150 K

H -4.40244198 3.25868177 -0.64169323  
H -3.41307306 -3.00236678 -3.19570446  
N -1.28413844 1.12625682 0.25440264  
N 0.11966471 3.99112105 1.81493378  
N -0.90969127 -1.35276496 -0.72809380  
N 1.35881436 -3.98766065 -1.29885447  
O 0.22084422 1.80339372 2.35539889  
O 0.74133879 -2.97826076 0.63185620  
C -1.41721809 2.36206913 0.73398364  
C -2.53606534 3.16616511 0.43403706  
H -2.64587092 4.15429449 0.88266647  
C -3.51367497 2.66600180 -0.40920487  
C -3.36803627 1.37955689 -0.96734411  
C -4.31427145 0.78734505 -1.86429763  
H -5.20459557 1.36056340 -2.13688755  
C -4.11770391 -0.46559548 -2.37278461  
H -4.84805822 -0.90446639 -3.05818391  
C -2.96075296 -1.23409045 -2.02253222  
C -2.70119667 -2.53093910 -2.51253557  
C -1.55588067 -3.20217490 -2.11697054  
H -1.34863412 -4.21248150 -2.47419572  
C -0.67702162 -2.57171345 -1.21409404

C -2.00850558 -0.68615514 -1.11939764  
 C -2.21213198 0.64456326 -0.58774304  
 C -0.30320626 2.71981955 1.69006324  
 C 0.53554475 -3.21013093 -0.57701182  
 C -0.13202247 5.12530756 0.90324992  
 H -0.95863622 5.75325632 1.28456926  
 C 1.19241536 5.89877892 0.94613802  
 H 1.91496265 5.42556190 0.26103160  
 H 1.06496716 6.95156717 0.65399671  
 C 1.64187205 5.71445799 2.40385652  
 H 1.07767880 6.39301395 3.06543946  
 H 2.71468210 5.90551090 2.55087399  
 C 1.28370357 4.25356960 2.69968009  
 H 2.09403539 3.55277848 2.43452525  
 H 1.01262856 4.06190252 3.74927926  
 C 2.61076951 -4.46421146 -0.65413189  
 H 2.38411164 -5.25386286 0.07891608  
 H 3.06398892 -3.62048531 -0.10603948  
 C 3.47074604 -4.93810749 -1.83296466  
 C 2.97722363 -4.07140970 -3.00223994  
 C 1.46139336 -4.03420115 -2.77181602  
 H 3.23651576 -4.47710419 -3.99123836  
 H 3.37837148 -3.04824209 -2.91554070  
 H 3.28826690 -6.00524998 -2.04434252  
 H 4.54284906 -4.80781698 -1.62542331  
 H 0.98003703 -3.15418673 -3.22099733  
 La 0.83872336 -0.46217763 1.29230678  
 N -0.96805716 -1.34064329 3.55371356  
 O 0.29452103 -1.19688201 3.71573591  
 O -1.40721273 -1.08877599 2.33716226  
 O -1.72797155 -1.68466699 4.43856907

N 3.58087325 -0.61733431 2.45621586  
 O 2.91281843 0.49729642 2.38420439  
 O 2.96445417 -1.66243231 1.99473536  
 O 4.70384836 -0.67272466 2.91961813  
 N 2.11687970 0.50705326 -1.28090858  
 O 2.58952880 0.88975298 -2.33803654  
 O 2.10633969 -0.74841261 -0.94637394  
 O 1.58814120 1.32107091 -0.42463127  
 H 0.98229730 -4.95095587 -3.16301823  
 H -0.38861269 4.76534939 -0.10323061  
 O -4.03421736 -0.96977693 1.34852934  
 H -3.18674946 -1.04227376 1.84901178  
 H -4.50020266 -1.78532612 1.59976244

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -10633.318784, E0 = -10632.848352, G= 245.6491 at T=298.150 K

H -4.69668531 2.89061546 -0.55803037  
 H -3.06045365 -3.23533607 -3.09341645  
 N -1.43171453 1.05112183 0.44338444  
 N -0.42989889 4.04776287 2.11610460  
 N -0.78011554 -1.37585735 -0.56420475  
 N 1.69958365 -3.85004592 -1.23345435  
 O -0.00780323 1.87785232 2.55906487  
 O 1.25308287 -2.63121057 0.62163615  
 C -1.69314098 2.26601577 0.92538214  
 C -2.87343287 2.96114945 0.58726591  
 H -3.10021973 3.92626595 1.03984082  
 C -3.76585841 2.38043833 -0.29600328  
 C -3.48011088 1.12032199 -0.86163914  
 C -4.33496523 0.45719248 -1.79907405  
 H -5.25892162 0.95374733 -2.10697198  
 C -4.00641537 -0.77023125 -2.30281210

H -4.66468143 -1.26702905 -3.02059841  
C -2.79844785 -1.43285310 -1.91256917  
C -2.41032624 -2.70112467 -2.39582586  
C -1.20881951 -3.25118351 -1.99554563  
H -0.89680034 -4.22665739 -2.36701918  
C -0.39859053 -2.54187393 -1.08379507  
C -1.92925191 -0.80925018 -0.97970450  
C -2.27562380 0.48895073 -0.44287571  
C -0.65413231 2.73217916 1.92099690  
C 0.92065793 -3.02115440 -0.52303910  
C -0.83307308 5.18720722 1.26615894  
H -1.77708447 5.63063049 1.63324344  
C 0.32264319 6.18026066 1.44763148  
H 1.15318751 5.90986729 0.77502513  
H 0.01393161 7.21242523 1.22624874  
C 0.72689164 5.95955658 2.91301203  
H 0.01278555 6.46390533 3.58511043  
H 1.73541641 6.33157635 3.14386487  
C 0.63168365 4.43881989 3.07581067  
H 1.56878924 3.92556095 2.79992199  
H 0.36264125 4.11186314 4.09206200  
C 3.01551318 -4.22041941 -0.65718055  
H 2.87487721 -4.86275434 0.22628568  
H 3.52310801 -3.29816413 -0.32648078  
C 3.74830914 -4.89443111 -1.82060528  
C 3.16947412 -4.17721987 -3.04834175  
C 1.68088627 -4.04632187 -2.70661616  
H 3.32601357 -4.72295856 -3.99047923  
H 3.58687472 -3.16177750 -3.14002800  
H 3.51234913 -5.97163916 -1.85356104  
H 4.83879280 -4.78436899 -1.72702336



H 1.22541404 -3.17285299 -3.20342374  
 La 0.40292335 -0.52967852 1.75472796  
 N 2.65807152 -0.75194389 3.67935705  
 O 3.58983350 -0.84540302 4.45099115  
 O 2.79707003 -0.25040156 2.48118258  
 O 1.45632243 -1.13700736 3.97999644  
 O 1.64724851 0.84116006 0.04533392  
 H 1.37645638 0.77681959 -0.97478098  
 H 2.60638618 0.65836483 0.06556714  
 N -2.04959011 -1.70822787 3.00809169  
 O -1.22287965 -2.41998005 2.30362034  
 O -1.74765527 -0.44647440 3.11326432  
 O -3.04210997 -2.18243718 3.52526236  
 H 1.14009130 -4.97767735 -2.95514321  
 H -0.96842623 4.86835241 0.22270632  
 N 1.31762779 -0.51052809 -2.78470755  
 O 0.70740825 -1.10725427 -3.70130491  
 O 0.82832462 0.61199808 -2.33971334  
 O 2.36655807 -0.96825194 -2.26218581

**L3\*La(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -10276.351556, E0 = -10275.920018, G= 227.2322 at T=298.150 K

H -4.10866928 3.40019989 -0.92950660  
 H -3.04102516 -2.82888055 -3.47213149  
 N -1.12121403 1.20764053 0.22194979  
 N 0.02636522 4.01343012 2.13759828  
 N -0.69360214 -1.28440154 -0.79593533  
 N 1.42521286 -4.15042591 -1.19464278  
 O 0.26618662 1.78773975 2.39449954  
 O 1.04838634 -2.75763583 0.53595656  
 C -1.29434586 2.43395352 0.72862732  
 C -2.37321115 3.25203133 0.33638731

H	-2.53719330	4.22241402	0.80239320
C	-3.25540423	2.78933191	-0.62356150
C	-3.06326151	1.51887465	-1.20438302
C	-3.92682624	0.97566676	-2.20951509
H	-4.76682568	1.58053052	-2.56040955
C	-3.71281719	-0.27314147	-2.71925712
H	-4.37919331	-0.68094587	-3.48360133
C	-2.61834216	-1.07686150	-2.26401472
C	-2.36879468	-2.38235664	-2.73487449
C	-1.28471708	-3.09562778	-2.25541401
H	-1.10786235	-4.11286163	-2.60125375
C	-0.44726819	-2.50415397	-1.28800809
C	-1.73492968	-0.57121724	-1.26977539
C	-1.96203196	0.75346804	-0.72896570
C	-0.28540567	2.75573230	1.80730450
C	0.73110735	-3.16714644	-0.61196929
C	-0.30438423	5.27897978	1.43985784
H	-1.26099467	5.68032265	1.81948185
C	0.85199142	6.20470524	1.83753121
H	1.72078001	6.01898718	1.18507302
H	0.57135433	7.26409292	1.75180471
C	1.15512359	5.76589870	3.27736950
H	0.40645963	6.18160582	3.97125673
H	2.15115857	6.07757187	3.62168336
C	1.03270125	4.24107599	3.21131921
H	1.97906888	3.75652552	2.91597629
H	0.69286066	3.77065301	4.14620590
C	2.57262421	-4.74826145	-0.45743021
H	2.22433901	-5.16356230	0.50017655
H	3.30144429	-3.95077491	-0.23275627
C	3.12950683	-5.78788376	-1.43385017

C 2.79974580 -5.18937159 -2.80877852  
 C 1.39005888 -4.62243080 -2.59960532  
 H 2.82387424 -5.92551804 -3.62481117  
 H 3.49862289 -4.37284470 -3.05342793  
 H 2.61428714 -6.75320578 -1.30153203  
 H 4.20567989 -5.95069981 -1.28179312  
 H 1.14786255 -3.79565310 -3.28256583  
 La 0.55218887 -0.50521076 1.47059381  
 N -1.41602159 -1.61648047 3.36703086  
 O -0.14041120 -1.50565302 3.63543844  
 O -1.76673853 -1.19340658 2.17958903  
 O -2.20737839 -2.07332087 4.15365648  
 N 3.19452691 0.36771548 0.46668297  
 O 2.10955834 0.48177344 -0.25447902  
 O 3.01897597 -0.15623216 1.65001655  
 O 4.27866697 0.72096592 0.06772143  
 H 0.63751686 -5.42354965 -2.70988154  
 H -0.37936839 5.11782980 0.35494775

**L3\*Ce(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -11000.743712, E0 = -11000.274750, G= 243.7494 at T=298.150 K

H -4.37681055 3.29184222 -0.65753949  
 H -3.28175306 -2.92088914 -3.32264924  
 N -1.21526372 1.20165241 0.17144923  
 N 0.04982640 4.04125786 1.95453119  
 N -0.79736328 -1.25539315 -0.83225995  
 N 1.32151568 -4.11520958 -1.21148539  
 O 0.43522659 1.82950664 2.10061288  
 O 0.89825803 -2.72901678 0.52185041  
 C -1.36905563 2.42405486 0.69335395  
 C -2.51530647 3.20465803 0.41854402

H -2.66347432 4.16779613 0.90597826  
 C -3.47420025 2.71253371 -0.44567797  
 C -3.30269933 1.44688904 -1.05067062  
 C -4.22581244 0.86333567 -1.96192336  
 H -5.12394619 1.42476726 -2.23248482  
 C -4.00205755 -0.38642392 -2.48978353  
 H -4.72196388 -0.82521814 -3.18630815  
 C -2.84717417 -1.14514446 -2.14184999  
 C -2.57734656 -2.44780946 -2.63372111  
 C -1.44244719 -3.11895132 -2.21732140  
 H -1.25017464 -4.13628292 -2.56057405  
 C -0.56236964 -2.49755478 -1.30902064  
 C -1.90106058 -0.59790468 -1.22877991  
 C -2.13017750 0.72140288 -0.68164784  
 C -0.24827828 2.76894736 1.62360990  
 C 0.60115439 -3.13427186 -0.63455802  
 C -0.37572780 5.28644085 1.28564715  
 H -1.27158606 5.70686626 1.77916515  
 C 0.82916754 6.21625805 1.48363245  
 H 1.58617651 6.00900078 0.70942152  
 H 0.54430264 7.27686310 1.42144632  
 C 1.35405385 5.79969931 2.86576056  
 H 0.72404480 6.23444080 3.65970993  
 H 2.39376211 6.10989952 3.04376101  
 C 1.21422672 4.27422523 2.84554148  
 H 2.09850907 3.77147555 2.41729903  
 H 1.02867329 3.82736635 3.83426857  
 C 2.50603032 -4.63592577 -0.48368943  
 H 2.18820763 -5.20008850 0.40683421  
 H 3.11220813 -3.78190851 -0.13583454  
 C 3.22981882 -5.48833132 -1.53263700

C 2.85753965 -4.80529547 -2.85766363  
 C 1.38007808 -4.44904900 -2.64741087  
 H 3.00740695 -5.44453192 -3.74026537  
 H 3.44149041 -3.87913775 -2.98663664  
 H 2.85211229 -6.52455187 -1.51864457  
 H 4.31427765 -5.51577044 -1.35252309  
 H 1.05165303 -3.59306598 -3.25459290  
 Ce 0.92008507 -0.31070215 0.95630401  
 N -0.59255695 -1.15986753 3.35321474  
 O 0.68149406 -0.97854692 3.35616589  
 O -1.16957474 -0.93649876 2.19812036  
 O -1.22226095 -1.51389813 4.32824993  
 N 3.72335768 -0.31590542 1.83969462  
 O 3.04379916 0.77659845 1.63232660  
 O 3.05918050 -1.40760005 1.63811111  
 O 4.88517141 -0.30347922 2.19023490  
 N 2.10047984 0.55293185 -1.61599255  
 O 2.59556246 0.90896934 -2.66663265  
 O 2.21643376 -0.66093493 -1.16596866  
 O 1.41104841 1.35000968 -0.86244142  
 H 0.73562145 -5.31951523 -2.87245989  
 H -0.60416710 5.09956264 0.22651938  
 O -3.89806724 -0.93616831 1.37377274  
 H -3.02588677 -0.97061294 1.82751644  
 H -4.20339108 -1.85779572 1.42900014

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11000.736938, E0 = -11000.269123, G= 245.2978 at T=298.150 K

H -4.78746080 2.93525434 -0.45032835  
 H -3.15612912 -3.14882779 -3.15215182  
 N -1.44553149 1.12353241 0.36957580  
 N -0.48222628 4.11069059 2.17546940

N -0.83973849 -1.29287338 -0.65990347  
 N 1.63689530 -3.80466962 -1.24866629  
 O 0.29370081 2.00383639 2.10641265  
 O 1.21748996 -2.42839932 0.48566243  
 C -1.69726908 2.35284781 0.88096952  
 C -2.91578531 3.01365209 0.60818344  
 H -3.15107107 3.96268106 1.08652163  
 C -3.83727837 2.43680477 -0.24280830  
 C -3.55423331 1.18570411 -0.85244566  
 C -4.42184782 0.53187001 -1.77277935  
 H -5.35988903 1.02404106 -2.04378629  
 C -4.10106134 -0.69107187 -2.31602693  
 H -4.77929783 -1.17787647 -3.02157664  
 C -2.88740420 -1.34778416 -1.96796215  
 C -2.49587369 -2.61415195 -2.46424985  
 C -1.29223895 -3.17027140 -2.08040857  
 H -1.00090086 -4.15100765 -2.45278454  
 C -0.46377853 -2.46801686 -1.17655730  
 C -1.99626803 -0.72710085 -1.04405260  
 C -2.32781005 0.56497955 -0.48142636  
 C -0.59053677 2.83089089 1.75236142  
 C 0.85119164 -2.92450237 -0.61642337  
 C -1.15650070 5.32053995 1.66717768  
 H -2.11013746 5.48918200 2.20111132  
 C -0.16058879 6.44279051 1.99240029  
 H 0.59930098 6.50704145 1.19629836  
 H -0.65851319 7.41957235 2.07972169  
 C 0.47889844 5.95868254 3.30156136  
 H -0.20510438 6.13492537 4.14837408  
 H 1.43606544 6.45160627 3.52424884  
 C 0.65369427 4.45665741 3.06298804

H	1.60274243	4.22271681	2.54956698
H	0.61479765	3.84699035	3.97869539
C	2.96492577	-4.11357784	-0.65676868
H	2.83924770	-4.50615215	0.36317042
H	3.53905797	-3.17263031	-0.60824841
C	3.58156872	-5.10081387	-1.65014827
C	2.98543167	-4.65302896	-2.99145770
C	1.53110969	-4.32064247	-2.63450503
H	3.04339981	-5.42088842	-3.77685428
H	3.46636677	-3.72942495	-3.35151315
H	3.27518320	-6.13304043	-1.40960944
H	4.68002462	-5.05314112	-1.63209462
H	1.11978960	-3.55023956	-3.30264282
Ce	0.45427093	-0.32532194	1.43842065
N	2.74448180	-0.69469094	3.21122861
O	3.69933724	-0.86934674	3.93402243
O	2.81665659	-0.01356956	2.10284925
O	1.56318545	-1.16666186	3.47600651
O	1.68500769	0.57326871	-0.38883540
H	1.58455396	0.23059507	-1.45504189
H	2.64899874	0.50840813	-0.22937250
N	-1.77284443	-1.24091327	3.12655282
O	-1.25227869	-1.96488893	2.17569470
O	-1.27179492	-0.05052297	3.23386741
O	-2.65925932	-1.64998138	3.84463024
H	0.89999264	-5.22789764	-2.64971995
H	-1.35992193	5.23036861	0.58988541
N	2.45244908	-1.01070619	-2.97798681
O	2.41477728	-1.64529753	-4.04599953
O	1.42327547	-0.22315802	-2.70096540
O	3.39270473	-1.08703983	-2.15752697

**L3\*Ce(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -10643.772031, E0 = -10643.341444, G= 225.9392 at T=298.150 K

H	-4.08151007	3.42509866	-0.95274878
H	-3.00676990	-2.81676817	-3.50926137
N	-1.09072149	1.21191061	0.18067843
N	0.04468916	3.98767900	2.16636157
N	-0.66813868	-1.24950993	-0.82533854
N	1.43818927	-4.14746094	-1.15467978
O	0.37644923	1.76262367	2.25258112
O	1.12777877	-2.61315370	0.46310401
C	-1.25581038	2.44946527	0.68574029
C	-2.33142734	3.26790261	0.29827714
H	-2.48777604	4.24096775	0.76000524
C	-3.23119760	2.80754113	-0.65357238
C	-3.05324507	1.53394210	-1.22869194
C	-3.92481923	0.98360109	-2.22435832
H	-4.77043152	1.58428645	-2.56902266
C	-3.70975566	-0.26531398	-2.73576355
H	-4.38132143	-0.67541671	-3.49438453
C	-2.60605812	-1.06488943	-2.29253340
C	-2.34138918	-2.36335492	-2.77059746
C	-1.24270320	-3.06504345	-2.29310417
H	-1.05745327	-4.07808161	-2.64494777
C	-0.41048318	-2.47290039	-1.32686973
C	-1.72630942	-0.54767060	-1.30333614
C	-1.95168340	0.76345909	-0.76707000
C	-0.23805629	2.75119758	1.74627757
C	0.76691473	-3.10885167	-0.64852047
C	-0.35331535	5.28992939	1.58216000
H	-1.32688546	5.60710287	1.99654329
C	0.75871938	6.23594761	2.05216050



H	1.62587321	6.15873146	1.37615919
H	0.42120361	7.28197908	2.06743050
C	1.10776460	5.68523741	3.44209146
H	0.35030028	5.99594021	4.17996168
H	2.09217525	6.01604748	3.80160880
C	1.06187749	4.16858387	3.23844957
H	2.02525616	3.76361251	2.88388228
H	0.76673675	3.59868264	4.13210773
C	2.58076429	-4.71014404	-0.38349271
H	2.23989892	-5.01793766	0.61630505
H	3.34129214	-3.92143846	-0.25179902
C	3.08035564	-5.85934305	-1.26296556
C	2.74613214	-5.38397360	-2.68397212
C	1.36426735	-4.74158955	-2.51007509
H	2.72510266	-6.19629908	-3.42425323
H	3.47180557	-4.62503386	-3.01909041
H	2.53263807	-6.78676414	-1.02920234
H	4.15264511	-6.04757214	-1.11293781
H	1.14697695	-3.96765208	-3.26025248
Ce	0.57178766	-0.41936344	1.26664388
N	-1.25991213	-1.52688122	3.21201587
O	0.03192604	-1.38280272	3.40297627
O	-1.67339110	-1.12144721	2.04354119
O	-1.99057841	-1.99251378	4.04597998
N	3.06381559	0.49115527	0.10057159
O	1.93434763	0.56661242	-0.54885477
O	2.96261358	-0.02414501	1.30063510
O	4.11319304	0.86259741	-0.36010227
H	0.57568675	-5.51450062	-2.54011297
H	-0.42803469	5.21598244	0.48766270

**L3\*Pr(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -11377.813864, E0 = -11377.344314, G= 243.9662 at T=298.150 K

H	-4.37773466	3.28027821	-0.66526723
H	-3.35062456	-2.97164583	-3.24074864
N	-1.24139524	1.16466844	0.20590524
N	0.08835694	4.01317406	1.89627349
N	-0.84503657	-1.29958498	-0.77704549
N	1.34117985	-4.05942774	-1.23694134
O	0.33389434	1.79765332	2.21626067
O	0.80984378	-2.84756589	0.59722066
C	-1.38516045	2.39384604	0.70318383
C	-2.51275373	3.18990302	0.41193932
H	-2.63882041	4.16829586	0.87576151
C	-3.48348975	2.69274235	-0.44111907
C	-3.32686853	1.41540778	-1.01659989
C	-4.26552105	0.82271737	-1.91710985
H	-5.16017962	1.38932860	-2.18894625
C	-4.05744553	-0.42952245	-2.42835522
H	-4.78475523	-0.87243861	-3.11450911
C	-2.89922953	-1.19349551	-2.07784772
C	-2.64055300	-2.49543834	-2.55955982
C	-1.49931681	-3.16566229	-2.14833355
H	-1.30042374	-4.18277359	-2.48974657
C	-0.61934149	-2.53351474	-1.25046325
C	-1.94822347	-0.63927335	-1.17723751
C	-2.16375279	0.68473780	-0.64391255
C	-0.26800358	2.73736715	1.65342212
C	0.56741130	-3.17238188	-0.58731079
C	-0.24690938	5.22273779	1.11807728
H	-1.11980152	5.73908567	1.55894876
C	1.01363635	6.08597326	1.26278126

H	1.76789677	5.76154709	0.52714807
H	0.80162019	7.15333414	1.10241544
C	1.48562229	5.75892448	2.68768430
H	0.87299418	6.30209446	3.42658877
H	2.54066443	6.01522446	2.86116242
C	1.24571300	4.24952507	2.79626584
H	2.10284019	3.65474200	2.43625069
H	1.00936604	3.90369081	3.81415939
C	2.56048512	-4.55675459	-0.54882956
H	2.28353262	-5.23769712	0.27084765
H	3.08620858	-3.69541192	-0.10223686
C	3.36251831	-5.22854328	-1.67034411
C	2.93160319	-4.45350409	-2.92537785
C	1.42723608	-4.25865936	-2.69729352
H	3.14272904	-4.98463821	-3.86526179
H	3.42409158	-3.46759415	-2.95289922
H	3.08431697	-6.29178143	-1.76419985
H	4.44436407	-5.17242336	-1.48121691
H	1.01994169	-3.38740110	-3.22966123
Pr	0.85940075	-0.37965205	1.08155787
N	-0.76601428	-1.19763494	3.40973759
O	0.50070572	-1.00843084	3.48626351
O	-1.27753603	-1.01044810	2.21413970
O	-1.45669460	-1.52798343	4.35306120
N	3.61633635	-0.44673792	2.06783438
O	2.96772194	0.66365999	1.87746203
O	2.94244289	-1.52103949	1.79793501
O	4.76450062	-0.47374773	2.46378994
N	2.08562827	0.48739699	-1.46942294
O	2.58943820	0.84939963	-2.51686215
O	2.14633012	-0.74171841	-1.05710256

O 1.44165754 1.29831684 -0.69073069  
H 0.86647797 -5.16291285 -2.99934435  
H -0.47292036 4.96286774 0.07397532  
O -3.96804309 -0.95537806 1.34826779  
H -3.09900999 -1.00532258 1.81036460  
H -4.35314703 -1.83050108 1.52515161

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11377.809424, E0 = -11377.339496 , G= 245.8723 at T=298.150 K

H -4.65733767 2.93883538 -0.58688498  
H -3.05994654 -3.21563101 -3.11548376  
N -1.41084480 1.05791438 0.41955683  
N -0.40730691 4.02854156 2.16134167  
N -0.78893518 -1.36145663 -0.57427919  
N 1.69219232 -3.85310817 -1.20077479  
O 0.06100168 1.84736311 2.47601366  
O 1.26811206 -2.53614187 0.58859247  
C -1.66036808 2.28132606 0.90134287  
C -2.83230495 2.98589802 0.56055647  
H -3.05062675 3.95324922 1.01175380  
C -3.73389935 2.41626382 -0.32419318  
C -3.46305871 1.15086496 -0.88628560  
C -4.32143736 0.49094620 -1.82418931  
H -5.24007177 0.99538994 -2.13559580  
C -4.00438738 -0.74084371 -2.32678843  
H -4.66576624 -1.23102689 -3.04625058  
C -2.80297661 -1.41369176 -1.93338144  
C -2.41431642 -2.68164325 -2.41367388  
C -1.21299183 -3.23477817 -2.00783062  
H -0.90259671 -4.20962477 -2.38144469  
C -0.40483391 -2.52946568 -1.09322631  
C -1.93593109 -0.79092866 -0.99779415

C	-2.26733708	0.50721806	-0.46707010
C	-0.61661357	2.72241879	1.89408588
C	0.91806763	-2.98750353	-0.53035378
C	-0.84066236	5.20970964	1.38833106
H	-1.79596436	5.60378027	1.78196466
C	0.28848910	6.21937561	1.63450181
H	1.12298667	6.01885319	0.94253260
H	-0.04810183	7.25588036	1.48601270
C	0.70642471	5.90943098	3.07969165
H	-0.01924780	6.34405279	3.78715777
H	1.70486641	6.29352808	3.33333468
C	0.65500617	4.37915373	3.13518620
H	1.60329449	3.91454387	2.81410146
H	0.40780634	3.97214651	4.12771082
C	3.01131487	-4.19284439	-0.61297882
H	2.87498260	-4.77079010	0.31433985
H	3.52959013	-3.25382805	-0.35352397
C	3.72659802	-4.95112276	-1.73433316
C	3.14678812	-4.30830574	-3.00176477
C	1.66217554	-4.13786983	-2.65902638
H	3.28934526	-4.91558218	-3.90773559
H	3.57443023	-3.30574656	-3.16195059
H	3.47636318	-6.02490425	-1.69464099
H	4.81904650	-4.84962606	-1.65568960
H	1.21606982	-3.29079008	-3.20692229
Pr	0.36689812	-0.47777480	1.61575675
N	2.54560781	-0.48822463	3.54788208
O	3.47110271	-0.47619814	4.33075523
O	2.69332933	-0.15394701	2.29142475
O	1.34211791	-0.82478935	3.88001037
O	1.55509782	0.75992912	-0.12115735

H 1.30542421 0.67811179 -1.15677953  
 H 2.51741004 0.59799492 -0.07188915  
 N -1.89789844 -1.71592724 2.99375272  
 O -1.01445937 -2.40495992 2.33471012  
 O -1.72465253 -0.42747033 2.95420432  
 O -2.81702638 -2.23289299 3.59340763  
 H 1.10728884 -5.07500696 -2.84755635  
 H -0.96884221 4.95568943 0.32615891  
 N 1.34449053 -0.62474853 -2.93156028  
 O 0.76624513 -1.24576867 -3.85053754  
 O 0.81561565 0.49207693 -2.50782633  
 O 2.39516449 -1.04552448 -2.38479805

**L3\*Pr(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11020.845953, E0 = -11020.414648, G= 227.7836 at T=298.150 K

H -4.07345963 3.41683006 -0.93772948  
 H -3.00333548 -2.82424593 -3.48538113  
 N -1.08443761 1.21185768 0.19658180  
 N 0.04305416 3.98701978 2.18160462  
 N -0.66170454 -1.26006854 -0.81112224  
 N 1.43852603 -4.15741730 -1.14205921  
 O 0.36880493 1.76210213 2.29633880  
 O 1.12484789 -2.64639163 0.49729148  
 C -1.25563157 2.43881845 0.71115845  
 C -2.33556914 3.25708747 0.32520235  
 H -2.50065351 4.22447300 0.79614639  
 C -3.22133255 2.80182099 -0.63766688  
 C -3.03229928 1.53421259 -1.22479677  
 C -3.89658999 0.98925549 -2.22926331  
 H -4.73843908 1.59245992 -2.57869434  
 C -3.68248367 -0.26016918 -2.73921537  
 H -4.35087299 -0.66841584 -3.50161028

C -2.58702874 -1.06442750 -2.28528905  
 C -2.33452702 -2.37143159 -2.74912095  
 C -1.24914718 -3.08084083 -2.26163840  
 H -1.07352531 -4.09967184 -2.60214496  
 C -0.41212189 -2.48489118 -1.29773879  
 C -1.70608521 -0.55290592 -1.29364860  
 C -1.93178630 0.76612437 -0.75573057  
 C -0.23734096 2.74294686 1.77869010  
 C 0.76856136 -3.12618399 -0.61611205  
 C -0.34663561 5.28203964 1.57561457  
 H -1.31669736 5.61460829 1.98630476  
 C 0.77332634 6.22767639 2.02749753  
 H 1.63937640 6.13057375 1.35264039  
 H 0.44448921 7.27659035 2.02351832  
 C 1.11875999 5.69944191 3.42704225  
 H 0.36434534 6.02972317 4.15952206  
 H 2.10595465 6.02911377 3.77990603  
 C 1.06092727 4.17975521 3.25090766  
 H 2.02116656 3.76031160 2.90483904  
 H 0.76066041 3.62836885 4.15448093  
 C 2.58728361 -4.72464323 -0.38354397  
 H 2.25011778 -5.05580568 0.61007297  
 H 3.33978891 -3.93111777 -0.23585553  
 C 3.09775543 -5.85076189 -1.28633082  
 C 2.75606894 -5.35085011 -2.69711614  
 C 1.36745727 -4.72723484 -2.50825167  
 H 2.74286652 -6.14824772 -3.45366192  
 H 3.47268343 -4.57715750 -3.01765823  
 H 2.56089711 -6.78879213 -1.07038462  
 H 4.17233706 -6.03015566 -1.14195836  
 H 1.14096713 -3.94302750 -3.24481058

Pr 0.58531177 -0.43401033 1.31058729  
 N -1.32202232 -1.51752484 3.18557501  
 O -0.03382376 -1.39867878 3.41276002  
 O -1.69999623 -1.09800506 2.01141453  
 O -2.08220482 -1.97606361 3.99851799  
 N 3.01759291 0.48787996 0.05144220  
 O 1.87364376 0.53866285 -0.57077140  
 O 2.95492411 -0.00585389 1.26423848  
 O 4.05219698 0.86242098 -0.44184041  
 H 0.58825547 -5.50909042 -2.55127215  
 H -0.42319751 5.19190645 0.48252252

**L3\*Nd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -11764.716923, E0 = -11764.246970, G= 244.1630 at T=298.150 K

H -4.37421703 3.27296662 -0.63751692  
 H -3.40208578 -2.99222827 -3.20453453  
 N -1.24946666 1.13495719 0.22457074  
 N 0.13054498 3.99160385 1.85215843  
 N -0.88888669 -1.33701384 -0.74831402  
 N 1.34009898 -4.02541733 -1.23423886  
 O 0.32571733 1.78174412 2.25031447  
 O 0.71295834 -2.94625664 0.65649962  
 C -1.37739980 2.36878753 0.71214485  
 C -2.50111365 3.17192245 0.42589056  
 H -2.61292887 4.15510368 0.88392484  
 C -3.48348188 2.67895842 -0.41660288  
 C -3.34004784 1.39735174 -0.98623270  
 C -4.28902435 0.80750036 -1.88207805  
 H -5.18000221 1.38159966 -2.15064883  
 C -4.09598637 -0.44573805 -2.39197350  
 H -4.82981110 -0.88332921 -3.07446003



C -2.94096041 -1.21813464 -2.04333377  
 C -2.68861198 -2.51967645 -2.52387190  
 C -1.55031669 -3.19696450 -2.11619830  
 H -1.35090184 -4.21286774 -2.46181583  
 C -0.66887927 -2.56615877 -1.21675098  
 C -1.98466277 -0.66833270 -1.14616358  
 C -2.18278527 0.66079813 -0.61584014  
 C -0.25085828 2.71414328 1.65528417  
 C 0.52225846 -3.20967174 -0.54808670  
 C -0.18062587 5.17469883 1.02589571  
 H -1.02950048 5.73793459 1.45654535  
 C 1.10859108 6.00277233 1.11091566  
 H 1.84109104 5.61776781 0.38255057  
 H 0.92900407 7.06761360 0.90146732  
 C 1.58991241 5.73002577 2.54423428  
 H 1.00701392 6.33054352 3.26252484  
 H 2.65538263 5.95830584 2.69127584  
 C 1.30080938 4.23666859 2.73277736  
 H 2.13442278 3.59402299 2.40086532  
 H 1.06041276 3.95436215 3.76928282  
 C 2.57522130 -4.50275898 -0.55835032  
 H 2.32669735 -5.27658558 0.18455373  
 H 3.02578020 -3.65310478 -0.01743266  
 C 3.45120263 -5.01049900 -1.71165729  
 C 2.98031902 -4.17357826 -2.91186428  
 C 1.46191692 -4.11786175 -2.70296812  
 H 3.24980211 -4.60985804 -3.88501549  
 H 3.38830996 -3.15146065 -2.84914804  
 H 3.26855922 -6.08233023 -1.89752638  
 H 4.52046013 -4.87830591 -1.49103606  
 H 0.99319118 -3.24855065 -3.18513107

Nd 0.82353902 -0.43295348 1.15504837  
 N -0.88315755 -1.25778794 3.41432023  
 O 0.38837785 -1.12972081 3.51758885  
 O -1.36792827 -0.97643369 2.22668266  
 O -1.60248339 -1.61218977 4.32783127  
 N 3.54973769 -0.57462341 2.17375612  
 O 2.90419674 0.54592991 2.02976155  
 O 2.87483287 -1.63331389 1.85638630  
 O 4.69695568 -0.61984873 2.57252598  
 N 2.07992816 0.45613533 -1.37105167  
 O 2.60142040 0.80296397 -2.41648340  
 O 2.10580802 -0.77962673 -0.96367389  
 O 1.45787084 1.27808881 -0.59493721  
 H 0.98025036 -5.04216290 -3.07303786  
 H -0.43230245 4.87599134 -0.00176403  
 O -4.03170109 -1.00555360 1.30717969  
 H -3.17111683 -1.02400613 1.78849864  
 H -4.42135000 -1.86635709 1.53648341

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11764.713775, E0 = -11764.243346, G= 246.0925 at T=298.150 K

H -4.67651796 2.91749692 -0.56148529  
 H -3.05279732 -3.22900248 -3.09336615  
 N -1.41391945 1.06376159 0.42040280  
 N -0.40841421 4.03732872 2.14777327  
 N -0.77483904 -1.35272741 -0.57612461  
 N 1.70532441 -3.84474325 -1.19131315  
 O 0.07559377 1.86010468 2.46616769  
 O 1.27698088 -2.52966714 0.60005480  
 C -1.66635776 2.27986479 0.90667582  
 C -2.84742904 2.97752738 0.57552069  
 H -3.07133603 3.94196725 1.03025174

C -3.74680448 2.40224910 -0.30567813  
 C -3.46945047 1.14146745 -0.87459505  
 C -4.32713223 0.47645688 -1.80893981  
 H -5.25075817 0.97355336 -2.11710501  
 C -4.00278950 -0.75391644 -2.31024027  
 H -4.66431189 -1.24982047 -3.02568603  
 C -2.79561663 -1.41960061 -1.92111063  
 C -2.40513587 -2.68980408 -2.39743900  
 C -1.20235431 -3.23698401 -1.99314654  
 H -0.89087176 -4.21376467 -2.36109161  
 C -0.39102903 -2.52259469 -1.08640432  
 C -1.92536879 -0.79137689 -0.99377418  
 C -2.26605344 0.50710297 -0.46122938  
 C -0.61101550 2.72841454 1.89004052  
 C 0.93174928 -2.97893023 -0.51984799  
 C -0.85684788 5.21205044 1.37276697  
 H -1.80769956 5.60541677 1.77762032  
 C 0.27271518 6.22665739 1.59571028  
 H 1.09789228 6.02293110 0.89368719  
 H -0.06904889 7.26098967 1.44413352  
 C 0.71153808 5.92904949 3.03730583  
 H -0.00458206 6.36802864 3.75176096  
 H 1.71277523 6.31713820 3.27317286  
 C 0.66469449 4.39911842 3.10600114  
 H 1.60957384 3.93322420 2.77718639  
 H 0.42948878 4.00021410 4.10472107  
 C 3.02364635 -4.18678188 -0.60321027  
 H 2.88597536 -4.77688313 0.31631795  
 H 3.53662133 -3.24902630 -0.32916164  
 C 3.74612403 -4.92890596 -1.73088098  
 C 3.16554260 -4.27653790 -2.99324799

C 1.67942393 -4.11703205 -2.65206385  
 H 3.31360936 -4.87404823 -3.90483189  
 H 3.58869267 -3.27040720 -3.14278793  
 H 3.50285101 -6.00460291 -1.70307195  
 H 4.83772945 -4.82128572 -1.64886487  
 H 1.22982705 -3.26735306 -3.19329309  
 Nd 0.37742120 -0.47915444 1.63589275  
 N 2.56441927 -0.66245556 3.52451324  
 O 3.48750496 -0.74011779 4.30701733  
 O 2.70841789 -0.18062074 2.32111335  
 O 1.36055064 -1.04704833 3.81597209  
 O 1.57259870 0.78248358 -0.08551277  
 H 1.30936408 0.70384663 -1.10972619  
 H 2.52684140 0.57488418 -0.05550056  
 N -1.95086670 -1.64918470 2.95955133  
 O -1.12731504 -2.35406280 2.24612951  
 O -1.68430161 -0.37745178 3.00726247  
 O -2.90428996 -2.13694572 3.53249860  
 H 1.13017714 -5.05560875 -2.84991360  
 H -0.99844682 4.95120478 0.31404710  
 N 1.32044411 -0.59886330 -2.90033078  
 O 0.73714709 -1.22355342 -3.81503105  
 O 0.79600298 0.51725197 -2.47655582  
 O 2.37444186 -1.02092087 -2.35870743

**L3\*Nd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11407.749948, E0 = -11407.318288, G= 227.9701 at T=298.150 K

H -4.08252954 3.41308284 -0.93163258  
 H -3.01446986 -2.82961273 -3.47784734  
 N -1.08466530 1.21741021 0.18573795  
 N 0.04474495 3.98403192 2.17735386  
 N -0.66065377 -1.25642562 -0.82426769

N	1.43760002	-4.15336323	-1.14290261
O	0.37203282	1.75952935	2.28664851
O	1.12644112	-2.63651848	0.49105674
C	-1.25702477	2.43898416	0.70565295
C	-2.34175897	3.25586414	0.32605681
H	-2.50893736	4.22128916	0.80035377
C	-3.22725439	2.80027080	-0.63563836
C	-3.03615880	1.53472567	-1.22744155
C	-3.90244818	0.98824465	-2.22927666
H	-4.74656916	1.58972478	-2.57616067
C	-3.68865108	-0.26141298	-2.73897886
H	-4.35982561	-0.67099762	-3.49819613
C	-2.59134459	-1.06459188	-2.28777766
C	-2.34178233	-2.37443113	-2.74644446
C	-1.25684249	-3.08356524	-2.26006031
H	-1.08429861	-4.10454702	-2.59586787
C	-0.41438648	-2.48236251	-1.30255592
C	-1.70503533	-0.55139148	-1.30180550
C	-1.93140376	0.77034581	-0.76239944
C	-0.23415212	2.74017954	1.77338147
C	0.76966548	-3.12040210	-0.61854005
C	-0.34885684	5.28009272	1.57573307
H	-1.31711709	5.61097193	1.99200678
C	0.77258742	6.22561502	2.02444816
H	1.63557374	6.13018608	1.34548354
H	0.44300726	7.27430296	2.02370977
C	1.12459433	5.69526005	3.42155337
H	0.37360331	6.02422190	4.15811110
H	2.11333919	6.02471447	3.77020335
C	1.06641972	4.17582846	3.24341917
H	2.02514815	3.75640583	2.89323735

H 0.76911885 3.62302899 4.14711523  
 C 2.58914685 -4.71687031 -0.38558868  
 H 2.25452471 -5.04570484 0.60966927  
 H 3.34024882 -3.92138886 -0.24154098  
 C 3.09910607 -5.84479713 -1.28641975  
 C 2.75160718 -5.35044861 -2.69780874  
 C 1.36233640 -4.72888422 -2.50662684  
 H 2.73736644 -6.15050030 -3.45152378  
 H 3.46551204 -4.57640314 -3.02345705  
 H 2.56517625 -6.78333044 -1.06553638  
 H 4.17455578 -6.02126598 -1.14507961  
 H 1.13181305 -3.94858527 -3.24601793  
 Nd 0.59079611 -0.43181160 1.30592978  
 N -1.31829381 -1.51877582 3.16802573  
 O -0.03614003 -1.39457679 3.40717411  
 O -1.69122994 -1.10400081 1.98979652  
 O -2.08534193 -1.97954845 3.97513843  
 N 3.03683925 0.48966163 0.09510585  
 O 1.90087759 0.55934232 -0.53957880  
 O 2.95915508 -0.02362769 1.29671717  
 O 4.07942009 0.86657417 -0.38150439  
 H 0.58471853 -5.51263809 -2.54313254  
 H -0.42990488 5.19289112 0.48278889

**L3\*Pm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12161.580205, E0 = -12161.109911, G= 244.9319 at T=298.150 K

H -4.36813641 3.29523277 -0.64048368  
 H -3.37702370 -2.96169400 -3.21804905  
 N -1.25432324 1.15512776 0.24155390  
 N 0.12112387 3.98978472 1.90208852  
 N -0.86822945 -1.30489242 -0.76153207

N 1.32537520 -4.04053497 -1.18317008  
 O 0.30822450 1.77509117 2.27720022  
 O 0.69877720 -2.91096187 0.68058729  
 C -1.38829827 2.38390326 0.73884171  
 C -2.50828195 3.18915439 0.44459099  
 H -2.62885427 4.16751814 0.91050094  
 C -3.47828269 2.70151949 -0.41532123  
 C -3.32503629 1.42650616 -0.99692965  
 C -4.26461077 0.84178603 -1.90594280  
 H -5.15367794 1.41646028 -2.17934775  
 C -4.06782103 -0.41028324 -2.41721702  
 H -4.79718304 -0.84644598 -3.10538483  
 C -2.91605878 -1.18467033 -2.06131673  
 C -2.66598868 -2.48975492 -2.53440166  
 C -1.53717899 -3.17306113 -2.11185312  
 H -1.34375095 -4.19358540 -2.44705009  
 C -0.65455794 -2.54116297 -1.21359932  
 C -1.96331465 -0.63563204 -1.16082442  
 C -2.17072272 0.68826908 -0.62082660  
 C -0.26600179 2.71742606 1.69239020  
 C 0.51998621 -3.19212461 -0.52058744  
 C -0.19812997 5.18787289 1.10014224  
 H -1.04814076 5.73735714 1.54563916  
 C 1.08761382 6.01977253 1.19766521  
 H 1.81945443 5.65355015 0.45901579  
 H 0.90224236 7.08768749 1.01040268  
 C 1.57560813 5.72066641 2.62347698  
 H 0.99330688 6.30451965 3.35577369  
 H 2.64072752 5.95029211 2.77056098  
 C 1.29343939 4.22281694 2.78419662  
 H 2.12839723 3.59012270 2.43672395

H	1.05644584	3.91960788	3.81547761
C	2.54786611	-4.51916695	-0.48549688
H	2.28563881	-5.28888512	0.25702000
H	2.99249554	-3.66725969	0.05684718
C	3.44117618	-5.03435278	-1.62202442
C	2.99632072	-4.19545460	-2.83039188
C	1.47461236	-4.13457537	-2.64972353
H	3.28241944	-4.63180017	-3.79882669
H	3.40548277	-3.17447901	-2.75819969
H	3.25507402	-6.10522747	-1.81017196
H	4.50703621	-4.90815306	-1.38224304
H	1.01981628	-3.26331925	-3.14160132
Pm	0.80693865	-0.38754913	1.10570478
N	-0.85273081	-1.35071242	3.33553123
O	0.42090154	-1.23297822	3.41805410
O	-1.36203134	-1.00643623	2.17652035
O	-1.55367780	-1.75090587	4.24524498
N	3.59366250	-0.40757221	1.93435001
O	2.94159865	0.68599761	1.65096819
O	2.89830208	-1.49099123	1.84785521
O	4.76705027	-0.39720163	2.25404835
N	2.02131677	0.24191079	-1.50864422
O	2.53332210	0.51130027	-2.58222651
O	2.14425421	-0.92424709	-0.95639735
O	1.30643630	1.09269536	-0.84783208
H	0.99598342	-5.05695629	-3.02858782
H	-0.45233631	4.90842724	0.06774496
O	-4.03152657	-0.95352888	1.29089272
H	-3.16703844	-1.00916207	1.76281726
H	-4.44548225	-1.80665755	1.50577700

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**



E= -12161.576087, E0 = -12161.105417, G= 246.738 at T=298.150 K

H	-4.66012335	2.92413735	-0.56299210
H	-3.07295680	-3.22779846	-3.11190271
N	-1.40698624	1.04758346	0.40889454
N	-0.39200255	4.00352526	2.16003704
N	-0.78631210	-1.36791611	-0.59400350
N	1.69335198	-3.85639524	-1.21910322
O	0.07045060	1.82097149	2.47670627
O	1.27414072	-2.53260827	0.56766927
C	-1.65377569	2.26064706	0.90291625
C	-2.83122969	2.96677756	0.57500935
H	-3.04931808	3.92968440	1.03588307
C	-3.73330951	2.40234661	-0.30991054
C	-3.46311879	1.14251220	-0.88430953
C	-4.32584333	0.48427778	-1.81933379
H	-5.24734354	0.98733097	-2.12425828
C	-4.01042223	-0.74697173	-2.32428217
H	-4.67669010	-1.23732841	-3.03911376
C	-2.80652070	-1.42061698	-1.93837345
C	-2.42194343	-2.69226718	-2.41617227
C	-1.22090936	-3.24626994	-2.01498318
H	-0.91409391	-4.22309256	-2.38675618
C	-0.40554500	-2.53738308	-1.10745740
C	-1.93280363	-0.79918861	-1.00989676
C	-2.26321197	0.50070602	-0.47408962
C	-0.60088581	2.69595861	1.89648736
C	0.92186725	-2.99026847	-0.54695445
C	-0.82132417	5.18275547	1.38138235
H	-1.77164984	5.58643198	1.77746999
C	0.31663474	6.18576622	1.61477649
H	1.14578474	5.97372818	0.91990900

H	-0.01301390	7.22368574	1.46071136
C	0.73992521	5.88277674	3.05993676
H	0.02188808	6.32829809	3.76841569
H	1.74282837	6.26081753	3.30489850
C	0.67744583	4.35333395	3.12665915
H	1.62024856	3.87843966	2.80466843
H	0.43145084	3.95524597	4.12309551
C	3.01652670	-4.19190025	-0.63790774
H	2.88588238	-4.77063704	0.28974888
H	3.53210473	-3.25079322	-0.38074976
C	3.72867155	-4.94740486	-1.76304603
C	3.14096642	-4.30506325	-3.02738929
C	1.65755224	-4.13816071	-2.67779732
H	3.28089595	-4.91157007	-3.93427634
H	3.56600666	-3.30154037	-3.18819451
H	3.48248315	-6.02203846	-1.72289634
H	4.82110405	-4.84179640	-1.68999481
H	1.20738471	-3.28943920	-3.22052050
Pm	0.38046807	-0.50163537	1.60467207
N	2.42773223	-0.34286311	3.63007832
O	3.29308629	-0.23954880	4.47450256
O	2.63944173	-0.04525206	2.37673092
O	1.22888291	-0.74969912	3.89468002
O	1.56677616	0.79310918	-0.08928984
H	1.33344996	0.69963551	-1.11667573
H	2.53393102	0.67757004	-0.02244898
N	-1.86017859	-1.73471808	2.98854160
O	-0.92117649	-2.42417264	2.41648459
O	-1.75151646	-0.44790533	2.85214162
O	-2.77586532	-2.25216722	3.59613323
H	1.10378122	-5.07606411	-2.86589384

H -0.95603937 4.92426920 0.32113740  
 N 1.32932341 -0.61970735 -2.90934086  
 O 0.72722179 -1.24761534 -3.81134868  
 O 0.81881696 0.50274658 -2.48794889  
 O 2.38760304 -1.04527092 -2.38076544

**L3\*Pm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11804.614976, E0 = -11804.183023, G= 227.3258 at T=298.150 K

H -4.07549524 3.41541338 -0.93220186  
 H -3.00618052 -2.82684064 -3.48104572  
 N -1.09333348 1.20852697 0.20354927  
 N 0.04528496 3.97133493 2.18856192  
 N -0.66950351 -1.26467371 -0.80641615  
 N 1.43578184 -4.15198946 -1.12627852  
 O 0.33711800 1.74219906 2.32817268  
 O 1.09221864 -2.66342354 0.52882969  
 C -1.26491034 2.42950869 0.72333986  
 C -2.34374595 3.25110626 0.33713335  
 H -2.50982833 4.21682215 0.81154764  
 C -3.22424364 2.79955006 -0.63092721  
 C -3.03310275 1.53409207 -1.22287333  
 C -3.89329624 0.99148321 -2.23205948  
 H -4.73290014 1.59600687 -2.58459139  
 C -3.67925453 -0.25795972 -2.74221587  
 H -4.34573460 -0.66410387 -3.50740647  
 C -2.58780527 -1.06530404 -2.28423190  
 C -2.33790541 -2.37480593 -2.74365544  
 C -1.25822937 -3.08720374 -2.25054765  
 H -1.08422375 -4.10788679 -2.58698392  
 C -0.42244229 -2.48961449 -1.28492725  
 C -1.70767689 -0.55637628 -1.29033196  
 C -1.93418980 0.76551712 -0.75055075

C	-0.24726905	2.72598243	1.79886138
C	0.75583029	-3.13169241	-0.59238434
C	-0.32530081	5.26394606	1.56487560
H	-1.29070771	5.61559296	1.97054195
C	0.80754584	6.19907331	2.00644946
H	1.67366397	6.07957077	1.33530712
H	0.49440718	7.25260544	1.98695028
C	1.14146817	5.68526983	3.41422963
H	0.38995424	6.03673172	4.13978338
H	2.13236594	6.00549126	3.76535845
C	1.06195033	4.16420937	3.25908470
H	2.01687813	3.72558856	2.92232990
H	0.75007510	3.62951756	4.16872883
C	2.58273506	-4.72073269	-0.36614421
H	2.23926163	-5.06970215	0.61918277
H	3.32631445	-3.92264938	-0.19934210
C	3.11127973	-5.82818651	-1.28162062
C	2.77633643	-5.31038666	-2.68771648
C	1.38016522	-4.70315075	-2.50113249
H	2.77711821	-6.09643078	-3.45616007
H	3.48793554	-4.52507019	-2.99067426
H	2.58175445	-6.77443504	-1.08432448
H	4.18629742	-5.99960947	-1.13108003
H	1.15110958	-3.91151619	-3.22880220
Pm	0.58031493	-0.43591371	1.31142616
N	-1.32078576	-1.51583672	3.16073823
O	-0.03869779	-1.39270484	3.39757776
O	-1.68789506	-1.09858978	1.98283494
O	-2.08932757	-1.97600067	3.96664596
N	2.96291709	0.50457847	0.01822838
O	1.80577374	0.55227596	-0.57680982

O 2.92798901 0.00044984 1.22530580  
O 3.98464918 0.89111716 -0.49460378  
H 0.60946864 -5.49227190 -2.56050444  
H -0.40197730 5.16149998 0.47296867

**L3\*Sm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12568.516240, E0 = -12568.046319, G= 244.140 at T=298.150 K

H -4.36221457 3.29610395 -0.65835512  
H -3.40557003 -2.97807360 -3.20422411  
N -1.22681069 1.16736555 0.18630789  
N 0.11675554 4.01742935 1.86870825  
N -0.88379687 -1.31805778 -0.76185894  
N 1.31539750 -4.04264164 -1.20101202  
O 0.35220462 1.80110514 2.20580435  
O 0.69836897 -2.91265678 0.66591662  
C -1.36019504 2.39654684 0.68297392  
C -2.48883486 3.19581437 0.40385830  
H -2.60665941 4.17436457 0.86987889  
C -3.46959901 2.70372963 -0.44045961  
C -3.32479095 1.42349517 -1.01261890  
C -4.27660608 0.83224702 -1.90456963  
H -5.16775322 1.40638900 -2.17243981  
C -4.08669758 -0.42323494 -2.40990615  
H -4.82289410 -0.86240345 -3.08881474  
C -2.93396306 -1.19743764 -2.05795264  
C -2.68985391 -2.50495172 -2.52628493  
C -1.55745327 -3.18658590 -2.11053300  
H -1.36575460 -4.20754147 -2.44539762  
C -0.67300743 -2.55428171 -1.21486974  
C -1.97362018 -0.64539981 -1.16654241  
C -2.16495085 0.68902427 -0.64565802

C	-0.23844638	2.73761272	1.63388848
C	0.50966978	-3.20020700	-0.53185672
C	-0.20565274	5.21669960	1.07051647
H	-1.07177782	5.75158739	1.50307047
C	1.06468129	6.06824160	1.19874513
H	1.81616485	5.72045851	0.47096801
H	0.86563456	7.13475800	1.01723075
C	1.53016675	5.76406050	2.63096809
H	0.92320734	6.33071852	3.35677338
H	2.58801031	6.01052094	2.80163741
C	1.27019346	4.26013851	2.77156711
H	2.12170315	3.64488053	2.43346071
H	1.02238262	3.94207883	3.79589367
C	2.54446292	-4.51829338	-0.51295823
H	2.28628230	-5.26643658	0.25243011
H	3.00960493	-3.65937662	0.00053272
C	3.41059923	-5.06931496	-1.65284860
C	2.96414828	-4.23997879	-2.86718726
C	1.44590616	-4.14929533	-2.66864419
H	3.22976017	-4.69444036	-3.83310676
H	3.39254642	-3.22570658	-2.81498623
H	3.19989133	-6.13885593	-1.82171273
H	4.48229313	-4.96126556	-1.43086755
H	1.00229526	-3.27225256	-3.16058731
Sm	0.84537745	-0.39429829	1.09036517
N	-0.77379304	-1.36283481	3.33049273
O	0.50799739	-1.35395682	3.35032725
O	-1.30904543	-0.85533649	2.24774075
O	-1.45780015	-1.80613840	4.23368740
N	3.56158638	-0.47852126	2.12094998
O	2.84640312	0.60753316	2.05741835

O 2.96646833 -1.54132617 1.70372808  
 O 4.70349550 -0.47810847 2.54182625  
 N 2.06342006 0.30846471 -1.49729240  
 O 2.53623962 0.62292707 -2.57652521  
 O 2.11300206 -0.89987218 -1.04214215  
 O 1.46704042 1.16499949 -0.72899532  
 H 0.94573754 -5.06473827 -3.03612328  
 H -0.43633556 4.94262457 0.03106744  
 O -3.96126556 -1.00677252 1.31272829  
 H -3.10469913 -0.98348463 1.80123293  
 H -4.31925678 -1.87784111 1.55463672

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12568.512537, E0 = -12568.042363, G= 247.1782 at T=298.150 K

H -4.69042730 2.92362523 -0.55870408  
 H -3.05572081 -3.22006750 -3.10248256  
 N -1.41299140 1.08278501 0.39233992  
 N -0.42593652 4.03395700 2.16658759  
 N -0.77219558 -1.32771611 -0.60365492  
 N 1.69248116 -3.84885168 -1.17567980  
 O 0.07830016 1.85628176 2.44482660  
 O 1.27905893 -2.49146318 0.58597392  
 C -1.67324185 2.28836703 0.89683956  
 C -2.86111975 2.98149443 0.57777095  
 H -3.09322953 3.93710423 1.04693103  
 C -3.75662661 2.41169214 -0.31101963  
 C -3.47272801 1.15869665 -0.89446962  
 C -4.32918978 0.49334040 -1.82996404  
 H -5.25613928 0.98683947 -2.13404632  
 C -4.00261307 -0.73586339 -2.33355927  
 H -4.66602087 -1.23331034 -3.04623604  
 C -2.79426408 -1.40081072 -1.94590902

C -2.40646577 -2.67596149 -2.41179276  
 C -1.20732403 -3.22525406 -1.99901855  
 H -0.90177315 -4.20825148 -2.35513902  
 C -0.39305013 -2.50480103 -1.09883785  
 C -1.92173898 -0.76953232 -1.02303112  
 C -2.26464009 0.52896762 -0.48881072  
 C -0.61715555 2.72782135 1.88564551  
 C 0.92753696 -2.96016979 -0.52268642  
 C -0.88733679 5.21804905 1.41396904  
 H -1.84149885 5.59432268 1.82717109  
 C 0.23213372 6.23999596 1.65407681  
 H 1.05792129 6.05854130 0.94668323  
 H -0.12078928 7.27339745 1.52298951  
 C 0.67745000 5.91956711 3.08882761  
 H -0.04128152 6.33768415 3.81307316  
 H 1.67532766 6.31321049 3.32962012  
 C 0.64610624 4.38822603 3.12860489  
 H 1.59482825 3.93809223 2.78897238  
 H 0.41767338 3.96811342 4.12018347  
 C 3.00524926 -4.19419479 -0.57742494  
 H 2.85826993 -4.75871849 0.35659924  
 H 3.53173923 -3.25743222 -0.32655492  
 C 3.71800232 -4.97470570 -1.68515754  
 C 3.14965248 -4.34389830 -2.96406555  
 C 1.66551697 -4.15412760 -2.62945604  
 H 3.29007435 -4.96514845 -3.86088467  
 H 3.58941197 -3.34869647 -3.13669920  
 H 3.45768094 -6.04544973 -1.63218141  
 H 4.81100321 -4.88204575 -1.60397518  
 H 1.22889268 -3.31185102 -3.19154310  
 Sm 0.38951811 -0.45273370 1.60224450



N 2.61480498 -0.62277287 3.42660141  
 O 3.55340147 -0.69826514 4.19259596  
 O 2.72019792 -0.09366890 2.24340129  
 O 1.43165243 -1.05791700 3.72078800  
 O 1.58083987 0.79957879 -0.11660529  
 H 1.35574186 0.70170379 -1.13491774  
 H 2.54229927 0.64430469 -0.04533114  
 N -1.89457858 -1.64293122 2.96686316  
 O -1.06947327 -2.34209752 2.25346875  
 O -1.64615560 -0.36819971 2.99929166  
 O -2.83618855 -2.13856411 3.55540085  
 H 1.10302055 -5.08884430 -2.80764580  
 H -1.02782714 4.97593737 0.35066721  
 N 1.37863731 -0.62528211 -2.94866133  
 O 0.79267710 -1.25805652 -3.85774493  
 O 0.86549699 0.49751416 -2.54377890  
 O 2.42712307 -1.05155551 -2.40133834

**L3\*Sm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12211.554264, E0 = -12211.122377, G= 227.4215 at T=298.150 K

H -4.07222462 3.41890526 -0.93502885  
 H -3.00370860 -2.82820439 -3.48292446  
 N -1.07616162 1.22052026 0.17558667  
 N 0.05095728 3.96995807 2.19079757  
 N -0.65330857 -1.24933934 -0.83214784  
 N 1.44033515 -4.15148354 -1.12221372  
 O 0.39365286 1.74707317 2.26531219  
 O 1.13834059 -2.60940719 0.48883396  
 C -1.24829078 2.43805957 0.70119393  
 C -2.33361506 3.25656056 0.32474992  
 H -2.50306559 4.21963596 0.80289334  
 C -3.21717262 2.80487084 -0.64083540

C -3.02540803 1.54175377 -1.23781335  
 C -3.88962221 0.99589843 -2.24207282  
 H -4.73315907 1.59745610 -2.59032869  
 C -3.67581773 -0.25402176 -2.75187778  
 H -4.34660912 -0.66249937 -3.51206827  
 C -2.58046532 -1.05913508 -2.29868913  
 C -2.33178043 -2.37112045 -2.75197077  
 C -1.24952483 -3.08092332 -2.26008177  
 H -1.07920778 -4.10369396 -2.59147334  
 C -0.40747097 -2.47641540 -1.30348980  
 C -1.69473422 -0.54563326 -1.31265557  
 C -1.92101705 0.77693915 -0.77307731  
 C -0.22111028 2.73053193 1.76866460  
 C 0.77752042 -3.10777521 -0.61261910  
 C -0.35678941 5.27255678 1.61316442  
 H -1.32817805 5.58576965 2.03565741  
 C 0.75538111 6.22167492 2.07741189  
 H 1.61740911 6.14942026 1.39440012  
 H 0.41398761 7.26636505 2.09792018  
 C 1.11740983 5.66844130 3.46297789  
 H 0.36500803 5.97469664 4.20781755  
 H 2.10340762 6.00213718 3.81518316  
 C 1.07530987 4.15225410 3.25574017  
 H 2.03699064 3.75008297 2.89351058  
 H 0.78794485 3.57880759 4.14973831  
 C 2.59061360 -4.70825005 -0.35837728  
 H 2.25701404 -5.01611662 0.64390314  
 H 3.34754944 -3.91532540 -0.23164396  
 C 3.08997822 -5.85630465 -1.23949134  
 C 2.74240398 -5.38538837 -2.65878987  
 C 1.35841501 -4.74954176 -2.47582603

H 2.71989655 -6.19907141 -3.39756417  
 H 3.46147370 -4.62321186 -3.00058174  
 H 2.54972935 -6.78660440 -0.99997020  
 H 4.16448402 -6.03806210 -1.09773874  
 H 1.13392889 -3.98002172 -3.22819281  
 Sm 0.61287695 -0.41675252 1.27772152  
 N -1.28875363 -1.49635053 3.13157082  
 O -0.00683425 -1.37079966 3.36178970  
 O -1.66328716 -1.08321607 1.95872521  
 O -2.05079269 -1.95739353 3.94451594  
 N 2.97029567 0.53356361 -0.05580518  
 O 1.81048751 0.57543474 -0.63758475  
 O 2.95143843 0.03300405 1.15189910  
 O 3.98677850 0.92255104 -0.57926971  
 H 0.57435185 -5.52734375 -2.49831963  
 H -0.43726173 5.20448399 0.51884389

**L3\*Eu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12985.714441, E0 = -12985.244662, G= 244.4690 at T=298.150 K

H -4.35237360 3.29831791 -0.65558147  
 H -3.38114905 -2.97175097 -3.20890784  
 N -1.23254764 1.16241395 0.21583708  
 N 0.11072682 3.99131584 1.92355692  
 N -0.86176682 -1.30697787 -0.77021635  
 N 1.31915772 -4.05622911 -1.18277669  
 O 0.31728953 1.77157104 2.26556182  
 O 0.72166181 -2.89658022 0.67283010  
 C -1.37118459 2.38690996 0.72221154  
 C -2.49391317 3.19010472 0.43127233  
 H -2.61756563 4.16555500 0.90229344  
 C -3.46254563 2.70435214 -0.43081298

C -3.31004238 1.42919242 -1.01256871  
C -4.25244713 0.84352744 -1.91823626  
H -5.14027500 1.41982639 -2.19230366  
C -4.06018639 -0.41093260 -2.42544723  
H -4.79196310 -0.84721607 -3.11098003  
C -2.91094375 -1.18756258 -2.06688857  
C -2.66713452 -2.49748349 -2.52995777  
C -1.54000938 -3.18217182 -2.10464406  
H -1.35329592 -4.20671034 -2.43127632  
C -0.65328854 -2.54723740 -1.21220183  
C -1.95389950 -0.63641834 -1.17232049  
C -2.15437436 0.69190812 -0.63910496  
C -0.25829035 2.71612930 1.68904865  
C 0.52604175 -3.19395924 -0.52087486  
C -0.20259295 5.19480801 1.12746179  
H -1.06610131 5.73338079 1.56034946  
C 1.07318425 6.03756523 1.25922751  
H 1.82253468 5.68769264 0.53029650  
H 0.88099432 7.10594559 1.08158064  
C 1.53705299 5.72544622 2.69024611  
H 0.93409544 6.29326963 3.41843820  
H 2.59651780 5.96460676 2.86114454  
C 1.26772344 4.22279978 2.82519555  
H 2.11442447 3.60447454 2.48016357  
H 1.01961100 3.90223575 3.84861088  
C 2.54351091 -4.53700256 -0.49159071  
H 2.28006458 -5.27696896 0.28002247  
H 3.01596045 -3.67771792 0.01439929  
C 3.40592408 -5.10330248 -1.62680185  
C 2.96958351 -4.27566767 -2.84580088  
C 1.45199060 -4.17038536 -2.64989519

H 3.23259401 -4.73743773 -3.80897236  
 H 3.40750933 -3.26527619 -2.79795766  
 H 3.18340182 -6.17135715 -1.78991187  
 H 4.47838259 -5.00606108 -1.40363514  
 H 1.01749706 -3.29176569 -3.14713693  
 Eu 0.81429547 -0.36967418 1.07306361  
 N -0.82033473 -1.30595517 3.32462025  
 O 0.45651051 -1.19970810 3.38064837  
 O -1.35038686 -0.96673775 2.17926574  
 O -1.50170577 -1.69398928 4.25616980  
 N 3.60184169 -0.28072315 1.91383076  
 O 2.94318771 0.78159010 1.57321370  
 O 2.93229651 -1.37983990 1.86476028  
 O 4.77147675 -0.23814335 2.25464988  
 N 2.03645635 0.22176015 -1.54943430  
 O 2.52846789 0.48454800 -2.63587427  
 O 2.17195058 -0.93453616 -0.98990023  
 O 1.33234525 1.08103085 -0.88836420  
 H 0.94420630 -5.08263397 -3.01488400  
 H -0.43327910 4.92442036 0.08708664  
 O -4.01529837 -0.97577184 1.28097975  
 H -3.15456605 -1.00624120 1.76169646  
 H -4.39700842 -1.84857285 1.47552598

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12985.712184, E0 = -12985.241966, G= 245.7084 at T=298.150 K

H -4.70339489 2.90865397 -0.56187856  
 H -3.01686358 -3.17925763 -3.17403007  
 N -1.44167566 1.06345308 0.43115607  
 N -0.46477857 4.04685974 2.17578840  
 N -0.75529045 -1.32052541 -0.62642848  
 N 1.69201982 -3.86564398 -1.15845525

O 0.10025242 1.88172781 2.42482281  
 O 1.22110128 -2.55349636 0.62265998  
 C -1.69956338 2.27707911 0.92178345  
 C -2.88350916 2.97004080 0.58946818  
 H -3.12005758 3.92687225 1.05328643  
 C -3.77068567 2.39842653 -0.30642548  
 C -3.47518516 1.15164661 -0.89566255  
 C -4.31715012 0.49924156 -1.85283506  
 H -5.24061203 0.99573696 -2.16251969  
 C -3.97886682 -0.72034526 -2.36975861  
 H -4.63027620 -1.21072865 -3.09828949  
 C -2.77091002 -1.38378394 -1.97860932  
 C -2.37623763 -2.64842224 -2.46520686  
 C -1.18460369 -3.20609117 -2.04345131  
 H -0.87709284 -4.18609810 -2.40632701  
 C -0.38148028 -2.49758863 -1.12420011  
 C -1.90888429 -0.76444709 -1.03685057  
 C -2.27230191 0.51810122 -0.47665370  
 C -0.63140309 2.73593450 1.89121616  
 C 0.91244125 -2.98454762 -0.51313275  
 C -0.96516883 5.22880888 1.44525170  
 H -1.92308414 5.57640791 1.87495780  
 C 0.13106076 6.27643442 1.68341053  
 H 0.94918042 6.12855291 0.95950586  
 H -0.25149962 7.30188274 1.57466853  
 C 0.60947543 5.94564295 3.10481167  
 H -0.10755158 6.33243608 3.84793639  
 H 1.60048521 6.36233711 3.33504558  
 C 0.61971909 4.41392994 3.11887050  
 H 1.57243359 3.99526739 2.75124812  
 H 0.42508695 3.97078824 4.10754585

C 2.97849584 -4.24147272 -0.52262527  
 H 2.79286766 -4.81012440 0.40182620  
 H 3.51501775 -3.31745768 -0.24694104  
 C 3.71036291 -5.02685642 -1.61479056  
 C 3.18783116 -4.38286781 -2.90688896  
 C 1.69875705 -4.16951561 -2.61163712  
 H 3.34218669 -5.00438976 -3.80120778  
 H 3.65008998 -3.39566970 -3.06600690  
 H 3.43283010 -6.09376383 -1.57452059  
 H 4.80188990 -4.95132065 -1.50251722  
 H 1.28763211 -3.32389474 -3.18648171  
 Eu 0.38833588 -0.45345041 1.60558128  
 N 2.77288866 -0.87460160 3.18442988  
 O 3.79954600 -1.08499014 3.80042601  
 O 2.71280193 -0.00873114 2.21279645  
 O 1.66496360 -1.48260272 3.43847466  
 O 1.54366744 0.83625197 -0.13588427  
 H 1.37072289 0.71331996 -1.14506710  
 H 2.50533700 0.71973139 -0.01180292  
 N -1.92582202 -1.36897171 3.12783861  
 O -1.62168884 -1.85338295 1.96002185  
 O -1.16305161 -0.41275927 3.53709126  
 O -2.86837077 -1.78473949 3.77561426  
 H 1.12740815 -5.09603071 -2.80482888  
 H -1.11289692 4.99836445 0.38031942  
 N 1.44105852 -0.64083791 -2.99760127  
 O 0.89535099 -1.28096735 -3.92828608  
 O 0.92153704 0.47926790 -2.62295461  
 O 2.46512175 -1.07282305 -2.40709686

**L3\*Eu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12628.752062, E0 = -12628.320471, G= 227.1595 at T=298.150 K

H	-4.07702160	3.41157794	-0.92826158
H	-2.99878168	-2.82586575	-3.48865318
N	-1.08251655	1.21535015	0.18599394
N	0.04377043	3.97098088	2.19049549
N	-0.65115005	-1.25646770	-0.82967985
N	1.43910766	-4.16305161	-1.13423443
O	0.35974950	1.74376154	2.31059527
O	1.13159800	-2.64129925	0.49654049
C	-1.25721228	2.42993975	0.71510154
C	-2.34170747	3.24867010	0.33609578
H	-2.51289320	4.21084595	0.81579047
C	-3.22223783	2.79790592	-0.63246226
C	-3.02807736	1.53574026	-1.23119545
C	-3.88998437	0.99159962	-2.23819089
H	-4.73374414	1.59294569	-2.58631992
C	-3.67373872	-0.25686428	-2.75013041
H	-4.34260321	-0.66512799	-3.51213384
C	-2.57807755	-1.06152916	-2.29672146
C	-2.32809305	-2.37181187	-2.75458980
C	-1.24675679	-3.08339763	-2.26356244
H	-1.07591236	-4.10503435	-2.59824038
C	-0.40613163	-2.48353148	-1.30299306
C	-1.69376183	-0.55042225	-1.30783820
C	-1.92374074	0.77145356	-0.76540720
C	-0.23592252	2.72428203	1.79144084
C	0.77685499	-3.12367153	-0.60984623
C	-0.34037176	5.26444817	1.57727611
H	-1.31033278	5.60265970	1.98356938
C	0.78096104	6.20902586	2.02826095
H	1.64886177	6.10627270	1.35669649
H	0.45526871	7.25889492	2.01852298



C	1.12021005	5.68605852	3.43131065
H	0.36348057	6.02083158	4.15934324
H	2.10663772	6.01526546	3.78671718
C	1.05942500	4.16577673	3.26069498
H	2.01991224	3.74376845	2.91836929
H	0.75638205	3.61853075	4.16583443
C	2.58513212	-4.73067141	-0.37266198
H	2.24729705	-5.04968405	0.62466484
H	3.34311604	-3.94094896	-0.23278114
C	3.08615851	-5.86892843	-1.26543403
C	2.74679303	-5.37914467	-2.68030238
C	1.36304796	-4.74285221	-2.49572182
H	2.72675395	-6.18297768	-3.42988491
H	3.46911669	-4.61396599	-3.00833821
H	2.54193163	-6.80063534	-1.04074097
H	4.15938234	-6.05580235	-1.12056041
H	1.14382720	-3.96461940	-3.24075627
Eu	0.59513074	-0.42153198	1.28488255
N	-1.28533566	-1.50703132	3.15495777
O	0.00899591	-1.50430882	3.32033753
O	-1.68318892	-0.97553611	2.04048586
O	-2.04222155	-1.96794164	3.97398424
N	2.96959043	0.59594697	0.03674282
O	1.80302942	0.77111822	-0.50198603
O	2.95440149	-0.08702952	1.14821362
O	3.99084020	1.02669644	-0.44429556
H	0.57821971	-5.51943111	-2.53333688
H	-0.41346949	5.17076826	0.48434222

**L3\*Gd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13413.273332, E0 = -13412.802524, G= 245.5743 at T=298.150 K

H	-4.37378073	3.29281449	-0.67070132
H	-3.37650776	-2.97287130	-3.24790621
N	-1.24720514	1.15863585	0.17996809
N	0.10659364	3.97900820	1.89750886
N	-0.86986995	-1.29735816	-0.80070525
N	1.32242000	-4.04438448	-1.19186866
O	0.35395080	1.75773156	2.16832519
O	0.72178483	-2.84981751	0.63543648
C	-1.38071203	2.38353825	0.68423134
C	-2.50716114	3.18549752	0.40271026
H	-2.63001418	4.16084576	0.87394303
C	-3.48206258	2.69905806	-0.45290729
C	-3.33138466	1.42485845	-1.03727341
C	-4.27385139	0.83460820	-1.94027770
H	-5.16622782	1.40537679	-2.21133780
C	-4.07532024	-0.41796723	-2.45091867
H	-4.80665827	-0.85652423	-3.13548040
C	-2.92009139	-1.18936491	-2.09869146
C	-2.66609478	-2.49468255	-2.56795073
C	-1.53226483	-3.17125726	-2.14642572
H	-1.33811581	-4.19270468	-2.47792196
C	-0.65155852	-2.53311563	-1.25081444
C	-1.96634328	-0.63545525	-1.20236742
C	-2.17296171	0.69093889	-0.66806829
C	-0.25057584	2.70793271	1.63171089
C	0.52711535	-3.17021132	-0.55448967
C	-0.24367987	5.20435476	1.15269613
H	-1.10912156	5.70978546	1.62034941
C	1.01873827	6.06602716	1.29287982
H	1.75949323	5.75890970	0.53648293
H	0.80285317	7.13643217	1.16029680

C	1.51727474	5.70845699	2.70142293
H	0.91923130	6.23687553	3.46258187
H	2.57551813	5.96073294	2.86035848
C	1.27788508	4.19715261	2.78434157
H	2.12764859	3.60646653	2.40086699
H	1.05611145	3.83271670	3.79901314
C	2.53795552	-4.52291298	-0.48188815
H	2.25862932	-5.23301935	0.31180185
H	3.02238703	-3.65654254	0.00053100
C	3.39046407	-5.14224911	-1.59677148
C	2.96381474	-4.35634327	-2.84671044
C	1.44839537	-4.21757126	-2.65298533
H	3.21630049	-4.86027098	-3.79136539
H	3.42030430	-3.35304260	-2.84084129
H	3.15409112	-6.21264267	-1.71951652
H	4.46444225	-5.05060530	-1.37905312
H	1.02668273	-3.35149813	-3.18231487
Gd	0.84829372	-0.38418272	1.04976654
N	-0.70635915	-1.17176998	3.36433697
O	0.56262332	-1.00738275	3.41277504
O	-1.23902047	-0.95683694	2.18049645
O	-1.38556945	-1.50050282	4.31687307
N	3.56939292	-0.46900052	1.96100473
O	2.90941834	0.63820100	1.76706743
O	2.89497614	-1.54508078	1.71895421
O	4.72568178	-0.48079279	2.33621836
N	2.02399492	0.40035498	-1.49027598
O	2.511110387	0.71680605	-2.56087685
O	2.09661794	-0.81229234	-1.02649283
O	1.39058304	1.23659587	-0.73589855
H	0.92523360	-5.13518000	-2.98086143

H -0.48727572 4.96820784 0.10693965  
O -3.91360259 -0.97638750 1.30768621  
H -3.04583216 -0.99767303 1.77647579  
H -4.29878235 -1.83942616 1.53590739

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13413.273675, E0 = -13412.802389, G= 247.4694 at T=298.150 K

H -4.66243505 2.93480635 -0.56832421  
H -3.04639769 -3.23188376 -3.08954072  
N -1.40151215 1.07462144 0.39382973  
N -0.38904995 4.03038740 2.16034961  
N -0.77422255 -1.33837020 -0.58433223  
N 1.71270120 -3.83702826 -1.16145539  
O 0.15277053 1.85678613 2.37603450  
O 1.30375528 -2.45324826 0.57999277  
C -1.64437568 2.29040265 0.88318378  
C -2.82800102 2.98864532 0.55950117  
H -3.05109668 3.95202661 1.01596463  
C -3.73293877 2.41616774 -0.31858775  
C -3.46264505 1.15515471 -0.89036769  
C -4.32231760 0.48710734 -1.82124507  
H -5.24638033 0.98320997 -2.12968969  
C -4.00005674 -0.74601066 -2.31885409  
H -4.66425180 -1.24302268 -3.03106236  
C -2.79350138 -1.41355479 -1.92923439  
C -2.40068507 -2.68662596 -2.39656854  
C -1.19688773 -3.22978902 -1.98827088  
H -0.88516134 -4.20791864 -2.35179639  
C -0.38528305 -2.50974202 -1.08541882  
C -1.92355764 -0.78194636 -1.00577044  
C -2.26014972 0.51953572 -0.47958064  
C -0.57025003 2.72891617 1.85401678

C	0.94488072	-2.94638419	-0.51622730
C	-0.88922942	5.22930574	1.45788372
H	-1.84552288	5.56733847	1.89833462
C	0.20936684	6.26909494	1.71796393
H	1.02579761	6.13645697	0.98926884
H	-0.17161082	7.29734278	1.63332474
C	0.68967873	5.90558290	3.13084531
H	-0.02485368	6.27745867	3.88383579
H	1.68214810	6.31466579	3.36808658
C	0.69625819	4.37385559	3.11171174
H	1.64763665	3.96090150	2.73448634
H	0.49973074	3.90936971	4.09008455
C	3.03707242	-4.15253258	-0.57170379
H	2.90798450	-4.69559860	0.37737575
H	3.55459356	-3.20339131	-0.35089025
C	3.74497223	-4.95099401	-1.66939473
C	3.15585017	-4.35479689	-2.95534062
C	1.67353463	-4.17047548	-2.60893130
H	3.29161096	-4.99491549	-3.83946323
H	3.58318424	-3.35933471	-3.15530586
H	3.49658108	-6.02281189	-1.58892512
H	4.83777142	-4.84511948	-1.60289395
H	1.22635722	-3.34119678	-3.18281913
Gd	0.37692547	-0.44008780	1.55175543
N	2.50520372	-0.63332826	3.42573380
O	3.42116785	-0.71029437	4.21596050
O	2.65012813	-0.12211217	2.23346877
O	1.30496097	-1.04493666	3.69094276
O	1.53406525	0.74295980	-0.17117059
H	1.28509450	0.64550042	-1.19810176
H	2.49298429	0.56408334	-0.12103509

N -1.88403153 -1.58026457 2.92052031  
 O -1.08569419 -2.28671145 2.18140912  
 O -1.61722505 -0.30733761 2.94243526  
 O -2.81157231 -2.06435442 3.53714514  
 H 1.11601520 -5.11241388 -2.76297116  
 H -1.03919184 5.02259159 0.38840139  
 N 1.32643712 -0.67141044 -2.97713804  
 O 0.74747127 -1.31873858 -3.87939787  
 O 0.78312218 0.43988478 -2.56282902  
 O 2.39227676 -1.06547785 -2.43920922

**L3\*Gd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13056.311580, E0 = -13055.879189, G= 227.6496 at T=298.150 K

H -4.07403088 3.45650625 -1.02098346  
 H -3.01132607 -2.80111408 -3.56156278  
 N -1.10055101 1.23988247 0.11093028  
 N 0.01755770 3.96933055 2.16264224  
 N -0.67899173 -1.22625446 -0.89408034  
 N 1.40520513 -4.14157343 -1.14607358  
 O 0.36310616 1.74638820 2.20239115  
 O 1.10773766 -2.57109165 0.43729138  
 C -1.27009535 2.45691180 0.64015996  
 C -2.34657478 3.28193116 0.25206718  
 H -2.51178026 4.24748039 0.72686309  
 C -3.22652888 2.83553553 -0.71947592  
 C -3.04056168 1.57022655 -1.31409609  
 C -3.90011191 1.02692986 -2.32397532  
 H -4.73903894 1.63137817 -2.67819929  
 C -3.68734407 -0.22403777 -2.83233690  
 H -4.35451651 -0.62998760 -3.59700561  
 C -2.59754729 -1.03306711 -2.37228179  
 C -2.34566855 -2.34515214 -2.82409477

C -1.26802278 -3.05671430 -2.32387757  
 H -1.09703720 -4.07928610 -2.65505981  
 C -0.43212700 -2.45604110 -1.35967612  
 C -1.71781838 -0.52171278 -1.38078785  
 C -1.94330573 0.80065942 -0.84263164  
 C -0.24830557 2.73642373 1.71894324  
 C 0.74853373 -3.08532357 -0.65554941  
 C -0.39429095 5.28215408 1.61141360  
 H -1.37499857 5.57469320 2.02721214  
 C 0.70091641 6.23075294 2.11615467  
 H 1.57220078 6.18719101 1.44262457  
 H 0.34690392 7.27047396 2.16067767  
 C 1.05244994 5.64367247 3.49039483  
 H 0.28642997 5.91878462 4.23352337  
 H 2.02946711 5.97976828 3.86465406  
 C 1.03291678 4.13397598 3.23962283  
 H 2.00214243 3.75605249 2.87148309  
 H 0.74835396 3.52923131 4.11343336  
 C 2.54837632 -4.69267607 -0.36660355  
 H 2.21158886 -4.96338844 0.64509523  
 H 3.31724882 -3.90766811 -0.26515615  
 C 3.02797723 -5.87332487 -1.21431541  
 C 2.69247055 -5.43461561 -2.64672828  
 C 1.31897807 -4.77021980 -2.48558426  
 H 2.65814281 -6.26688814 -3.36399364  
 H 3.42531180 -4.69394207 -3.00613713  
 H 2.46940207 -6.78624249 -0.95107299  
 H 4.09847975 -6.07129955 -1.06456065  
 H 1.11263824 -4.01525927 -3.25771260  
 Gd 0.57183862 -0.38253820 1.17772245  
 N -0.96924049 -1.49493372 3.24953628

O 0.31847668 -1.30654955 3.33787727  
 O -1.49243450 -1.11944306 2.10430169  
 O -1.62705064 -1.97164166 4.13794184  
 N 3.09917593 0.44137338 0.24278902  
 O 2.00638556 0.54981965 -0.47841486  
 O 2.91581821 -0.07962209 1.42232227  
 O 4.17867422 0.79662019 -0.15975346  
 H 0.52113163 -5.53420019 -2.49278355  
 H -0.45673716 5.24166059 0.51449668

**L3\*Tb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13851.216728, E0 = -13850.746007, G= 245.6919 at T=298.150 K

H -4.36078978 3.30420899 -0.68751687  
 H -3.36455083 -2.97470665 -3.24469566  
 N -1.23306370 1.16710281 0.16741605  
 N 0.09816170 3.98139429 1.92267990  
 N -0.85361874 -1.28039074 -0.81539339  
 N 1.32056999 -4.05533028 -1.16862226  
 O 0.36685693 1.75647640 2.14280128  
 O 0.76007885 -2.78780389 0.62046599  
 C -1.36916769 2.39513421 0.67342317  
 C -2.49551010 3.19532013 0.38823751  
 H -2.61978650 4.17038345 0.85948586  
 C -3.46963310 2.71023512 -0.46873888  
 C -3.31811571 1.43436766 -1.05252814  
 C -4.25888824 0.84217268 -1.95474756  
 H -5.15130138 1.41252923 -2.22668886  
 C -4.06194353 -0.41281208 -2.46362209  
 H -4.79437065 -0.85250646 -3.14616346  
 C -2.90771270 -1.18236303 -2.10977578  
 C -2.65321875 -2.49112272 -2.56952453



C -1.51985025 -3.16517329 -2.14306974  
 H -1.32936811 -4.19035244 -2.46452594  
 C -0.63549608 -2.51991940 -1.25559199  
 C -1.95260561 -0.62286592 -1.21713161  
 C -2.15952897 0.70167506 -0.68233031  
 C -0.24841279 2.71392679 1.62503564  
 C 0.54416794 -3.14659882 -0.55497104  
 C -0.25759822 5.21898031 1.20223284  
 H -1.13434637 5.70380735 1.67059803  
 C 0.99217612 6.09414148 1.37335122  
 H 1.74221230 5.82286739 0.61218715  
 H 0.75988048 7.16437244 1.27128088  
 C 1.48863697 5.70431948 2.77408648  
 H 0.88299358 6.20699739 3.54652214  
 H 2.54384947 5.96261406 2.94326615  
 C 1.26422572 4.18900824 2.81795430  
 H 2.12126589 3.61695075 2.42248225  
 H 1.04351211 3.79765058 3.82280278  
 C 2.53278065 -4.53114128 -0.45172453  
 H 2.24615622 -5.19993877 0.37459338  
 H 3.04270625 -3.65720320 -0.01132792  
 C 3.35749316 -5.21839857 -1.54755509  
 C 2.93562460 -4.47710466 -2.82602334  
 C 1.42653537 -4.29072285 -2.62230182  
 H 3.16349125 -5.02838993 -3.75028753  
 H 3.41926074 -3.48756266 -2.87055993  
 H 3.09381509 -6.28684616 -1.62138462  
 H 4.43582153 -5.14433002 -1.34542716  
 H 1.02057743 -3.43683863 -3.18285656  
 Tb 0.84488869 -0.32894078 0.99200594  
 N -0.65134889 -1.16915476 3.30151796

O 0.61847001 -0.98971236 3.31982040  
 O -1.21220195 -0.93788218 2.13700914  
 O -1.29999411 -1.52254760 4.26587105  
 N 3.57190728 -0.40172505 1.85762429  
 O 2.89194894 0.69579816 1.66378689  
 O 2.90794563 -1.48379421 1.63478386  
 O 4.73346329 -0.39093161 2.21545720  
 N 2.00308967 0.47567362 -1.52837658  
 O 2.49984932 0.78965020 -2.59421039  
 O 2.07497001 -0.73771143 -1.05991054  
 O 1.36005938 1.30719173 -0.78059727  
 H 0.87750351 -5.20746279 -2.90773630  
 H -0.48678681 5.00259495 0.14887629  
 O -3.90231967 -1.01591623 1.29404032  
 H -3.03109121 -1.01491940 1.75541580  
 H -4.25432587 -1.89642453 1.50880563

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13851.216413, E0 = -13850.745715, G= 249.7572 at T=298.150 K

H -4.74535131 2.96289039 -0.47752759  
 H -3.14900517 -3.18049955 -3.09415674  
 N -1.45465219 1.10359251 0.39308396  
 N -0.42231491 4.04675436 2.18724942  
 N -0.85582423 -1.30498862 -0.59806573  
 N 1.67675567 -3.74839115 -1.22657955  
 O 0.20551635 1.88961577 2.25649595  
 O 1.27551627 -2.34148574 0.48617867  
 C -1.68823767 2.32060862 0.89536816  
 C -2.88499951 3.01247096 0.60600019  
 H -3.10278773 3.97119761 1.07392144  
 C -3.80904317 2.44478178 -0.25408059  
 C -3.54776621 1.18702888 -0.84298438

C -4.42023134 0.52518767 -1.76399326  
 H -5.35260010 1.01991308 -2.04894638  
 C -4.10235786 -0.70191330 -2.28510618  
 H -4.77852678 -1.19247139 -2.99046302  
 C -2.88922477 -1.36931336 -1.92316389  
 C -2.49498510 -2.63632035 -2.40785933  
 C -1.28362870 -3.18029475 -2.01965427  
 H -0.98161590 -4.15719938 -2.39324427  
 C -0.46092218 -2.46745992 -1.12073421  
 C -2.00858808 -0.74727654 -1.00016153  
 C -2.33614206 0.55192608 -0.45901808  
 C -0.58171076 2.75775766 1.82153261  
 C 0.88859183 -2.87742233 -0.58274812  
 C -1.00166631 5.26555681 1.58846557  
 H -1.95226038 5.52989912 2.08770370  
 C 0.06200820 6.33509302 1.87375677  
 H 0.84747100 6.29266214 1.10150850  
 H -0.36749592 7.34754181 1.88036180  
 C 0.62630469 5.89713097 3.23326254  
 H -0.06581686 6.18103743 4.04333115  
 H 1.61070561 6.33444738 3.45303559  
 C 0.69841415 4.37297297 3.10307550  
 H 1.64512265 4.03317404 2.64859533  
 H 0.57630855 3.83167839 4.05364180  
 C 3.04122901 -3.98096061 -0.68422997  
 H 2.97607565 -4.34178638 0.35284317  
 H 3.57188869 -3.01319337 -0.69176185  
 C 3.65630317 -4.97437048 -1.67126167  
 C 2.99216151 -4.58874846 -2.99963188  
 C 1.54007339 -4.29820108 -2.59671831  
 H 3.04969811 -5.37549019 -3.76617599

H 3.42015147 -3.65589571 -3.40086603  
 H 3.39869428 -6.00940037 -1.38901842  
 H 4.75203419 -4.88570261 -1.69838727  
 H 1.08860099 -3.55219316 -3.26684117  
 Tb 0.35752183 -0.38047963 1.45768201  
 N 2.50889206 -0.50904983 3.28811193  
 O 3.42686319 -0.55351996 4.07739162  
 O 2.62562132 0.00746694 2.09940720  
 O 1.32354176 -0.96842319 3.55501437  
 O 1.47773778 0.65669465 -0.33047393  
 H 1.36980712 0.29686594 -1.34023786  
 H 2.44286847 0.58202082 -0.18428646  
 N -1.81378305 -1.50601280 2.94952774  
 O -1.05654097 -2.20932889 2.16324353  
 O -1.55502927 -0.23331112 2.94828486  
 O -2.69560885 -1.99621582 3.62444091  
 H 0.93845326 -5.22514868 -2.57122755  
 H -1.18665600 5.12408209 0.51374388  
 N 2.27130556 -0.94271314 -2.94077063  
 O 2.26535940 -1.61302328 -3.99392152  
 O 1.19295681 -0.24805225 -2.65057707  
 O 3.24481940 -0.91578519 -2.15138245

**L3\*Tb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13494.256490, E0 = -13493.824157, G= 227.9087 at T=298.150 K

H -4.09701490 3.43817496 -0.96801138  
 H -3.02350593 -2.81630731 -3.53552341  
 N -1.09430635 1.23270798 0.11184809  
 N 0.04062942 3.95587921 2.16309333  
 N -0.67506444 -1.22093630 -0.89173031  
 N 1.42229593 -4.12884331 -1.14126301  
 O 0.40765584 1.73591626 2.16507435

O 1.14672995 -2.51965308 0.40672332  
 C -1.25932407 2.45100522 0.64369851  
 C -2.34576893 3.26995063 0.27441075  
 H -2.50755930 4.23467541 0.75154185  
 C -3.24234557 2.81988573 -0.68193388  
 C -3.06251740 1.55483258 -1.27861524  
 C -3.93437028 1.00421429 -2.27438617  
 H -4.78340054 1.60207009 -2.61550784  
 C -3.71956158 -0.24497901 -2.78735685  
 H -4.39536667 -0.65490234 -3.54227805  
 C -2.61577964 -1.04625511 -2.34622693  
 C -2.35462642 -2.35384321 -2.80526519  
 C -1.26115048 -3.05405354 -2.32039571  
 H -1.08287442 -4.07321024 -2.65784192  
 C -0.42020589 -2.44822931 -1.36488163  
 C -1.72842634 -0.52698880 -1.36681628  
 C -1.95439076 0.79049832 -0.82674944  
 C -0.22265334 2.72801924 1.70518970  
 C 0.77055657 -3.06116033 -0.66979033  
 C -0.39031714 5.27156353 1.63467407  
 H -1.36694992 5.55089951 2.06875634  
 C 0.70519274 6.22285938 2.13368297  
 H 1.56561375 6.19528103 1.44553876  
 H 0.34335610 7.25888634 2.19737291  
 C 1.08403540 5.62171173 3.49457407  
 H 0.32881495 5.88219261 4.25382614  
 H 2.06476808 5.96053886 3.85648537  
 C 1.07130432 4.11487865 3.22598815  
 H 2.03738856 3.74823904 2.83869267  
 H 0.80455416 3.49819565 4.09709167  
 C 2.57299519 -4.66319323 -0.36165777

H 2.24751139 -4.90679407 0.66057396  
 H 3.34545755 -3.87844181 -0.28949669  
 C 3.03868008 -5.86747599 -1.18352628  
 C 2.68774986 -5.46541500 -2.62297988  
 C 1.31975400 -4.78894472 -2.46399832  
 H 2.63997173 -6.31673670 -3.31672263  
 H 3.42039990 -4.73946238 -3.01137257  
 H 2.48045230 -6.77118158 -0.88961536  
 H 4.11025190 -6.06527042 -1.04135191  
 H 1.11069655 -4.05093288 -3.25171781  
 Tb 0.56704527 -0.36208910 1.12513220  
 N -0.97936207 -1.48085165 3.16635561  
 O 0.30781773 -1.27870512 3.25977588  
 O -1.49720490 -1.11009502 2.01912761  
 O -1.63491011 -1.96469808 4.05167150  
 N 3.03874803 0.52119082 0.14950199  
 O 1.92737854 0.64765286 -0.53562564  
 O 2.88866258 -0.04865601 1.31311548  
 O 4.10521030 0.90058851 -0.26363486  
 H 0.51688111 -5.54744768 -2.44567370  
 H -0.46960247 5.24324512 0.53842926

**L3\*Dy(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14299.825833, E0 = -14299.354900, G= 245.9776 at T=298.150 K

H -4.36961746 3.29793930 -0.67329466  
 H -3.37064934 -2.97203350 -3.25002170  
 N -1.23733056 1.16387451 0.16419689  
 N 0.10780333 3.97194314 1.91141939  
 N -0.86032206 -1.28323543 -0.81499112  
 N 1.32131636 -4.04675484 -1.17086470  
 O 0.37460902 1.74768794 2.13223505

O 0.73322505 -2.80437922 0.62787861  
 C -1.37227404 2.38729763 0.67303371  
 C -2.50059700 3.18824863 0.39615700  
 H -2.62411189 4.16161680 0.87102580  
 C -3.47704744 2.70414066 -0.45934334  
 C -3.32612872 1.43154335 -1.04727948  
 C -4.26926374 0.83946550 -1.94865477  
 H -5.16326284 1.40859580 -2.21835375  
 C -4.07069302 -0.41340557 -2.45920563  
 H -4.80345631 -0.85294002 -3.14158964  
 C -2.91421580 -1.18368220 -2.10882688  
 C -2.65961933 -2.49034476 -2.57317305  
 C -1.52466595 -3.16439223 -2.14949107  
 H -1.33154714 -4.18766546 -2.47568750  
 C -0.64264303 -2.52156663 -1.25869286  
 C -1.95888972 -0.62565476 -1.21688890  
 C -2.16574001 0.69922370 -0.68258983  
 C -0.24091543 2.70409679 1.61920202  
 C 0.53396237 -3.15104437 -0.55416471  
 C -0.25698450 5.21092892 1.19736803  
 H -1.12674999 5.69580317 1.67870247  
 C 0.99654937 6.08262253 1.35508382  
 H 1.73749292 5.80355453 0.58811778  
 H 0.76831740 7.15361738 1.25093079  
 C 1.50499403 5.69476843 2.75200868  
 H 0.90547913 6.19812489 3.52881622  
 H 2.56147122 5.95351458 2.91229534  
 C 1.28074598 4.17954111 2.79827285  
 H 2.13437891 3.60654378 2.39704466  
 H 1.06680620 3.78811359 3.80453467  
 C 2.53338265 -4.51910448 -0.45082644

H 2.24804091 -5.20405149 0.36254567  
 H 3.02825880 -3.64533639 0.00691781  
 C 3.37578106 -5.17870760 -1.55022800  
 C 2.95464182 -4.42347574 -2.82079768  
 C 1.44161367 -4.26019001 -2.62696385  
 H 3.19754386 -4.95752621 -3.75131941  
 H 3.42438102 -3.42663479 -2.84575415  
 H 3.12699819 -6.24930525 -1.64251077  
 H 4.45133209 -5.09327793 -1.33799505  
 H 1.02934802 -3.40326118 -3.17815399  
 Dy 0.84366512 -0.36039481 0.99712390  
 N -0.66370273 -1.14592540 3.30970979  
 O 0.60609436 -0.97497237 3.33258963  
 O -1.21819711 -0.92678142 2.13945389  
 O -1.32021260 -1.48282194 4.27535582  
 N 3.55385995 -0.43414128 1.87923026  
 O 2.87901354 0.66474402 1.68091798  
 O 2.88753796 -1.51506722 1.65691006  
 O 4.71466923 -0.42679253 2.24157548  
 N 2.00284648 0.42351222 -1.51988411  
 O 2.49891996 0.73072582 -2.58885431  
 O 2.07363415 -0.78729302 -1.04547071  
 O 1.36227512 1.25969613 -0.77626991  
 H 0.90638137 -5.17962599 -2.92926240  
 H -0.50025535 4.99759054 0.14662050  
 O -3.90171552 -0.99415779 1.29601192  
 H -3.03030920 -0.99752724 1.75807154  
 H -4.26625395 -1.86560404 1.52604699

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14299.827000, E0 = -14299.355518, G= 247.8696 at T=298.150 K

H -4.64992476 2.95819378 -0.59938622



H	-3.03016138	-3.22632527	-3.10502267
N	-1.41229272	1.07231629	0.39116254
N	-0.38317674	4.01281404	2.17447329
N	-0.78677863	-1.33089042	-0.57312578
N	1.71626878	-3.82161593	-1.12393177
O	0.15975840	1.83617949	2.34523892
O	1.30169928	-2.39632297	0.58186710
C	-1.64587557	2.29327416	0.87376273
C	-2.82143354	2.99971962	0.53895849
H	-3.03880525	3.96800780	0.98749810
C	-3.72765923	2.43085599	-0.34140143
C	-3.46604586	1.16440129	-0.90530705
C	-4.32071447	0.49597391	-1.84084702
H	-5.24052095	0.99404615	-2.15870547
C	-3.99776697	-0.73922431	-2.33439732
H	-4.65776253	-1.23396182	-3.05209160
C	-2.79564595	-1.41036987	-1.93614364
C	-2.39410663	-2.68045521	-2.40377235
C	-1.18995142	-3.21885562	-1.98736572
H	-0.87090403	-4.19359398	-2.35334826
C	-0.38766664	-2.49896789	-1.07657337
C	-1.93505204	-0.77941924	-1.00459254
C	-2.27166295	0.52189630	-0.48417461
C	-0.56813818	2.71859646	1.84393668
C	0.94382626	-2.91860056	-0.50224781
C	-0.88769484	5.22542572	1.49943876
H	-1.84548974	5.54943895	1.94702566
C	0.20728859	6.26303768	1.78274465
H	1.02297413	6.15110445	1.04976285
H	-0.17793952	7.29145432	1.72341740
C	0.69162452	5.86775255	3.18572640

H	-0.02340322	6.21835947	3.94838476
H	1.68256199	6.27572012	3.43090677
C	0.70493031	4.33716965	3.12936330
H	1.65648687	3.93794990	2.73799443
H	0.51431197	3.84802222	4.09680891
C	3.04175782	-4.11480093	-0.52518916
H	2.91467476	-4.63730526	0.43567413
H	3.55217814	-3.15739894	-0.32454351
C	3.75724435	-4.93285370	-1.60340953
C	3.16663170	-4.36939669	-2.90325713
C	1.68255854	-4.18729019	-2.56371212
H	3.30845118	-5.02789736	-3.77280831
H	3.58757496	-3.37567067	-3.12452650
H	3.51566911	-6.00424719	-1.49966502
H	4.84913683	-4.81814051	-1.53717518
H	1.23241246	-3.37446666	-3.15830088
Dy	0.34615377	-0.41617826	1.50646257
N	2.51850486	-0.61929798	3.29355454
O	3.45763755	-0.70478529	4.05508757
O	2.62364864	-0.09593574	2.10504580
O	1.32663238	-1.03506911	3.58882356
O	1.45728683	0.74824220	-0.23048937
H	1.21386409	0.62731194	-1.25387061
H	2.41624188	0.57057416	-0.17459732
N	-1.85951233	-1.57023680	2.90396404
O	-1.07465684	-2.27329826	2.15257144
O	-1.60084724	-0.29326537	2.90721631
O	-2.76828194	-2.05272961	3.54859948
H	1.13107133	-5.13588047	-2.69771576
H	-1.03604078	5.04233503	0.42546013
N	1.30566430	-0.71071804	-3.02207971

O 0.76002669 -1.37897229 -3.92969561  
O 0.72874504 0.38995013 -2.62689185  
O 2.37041402 -1.07568479 -2.46056914

**L3\*Dy(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13942.867702, E0 = -13942.435221, G= 228.1115 at T=298.150 K

H -4.09385490 3.44145060 -0.98281872  
H -3.03085232 -2.82197070 -3.52883768  
N -1.09155309 1.23945415 0.09995173  
N 0.03378637 3.95766735 2.16275716  
N -0.67671323 -1.22055483 -0.89734107  
N 1.41385388 -4.13005257 -1.13061702  
O 0.41854870 1.74157465 2.14544797  
O 1.12347364 -2.53444600 0.42889392  
C -1.25896645 2.45472145 0.63344455  
C -2.34675217 3.27336216 0.26436529  
H -2.51247597 4.23610020 0.74408245  
C -3.23827291 2.82452798 -0.69625551  
C -3.05405426 1.56146729 -1.29632592  
C -3.92429328 1.01065576 -2.29332209  
H -4.77175903 1.60913813 -2.63727736  
C -3.71218276 -0.24076855 -2.80192828  
H -4.38839531 -0.65130025 -3.55616474  
C -2.61249685 -1.04420888 -2.35488415  
C -2.35930848 -2.35783672 -2.80194521  
C -1.27328026 -3.06224155 -2.30837393  
H -1.10141313 -4.08591318 -2.63584518  
C -0.42947018 -2.45199180 -1.35699379  
C -1.72268188 -0.52392834 -1.37786555  
C -1.94604695 0.79844713 -0.84125745  
C -0.22049136 2.73098826 1.69636559  
C 0.75809264 -3.06778455 -0.65320283

C	-0.40879491	5.27489948	1.64769626
H	-1.38523746	5.54364443	2.08885789
C	0.68273067	6.22919559	2.14969683
H	1.53996909	6.21329355	1.45723510
H	0.31403518	7.26210785	2.22371840
C	1.07251441	5.61953020	3.50373173
H	0.32061869	5.87050629	4.26942253
H	2.05363488	5.96089745	3.86216259
C	1.06653559	4.11464167	3.22425127
H	2.03310537	3.75413871	2.83265734
H	0.80439085	3.49088740	4.09174728
C	2.56494021	-4.66485310	-0.35180849
H	2.23575473	-4.92500257	0.66520387
H	3.32982230	-3.87431860	-0.26460636
C	3.04613757	-5.85389614	-1.18705487
C	2.69548869	-5.43863249	-2.62288475
C	1.32016671	-4.77818108	-2.46016407
H	2.65850210	-6.28219414	-3.32670832
H	3.42137027	-4.70040083	-3.00070381
H	2.49736977	-6.76734877	-0.90588671
H	4.11945295	-6.04130173	-1.04393649
H	1.10465252	-4.03531170	-3.24144530
Dy	0.57735169	-0.36469552	1.12914050
N	-0.94877607	-1.44948125	3.19331479
O	0.35033190	-1.34721696	3.23594451
O	-1.48207426	-1.00257850	2.08042455
O	-1.60486627	-1.91009939	4.09116268
N	3.05099988	0.44081727	0.11683001
O	1.95110154	0.46373683	-0.59802347
O	2.88212132	0.02314406	1.33878589
O	4.12137794	0.77662170	-0.32428256

H 0.52558327 -5.54552126 -2.45021629

H -0.49275213 5.25641441 0.55168533

**L3\*Ho(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14759.269059, E0 = -14758.798090, G= 245.9377 at T=298.150 K

H -4.36896896 3.29457736 -0.66742963

H -3.36200881 -2.97459722 -3.24265790

N -1.23566985 1.16532004 0.17035595

N 0.11096314 3.97619224 1.91261446

N -0.85190475 -1.28165185 -0.80862540

N 1.32677901 -4.05003119 -1.16982245

O 0.38141048 1.75223076 2.13387203

O 0.74740583 -2.80602574 0.63049316

C -1.36961675 2.38873172 0.67762309

C -2.49901462 3.18841267 0.40064287

H -2.62325740 4.16238022 0.87412596

C -3.47554255 2.70200872 -0.45348829

C -3.32391715 1.42919040 -1.04066086

C -4.26656389 0.83576459 -1.94157004

H -5.16120195 1.40375042 -2.21105170

C -4.06569290 -0.41694081 -2.45136547

H -4.79768610 -0.85810608 -3.13352776

C -2.90773129 -1.18542027 -2.10112596

C -2.65164471 -2.49162483 -2.56605911

C -1.51544094 -3.16353583 -2.14299417

H -1.32120228 -4.18664026 -2.46903849

C -0.63308483 -2.51967573 -1.25305319

C -1.95266283 -0.62638515 -1.20969701

C -2.16271472 0.69827878 -0.67577344

C -0.23587570 2.70712805 1.62207496

C 0.54385406 -3.15098858 -0.55034238

C	-0.25696477	5.21390343	1.19810653
H	-1.12589657	5.69882488	1.68094552
C	0.99622619	6.08698559	1.35119426
H	1.73528266	5.80745745	0.58259141
H	0.76681638	7.15764952	1.24622130
C	1.50886309	5.70148134	2.74722290
H	0.91115642	6.20550680	3.52499032
H	2.56558394	5.96126413	2.90422606
C	1.28579724	4.18613482	2.79621196
H	2.13882971	3.61311674	2.39373541
H	1.07470953	3.79632425	3.80371428
C	2.53631258	-4.52949429	-0.45076916
H	2.24759030	-5.21211147	0.36338678
H	3.03726268	-3.65876007	0.00613213
C	3.37313724	-5.19565058	-1.55048370
C	2.95635748	-4.43785906	-2.82095075
C	1.44462550	-4.26368666	-2.62592316
H	3.19459248	-4.97388172	-3.75156736
H	3.43372273	-3.44465613	-2.84680557
H	3.11618114	-6.26436329	-1.64221466
H	4.44948673	-5.11838484	-1.33924663
H	1.03803039	-3.40386271	-3.17684102
Ho	0.84175992	-0.35513917	0.99706960
N	-0.67794830	-1.16324663	3.28029346
O	0.59149230	-0.99461305	3.31167912
O	-1.22404552	-0.92714512	2.10940790
O	-1.34078443	-1.51232243	4.23699903
N	3.54628205	-0.43197513	1.86645293
O	2.87545133	0.66774744	1.67467690
O	2.87257385	-1.50930190	1.64142823
O	4.70815802	-0.43431348	2.22497988

N 1.99287868 0.45972791 -1.50238311  
 O 2.49172044 0.78570682 -2.56436253  
 O 2.06858897 -0.75480938 -1.04221833  
 O 1.34291565 1.28167474 -0.74970859  
 H 0.90305966 -5.17927933 -2.92883444  
 H -0.50250381 4.99916315 0.14817905  
 O -3.92015243 -0.99239141 1.29325950  
 H -3.04252410 -0.99608606 1.74279630  
 H -4.28363419 -1.86167765 1.53288841

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14759.272419, E0 = -14758.800833, G= 248.1065 at T=298.150 K

H -4.65021944 2.95253348 -0.58722156  
 H -3.03784060 -3.23287296 -3.09387422  
 N -1.40049720 1.07626271 0.38086978  
 N -0.37742829 4.01174831 2.17637920  
 N -0.78182209 -1.33162344 -0.58081895  
 N 1.71632409 -3.82801628 -1.12985504  
 O 0.17631242 1.83625245 2.33049083  
 O 1.31412840 -2.38898182 0.56767070  
 C -1.63646984 2.29387403 0.86891484  
 C -2.81696153 2.99695039 0.54308975  
 H -3.03511262 3.96300149 0.99609041  
 C -3.72476268 2.42793512 -0.33505982  
 C -3.46195531 1.16331267 -0.90293652  
 C -4.32056999 0.49368536 -1.83422005  
 H -5.24254751 0.99066752 -2.14751697  
 C -3.99926281 -0.74146479 -2.32884526  
 H -4.66300631 -1.23786294 -3.04192185  
 C -2.79531264 -1.41184735 -1.93475711  
 C -2.39765382 -2.68489408 -2.39795303  
 C -1.19243956 -3.22358489 -1.98558331

H	-0.87716967	-4.20074463	-2.34832668
C	-0.38507977	-2.50108933	-1.08080065
C	-1.92973959	-0.77888471	-1.00923085
C	-2.26360154	0.52396703	-0.48892745
C	-0.55669284	2.71808147	1.83830643
C	0.94919026	-2.91906404	-0.50924611
C	-0.88811064	5.22614431	1.50948453
H	-1.84373891	5.54665232	1.96432173
C	0.20672220	6.26475143	1.79030943
H	1.01776350	6.15780497	1.05148828
H	-0.18102621	7.29261541	1.73786211
C	0.70137310	5.86474419	3.18828321
H	-0.00750886	6.21262217	3.95782280
H	1.69426894	6.27173853	3.42728376
C	0.71464342	4.33416700	3.12728095
H	1.66434765	3.93533397	2.73111200
H	0.52821410	3.84262180	4.09433699
C	3.04416156	-4.12005758	-0.53550470
H	2.92071915	-4.64004898	0.42718494
H	3.55536103	-3.16217566	-0.33919191
C	3.75545907	-4.94090700	-1.61419487
C	3.15944433	-4.38171864	-2.91345811
C	1.67657566	-4.19813538	-2.56843281
H	3.29784918	-5.04334927	-3.78116059
H	3.57962036	-3.38881397	-3.13952041
H	3.51506758	-6.01211500	-1.50600207
H	4.84757090	-4.82541943	-1.55284452
H	1.22591305	-3.38566327	-3.16307998
Ho	0.35402527	-0.41475201	1.49040437
N	2.45826483	-0.55628121	3.33795214
O	3.37177444	-0.60846156	4.13292408



O 2.60285830 -0.08514070 2.13143277  
 O 1.25685942 -0.95811754 3.61148524  
 O 1.47009206 0.73234814 -0.23211667  
 H 1.22390187 0.61936390 -1.25652492  
 H 2.42760611 0.54604149 -0.17965090  
 N -1.83996034 -1.57165849 2.88051486  
 O -1.02331996 -2.26979303 2.15583062  
 O -1.61196661 -0.29192948 2.86367774  
 O -2.74705958 -2.06738162 3.51777196  
 H 1.12382162 -5.14648724 -2.69814014  
 H -1.04271030 5.04761934 0.43557388  
 N 1.31013191 -0.71516728 -3.02492166  
 O 0.75529027 -1.38519740 -3.92574024  
 O 0.73730594 0.38724700 -2.62740374  
 O 2.37858558 -1.08039200 -2.47116661

**L3\*Ho(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -14402.310913, E0 = -14401.878517, G= 229.3640 at T=298.150 K

H -4.08853197 3.46860027 -1.04042482  
 H -3.01900315 -2.79602218 -3.59083748  
 N -1.10689998 1.25047636 0.06644182  
 N 0.01439119 3.95240545 2.15056276  
 N -0.68713868 -1.20313644 -0.93430376  
 N 1.39517415 -4.12299204 -1.14285254  
 O 0.38041756 1.73265338 2.12657309  
 O 1.10883844 -2.50908232 0.39759082  
 C -1.27510488 2.46447158 0.60314852  
 C -2.35497117 3.28903627 0.22375800  
 H -2.51967049 4.25239849 0.70257467  
 C -3.23970556 2.84604740 -0.74592865  
 C -3.05672956 1.58256328 -1.34603441  
 C -3.91930199 1.03627658 -2.35232711

H -4.76172733 1.63796711 -2.70295215  
C -3.70547724 -0.21457042 -2.86202812  
H -4.37561178 -0.62142998 -3.62361336  
C -2.61154461 -1.02179170 -2.40748191  
C -2.35454822 -2.33437657 -2.85586643  
C -1.27313197 -3.04061675 -2.35463309  
H -1.09956348 -4.06360626 -2.68305779  
C -0.43687809 -2.43460894 -1.39375603  
C -1.73025382 -0.50567842 -1.42116451  
C -1.95602179 0.81476963 -0.88268995  
C -0.24519955 2.72960353 1.67682874  
C 0.74434000 -3.05079341 -0.68001252  
C -0.41884109 5.27496910 1.64150834  
H -1.40046287 5.54179335 2.07223582  
C 0.66791469 6.22298002 2.16579890  
H 1.53289580 6.21324682 1.48293293  
H 0.29958892 7.25553322 2.24619722  
C 1.04194355 5.59892845 3.51772141  
H 0.28116783 5.84171152 4.27731180  
H 2.01899576 5.93607092 3.89094615  
C 1.03871155 4.09731674 3.22176576  
H 2.00847888 3.74227834 2.83288264  
H 0.77074087 3.46292758 4.07961082  
C 2.53571725 -4.65848112 -0.34905705  
H 2.19817328 -4.89920759 0.66990697  
H 3.30842042 -3.87481546 -0.26895535  
C 3.00820065 -5.86502504 -1.16342652  
C 2.67086220 -5.46756315 -2.60761046  
C 1.30248749 -4.78828478 -2.46370959  
H 2.62797475 -6.32130241 -3.29871726  
H 3.40803361 -4.74415684 -2.99216890

H 2.44761801 -6.76808834 -0.87202901  
 H 4.07854557 -6.06195831 -1.01134443  
 H 1.10279071 -4.05343866 -3.25676918  
 Ho 0.54502684 -0.35185656 1.08983934  
 N -0.79344702 -1.45585692 3.24932933  
 O 0.49008000 -1.24140680 3.23800874  
 O -1.40299463 -1.09870315 2.13832831  
 O -1.37850344 -1.93633711 4.18482113  
 N 3.09610343 0.39731237 0.30702940  
 O 2.03165340 0.53720111 -0.45878455  
 O 2.84890199 -0.12527284 1.46859384  
 O 4.19664288 0.72985560 -0.05450989  
 H 0.49813882 -5.54545212 -2.44938493  
 H -0.48770598 5.26651907 0.54418343

**L3\*Er(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15229.645638, E0 = -15229.174599, G= 246.0011 at T=298.150 K

H -4.37257147 3.29144073 -0.67680854  
 H -3.36761117 -2.97536016 -3.26832056  
 N -1.24094272 1.15457141 0.15524898  
 N 0.10360601 3.96268535 1.90735793  
 N -0.86710453 -1.29052913 -0.82014441  
 N 1.31786883 -4.05374432 -1.17699754  
 O 0.37502822 1.73825359 2.12015104  
 O 0.73228180 -2.80068302 0.61537319  
 C -1.37310088 2.37799835 0.66416788  
 C -2.50196218 3.17919803 0.38951829  
 H -2.62359262 4.15252590 0.86497182  
 C -3.48035574 2.69646263 -0.46453679  
 C -3.33164787 1.42414403 -1.05300188  
 C -4.27460909 0.83234739 -1.95500100

H -5.16854429 1.40171766 -2.22364140  
C -4.07496977 -0.41932079 -2.46830273  
H -4.80697250 -0.85746306 -3.15238094  
C -2.91782594 -1.18959439 -2.11938334  
C -2.65928960 -2.49400091 -2.58840537  
C -1.52294219 -3.16637492 -2.16592288  
H -1.32639456 -4.18741941 -2.49699759  
C -0.64468747 -2.52567768 -1.26959097  
C -1.96496117 -0.63363045 -1.22389495  
C -2.17159653 0.69095582 -0.68920827  
C -0.24096856 2.69419622 1.61009717  
C 0.53193152 -3.15338969 -0.56350666  
C -0.25933346 5.20253897 1.19450426  
H -1.12885690 5.68860817 1.67529213  
C 0.99525321 6.07273722 1.35362446  
H 1.73593724 5.79360056 0.58648717  
H 0.76826268 7.14412975 1.25070167  
C 1.50297725 5.68276691 2.75023127  
H 0.90457517 6.18677616 3.52748108  
H 2.55995989 5.93940258 2.91058111  
C 1.27595389 4.16789103 2.79524446  
H 2.12868762 3.59318304 2.39458394  
H 1.06063163 3.77632737 3.80119276  
C 2.52702498 -4.52746534 -0.45302165  
H 2.23770118 -5.20865297 0.36213264  
H 3.02399969 -3.65401554 0.00297668  
C 3.36880255 -5.19489765 -1.54823995  
C 2.95154238 -4.44481134 -2.82318330  
C 1.43888474 -4.27479744 -2.63173699  
H 3.19329715 -4.98472357 -3.75061393  
H 3.42563415 -3.45016050 -2.85321093

H 3.11681247 -6.26512241 -1.63568974  
 H 4.44436312 -5.11188364 -1.33525157  
 H 1.03020048 -3.41937304 -3.18795967  
 Er 0.82794672 -0.35711309 0.98179841  
 N -0.61279297 -1.09793127 3.32414317  
 O 0.65507370 -0.93172318 3.32483435  
 O -1.18295705 -0.89345819 2.15607643  
 O -1.25956070 -1.41912639 4.30158758  
 N 3.51332092 -0.45055774 1.88711131  
 O 2.84587383 0.65109152 1.71127963  
 O 2.84534526 -1.52160227 1.61921227  
 O 4.66871023 -0.46303329 2.26767159  
 N 2.00689769 0.50603449 -1.47766447  
 O 2.51049471 0.85500705 -2.53004813  
 O 2.06064391 -0.72298193 -1.05458355  
 O 1.37332487 1.31748474 -0.69983286  
 H 0.90096390 -5.19387150 -2.93050742  
 H -0.50155050 4.99096251 0.14313263  
 O -3.86856318 -0.98694217 1.31743598  
 H -2.99704027 -0.97709501 1.77910495  
 H -4.21650839 -1.86651182 1.54228199

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15229.648795, E0 = -15229.177172, G= 248.2065 at T=298.150 K

H -4.66377878 2.95139503 -0.59014869  
 H -3.01892090 -3.21799278 -3.11282158  
 N -1.40168905 1.09467280 0.36539403  
 N -0.39153674 4.03594828 2.17048359  
 N -0.76744187 -1.30735898 -0.60066849  
 N 1.71318662 -3.83339238 -1.10486686  
 O 0.23081037 1.87712586 2.24916315  
 O 1.30320776 -2.38088322 0.57938725

C -1.64042389 2.31194782 0.85470837  
C -2.82727003 3.00642228 0.53382540  
H -3.05301571 3.96994185 0.98767060  
C -3.73431134 2.43183494 -0.34217632  
C -3.46513128 1.17132974 -0.91526669  
C -4.32085896 0.49858770 -1.84684360  
H -5.24678421 0.99000156 -2.15719748  
C -3.99160910 -0.73367292 -2.34323072  
H -4.65248775 -1.23416996 -3.05615830  
C -2.78255296 -1.39698446 -1.95225656  
C -2.38074493 -2.66819000 -2.41654587  
C -1.17737150 -3.20552468 -1.99796641  
H -0.85992616 -4.18289709 -2.35810494  
C -0.37305203 -2.48118782 -1.09165716  
C -1.91838360 -0.76048028 -1.02826822  
C -2.26167846 0.53859228 -0.50461978  
C -0.54507113 2.74675012 1.80312920  
C 0.94948542 -2.90947223 -0.50100380  
C -0.96132189 5.25535965 1.56361246  
H -1.92180860 5.51702833 2.04498863  
C 0.09503212 6.32601547 1.87164962  
H 0.89402503 6.28772116 1.11322773  
H -0.33657965 7.33757830 1.87383795  
C 0.63614148 5.88481998 3.23949003  
H -0.07065079 6.16491938 4.03806925  
H 1.61552691 6.32349443 3.47806931  
C 0.71296334 4.36118412 3.10589170  
H 1.66755688 4.02370024 2.66656566  
H 0.57471728 3.81687427 4.05246496  
C 3.02717400 -4.14117670 -0.48843107  
H 2.88159347 -4.65129185 0.47649249

H 3.55084515 -3.19022226 -0.29104805  
 C 3.74133468 -4.98155451 -1.55020142  
 C 3.17268682 -4.42440224 -2.86262083  
 C 1.68799210 -4.21701241 -2.53992629  
 H 3.31364465 -5.09495115 -3.72307825  
 H 3.61044431 -3.43965220 -3.09105706  
 H 3.48275447 -6.04803324 -1.43725312  
 H 4.83409929 -4.88247490 -1.47397697  
 H 1.25509655 -3.40680194 -3.15035892  
 Er 0.37253773 -0.37310246 1.44957697  
 N 2.53425193 -0.76249081 3.18247676  
 O 3.48667002 -0.94890070 3.90948200  
 O 2.63146996 -0.12552525 2.04858088  
 O 1.33871877 -1.17172360 3.45917892  
 O 1.49127150 0.72323024 -0.28655574  
 H 1.24911845 0.60330969 -1.31214559  
 H 2.44860744 0.53808874 -0.22743185  
 N -1.79745770 -1.43462217 2.93479204  
 O -1.13515675 -2.13383579 2.06851935  
 O -1.43022275 -0.19065532 3.01043582  
 O -2.69189095 -1.89783537 3.61353302  
 H 1.12548113 -5.16014194 -2.66722679  
 H -1.12468636 5.11730194 0.48496887  
 N 1.34332883 -0.74665862 -3.06412292  
 O 0.79916728 -1.41848743 -3.96954107  
 O 0.76949543 0.36056468 -2.68003225  
 O 2.40337896 -1.11198282 -2.49485660

**L3\*Er(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -14872.689825, E0 = -14872.257121, G= 228.5721 at T=298.150 K

H -4.08139801 3.44147348 -0.96787697  
 H -3.00881958 -2.82408571 -3.52292681

N -1.08404922 1.23223245 0.11228622  
 N 0.05018094 3.93662238 2.18623042  
 N -0.66522866 -1.21638477 -0.88580167  
 N 1.43011940 -4.12544584 -1.10205114  
 O 0.43854299 1.72125900 2.14146590  
 O 1.15982258 -2.49382305 0.42306781  
 C -1.24892843 2.44661140 0.64871860  
 C -2.33555532 3.26717091 0.28032073  
 H -2.50030041 4.22933722 0.76148516  
 C -3.22717619 2.82219672 -0.68248546  
 C -3.04416132 1.56050849 -1.28570664  
 C -3.91212511 1.00978887 -2.28507090  
 H -4.75971794 1.60763943 -2.62980127  
 C -3.69800639 -0.24103041 -2.79515004  
 H -4.37310600 -0.65081853 -3.55079031  
 C -2.59822869 -1.04475391 -2.34805179  
 C -2.34053421 -2.35752630 -2.79466486  
 C -1.25279403 -3.05838466 -2.29906344  
 H -1.07768834 -4.08114290 -2.62734079  
 C -0.41157708 -2.44650936 -1.34632480  
 C -1.71208477 -0.52363890 -1.36897802  
 C -1.93784380 0.79583573 -0.83104622  
 C -0.20557776 2.71497917 1.70803654  
 C 0.78117085 -3.05094481 -0.64300907  
 C -0.39743140 5.25881100 1.68831491  
 H -1.37340462 5.51922989 2.13539886  
 C 0.69318128 6.21009207 2.19825006  
 H 1.54782832 6.20449972 1.50238895  
 H 0.32252541 7.24128962 2.28526759  
 C 1.08976686 5.58482790 3.54297686  
 H 0.33936188 5.82253075 4.31438446



H	2.07083988	5.92527485	3.90243292
C	1.08874810	4.08380318	3.24328828
H	2.05462670	3.73392320	2.84046173
H	0.83485663	3.44677758	4.10351706
C	2.58380842	-4.64859009	-0.31911203
H	2.26098895	-4.88044786	0.70669985
H	3.35502672	-3.86176729	-0.25807053
C	3.04924345	-5.86184645	-1.12799466
C	2.69281983	-5.47792006	-2.57098532
C	1.32375526	-4.80276251	-2.41592121
H	2.64532328	-6.33683300	-3.25534058
H	3.42223024	-4.75436163	-2.96984935
H	2.49425292	-6.76325798	-0.82119870
H	4.12185431	-6.05498171	-0.98722667
H	1.11069727	-4.07584047	-3.21267629
Er	0.57878327	-0.34344599	1.08476198
N	-0.99206078	-1.43018472	3.09043741
O	0.29728949	-1.24897861	3.18721104
O	-1.49604619	-1.04891992	1.94401658
O	-1.65762353	-1.90452635	3.97438359
N	2.92572880	0.54243034	-0.09914268
O	1.77236104	0.59620321	-0.71452069
O	2.86271119	0.04008264	1.10344124
O	3.95455241	0.92313981	-0.59906346
H	0.52257913	-5.56257629	-2.38437128
H	-0.48411003	5.25315857	0.59236908

**L3\*Tm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15711.145698, E0 = -15710.674892, G= 245.8307 at T=298.150 K

H	-4.35207415	3.31162238	-0.70123279
H	-3.37195897	-2.97982430	-3.23333454

N	-1.21792865	1.18228710	0.13417481
N	0.10057260	3.97840762	1.93064713
N	-0.85192555	-1.27610230	-0.81779569
N	1.30864120	-4.06240749	-1.13836491
O	0.39533785	1.75242794	2.09505987
O	0.73181790	-2.78695083	0.64308655
C	-1.35470593	2.40324974	0.64711714
C	-2.48481226	3.20235515	0.37075877
H	-2.61152005	4.17464924	0.84682292
C	-3.45958543	2.71797061	-0.48640031
C	-3.30964088	1.44422340	-1.07185912
C	-4.25469589	0.84863770	-1.96886468
H	-5.14776325	1.41780972	-2.24098873
C	-4.05907202	-0.40824586	-2.47055793
H	-4.79351330	-0.85126287	-3.14887929
C	-2.90527034	-1.17994046	-2.11370754
C	-2.65846372	-2.49369192	-2.56229615
C	-1.52814186	-3.16912627	-2.12907028
H	-1.34093320	-4.19759893	-2.44219303
C	-0.64195156	-2.52148581	-1.24578953
C	-1.94659257	-0.61707586	-1.22888124
C	-2.14855003	0.71324950	-0.70702267
C	-0.22854581	2.71277428	1.60291958
C	0.53003138	-3.15022492	-0.53173196
C	-0.27025652	5.23025942	1.24311030
H	-1.15089929	5.69399214	1.72566652
C	0.97119379	6.11228514	1.43630660
H	1.72354996	5.86192465	0.67056102
H	0.73132908	7.18286276	1.35684454
C	1.46957874	5.69523144	2.82842636
H	0.85672820	6.17285347	3.61101198

H	2.52142215	5.96135330	3.00613666
C	1.26118267	4.17697620	2.83509326
H	2.12543273	3.62245679	2.43071795
H	1.04032433	3.75969672	3.82944322
C	2.51947236	-4.53060436	-0.41410905
H	2.23279595	-5.20446730	0.40798858
H	3.01915622	-3.65302706	0.03095956
C	3.35804439	-5.20733738	-1.50594962
C	2.94142008	-4.46273375	-2.78420258
C	1.42923200	-4.28901052	-2.59245205
H	3.18165922	-5.00742006	-3.70926046
H	3.41645360	-3.46874452	-2.81876922
H	3.10282326	-6.27734661	-1.58706617
H	4.43408251	-5.12613058	-1.29447222
H	1.02316773	-3.43434930	-3.15170932
Tm	0.84215516	-0.33035347	0.93308592
N	-0.59450102	-1.17537129	3.23812652
O	0.68258333	-1.07915640	3.20357394
O	-1.18984723	-0.83627337	2.12080836
O	-1.22003341	-1.54899430	4.21151829
N	3.55238199	-0.36318815	1.78599584
O	2.83879590	0.71613842	1.64355004
O	2.92510772	-1.45160270	1.51608574
O	4.71561909	-0.33080646	2.14418101
N	1.97319961	0.35401717	-1.60341132
O	2.44291592	0.65662724	-2.68614316
O	2.06585121	-0.83935148	-1.11022913
O	1.33489656	1.19806373	-0.85962874
H	0.88886660	-5.20773077	-2.88798904
H	-0.49885193	5.04086256	0.18448389
O	-3.87807155	-0.97135359	1.29887748

H -3.00479794 -0.95020849 1.75667107

H -4.21291828 -1.85576653 1.52455103

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15711.148628, E0 = -15710.677500, G= 248.7671 at T=298.150 K

H -4.66133642 2.95834041 -0.58265585

H -3.04410815 -3.22385335 -3.10055280

N -1.38916671 1.10099566 0.34377280

N -0.39065152 4.01858807 2.18973160

N -0.76987630 -1.30208480 -0.62010229

N 1.70563889 -3.83515167 -1.11644304

O 0.22002761 1.85549009 2.26063633

O 1.31624568 -2.35447001 0.54594111

C -1.63218820 2.31069827 0.84742504

C -2.82166576 3.00618672 0.53673577

H -3.04796839 3.96461105 1.00136173

C -3.73009014 2.43856120 -0.34197941

C -3.46200442 1.18064070 -0.92239881

C -4.32388544 0.50804996 -1.84884965

H -5.25152302 1.00018024 -2.15318894

C -4.00169611 -0.72632885 -2.34541607

H -4.66992855 -1.22624075 -3.05187225

C -2.79302216 -1.39282870 -1.95879805

C -2.39909673 -2.67021871 -2.41352582

C -1.19599235 -3.21096349 -1.99670851

H -0.88859099 -4.19478416 -2.34805727

C -0.38219002 -2.48138928 -1.10284770

C -1.92036474 -0.75389338 -1.04391432

C -2.25552344 0.54863721 -0.52135354

C -0.54468864 2.73242140 1.81044424

C 0.94702268 -2.90253782 -0.51961446

C -0.94477099 5.24368858 1.58024037

H	-1.90820253	5.51174164	2.05224967
C	0.11614855	6.30543089	1.90289557
H	0.92408228	6.26241779	1.15425062
H	-0.30744812	7.32040787	1.90220380
C	0.63665724	5.85714197	3.27655697
H	-0.07785740	6.14170027	4.06664848
H	1.61638463	6.28759050	3.52839875
C	0.70293182	4.33300972	3.14113140
H	1.66103077	3.98883891	2.71476889
H	0.54738230	3.78828382	4.08483076
C	3.02427411	-4.13601780	-0.50732142
H	2.88594484	-4.61861372	0.47265145
H	3.55789399	-3.18439674	-0.34276447
C	3.71884561	-5.01137972	-1.55370545
C	3.14014173	-4.48500347	-2.87442493
C	1.66138470	-4.25321436	-2.54078770
H	3.26404071	-5.18093634	-3.71716666
H	3.58718920	-3.51267409	-3.13568878
H	3.45216417	-6.07192373	-1.40854561
H	4.81321144	-4.92042923	-1.49278176
H	1.23030186	-3.45319152	-3.16493511
Tm	0.38107756	-0.37748626	1.43873858
N	2.52438545	-0.52659345	3.22749734
O	3.45783758	-0.59093940	3.99991202
O	2.63688302	-0.02961588	2.03065944
O	1.33423221	-0.94024360	3.51911211
O	1.49628258	0.73708665	-0.29911759
H	1.28621387	0.60028654	-1.31448507
H	2.45802379	0.59224802	-0.21003592
N	-1.78592479	-1.50585151	2.88534093
O	-1.00698137	-2.21014953	2.12693596

O -1.52950037 -0.23311707 2.88217068  
 O -2.68657804 -1.99256301 3.54096603  
 H 1.08612967 -5.19181871 -2.64072347  
 H -1.09846342 5.10945511 0.49966902  
 N 1.39650023 -0.76595843 -3.10346818  
 O 0.84484750 -1.44803035 -3.99828482  
 O 0.82960469 0.34133577 -2.72948241  
 O 2.46032596 -1.12917161 -2.54187918

**L3\*Tm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15354.191187, E0 = -15353.758722, G= 228.0095 at T=298.150 K

H -4.08928633 3.48240256 -1.06912804  
 H -3.01620030 -2.78331637 -3.62572646  
 N -1.10489833 1.26394606 0.02697230  
 N 0.00162726 3.94828796 2.14714384  
 N -0.68492490 -1.18413174 -0.97294396  
 N 1.38374829 -4.11977291 -1.14663458  
 O 0.41623434 1.74074697 2.05453587  
 O 1.14052379 -2.44922352 0.33766147  
 C -1.27353442 2.47503495 0.56956834  
 C -2.35552979 3.29925275 0.19423373  
 H -2.52240276 4.26064348 0.67578983  
 C -3.24011326 2.85908318 -0.77723533  
 C -3.05732203 1.59756887 -1.38157749  
 C -3.91967821 1.05123031 -2.38823652  
 H -4.76277733 1.65222764 -2.73847580  
 C -3.70543194 -0.19949542 -2.89868569  
 H -4.37599277 -0.60610628 -3.66006279  
 C -2.61116529 -1.00683224 -2.44451332  
 C -2.35288787 -2.31992531 -2.89079642  
 C -1.27169788 -3.02525854 -2.38730621  
 H -1.09879565 -4.04826117 -2.71535659

C -0.43466040 -2.41696167 -1.42803109  
 C -1.72902358 -0.48972133 -1.45998442  
 C -1.95532274 0.83058214 -0.92095053  
 C -0.23678543 2.73477221 1.63903356  
 C 0.75213480 -3.02349591 -0.71425921  
 C -0.46735001 5.27685595 1.68806958  
 H -1.45547748 5.50097513 2.12815332  
 C 0.59455067 6.23408413 2.24595881  
 H 1.45574403 6.27707577 1.55967677  
 H 0.19682102 7.25140238 2.36906672  
 C 0.99412173 5.56826019 3.57021093  
 H 0.23172197 5.75927114 4.34282589  
 H 1.96375120 5.91789865 3.95116949  
 C 1.03097308 4.08016014 3.21519470  
 H 2.00695944 3.76806927 2.80556130  
 H 0.78852838 3.40490532 4.04904413  
 C 2.52655101 -4.64102554 -0.34664348  
 H 2.20276856 -4.82108355 0.68907082  
 H 3.31875086 -3.87319469 -0.32062584  
 C 2.95498157 -5.89808559 -1.10651612  
 C 2.60793710 -5.56155920 -2.56371832  
 C 1.26030695 -4.83840132 -2.43666363  
 H 2.53255820 -6.44594765 -3.21216130  
 H 3.35902357 -4.87832451 -2.99214268  
 H 2.37402916 -6.76987362 -0.76408792  
 H 4.02167845 -6.11682367 -0.95891517  
 H 1.07508731 -4.13311815 -3.25952387  
 Tm 0.57448846 -0.31758726 1.02017939  
 N -0.58421320 -1.43340456 3.25697398  
 O 0.68274009 -1.18261600 3.18551922  
 O -1.25322449 -1.10637569 2.16716170

O -1.12220502 -1.91948116 4.21851110  
 N 3.13789678 0.42093277 0.31111270  
 O 2.08557343 0.56155634 -0.47273204  
 O 2.86754417 -0.10441027 1.46010697  
 O 4.24301958 0.75914794 -0.03283515  
 H 0.43488294 -5.57059669 -2.38325071  
 H -0.53635663 5.30803728 0.59121472

**L3\*Yb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16203.916575, E0 = -16203.445940, G= 245.7998 at T=298.150 K

H -4.34556150 3.31052256 -0.68713999  
 H -3.35518074 -2.97790337 -3.22467566  
 N -1.21337533 1.18203175 0.15317966  
 N 0.10211512 3.96748734 1.96269119  
 N -0.83044851 -1.26465046 -0.82251227  
 N 1.31750238 -4.06760788 -1.12915683  
 O 0.38405439 1.73853123 2.12968349  
 O 0.76843858 -2.76229310 0.63972288  
 C -1.35461664 2.39977813 0.67301100  
 C -2.48352742 3.19915915 0.39345974  
 H -2.61382532 4.16895628 0.87364107  
 C -3.45287919 2.71751785 -0.47145256  
 C -3.29786801 1.44731379 -1.06339586  
 C -4.23915243 0.85358793 -1.96567690  
 H -5.13195133 1.42273128 -2.23864794  
 C -4.04196119 -0.40242666 -2.46906590  
 H -4.77540255 -0.84491086 -3.14881802  
 C -2.88805842 -1.17383730 -2.11171389  
 C -2.64107752 -2.48925209 -2.55614495  
 C -1.51171362 -3.16434669 -2.11959291  
 H -1.32773066 -4.19518185 -2.42673469



C -0.62150759 -2.51277828 -1.24276638  
 C -1.92916763 -0.60935402 -1.22888613  
 C -2.13675904 0.71660131 -0.69893599  
 C -0.23283331 2.70353723 1.63588762  
 C 0.55291086 -3.13835263 -0.52819484  
 C -0.26415941 5.21998501 1.27325618  
 H -1.14304066 5.68712234 1.75557077  
 C 0.98044688 6.09776258 1.46490860  
 H 1.73156178 5.84404039 0.69906217  
 H 0.74426371 7.16907120 1.38452601  
 C 1.47814631 5.68034172 2.85715342  
 H 0.86714756 6.16029310 3.63974762  
 H 2.53092718 5.94329786 3.03401041  
 C 1.26521850 4.16276836 2.86475611  
 H 2.12692022 3.60670662 2.45693922  
 H 1.04510093 3.74629951 3.85957217  
 C 2.52770710 -4.53805256 -0.40672040  
 H 2.24043846 -5.19630718 0.42770675  
 H 3.04028797 -3.65938997 0.02112890  
 C 3.35194802 -5.23858309 -1.49413204  
 C 2.94091249 -4.50022078 -2.77764177  
 C 1.43177354 -4.30480814 -2.58230782  
 H 3.17044640 -5.05646420 -3.69854689  
 H 3.42941356 -3.51323605 -2.82315469  
 H 3.07931590 -6.30515385 -1.56299436  
 H 4.42997932 -5.17231464 -1.28766453  
 H 1.03614354 -3.44812465 -3.14594007  
 Yb 0.81833434 -0.30809838 0.92167509  
 N -0.64327168 -1.17559326 3.20912886  
 O 0.62895274 -1.02504301 3.20036840  
 O -1.22659266 -0.90302330 2.06999254

O	-1.27349985	-1.54267955	4.18331575
N	3.55767202	-0.22296333	1.69318926
O	2.86848307	0.83254689	1.39405382
O	2.90656090	-1.32776570	1.61460185
O	4.73074722	-0.16492140	2.02102828
N	1.95562482	0.30506280	-1.64008117
O	2.43195152	0.57475758	-2.73042846
O	2.09398580	-0.85612375	-1.08770359
O	1.26496053	1.15485585	-0.95498919
H	0.87847281	-5.21777296	-2.87159348
H	-0.49373186	5.02974558	0.21502249
O	-3.92089772	-0.95663983	1.27266061
H	-3.04312778	-0.96868587	1.72253716
H	-4.27594709	-1.83755326	1.48022044

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16203.921195, E0 = -16203.450024, G= 247.5264 at T=298.150 K

H	-4.67150068	2.94698429	-0.56647617
H	-3.02366161	-3.19829702	-3.13517714
N	-1.39132261	1.10255480	0.35587084
N	-0.40655956	4.04753542	2.18904543
N	-0.74516624	-1.28316760	-0.65029061
N	1.70654953	-3.84822392	-1.10780740
O	0.30552557	1.91690016	2.16608405
O	1.30238187	-2.36834025	0.55121154
C	-1.63287258	2.31750178	0.85235554
C	-2.82747602	3.00527239	0.54499775
H	-3.05848622	3.96302104	1.00749683
C	-3.73614025	2.43248963	-0.33022276
C	-3.46002579	1.18079436	-0.91838974
C	-4.31800795	0.51291680	-1.85155785
H	-5.24750948	1.00368595	-2.15224504

C -3.98914599 -0.71513659 -2.35794544  
 H -4.65472937 -1.21369660 -3.06788135  
 C -2.77597761 -1.37705338 -1.97754180  
 C -2.38038468 -2.65006804 -2.44222617  
 C -1.18042767 -3.19499755 -2.02252984  
 H -0.87524682 -4.17938423 -2.37415719  
 C -0.36677438 -2.46779180 -1.12660396  
 C -1.90254545 -0.74018502 -1.06123531  
 C -2.25049067 0.55170190 -0.51928908  
 C -0.52092886 2.76460338 1.77837551  
 C 0.94806445 -2.90668893 -0.52319992  
 C -1.03576159 5.26866102 1.64886773  
 H -1.99949765 5.46678448 2.15383387  
 C -0.02159201 6.36920500 1.99281812  
 H 0.76256555 6.40658569 1.21898723  
 H -0.49778900 7.35866070 2.05512071  
 C 0.56746805 5.88426781 3.32539010  
 H -0.13384277 6.09093142 4.15077639  
 H 1.53145814 6.35417366 3.56737375  
 C 0.70815289 4.37489557 3.11092138  
 H 1.66531062 4.10442257 2.63224268  
 H 0.62039065 3.77695870 4.03075790  
 C 3.01202250 -4.16305542 -0.47724819  
 H 2.85334063 -4.62891245 0.50760740  
 H 3.56029558 -3.21877766 -0.31865022  
 C 3.70368719 -5.06537724 -1.50251639  
 C 3.14948440 -4.55054522 -2.83823991  
 C 1.67140269 -4.28830671 -2.52459502  
 H 3.27032328 -5.26181602 -3.66851044  
 H 3.61678886 -3.59089684 -3.11059165  
 H 3.41691828 -6.11878443 -1.34447658

H 4.79866600 -4.99234581 -1.42981040  
 H 1.25895596 -3.49492717 -3.16866970  
 Yb 0.39466798 -0.35382459 1.41893637  
 N 2.59492779 -0.74503046 3.09415221  
 O 3.57164168 -0.94923341 3.78668833  
 O 2.63461900 0.01507680 2.03759241  
 O 1.43541169 -1.25660241 3.33918548  
 O 1.52864897 0.69931209 -0.35057703  
 H 1.35442543 0.56070900 -1.35696852  
 H 2.49232721 0.60745925 -0.22426216  
 N -1.79912043 -1.27079725 2.95888090  
 O -1.30122566 -1.95297229 1.97520244  
 O -1.26446807 -0.10318989 3.12693095  
 O -2.70123863 -1.68881512 3.65942955  
 H 1.08202720 -5.21914339 -2.61599588  
 H -1.20861983 5.17677307 0.56666183  
 N 1.47643077 -0.81236666 -3.18076897  
 O 0.94241112 -1.50769114 -4.07834053  
 O 0.91068476 0.29289556 -2.82925582  
 O 2.53055978 -1.17729056 -2.59954119

**L3\*Yb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15846.962677, E0 = -15846.530353, G= 228.2709 at T=298.150 K

H -4.04655600 3.47053313 -1.01229203  
 H -2.98394299 -2.80364776 -3.56094790  
 N -1.06880879 1.24598992 0.08729505  
 N 0.04981723 3.93245268 2.19616485  
 N -0.65551019 -1.20273268 -0.90982550  
 N 1.42356157 -4.12541437 -1.08571327  
 O 0.44816747 1.71965837 2.12436891  
 O 1.14852786 -2.48235726 0.42737150  
 C -1.23370695 2.45794034 0.62839305

C	-2.31366515	3.28418350	0.25214881
H	-2.47874928	4.24610758	0.73340553
C	-3.19901991	2.84538937	-0.71963739
C	-3.01845908	1.58332503	-1.32307768
C	-3.88025880	1.03742957	-2.33078146
H	-4.72124386	1.64011765	-2.68327355
C	-3.66862893	-0.21438070	-2.84009194
H	-4.33997488	-0.61866796	-3.60226893
C	-2.57729197	-1.02469885	-2.38391328
C	-2.32079244	-2.33943582	-2.82651854
C	-1.24116445	-3.04555845	-2.31971931
H	-1.06993759	-4.07019138	-2.64433050
C	-0.40484962	-2.43552732	-1.36065006
C	-1.69602990	-0.50732732	-1.39904654
C	-1.91906762	0.81354362	-0.86107850
C	-0.19619380	2.71501732	1.69909489
C	0.77820802	-3.04274035	-0.63936836
C	-0.40392587	5.25925064	1.71740961
H	-1.38878286	5.50227690	2.15480185
C	0.66977555	6.21216679	2.25965810
H	1.53151906	6.23315525	1.57299161
H	0.28502896	7.23633194	2.36621261
C	1.06074953	5.56289339	3.59471440
H	0.30066657	5.77649546	4.36369419
H	2.03465176	5.90637255	3.97044992
C	1.07833338	4.06865788	3.26381397
H	2.05124974	3.73722625	2.86212993
H	0.82495761	3.41128898	4.10870504
C	2.56510735	-4.65289068	-0.28915074
H	2.23198223	-4.87401104	0.73568994
H	3.34389043	-3.87346506	-0.22816098

C 3.02593541 -5.87712622 -1.08381605  
 C 2.68640804 -5.50146914 -2.53324509  
 C 1.32343137 -4.81007767 -2.39612126  
 H 2.63556290 -6.36622190 -3.20994544  
 H 3.42740870 -4.78982496 -2.93210196  
 H 2.45887303 -6.77035332 -0.77510023  
 H 4.09519243 -6.08002329 -0.93185443  
 H 1.12764382 -4.08574963 -3.19966888  
 Yb 0.57257980 -0.33600831 1.06219709  
 N -1.01730049 -1.42336571 3.05031967  
 O 0.25002530 -1.15701461 3.18598843  
 O -1.49899852 -1.11988544 1.87796581  
 O -1.68426359 -1.90591192 3.93128681  
 N 2.93524170 0.49606994 -0.12106804  
 O 1.80861092 0.47969621 -0.77514404  
 O 2.83522725 0.10751449 1.11760378  
 O 3.98011088 0.84103835 -0.61728656  
 H 0.51337934 -5.56059837 -2.36902761  
 H -0.47470233 5.27455378 0.62035078

**L3\*Lu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16708.119428, E0 = -16707.647810, G= 246.8703 at T=298.150 K

H -4.36776161 3.31028891 -0.69717026  
 H -3.34930801 -2.96595669 -3.26748776  
 N -1.23251867 1.18291616 0.12995955  
 N 0.09667175 3.95941830 1.94181621  
 N -0.83808279 -1.25041652 -0.85013163  
 N 1.31269670 -4.05742550 -1.13239241  
 O 0.40364727 1.73450613 2.06121898  
 O 0.75870973 -2.72427058 0.60905421  
 C -1.36984301 2.40018535 0.64907461

C	-2.50126314	3.19906950	0.37620494
H	-2.63227963	4.16783810	0.85824203
C	-3.47352624	2.71784544	-0.48645008
C	-3.31792092	1.44990289	-1.08346307
C	-4.25711060	0.85441238	-1.98700380
H	-5.15307617	1.41949201	-2.25818157
C	-4.05353498	-0.39919454	-2.49474502
H	-4.78493977	-0.84243464	-3.17620516
C	-2.89537811	-1.16670799	-2.14179730
C	-2.63948393	-2.47711706	-2.59453321
C	-1.50573456	-3.14696431	-2.16075754
H	-1.31596601	-4.17510748	-2.47290421
C	-0.62180835	-2.49472117	-1.27833962
C	-1.94016230	-0.60171449	-1.25514054
C	-2.15546584	0.72119349	-0.72082371
C	-0.23366426	2.70073843	1.59588468
C	0.54745728	-3.11659884	-0.55625838
C	-0.29967508	5.22427654	1.29371703
H	-1.17765105	5.66397762	1.80276513
C	0.93497276	6.11539030	1.48940122
H	1.67577040	5.89532995	0.70341390
H	0.68126506	7.18473196	1.44406259
C	1.46427870	5.66618776	2.85993195
H	0.86235887	6.11569834	3.66723680
H	2.51642394	5.93916130	3.02473736
C	1.27291214	4.14616728	2.82903647
H	2.13470292	3.61258864	2.39232612
H	1.07573533	3.69834328	3.81492496
C	2.51183414	-4.52727175	-0.38940164
H	2.20766449	-5.16052628	0.45819160
H	3.03309202	-3.64601374	0.02296040

C 3.33126664 -5.26806831 -1.45369494  
 C 2.93230891 -4.56527090 -2.76092625  
 C 1.42533946 -4.34352350 -2.57620215  
 H 3.15624928 -5.15353966 -3.66309071  
 H 3.43477464 -3.58718681 -2.83712530  
 H 3.04812002 -6.33338737 -1.49194801  
 H 4.40940666 -5.20678759 -1.24663031  
 H 1.04135168 -3.50058222 -3.16804218  
 Lu 0.86224383 -0.31642464 0.91250181  
 N -0.54158443 -1.10246861 3.22828412  
 O 0.72518229 -0.91543651 3.21263361  
 O -1.12636554 -0.89384383 2.06867194  
 O -1.16943932 -1.44303870 4.21054983  
 N 3.55812740 -0.35995275 1.71131289  
 O 2.86005878 0.72662765 1.52576423  
 O 2.89907432 -1.44895506 1.50511980  
 O 4.72654104 -0.33582312 2.04694033  
 N 1.94428825 0.44922629 -1.58935428  
 O 2.41494179 0.76268983 -2.66682339  
 O 2.04091740 -0.75558823 -1.10804152  
 O 1.30162072 1.27624881 -0.83327961  
 H 0.86078948 -5.25850201 -2.83589602  
 H -0.54275352 5.05974483 0.23418131  
 O -3.82945204 -0.98557580 1.28348935  
 H -2.94812441 -0.97753572 1.72600245  
 H -4.18892479 -1.85027313 1.54463017

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16708.120723, E0 = -16707.649789, G= 249.7340 at T=298.150 K

H -4.64258289 2.96658874 -0.59558582  
 H -3.02786350 -3.23209810 -3.10084319  
 N -1.39330530 1.08486140 0.35523155



N -0.36179805 4.00234079 2.18362355  
 N -0.78095227 -1.31463993 -0.59457827  
 N 1.72212827 -3.81736565 -1.09777057  
 O 0.24409246 1.83843195 2.23728967  
 O 1.32431233 -2.32698083 0.55415595  
 C -1.62159514 2.30289030 0.84580582  
 C -2.80396914 3.00608659 0.52579188  
 H -3.02125835 3.97179055 0.97913957  
 C -3.71747947 2.43891597 -0.34871376  
 C -3.46033239 1.17436814 -0.91933751  
 C -4.32004595 0.50125813 -1.84763527  
 H -5.24356270 0.99599212 -2.15988231  
 C -3.99890852 -0.73537660 -2.34042907  
 H -4.66428995 -1.23257470 -3.05140424  
 C -2.79380035 -1.40544987 -1.94789314  
 C -2.39094806 -2.67883635 -2.40615320  
 C -1.18494582 -3.21332836 -1.98856473  
 H -0.86752731 -4.19073057 -2.34836102  
 C -0.37965581 -2.48599505 -1.08542085  
 C -1.92949688 -0.76844686 -1.02561092  
 C -2.26196027 0.53482950 -0.50886089  
 C -0.52384442 2.71955395 1.79937518  
 C 0.95621008 -2.88920784 -0.50560981  
 C -0.92147028 5.23268270 1.58998060  
 H -1.87993932 5.49672270 2.07417059  
 C 0.14362881 6.29120016 1.90973783  
 H 0.94258708 6.25449085 1.15119898  
 H -0.27962601 7.30620861 1.92271078  
 C 0.68038464 5.83109426 3.27310562  
 H -0.02398804 6.10971975 4.07432747  
 H 1.66354609 6.25861263 3.51636028

C	0.74366450	4.30812931	3.12448883
H	1.69583106	3.96557283	2.68383598
H	0.59852856	3.75589728	4.06542873
C	3.04854941	-4.09455490	-0.49339709
H	2.92189288	-4.57539368	0.48892748
H	3.56636930	-3.13324428	-0.33520237
C	3.75270653	-4.96223593	-1.53954136
C	3.16154289	-4.44776773	-2.85920143
C	1.68024051	-4.23833513	-2.52187586
H	3.29382372	-5.14272642	-3.70143151
H	3.59078479	-3.46817398	-3.12316990
H	3.50267196	-6.02627993	-1.39046907
H	4.84576464	-4.85418749	-1.48241365
H	1.23727977	-3.44453287	-3.14658380
Lu	0.35499945	-0.37637538	1.41259861
N	2.44401979	-0.54511094	3.21944928
O	3.36524415	-0.61869061	4.00307274
O	2.57322741	-0.04242679	2.02336407
O	1.24364066	-0.95244652	3.49050546
O	1.42685688	0.71167582	-0.31464937
H	1.18765485	0.57326007	-1.34073997
H	2.38953710	0.55751026	-0.25359401
N	-1.79919374	-1.48438084	2.84815264
O	-1.02716219	-2.19004035	2.08232236
O	-1.53918517	-0.21073884	2.83453941
O	-2.69168568	-1.96672320	3.51543570
H	1.11894572	-5.18572807	-2.61788559
H	-1.08561563	5.10751152	0.50991118
N	1.31976974	-0.77921766	-3.08761907
O	0.78629786	-1.46720624	-3.98719025
O	0.72059739	0.31583220	-2.70439768

O 2.39065742 -1.11647975 -2.52202177

**L3\*Lu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15846.962677, E0 = -15846.530353, G= 228.2709 at T=298.150 K

H -4.04655600 3.47053313 -1.01229203

H -2.98394299 -2.80364776 -3.56094790

N -1.06880879 1.24598992 0.08729505

N 0.04981723 3.93245268 2.19616485

N -0.65551019 -1.20273268 -0.90982550

N 1.42356157 -4.12541437 -1.08571327

O 0.44816747 1.71965837 2.12436891

O 1.14852786 -2.48235726 0.42737150

C -1.23370695 2.45794034 0.62839305

C -2.31366515 3.28418350 0.25214881

H -2.47874928 4.24610758 0.73340553

C -3.19901991 2.84538937 -0.71963739

C -3.01845908 1.58332503 -1.32307768

C -3.88025880 1.03742957 -2.33078146

H -4.72124386 1.64011765 -2.68327355

C -3.66862893 -0.21438070 -2.84009194

H -4.33997488 -0.61866796 -3.60226893

C -2.57729197 -1.02469885 -2.38391328

C -2.32079244 -2.33943582 -2.82651854

C -1.24116445 -3.04555845 -2.31971931

H -1.06993759 -4.07019138 -2.64433050

C -0.40484962 -2.43552732 -1.36065006

C -1.69602990 -0.50732732 -1.39904654

C -1.91906762 0.81354362 -0.86107850

C -0.19619380 2.71501732 1.69909489

C 0.77820802 -3.04274035 -0.63936836

C -0.40392587 5.25925064 1.71740961

H -1.38878286 5.50227690 2.15480185

C	0.66977555	6.21216679	2.25965810
H	1.53151906	6.23315525	1.57299161
H	0.28502896	7.23633194	2.36621261
C	1.06074953	5.56289339	3.59471440
H	0.30066657	5.77649546	4.36369419
H	2.03465176	5.90637255	3.97044992
C	1.07833338	4.06865788	3.26381397
H	2.05124974	3.73722625	2.86212993
H	0.82495761	3.41128898	4.10870504
C	2.56510735	-4.65289068	-0.28915074
H	2.23198223	-4.87401104	0.73568994
H	3.34389043	-3.87346506	-0.22816098
C	3.02593541	-5.87712622	-1.08381605
C	2.68640804	-5.50146914	-2.53324509
C	1.32343137	-4.81007767	-2.39612126
H	2.63556290	-6.36622190	-3.20994544
H	3.42740870	-4.78982496	-2.93210196
H	2.45887303	-6.77035332	-0.77510023
H	4.09519243	-6.08002329	-0.93185443
H	1.12764382	-4.08574963	-3.19966888
Yb	0.57257980	-0.33600831	1.06219709
N	-1.01730049	-1.42336571	3.05031967
O	0.25002530	-1.15701461	3.18598843
O	-1.49899852	-1.11988544	1.87796581
O	-1.68426359	-1.90591192	3.93128681
N	2.93524170	0.49606994	-0.12106804
O	1.80861092	0.47969621	-0.77514404
O	2.83522725	0.10751449	1.11760378
O	3.98011088	0.84103835	-0.61728656
H	0.51337934	-5.56059837	-2.36902761
H	-0.47470233	5.27455378	0.62035078

## Ligand L4

E= -2142.322482, E0 = -2141.943196, G= 200.5447 at T=298.150 K

Cl	-4.65378714	3.99378085	-1.50815678
Cl	-3.47726941	-2.91266418	-4.40026712
N	-1.14455450	1.39452755	-0.23621914
N	0.88670796	2.73105788	1.38006496
N	-0.79553300	-1.14055133	-1.17604840
N	1.10540342	-2.95182633	0.03058689
O	-0.85728842	3.97260189	2.14610434
O	1.08520746	-4.01330662	-1.97929978
C	-1.33009493	2.60832334	0.26236436
C	-2.42187214	3.43653727	-0.08372008
H	-2.52922106	4.40148544	0.41146547
C	-3.31226492	2.97607946	-1.02582753
C	-3.15152264	1.68723452	-1.60143054
C	-4.02668715	1.14222491	-2.58644271
H	-4.86977339	1.74733448	-2.92395663
C	-3.81709337	-0.10515072	-3.10302877
H	-4.48735428	-0.50971705	-3.86325002
C	-2.72516727	-0.91062397	-2.66403961
C	-2.45182300	-2.21145511	-3.16556001
C	-1.37969708	-2.93052459	-2.69101501
H	-1.10991192	-3.91568112	-3.07168579
C	-0.58977431	-2.35310960	-1.67163599
C	-1.82774091	-0.41951004	-1.66471505
C	-2.03376675	0.92642987	-1.13683045
C	-0.40536746	3.15952706	1.33754981
C	0.59971559	-3.17912412	-1.21387267
C	1.64230227	1.92531943	0.39602691
H	1.82252121	2.51440001	-0.52340811
H	1.07744324	1.02638686	0.12127180

C	2.96258593	1.64891815	1.12331522
H	2.84569240	0.78314310	1.79736674
H	3.78192782	1.43285966	0.42153043
C	3.18250632	2.93188167	1.94123340
H	3.57358193	3.73075676	1.28954875
H	3.88324118	2.80015588	2.77879572
C	1.77009475	3.28874421	2.42266273
H	1.53722310	2.82401943	3.39750576
H	1.59305704	4.37080288	2.52540612
C	2.27824569	-3.73876595	0.45342606
H	3.10659552	-3.59952903	-0.25829107
H	2.02767897	-4.81510353	0.45896098
C	2.57850289	-3.21151686	1.86134076
C	1.18865013	-2.81811905	2.38543105
C	0.52001405	-2.19065738	1.15347350
H	1.22244620	-2.11917233	3.23442078
H	0.63421047	-3.71802306	2.69997644
H	3.22797132	-2.32190537	1.80266964
H	3.08224344	-3.96428776	2.48538494
H	-0.57460755	-2.28580070	1.16603982
H	0.75640196	-1.11840630	1.06477737

**L4\*La(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -11555.128220, E0 = -11554.677591, G= 228.5033 at T=298.150 K

Cl	-4.89738369	3.64537525	-0.73742729
Cl	-3.78762484	-3.34525824	-3.57334924
N	-1.28458834	1.11064088	0.26824898
N	0.14199445	3.97497582	1.80161405
N	-0.91210419	-1.35245550	-0.70037997
N	1.37783527	-3.96768093	-1.29094815
O	0.20017353	1.79666364	2.39211082

O 0.76285243 -2.97080779 0.64826882  
C -1.41124797 2.34744716 0.74511337  
C -2.52028918 3.16060495 0.45109200  
H -2.63071942 4.15168524 0.89022970  
C -3.50253701 2.66018414 -0.38768941  
C -3.37979627 1.36732125 -0.95128632  
C -4.32517815 0.76977229 -1.83875704  
H -5.21608829 1.33906376 -2.10832667  
C -4.12848711 -0.48474088 -2.34365702  
H -4.85941839 -0.92659765 -3.02270555  
C -2.97178435 -1.24832392 -1.99923146  
C -2.68610477 -2.54919434 -2.48054934  
C -1.53469765 -3.21210170 -2.08671045  
H -1.32696497 -4.21890163 -2.44964671  
C -0.66819733 -2.56803560 -1.18684459  
C -2.01661921 -0.69987273 -1.09671831  
C -2.22099090 0.63568914 -0.56780881  
C -0.29916516 2.70914268 1.70349860  
C 0.55471003 -3.19963312 -0.56032258  
C -0.08653336 5.09153986 0.86171877  
H -0.90519083 5.74110508 1.22338068  
C 1.24998534 5.84433651 0.89543235  
H 1.96903598 5.34275770 0.22710146  
H 1.14098763 6.89144230 0.57692027  
C 1.68632722 5.68868399 2.36048818  
H 1.12901652 6.39222670 3.00137520  
H 2.76112962 5.86575842 2.51026225  
C 1.30307317 4.24130964 2.68968964  
H 2.10406637 3.52161956 2.44778633  
H 1.02037477 4.07973719 3.74124885  
C 2.63642859 -4.44098949 -0.65527976

H 2.41698432 -5.23778629 0.07218103  
 H 3.08574080 -3.59840870 -0.10224037  
 C 3.49454045 -4.90017557 -1.84121943  
 C 2.98872757 -4.03040981 -3.00277805  
 C 1.47382200 -4.00512218 -2.76532459  
 H 3.24536610 -4.42871237 -3.99539232  
 H 3.38318491 -3.00494409 -2.91281438  
 H 3.32069635 -5.96755648 -2.05807447  
 H 4.56636524 -4.76178360 -1.63765669  
 H 0.98460573 -3.12607026 -3.20759106  
 La 0.84659690 -0.46117336 1.32462835  
 N -0.95491135 -1.39926553 3.56271911  
 O 0.30802971 -1.27091157 3.72720313  
 O -1.39359009 -1.10355890 2.35466981  
 O -1.71744430 -1.76610327 4.43542671  
 N 3.58035398 -0.59539592 2.50373173  
 O 2.87603283 0.49861664 2.49362230  
 O 3.00161028 -1.62980115 1.97123408  
 O 4.69964600 -0.64429563 2.97490120  
 N 2.10535836 0.55871612 -1.23859715  
 O 2.57142901 0.96606803 -2.28887010  
 O 2.06194949 -0.70679313 -0.94908088  
 O 1.61918092 1.35707319 -0.34186357  
 H 0.99935555 -4.92305470 -3.15908909  
 H -0.34225461 4.71270084 -0.13802040  
 O -4.00360823 -0.94416296 1.34744322  
 H -3.16719460 -1.04560661 1.86149848  
 H -4.51685286 -1.72657275 1.61141205

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11555.122669, E0 = -11554.671427, G= 231.0993 at T=298.150 K

Cl -5.20045567 3.24251842 -0.69036120



Cl -3.40397215 -3.61800528 -3.46291733  
 N -1.42220354 1.03468645 0.45163086  
 N -0.39966443 4.03238297 2.10701561  
 N -0.77784383 -1.37794387 -0.54126942  
 N 1.71871459 -3.83047748 -1.23133826  
 O -0.02153555 1.86114931 2.59019852  
 O 1.27586663 -2.62016582 0.63142890  
 C -1.67500627 2.25226450 0.92889303  
 C -2.84230113 2.96190047 0.59136915  
 H -3.06880617 3.93009496 1.03477049  
 C -3.73830485 2.38432384 -0.29134253  
 C -3.47604394 1.11406767 -0.86172575  
 C -4.32597446 0.45049250 -1.79684365  
 H -5.24393892 0.94855189 -2.11197662  
 C -4.00083828 -0.78116083 -2.29268026  
 H -4.65597582 -1.27783716 -3.01007032  
 C -2.80108738 -1.44621909 -1.89773941  
 C -2.39392018 -2.72216105 -2.36457324  
 C -1.18921089 -3.26550508 -1.96272814  
 H -0.88024253 -4.24100018 -2.33367395  
 C -0.38923237 -2.54198766 -1.05930007  
 C -1.92895317 -0.82265598 -0.96508682  
 C -2.27340841 0.48193625 -0.43316415  
 C -0.64151156 2.71862841 1.93128347  
 C 0.93921953 -3.01261091 -0.51058352  
 C -0.77631444 5.16420507 1.23390114  
 H -1.72070479 5.62356663 1.57968020  
 C 0.38792232 6.14601851 1.42019498  
 H 1.22583413 5.85592270 0.76522619  
 H 0.09516925 7.17828417 1.17918742  
 C 0.76554531 5.94234133 2.89521098

H	0.04590090	6.46351242	3.54819512
H	1.77417409	6.30670166	3.13730526
C	0.65154725	4.42516756	3.07811856
H	1.58711731	3.89868927	2.82274842
H	0.36277196	4.11442280	4.09395695
C	3.04273820	-4.19297981	-0.66790420
H	2.91399598	-4.83715868	0.21594737
H	3.54703665	-3.26745892	-0.34125993
C	3.76840854	-4.86034441	-1.83943534
C	3.17485666	-4.14333439	-3.06021166
C	1.68845391	-4.02200556	-2.70548534
H	3.32571650	-4.68599319	-4.00494766
H	3.58644938	-3.12570405	-3.15341043
H	3.53793430	-5.93864012	-1.87255859
H	4.85902548	-4.74450016	-1.75540674
H	1.22231603	-3.14927149	-3.19364667
La	0.40490597	-0.54144663	1.78494990
N	2.63266110	-0.71060914	3.74317479
O	3.55127096	-0.77351713	4.53282166
O	2.78343892	-0.22389553	2.53997564
O	1.43316031	-1.11564279	4.02737093
O	1.64609587	0.84996283	0.08789846
H	1.37120795	0.79406869	-0.93129170
H	2.60716200	0.67803377	0.10549285
N	-2.03688979	-1.76311183	3.01214504
O	-1.17447758	-2.46543527	2.34168720
O	-1.78712487	-0.48593581	3.07149339
O	-3.01258397	-2.25752354	3.54040217
H	1.15127861	-4.95582247	-2.95231366
H	-0.89901561	4.83174658	0.19312771
N	1.28270352	-0.48357105	-2.74361777

O 0.64920139 -1.08505666 -3.64155054  
O 0.80239534 0.63873893 -2.28924012  
O 2.34534550 -0.93769270 -2.24714732

**L4\*La(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11198.152211, E0 = -11197.739891, G= 212.6490 at T=298.150 K

Cl -4.57999468 3.79377484 -1.04870248

Cl -3.39114976 -3.14701843 -3.88123965

N -1.12770307 1.18401659 0.24909462

N 0.05406790 3.99699116 2.13222551

N -0.70348066 -1.28873873 -0.76093841

N 1.44492805 -4.12877464 -1.18346667

O 0.25678095 1.77149355 2.42844868

O 1.03832126 -2.77262354 0.57083422

C -1.29176295 2.41263342 0.75268358

C -2.35771775 3.24223328 0.36747098

H -2.51960444 4.21443462 0.82869434

C -3.24904490 2.78657579 -0.59139526

C -3.07435513 1.50887644 -1.18356395

C -3.92978120 0.96777630 -2.19019365

H -4.76498508 1.57315421 -2.54539990

C -3.71577954 -0.28143057 -2.70007563

H -4.37811708 -0.68526995 -3.46717095

C -2.62953901 -1.08719885 -2.24327755

C -2.36037374 -2.40048242 -2.70856380

C -1.26993835 -3.10586834 -2.22387719

H -1.09167600 -4.12075186 -2.57359385

C -0.44853026 -2.50550842 -1.25548851

C -1.74846590 -0.58608437 -1.24333429

C -1.97613800 0.74177027 -0.70113540

C -0.27753183 2.73917651 1.82594109

C 0.73526347 -3.16688156 -0.58578247

C	-0.26052511	5.25555277	1.41317594
H	-1.21259522	5.67454624	1.78498876
C	0.90655488	6.17331362	1.79779422
H	1.77336478	5.96788740	1.14863706
H	0.63808191	7.23439932	1.69616854
C	1.20376885	5.75244141	3.24418068
H	0.45768896	6.18467808	3.93073773
H	2.20205665	6.05959988	3.58594298
C	1.06681609	4.22836876	3.19958496
H	2.00737834	3.73137975	2.90607023
H	0.72623736	3.77293205	4.14151382
C	2.59883189	-4.72289324	-0.45266628
H	2.25458860	-5.15542078	0.49868542
H	3.31758118	-3.91940141	-0.21688575
C	3.16949344	-5.74094152	-1.44337499
C	2.83851433	-5.12343454	-2.80959058
C	1.42138159	-4.57667828	-2.59727120
H	2.87442565	-5.84555387	-3.63757777
H	3.52866983	-4.29480410	-3.03768802
H	2.66311812	-6.71319628	-1.32878482
H	4.24662256	-5.89574194	-1.28989661
H	1.17201257	-3.74098349	-3.26666784
La	0.53446931	-0.52539086	1.51217866
N	-1.44549167	-1.63380980	3.39687562
O	-0.17043664	-1.52587581	3.67095280
O	-1.78940666	-1.20869005	2.20785618
O	-2.24121642	-2.08945274	4.17915297
N	3.17723560	0.34615192	0.50710952
O	2.09231472	0.45896161	-0.21476682
O	3.00091314	-0.17576624	1.69118333
O	4.26141262	0.69852668	0.10785739

H 0.67885017 -5.38456488 -2.72460151

H -0.33640340 5.07758474 0.33093241

**L4\*Ce(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -11922.549498, E0 = -11922.099577, G= 229.4037 at T=298.150 K

Cl -4.86945105 3.67636013 -0.75528437

Cl -3.64236045 -3.24267578 -3.73543525

N -1.20732653 1.18852544 0.17770723

N 0.06300719 4.03236866 1.95875609

N -0.79049182 -1.25260735 -0.82314038

N 1.34082890 -4.10539913 -1.20406735

O 0.44861877 1.82004380 2.10374546

O 0.90905398 -2.72668719 0.53318846

C -1.35475147 2.41249156 0.69965512

C -2.49227238 3.20105839 0.43077672

H -2.64602780 4.16441965 0.91309321

C -3.45137262 2.71186876 -0.43480903

C -3.30018568 1.44247627 -1.05194604

C -4.21690416 0.86126655 -1.96317720

H -5.11133432 1.42301273 -2.23571920

C -3.99344802 -0.38946810 -2.49151444

H -4.70943451 -0.82640827 -3.18931699

C -2.84445596 -1.14678895 -2.14216280

C -2.55046248 -2.45396137 -2.62451029

C -1.41634309 -3.12419701 -2.20527220

H -1.22970116 -4.13998222 -2.55186391

C -0.54823685 -2.49310160 -1.29757595

C -1.89668512 -0.60426390 -1.22436166

C -2.12680149 0.71848196 -0.67475587

C -0.23470546 2.76101732 1.62764573

C 0.61776590 -3.12988400 -0.62506849

C	-0.36517102	5.27982903	1.29442739
H	-1.26435423	5.69361830	1.78738606
C	0.83515549	6.21334362	1.50193799
H	1.59529006	6.01472616	0.72859824
H	0.54518062	7.27279520	1.44559312
C	1.35772991	5.79074669	2.88303256
H	0.72351879	6.21755648	3.67783999
H	2.39545560	6.10455227	3.06595564
C	1.22518718	4.26496458	2.85333300
H	2.11231160	3.76913404	2.42293572
H	1.03958273	3.81063485	3.83858132
C	2.52275014	-4.63032818	-0.47420549
H	2.20090175	-5.18558168	0.42034355
H	3.13536716	-3.77811289	-0.13326137
C	3.23793697	-5.49458504	-1.51895154
C	2.87119460	-4.81509972	-2.84728074
C	1.39674580	-4.44540119	-2.63934016
H	3.01496124	-5.46009064	-3.72658205
H	3.46304750	-3.89473128	-2.98130107
H	2.85043597	-6.52700377	-1.49883926
H	4.32216024	-5.53123617	-1.33940268
H	1.07597244	-3.58918023	-3.25023961
Ce	0.93451172	-0.31085441	0.96484810
N	-0.55679941	-1.16525197	3.36767793
O	0.71666402	-0.97443110	3.36085153
O	-1.14135718	-0.95149773	2.21446514
O	-1.17735004	-1.51802802	4.34791613
N	3.73957849	-0.30990776	1.83184254
O	3.05933261	0.78108943	1.61704302
O	3.07395577	-1.40272903	1.63841307
O	4.90097427	-0.29552400	2.18112516

N 2.10564303 0.54868454 -1.61023080  
 O 2.60022235 0.90419650 -2.66031003  
 O 2.22208405 -0.66515851 -1.15861917  
 O 1.41526628 1.34518898 -0.85637599  
 H 0.74506849 -5.31142807 -2.86002946  
 H -0.58880079 5.09774685 0.23341271  
 O -3.85433435 -0.89013427 1.36111963  
 H -2.99395561 -0.96371859 1.83206701  
 H -4.23858690 -1.77676046 1.46963644

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -11922.542964, E0 = -11922.093542, G= 230.4261 at T=298.150 K

Cl -5.14171219 3.32758212 -0.79864460  
 Cl -3.40777802 -3.61219645 -3.48094153  
 N -1.39745986 1.06006455 0.39618582  
 N -0.41226143 4.04711723 2.16453099  
 N -0.79120320 -1.34690917 -0.57626605  
 N 1.70289326 -3.83684993 -1.16867363  
 O 0.09788672 1.86535192 2.40103126  
 O 1.29545915 -2.46466756 0.57985944  
 C -1.63102698 2.31194925 0.85592043  
 C -2.78491688 3.02428460 0.49470270  
 H -3.00188470 4.00399733 0.91545457  
 C -3.69457936 2.44866157 -0.37887114  
 C -3.45549679 1.15801513 -0.92583317  
 C -4.30950689 0.49060309 -1.85080373  
 H -5.22136545 0.99789965 -2.16988897  
 C -4.00503254 -0.75551170 -2.33937287  
 H -4.66922903 -1.24880648 -3.05023980  
 C -2.81548262 -1.42387092 -1.93881512  
 C -2.40359426 -2.70347285 -2.38691187  
 C -1.20143390 -3.24934602 -1.97323930

H	-0.90042979	-4.23134232	-2.33172154
C	-0.40056869	-2.51950502	-1.07491684
C	-1.94280374	-0.79000193	-1.00621545
C	-2.26597881	0.51524448	-0.48488507
C	-0.60658848	2.75129747	1.84378183
C	0.93043917	-2.95804882	-0.51919663
C	-0.86650866	5.25252342	1.44413233
H	-1.84222865	5.59567022	1.83545911
C	0.22423986	6.28318214	1.76512194
H	1.07472217	6.15131235	1.07617784
H	-0.14572997	7.31447077	1.67000794
C	0.63199157	5.90668535	3.19731092
H	-0.11629377	6.27873516	3.91672373
H	1.61447430	6.30654716	3.48655295
C	0.62785059	4.37496948	3.16897225
H	1.59464228	3.95904493	2.83600378
H	0.38153937	3.90828705	4.13514233
C	3.02901697	-4.15539455	-0.58271360
H	2.90085793	-4.68617773	0.37335378
H	3.55451179	-3.20698094	-0.37808487
C	3.72386765	-4.97116375	-1.67561364
C	3.13394046	-4.38217592	-2.96434450
C	1.65466642	-4.18379450	-2.61358285
H	3.26025605	-5.03154659	-3.84290957
H	3.56914520	-3.39237809	-3.17485690
H	3.46592021	-6.03967476	-1.58263290
H	4.81780958	-4.87454557	-1.61529577
H	1.21027327	-3.35622597	-3.19096541
Ce	0.39055350	-0.40325338	1.56868470
N	2.63637209	-0.57923585	3.42687583
O	3.57845330	-0.65218413	4.18286562



O 2.74325705 -0.09486385 2.21860194  
 O 1.44121015 -0.96933514 3.74409652  
 O 1.59380007 0.73663753 -0.18309233  
 H 1.34200704 0.64514065 -1.24443841  
 H 2.55874324 0.59173918 -0.12631713  
 N -1.80897093 -1.64990878 3.05189514  
 O -1.01910245 -2.32444525 2.26827455  
 O -1.57921648 -0.36973298 3.07727361  
 O -2.69063616 -2.17036581 3.69944239  
 H 1.08873785 -5.12211227 -2.75543809  
 H -0.96487647 5.04708767 0.36798796  
 N 1.42182255 -0.67271203 -2.95782757  
 O 0.84715462 -1.29421091 -3.87374306  
 O 0.88553172 0.45173907 -2.54184318  
 O 2.46985054 -1.08289313 -2.40328646

**L4\*Ce(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11565.572850, E0 = -11565.161665, G= 211.0802 at T=298.150 K

Cl -4.54329586 3.82554245 -1.08012652  
 Cl -3.34653997 -3.13205433 -3.92779016  
 N -1.07949114 1.20096397 0.19028138  
 N 0.06126584 3.98259068 2.17093253  
 N -0.65948457 -1.24573123 -0.80945504  
 N 1.45306206 -4.14244318 -1.14561689  
 O 0.38721523 1.75671482 2.26710820  
 O 1.13795817 -2.61603022 0.47927701  
 C -1.24009430 2.43851423 0.69545859  
 C -2.30660057 3.26488924 0.31725493  
 H -2.46583557 4.23817015 0.77524614  
 C -3.21230006 2.80967426 -0.63528496  
 C -3.04981947 1.53100610 -1.22265625  
 C -3.91688657 0.98134291 -2.21568441

H -4.76017809 1.58148658 -2.56081533  
C -3.70193505 -0.26803076 -2.72683740  
H -4.37163067 -0.67707497 -3.48488259  
C -2.60318017 -1.06671202 -2.28525567  
C -2.32136822 -2.37284040 -2.75555348  
C -1.21834171 -3.06973290 -2.27340341  
H -1.03655434 -4.08152199 -2.62789130  
C -0.39775354 -2.46812701 -1.31008387  
C -1.72120452 -0.55234343 -1.29439950  
C -1.94700491 0.76183879 -0.75715548  
C -0.22283173 2.74514866 1.75679636  
C 0.78083223 -3.10776544 -0.63456368  
C -0.33311993 5.28435183 1.58156252  
H -1.30680752 5.60444403 1.99351609  
C 0.77972221 6.22958040 2.05102324  
H 1.64786625 6.14905214 1.37673557  
H 0.44365335 7.27607489 2.06242967  
C 1.12496662 5.68250608 3.44330549  
H 0.36655107 5.99649096 4.17876387  
H 2.10919714 6.01278973 3.80373740  
C 1.07725608 4.16540623 3.24453354  
H 2.04035878 3.75768948 2.89243960  
H 0.77940851 3.59848881 4.13917780  
C 2.59511328 -4.70824862 -0.37504372  
H 2.25253987 -5.02013731 0.62289125  
H 3.35488963 -3.91954398 -0.23914631  
C 3.09614301 -5.85341120 -1.25876760  
C 2.76412535 -5.37189674 -2.67820549  
C 1.38172698 -4.73076534 -2.50431895  
H 2.74418211 -6.18103504 -3.42192602  
H 3.48999262 -4.61136532 -3.00915956

H 2.54835486 -6.78193474 -1.02972257  
 H 4.16822720 -6.04196310 -1.10783327  
 H 1.16572821 -3.95354939 -3.25148296  
 Ce 0.58014679 -0.42538595 1.28496373  
 N -1.25539601 -1.53174973 3.22567868  
 O 0.03670657 -1.38845372 3.41842604  
 O -1.66605747 -1.12537146 2.05635309  
 O -1.98743463 -1.99699581 4.05806923  
 N 3.07466030 0.48320404 0.12469640  
 O 1.94608831 0.55956757 -0.52678245  
 O 2.97011256 -0.03244285 1.32451630  
 O 4.12495422 0.85382789 -0.33366522  
 H 0.59365088 -5.50407028 -2.53879809  
 H -0.40551013 5.20737267 0.48713359

**L4\*Pr(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12299.618839, E0 = -12299.168413, G= 229.4959 at T=298.150 K

Cl -4.87759018 3.66419935 -0.74198043  
 Cl -3.70807505 -3.28846693 -3.65770674  
 N -1.24044621 1.14925623 0.22293910  
 N 0.10597614 3.99943829 1.89623737  
 N -0.83983701 -1.29369819 -0.76534235  
 N 1.36177647 -4.04263115 -1.23273408  
 O 0.34152770 1.78456628 2.23478580  
 O 0.81393272 -2.84878922 0.60912466  
 C -1.37947667 2.37636995 0.72509563  
 C -2.50052333 3.17986822 0.44566068  
 H -2.63298821 4.15616941 0.90925437  
 C -3.47171187 2.68713880 -0.40977243  
 C -3.33269429 1.41002262 -1.00394261  
 C -4.26333523 0.82148385 -1.90766847

H -5.15507603 1.38803554 -2.17979860  
C -4.05223370 -0.42862794 -2.42439008  
H -4.77392387 -0.86808968 -3.11485600  
C -2.89833951 -1.19139099 -2.07597923  
C -2.61311388 -2.49503112 -2.55487704  
C -1.47073066 -3.16333890 -2.14299583  
H -1.27403009 -4.17633915 -2.49359560  
C -0.60495561 -2.52438712 -1.24179864  
C -1.94751000 -0.64380825 -1.16781497  
C -2.16715765 0.68076730 -0.62730932  
C -0.25762731 2.72406340 1.66882825  
C 0.58157855 -3.16622305 -0.57931256  
C -0.24102873 5.20558786 1.11773169  
H -1.10663188 5.72372580 1.57058299  
C 1.02216458 6.06849861 1.23867393  
H 1.76518023 5.73935699 0.49379364  
H 0.80818212 7.13492775 1.07535398  
C 1.51425183 5.74962044 2.65865517  
H 0.91371483 6.29913855 3.40264606  
H 2.57214761 6.00504351 2.81497169  
C 1.27348745 4.24142885 2.78250599  
H 2.12501383 3.64108658 2.41839314  
H 1.04665852 3.90465236 3.80560303  
C 2.57670331 -4.54698706 -0.54123026  
H 2.29284620 -5.22553587 0.27795324  
H 3.10614395 -3.68827891 -0.09393704  
C 3.37676334 -5.22358227 -1.66094100  
C 2.95493317 -4.44455004 -2.91650891  
C 1.45115662 -4.23896599 -2.69370294  
H 3.16478825 -4.97644663 -3.85613036  
H 3.45469570 -3.46229315 -2.94230509

H 3.09120321 -6.28466988 -1.75606155  
 H 4.45843458 -5.17518616 -1.46891737  
 H 1.05272114 -3.36332750 -3.22560334  
 Pr 0.86894482 -0.38740110 1.10097980  
 N -0.74328035 -1.21383703 3.43094373  
 O 0.52365166 -1.02195096 3.50242066  
 O -1.25885344 -1.02669096 2.23667717  
 O -1.42968547 -1.54559422 4.37602615  
 N 3.62020659 -0.46009403 2.09343028  
 O 2.96685028 0.65054196 1.91919672  
 O 2.95117044 -1.53224254 1.80198348  
 O 4.76602221 -0.48919401 2.49395251  
 N 2.09285069 0.49792060 -1.44178462  
 O 2.59656286 0.86640668 -2.48618793  
 O 2.15044022 -0.73508072 -1.03871989  
 O 1.45205295 1.30393231 -0.65524137  
 H 0.88478976 -5.13834667 -2.99941754  
 H -0.48334366 4.94097519 0.07857906  
 O -3.92966533 -0.91918057 1.33861399  
 H -3.07462192 -1.00110149 1.82167101  
 H -4.37103701 -1.76286447 1.53529882

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12299.613180, E0 = -12299.162519, G= 230.9470 at T=298.150 K

Cl -5.16419220 3.29152536 -0.71620572  
 Cl -3.38556194 -3.58216119 -3.51640177  
 N -1.39764857 1.04523754 0.41856086  
 N -0.39024690 4.02104568 2.15979218  
 N -0.77847570 -1.35309815 -0.57166177  
 N 1.71174467 -3.83995199 -1.17737794  
 O 0.08821510 1.84057403 2.46030164  
 O 1.27078259 -2.52044702 0.60725003

C -1.63988590 2.27284575 0.89794111  
 C -2.80403757 2.98599911 0.56325662  
 H -3.02735519 3.95304418 1.00968397  
 C -3.70786095 2.41983938 -0.32128337  
 C -3.45580339 1.14816082 -0.89643031  
 C -4.30608940 0.49059159 -1.83485842  
 H -5.22073984 0.99546826 -2.14921761  
 C -3.98915267 -0.74335980 -2.33646536  
 H -4.64715624 -1.23238587 -3.05636501  
 C -2.79521680 -1.41559386 -1.94093812  
 C -2.38431621 -2.69036579 -2.40663934  
 C -1.18328595 -3.23885059 -1.99507344  
 H -0.87671387 -4.21450663 -2.36671829  
 C -0.38794643 -2.52121353 -1.08352292  
 C -1.92684627 -0.79457957 -1.00234342  
 C -2.26005650 0.50613451 -0.46877265  
 C -0.59585947 2.71719003 1.88620424  
 C 0.93151516 -2.97739577 -0.51466316  
 C -0.83399457 5.20727587 1.39931762  
 H -1.79132724 5.58960724 1.79924822  
 C 0.28844365 6.22226524 1.65355325  
 H 1.12227952 6.03542089 0.95710713  
 H -0.05683975 7.25742483 1.51686406  
 C 0.71248990 5.90084410 3.09440136  
 H -0.01325440 6.32392263 3.80865479  
 H 1.70948029 6.28854132 3.34812641  
 C 0.67149740 4.36988258 3.13573909  
 H 1.62178934 3.91398668 2.80842686  
 H 0.42722178 3.95219612 4.12453651  
 C 3.02728772 -4.17997789 -0.58085471  
 H 2.88392544 -4.75513363 0.34711698

H 3.54418468 -3.24026752 -0.32112917  
 C 3.74770617 -4.94235754 -1.69600642  
 C 3.17448831 -4.30434418 -2.96911407  
 C 1.68855131 -4.13033962 -2.63515449  
 H 3.32047415 -4.91641521 -3.87117648  
 H 3.60574293 -3.30391574 -3.13258791  
 H 3.49771070 -6.01593494 -1.65321505  
 H 4.83962774 -4.83978605 -1.61264980  
 H 1.24502194 -3.28392482 -3.18664765  
 Pr 0.37157157 -0.47855127 1.62688589  
 N 2.59809208 -0.55074131 3.50236440  
 O 3.52519178 -0.58661807 4.28136826  
 O 2.72147441 -0.10769025 2.28445363  
 O 1.40056515 -0.94737893 3.81349230  
 O 1.57135105 0.77050138 -0.10178254  
 H 1.31128800 0.69246662 -1.13168561  
 H 2.52975392 0.58372766 -0.06705199  
 N -1.93560934 -1.66358066 2.98946643  
 O -1.10946286 -2.35963392 2.26350927  
 O -1.69510317 -0.38727531 3.01448369  
 O -2.86146641 -2.16750288 3.58896756  
 H 1.13351655 -5.06759739 -2.82196856  
 H -0.96168870 4.96278334 0.33489335  
 N 1.33649051 -0.61935502 -2.90301800  
 O 0.75182527 -1.24969697 -3.81204963  
 O 0.81322402 0.50201648 -2.48837113  
 O 2.38867044 -1.03859091 -2.35656548

**L4\*Pr(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -11942.646743, E0 = -11942.234687, G= 213.1257 at T=298.150 K

Cl -4.53877211 3.81441259 -1.06147969

Cl -3.34564376 -3.13799787 -3.90612936

N	-1.08117414	1.19405973	0.21344189
N	0.06908377	3.97814202	2.17635369
N	-0.66272318	-1.26162171	-0.78722042
N	1.45690250	-4.14424133	-1.13578653
O	0.37157443	1.75094914	2.31909442
O	1.11970460	-2.65915680	0.52385163
C	-1.24395728	2.42285132	0.72532034
C	-2.31310010	3.25099921	0.34803784
H	-2.47703958	4.22051144	0.81302470
C	-3.20823812	2.80099702	-0.61238205
C	-3.03786635	1.52603495	-1.20922804
C	-3.89532208	0.98331213	-2.21399117
H	-4.73241377	1.58745742	-2.56753373
C	-3.68089318	-0.26592749	-2.72498083
H	-4.34470844	-0.67027634	-3.49068284
C	-2.59249759	-1.07135010	-2.27114630
C	-2.31940055	-2.38420081	-2.73235035
C	-1.22773027	-3.08696246	-2.24190784
H	-1.05144250	-4.10266066	-2.58880854
C	-0.40611926	-2.48371458	-1.27642977
C	-1.71202528	-0.56452906	-1.27496243
C	-1.93819141	0.75750577	-0.73509264
C	-0.22227576	2.73210406	1.78975677
C	0.77602100	-3.12736487	-0.59804899
C	-0.31120384	5.27050352	1.55744386
H	-1.27962887	5.61306953	1.96385360
C	0.81372964	6.21313286	2.00321865
H	1.68058038	6.10466528	1.33118629
H	0.49107823	7.26382780	1.98876798
C	1.15219462	5.69555902	3.40834045
H	0.39725885	6.03604174	4.13558531



H	2.14004064	6.02310896	3.76131940
C	1.08705044	4.17481184	3.24543142
H	2.04541588	3.74792194	2.90323114
H	0.78292751	3.63205385	4.15288591
C	2.60517097	-4.71548605	-0.37873518
H	2.26549530	-5.05642605	0.61066085
H	3.35494304	-3.92108321	-0.22182316
C	3.12119508	-5.83138752	-1.29080820
C	2.78525209	-5.31703711	-2.69775844
C	1.39407372	-4.69916916	-2.50905228
H	2.77721834	-6.10628939	-3.46279931
H	3.50135779	-4.53828716	-3.00689721
H	2.58407617	-6.77197933	-1.08708024
H	4.19520235	-6.01137495	-1.14314997
H	1.16865432	-3.90759397	-3.23808479
Pr	0.57670742	-0.45161539	1.34403181
N	-1.34477150	-1.53983855	3.20054746
O	-0.05912225	-1.41081643	3.44037366
O	-1.71278381	-1.12749112	2.02084827
O	-2.10932422	-2.00141835	4.00712061
N	3.01942706	0.48873571	0.12104714
O	1.87863588	0.56266874	-0.50476223
O	2.94784021	-0.03850502	1.31934321
O	4.05813599	0.87239653	-0.35588703
H	0.61762303	-5.48303270	-2.56417060
H	-0.38620195	5.17100096	0.46505219

**L4\*Nd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -12686.521627, E0 = -12686.070821, G= 229.6118 at T=298.150 K

Cl	-4.87008715	3.66031504	-0.73161685
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Cl	-3.76875257	-3.32681537	-3.59673119
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N	-1.25004280	1.12002933	0.23800462
N	0.14445066	3.97984600	1.84641087
N	-0.88470292	-1.33243763	-0.73057896
N	1.36649179	-4.00161314	-1.23471785
O	0.31380722	1.77249753	2.27738261
O	0.73552710	-2.93785238	0.66408753
C	-1.37277055	2.35454440	0.72374189
C	-2.48723388	3.16596842	0.44344866
H	-2.60237002	4.15086222	0.89419866
C	-3.47218490	2.67315245	-0.39703500
C	-3.34976578	1.38668358	-0.97414821
C	-4.29472494	0.79409862	-1.86544883
H	-5.18445158	1.36585522	-2.13380218
C	-4.09984779	-0.45943174	-2.37417698
H	-4.83080959	-0.89775109	-3.05548668
C	-2.94613171	-1.22749460	-2.02919912
C	-2.66646314	-2.53170824	-2.50358558
C	-1.52258801	-3.20162964	-2.09783340
H	-1.32376242	-4.21429682	-2.44921565
C	-0.65336204	-2.55790710	-1.20122564
C	-1.98816180	-0.67857349	-1.13021934
C	-2.18976665	0.65341175	-0.59867734
C	-0.24748802	2.70447826	1.66812754
C	0.54575694	-3.19747066	-0.54111582
C	-0.15457056	5.15442944	1.00260150
H	-1.00042903	5.72984791	1.42271972
C	1.14102209	5.97282934	1.08209717
H	1.87324607	5.57186604	0.36218500
H	0.97045469	7.03593349	0.85729444
C	1.61403596	5.71644068	2.52125120
H	1.03338206	6.33171511	3.22870541

H	2.68080544	5.93776989	2.66925168
C	1.31232214	4.22831488	2.72991920
H	2.14202547	3.57420802	2.41099000
H	1.06390703	3.96219659	3.76875281
C	2.60090876	-4.48593187	-0.56248778
H	2.34838796	-5.24790573	0.19106165
H	3.06628418	-3.63584280	-0.03470168
C	3.46070719	-5.01564169	-1.71748686
C	2.99830675	-4.17543793	-2.91849279
C	1.48169601	-4.09397364	-2.70463991
H	3.25613523	-4.61900187	-3.89143610
H	3.42446089	-3.16039944	-2.86137676
H	3.25588894	-6.08441401	-1.89721525
H	4.53353071	-4.90312672	-1.50372112
H	1.02713335	-3.21566725	-3.18416715
Nd	0.83718175	-0.43214339	1.17912841
N	-0.85527730	-1.28487432	3.43459487
O	0.41627881	-1.15199757	3.53453732
O	-1.34404230	-0.99728251	2.24967575
O	-1.57034755	-1.64729571	4.34753942
N	3.55395603	-0.57084668	2.21804261
O	2.89135432	0.54397625	2.11036897
O	2.90134072	-1.62604356	1.84579456
O	4.69506168	-0.61422867	2.63285494
N	2.07805538	0.50156212	-1.33778441
O	2.59132099	0.86666679	-2.38044453
O	2.09378242	-0.74367625	-0.95910174
O	1.47579741	1.31273317	-0.53431487
H	0.98332232	-5.00930977	-3.07448053
H	-0.40442881	4.84388256	-0.02195549
O	-3.99284291	-0.96879971	1.30973792

H -3.14272285 -1.02025461 1.80706108

H -4.43799782 -1.79703641 1.55705345

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -12686.517753, E0 = -12686.066532, G= 231.4654 at T=298.150 K

Cl -5.18136549 3.26687717 -0.69776183

Cl -3.39267588 -3.61195588 -3.46663523

N -1.40425694 1.04813278 0.42498451

N -0.38504347 4.02298498 2.14067411

N -0.76977414 -1.35490763 -0.55682242

N 1.72663987 -3.82648921 -1.18731582

O 0.05827362 1.84178388 2.49866295

O 1.29126787 -2.52953839 0.61695021

C -1.65058184 2.26586032 0.90800393

C -2.81917691 2.97648931 0.57662195

H -3.04520512 3.94311833 1.02307618

C -3.72009468 2.40361524 -0.30569911

C -3.46399426 1.13386095 -0.87993199

C -4.31582642 0.46854806 -1.81286335

H -5.23380947 0.96704924 -2.12739468

C -3.99337912 -0.76533502 -2.30691266

H -4.65092325 -1.26206791 -3.02209044

C -2.79391837 -1.43207872 -1.91199291

C -2.38488626 -2.71006632 -2.37126517

C -1.17965269 -3.25127101 -1.96431446

H -0.87129593 -4.22841167 -2.33108211

C -0.37974894 -2.52357912 -1.06428337

C -1.92137134 -0.80394024 -0.98436117

C -2.26195312 0.50009555 -0.45625740

C -0.60316145 2.71448779 1.90119243

C 0.94855827 -2.97518587 -0.50450873

C -0.80887538 5.19293165 1.34372461

H	-1.75902796	5.60395098	1.73219097
C	0.33135605	6.19533491	1.56686497
H	1.16208708	5.97117329	0.87783325
H	0.00470492	7.23158264	1.39673686
C	0.74855298	5.91286325	3.01792479
H	0.03122517	6.37285471	3.71774673
H	1.75274062	6.28943014	3.25956368
C	0.67899334	4.38492775	3.10947490
H	1.62148964	3.90052414	2.80134463
H	0.42321366	4.00475836	4.11042452
C	3.05061507	-4.16333675	-0.60833359
H	2.92174840	-4.76088190	0.30758446
H	3.55807257	-3.22360992	-0.33064792
C	3.77216387	-4.89202452	-1.74528146
C	3.17989063	-4.23504448	-2.99995708
C	1.69446385	-4.08881426	-2.65017748
H	3.32692671	-4.82562160	-3.91610885
H	3.59576583	-3.22531676	-3.14515114
H	3.53693867	-5.96957207	-1.72379184
H	4.86332512	-4.77679110	-1.66857660
H	1.23427320	-3.23829365	-3.18127227
Nd	0.37640455	-0.49289730	1.66679537
N	2.54059768	-0.65475196	3.57988024
O	3.45357728	-0.72023350	4.37438583
O	2.69664478	-0.18210806	2.37385559
O	1.33466208	-1.04314291	3.85881662
O	1.57571363	0.79589742	-0.03418800
H	1.31226587	0.72894740	-1.05851924
H	2.53227806	0.60001040	-0.00297226
N	-1.95223212	-1.68707693	2.96135378
O	-1.10648358	-2.38518429	2.26705766

O -1.70998669 -0.40921888 2.99358988  
 O -2.90170670 -2.18471646 3.53072548  
 H 1.15146589 -5.03025675 -2.85136056  
 H -0.94112968 4.91933346 0.28703868  
 N 1.29216075 -0.56558573 -2.85249114  
 O 0.68216085 -1.19343424 -3.74792600  
 O 0.78287959 0.55446327 -2.42128849  
 O 2.35743904 -0.98914617 -2.33554292

**L4\*Nd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12329.550857, E0 = -12329.138320, G= 212.3969 at T=298.150 K

Cl -4.53976870 3.81310391 -1.05924988  
 Cl -3.35926461 -3.14432931 -3.89125705  
 N -1.09267735 1.18882251 0.22257991  
 N 0.07448998 3.96753454 2.17475224  
 N -0.66332674 -1.26130056 -0.79185593  
 N 1.45218742 -4.14133167 -1.12673390  
 O 0.34830678 1.73842609 2.34444118  
 O 1.09209526 -2.67735076 0.54735243  
 C -1.25183630 2.41490912 0.73439205  
 C -2.31819773 3.24734497 0.35489672  
 H -2.48072100 4.21712208 0.82017916  
 C -3.21040034 2.79976010 -0.60827076  
 C -3.03907776 1.52587581 -1.20815456  
 C -3.89542937 0.98403317 -2.21433806  
 H -4.73132324 1.58897018 -2.56888127  
 C -3.68336225 -0.26675457 -2.72282100  
 H -4.34854460 -0.67123860 -3.48721790  
 C -2.59617209 -1.07336676 -2.26801276  
 C -2.32759643 -2.38964534 -2.72361135  
 C -1.23968375 -3.09435987 -2.22994590  
 H -1.06707323 -4.11339664 -2.56955719

C -0.41388386 -2.48605275 -1.26991916  
 C -1.71204436 -0.56653792 -1.27497983  
 C -1.94088495 0.75706661 -0.73107260  
 C -0.22842354 2.72014260 1.80290139  
 C 0.76464868 -3.13299179 -0.58199775  
 C -0.29029909 5.25645876 1.53880405  
 H -1.25363839 5.61660004 1.94205391  
 C 0.84717339 6.19035244 1.97117782  
 H 1.71180880 6.06106520 1.29996300  
 H 0.53815955 7.24482632 1.94170725  
 C 1.18014610 5.68792152 3.38303447  
 H 0.43069583 6.04827118 4.10634518  
 H 2.17264962 6.00730419 3.73032594  
 C 1.09492385 4.16600323 3.24132085  
 H 2.04726696 3.72126842 2.90518808  
 H 0.78323811 3.64010000 4.15609312  
 C 2.59766340 -4.71671629 -0.36841655  
 H 2.25091600 -5.07752848 0.61146510  
 H 3.33878708 -3.91877937 -0.19031110  
 C 3.13161612 -5.81247234 -1.29468417  
 C 2.80194449 -5.27860737 -2.69596338  
 C 1.40341425 -4.67730427 -2.50840187  
 H 2.80778575 -6.05540657 -3.47366643  
 H 3.51279902 -4.48795319 -2.98648787  
 H 2.60218978 -6.76145983 -1.11079299  
 H 4.20615959 -5.98461723 -1.14181840  
 H 1.17445695 -3.87832189 -3.22806859  
 Nd 0.57395750 -0.46176621 1.36684608  
 N -1.36511087 -1.57908010 3.17813373  
 O -0.09417091 -1.41739428 3.45551705  
 O -1.70157611 -1.19134462 1.98050272

O -2.14809632 -2.04610729 3.96501756  
 N 2.98963451 0.53961110 0.14738575  
 O 1.83188009 0.65669149 -0.43859038  
 O 2.94660640 -0.05989091 1.30983174  
 O 4.01701164 0.94805175 -0.33601394  
 H 0.63559991 -5.46834373 -2.57904792  
 H -0.36762846 5.14411497 0.44793117

**L4\*Pm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13083.384056, E0 = -13082.933207, G= 232.1081 at T=298.150 K

Cl -4.90932274 3.64834094 -0.83989012  
 Cl -3.69141531 -3.38371086 -3.55224562  
 N -1.29265797 1.15450549 0.24835126  
 N 0.02743386 3.93065548 1.97498667  
 N -0.85839134 -1.28791618 -0.71133274  
 N 1.45256591 -3.94235659 -1.27749944  
 O -0.09094303 1.74238586 2.56633186  
 O 1.04263628 -2.65013266 0.52302581  
 C -1.46952617 2.37109852 0.76201510  
 C -2.57488847 3.17536116 0.43659610  
 H -2.70755005 4.15814924 0.88864285  
 C -3.51809478 2.67468739 -0.44665402  
 C -3.36608028 1.38413656 -1.01112211  
 C -4.28574419 0.76961553 -1.91418004  
 H -5.17868853 1.32607830 -2.20346117  
 C -4.06558514 -0.48651367 -2.40660644  
 H -4.78140831 -0.94335330 -3.09131384  
 C -2.90613699 -1.23354697 -2.03548622  
 C -2.60147095 -2.54175639 -2.48289514  
 C -1.43743145 -3.17431688 -2.07686114  
 H -1.22287524 -4.18627262 -2.41832781



C -0.57508689 -2.49590421 -1.19498837  
 C -1.96788704 -0.66099113 -1.13180554  
 C -2.20232916 0.66996562 -0.61295158  
 C -0.44955635 2.68451977 1.83287406  
 C 0.70181024 -3.05051422 -0.60640699  
 C 0.00172479 4.99169254 0.94884372  
 H -0.71421444 5.78478765 1.23467243  
 C 1.44268739 5.51745415 0.97170365  
 H 2.07909274 4.82955265 0.39125475  
 H 1.52212524 6.52936125 0.55032092  
 C 1.79676402 5.45024586 2.46652699  
 H 1.36091936 6.30959082 3.00297904  
 H 2.88058138 5.44529533 2.64665484  
 C 1.15237236 4.13506413 2.92841148  
 H 1.83375871 3.27112532 2.84537244  
 H 0.77130717 4.16613817 3.96083045  
 C 2.73933840 -4.35955477 -0.66126657  
 H 2.54939008 -4.93024874 0.25909233  
 H 3.30361056 -3.45445204 -0.37816194  
 C 3.42379189 -5.17057085 -1.76798582  
 C 2.87805963 -4.53901100 -3.05674052  
 C 1.40322578 -4.28354502 -2.71354055  
 H 2.98982501 -5.17949629 -3.94260073  
 H 3.38027477 -3.57795954 -3.25469255  
 H 3.12798333 -6.23164797 -1.70725024  
 H 4.51948357 -5.11511707 -1.69179118  
 H 0.96161765 -3.46060300 -3.29431581  
 Pm 0.77765888 -0.24273492 1.20458996  
 N -0.83038503 -1.46883607 3.33251882  
 O 0.41661471 -1.20784438 3.47182226  
 O -1.32600522 -1.16286302 2.15529609

O -1.51961517 -1.95561099 4.20714760  
 N 3.50094748 -0.11054466 2.21947169  
 O 2.55996656 0.64307147 2.67940760  
 O 3.12558675 -0.94662374 1.29091918  
 O 4.64961720 -0.05275642 2.61366987  
 N 1.85941672 1.35869348 -1.02458274  
 O 2.32259631 2.01886630 -1.93849206  
 O 1.54569221 0.11232580 -1.15642738  
 O 1.63912129 1.86279380 0.15069838  
 H 0.80480158 -5.19971800 -2.87395048  
 H -0.28844821 4.57757378 -0.02668540  
 O -3.96284842 -1.20418942 1.20206439  
 H -3.12027073 -1.26203156 1.71070492  
 H -4.62954140 -1.53988814 1.82471406

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13083.380097, E0 = -13082.928647, G= 232.1472 at T=298.150 K

Cl -5.17671490 3.26278281 -0.67236203  
 Cl -3.40457749 -3.59702873 -3.50422740  
 N -1.40092635 1.02711427 0.42036197  
 N -0.37154952 3.98761225 2.15354156  
 N -0.77954435 -1.37015283 -0.57681942  
 N 1.71407688 -3.84301758 -1.20996404  
 O 0.06055341 1.80340505 2.50970888  
 O 1.28181505 -2.53986454 0.59014434  
 C -1.64293909 2.24003363 0.91512775  
 C -2.81256771 2.95510101 0.59483135  
 H -3.03563595 3.91710591 1.05277085  
 C -3.71481133 2.39458346 -0.29341510  
 C -3.46084499 1.13134098 -0.88291389  
 C -4.31318188 0.47748172 -1.82379961  
 H -5.22859955 0.98250932 -2.13549352

C -3.99525452 -0.75325698 -2.32889867  
 H -4.65388870 -1.24057937 -3.04948878  
 C -2.79984140 -1.42889535 -1.93658423  
 C -2.39498186 -2.70662141 -2.40130329  
 C -1.19416726 -3.25744629 -1.99357414  
 H -0.89013183 -4.23422384 -2.36488008  
 C -0.39248028 -2.53807783 -1.08817136  
 C -1.92668879 -0.81093258 -1.00327754  
 C -2.26093459 0.49080533 -0.46514151  
 C -0.59248483 2.67908955 1.91128373  
 C 0.93691206 -2.98997188 -0.52951759  
 C -0.78708202 5.15910149 1.35501623  
 H -1.73273802 5.57962799 1.74469984  
 C 0.36211076 6.15235186 1.57352734  
 H 1.19017684 5.91783714 0.88466507  
 H 0.04502385 7.19101048 1.39986217  
 C 0.77796990 5.87039757 3.02511215  
 H 0.06418089 6.33794498 3.72352290  
 H 1.78502190 6.24013805 3.26549268  
 C 0.69618046 4.34327936 3.12057853  
 H 1.63433254 3.84979200 2.81353879  
 H 0.43835267 3.96757412 4.12271547  
 C 3.04036450 -4.17461824 -0.63277709  
 H 2.91383028 -4.76412725 0.28862447  
 H 3.54812574 -3.23205519 -0.36551809  
 C 3.75728869 -4.91283703 -1.76610970  
 C 3.16502452 -4.26081800 -3.02299643  
 C 1.68002808 -4.10882473 -2.67226100  
 H 3.30964804 -4.85467672 -3.93736196  
 H 3.58260512 -3.25233388 -3.17218041  
 H 3.51789021 -5.98932314 -1.73727047

H 4.84901714 -4.80142546 -1.69196391  
 H 1.22417068 -3.25599456 -3.20405340  
 Pm 0.38049844 -0.51554042 1.63029444  
 N 2.42481303 -0.37356156 3.65905333  
 O 3.28750157 -0.27311307 4.50600433  
 O 2.63328695 -0.04958897 2.41134000  
 O 1.23150945 -0.80243754 3.91391897  
 O 1.56651592 0.82782370 -0.03129913  
 H 1.33552468 0.73975086 -1.05869019  
 H 2.53214502 0.70538270 0.04391146  
 N -1.87978148 -1.73919284 2.98566484  
 O -0.95249271 -2.43286180 2.39838362  
 O -1.74144268 -0.45136312 2.88466144  
 O -2.80925012 -2.25234890 3.57407546  
 H 1.13336408 -5.04862642 -2.87114382  
 H -0.92420965 4.88545752 0.29896829  
 N 1.30619323 -0.58191168 -2.84909058  
 O 0.68545806 -1.21193182 -3.73791552  
 O 0.81133872 0.54718959 -2.42946196  
 O 2.36689472 -1.01404381 -2.33147717

**L4\*Pm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -12726.415740, E0 = -12726.003075, G= 212.6284 at T=298.150 K

Cl -4.53627205 3.81415892 -1.06143916  
 Cl -3.34444571 -3.13740349 -3.90188885  
 N -1.08750236 1.19282007 0.22079812  
 N 0.06906384 3.96612597 2.18604565  
 N -0.66633338 -1.26391327 -0.78283048  
 N 1.45659637 -4.13992357 -1.12186611  
 O 0.34820330 1.73617625 2.34554052  
 O 1.10240173 -2.66843748 0.54688865  
 C -1.25185490 2.41576815 0.73816049

C -2.31941009 3.24700046 0.35912761  
 H -2.48575258 4.21424866 0.82830691  
 C -3.20732093 2.80117464 -0.60835153  
 C -3.03303194 1.52876687 -1.21085382  
 C -3.88466930 0.98947072 -2.22236013  
 H -4.71814871 1.59588277 -2.58004093  
 C -3.67042542 -0.26013958 -2.73290968  
 H -4.33107424 -0.66206843 -3.50254750  
 C -2.58764672 -1.06930029 -2.27231336  
 C -2.31830215 -2.38564324 -2.72746611  
 C -1.23323286 -3.09166884 -2.23006535  
 H -1.05933595 -4.10971546 -2.57153916  
 C -0.41197091 -2.48629093 -1.26394141  
 C -1.70904183 -0.56567299 -1.27293336  
 C -1.93627059 0.75961053 -0.73148614  
 C -0.22991489 2.71896887 1.80900955  
 C 0.77138853 -3.12888932 -0.57847393  
 C -0.29875699 5.25662994 1.55497658  
 H -1.26561034 5.61018705 1.95551455  
 C 0.83190209 6.19404411 1.99739814  
 H 1.70019627 6.07424450 1.32923460  
 H 0.51665825 7.24683666 1.97395587  
 C 1.16169465 5.68455505 3.40767074  
 H 0.40619886 6.03532934 4.12940216  
 H 2.15028834 6.00799656 3.76223445  
 C 1.08662450 4.16317654 3.25548029  
 H 2.04253173 3.72762895 2.91738057  
 H 0.77741504 3.62816453 4.16571665  
 C 2.60451531 -4.71159124 -0.36453924  
 H 2.26248288 -5.06069899 0.62114841  
 H 3.34991956 -3.91477227 -0.19935443

C 3.12915373 -5.81810284 -1.28304684  
 C 2.79834366 -5.29326344 -2.68741441  
 C 1.40327084 -4.68356991 -2.50047064  
 H 2.79787302 -6.07588243 -3.45928836  
 H 3.51248765 -4.50862312 -2.98587513  
 H 2.59441161 -6.76227379 -1.08989465  
 H 4.20304537 -5.99539948 -1.13146603  
 H 1.17771387 -3.88737535 -3.22430372  
 Pm 0.57513154 -0.44982731 1.34317219  
 N -1.33950901 -1.52656651 3.18049479  
 O -0.05816809 -1.40646267 3.42434287  
 O -1.69855177 -1.10741138 2.00051689  
 O -2.11336875 -1.98536193 3.98152781  
 N 2.96937084 0.48456785 0.06742837  
 O 1.81652498 0.53536052 -0.53592616  
 O 2.92432952 -0.01964417 1.27392340  
 O 3.99570894 0.86850679 -0.43799171  
 H 0.63128328 -5.47099543 -2.56567788  
 H -0.37080756 5.14948654 0.46315852

**L4\*Sm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -13490.321048, E0 = -13489.870300, G= 229.4138 at T=298.150 K

Cl -4.85492325 3.67828751 -0.77527303  
 Cl -3.78973222 -3.35090709 -3.54380679  
 N -1.22432649 1.15158689 0.19503006  
 N 0.13379863 4.01453114 1.83757234  
 N -0.88431388 -1.32418096 -0.72230202  
 N 1.35784960 -4.00697899 -1.22381592  
 O 0.30630800 1.80453920 2.26012850  
 O 0.77242875 -2.89163923 0.66035801  
 C -1.35363960 2.38503790 0.68117887

C -2.47132087 3.19214153 0.40077204  
 H -2.58836937 4.17796135 0.84894544  
 C -3.45665407 2.69366980 -0.43517438  
 C -3.33701897 1.40123165 -0.99932516  
 C -4.28906965 0.79902250 -1.87663174  
 H -5.17933226 1.36898994 -2.14690733  
 C -4.10008764 -0.46164995 -2.36936355  
 H -4.83584309 -0.90778679 -3.04035378  
 C -2.94762707 -1.22857368 -2.01789665  
 C -2.67677760 -2.54200697 -2.47156620  
 C -1.53158855 -3.20774412 -2.06452775  
 H -1.33717501 -4.22553015 -2.40316653  
 C -0.65562552 -2.55383086 -1.18118894  
 C -1.98315799 -0.67086977 -1.13155603  
 C -2.17393708 0.67277467 -0.62355185  
 C -0.24308428 2.73579001 1.64286304  
 C 0.55572456 -3.18064499 -0.53167117  
 C -0.14552598 5.18761301 0.98530275  
 H -1.00398350 5.76147842 1.38147497  
 C 1.14487815 6.01030064 1.09974706  
 H 1.89823866 5.61069679 0.40116969  
 H 0.97755432 7.07261372 0.86879498  
 C 1.57757854 5.75692225 2.55207396  
 H 0.97455621 6.37097836 3.24163485  
 H 2.63871980 5.98258686 2.73079991  
 C 1.27473128 4.26793003 2.75380397  
 H 2.11548042 3.61594272 2.46096087  
 H 0.99741411 4.00271177 3.78558564  
 C 2.60653758 -4.47397804 -0.56617421  
 H 2.36921787 -5.20225477 0.22454646  
 H 3.09374356 -3.60699296 -0.08767737

C 3.42977428 -5.05560398 -1.72190785  
 C 2.95389843 -4.24366331 -2.93671227  
 C 1.44339514 -4.13162470 -2.69365072  
 H 3.18373442 -4.71886635 -3.90173507  
 H 3.39729428 -3.23465061 -2.91882157  
 H 3.20093799 -6.12526560 -1.86365604  
 H 4.50917864 -4.95711517 -1.53616846  
 H 0.99542248 -3.25525498 -3.18292165  
 Sm 0.85586876 -0.39164019 1.16402018  
 N -0.77631652 -1.49500561 3.32523298  
 O 0.50464475 -1.51302946 3.34643149  
 O -1.29904151 -0.89294505 2.28364277  
 O -1.47206879 -1.99167669 4.19012117  
 N 3.51242566 -0.49051470 2.32785726  
 O 2.70655918 0.51777881 2.47086763  
 O 3.04688573 -1.45262992 1.60328698  
 O 4.61744785 -0.51906794 2.83477187  
 N 2.09414744 0.49569455 -1.35122049  
 O 2.57643723 0.89988589 -2.39510226  
 O 1.98773086 -0.75962573 -1.07303846  
 O 1.64643896 1.30544841 -0.43933776  
 H 0.92283672 -5.04546070 -3.03560996  
 H -0.36680356 4.87672853 -0.04575050  
 O -3.94288039 -0.94845837 1.32914150  
 H -3.09277487 -0.96971518 1.82893062  
 H -4.36681938 -1.78349006 1.59051478

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13490.316599, E0 = -13489.865648, G= 232.5921 at T=298.150 K

Cl -5.19620228 3.27002025 -0.68644023  
 Cl -3.39916968 -3.60503101 -3.47056460  
 N -1.39831507 1.06811178 0.39415771



N -0.39842486 4.02161884 2.15719914  
 N -0.76671082 -1.33173156 -0.58371449  
 N 1.71374857 -3.83283520 -1.17164803  
 O 0.07184003 1.83962619 2.46969271  
 O 1.29094458 -2.49607706 0.60528541  
 C -1.65222681 2.27525306 0.89596587  
 C -2.82886219 2.98072529 0.57914704  
 H -3.06263852 3.93899369 1.03936720  
 C -3.72760367 2.41235399 -0.30818743  
 C -3.46656585 1.14967787 -0.89609653  
 C -4.31929588 0.48335171 -1.82772517  
 H -5.24128819 0.97814959 -2.13648009  
 C -3.99549437 -0.74953735 -2.32434201  
 H -4.65620947 -1.24805820 -3.03540659  
 C -2.79410958 -1.41519260 -1.93272889  
 C -2.38795686 -2.69773769 -2.38229227  
 C -1.18581903 -3.24129152 -1.96886551  
 H -0.88417053 -4.22459316 -2.32478356  
 C -0.38192835 -2.50768709 -1.07617259  
 C -1.91767478 -0.78377533 -1.01130509  
 C -2.25872469 0.52110541 -0.48223543  
 C -0.60270882 2.71551204 1.89257514  
 C 0.94376642 -2.95914507 -0.50650823  
 C -0.84074432 5.20217037 1.38655436  
 H -1.79596901 5.59097052 1.78528690  
 C 0.28507963 6.21627235 1.62956274  
 H 1.11727750 6.02053881 0.93367434  
 H -0.05762599 7.25104332 1.48375571  
 C 0.71050847 5.90737343 3.07289886  
 H -0.01208261 6.34040356 3.78431320  
 H 1.70940995 6.29398489 3.32058311

C	0.66435730	4.37694025	3.12964034
H	1.61296022	3.91424346	2.80712938
H	0.41841140	3.96984172	4.12242079
C	3.03179836	-4.17437458	-0.58233720
H	2.89252114	-4.74814606	0.34715077
H	3.55247045	-3.23588920	-0.32571486
C	3.74458766	-4.94004869	-1.70035183
C	3.16525698	-4.30310965	-2.97133350
C	1.68148124	-4.12617397	-2.62829351
H	3.30479431	-4.91692781	-3.87328863
H	3.59836030	-3.30413342	-3.13892674
H	3.49295163	-6.01309013	-1.65471411
H	4.83718872	-4.83955431	-1.62382782
H	1.23545790	-3.28154516	-3.17957354
Sm	0.39437273	-0.46508390	1.63064134
N	2.59376025	-0.61318070	3.48464751
O	3.51874542	-0.67424941	4.26753616
O	2.72271657	-0.12204419	2.28743339
O	1.40100169	-1.02754629	3.77272749
O	1.59182799	0.80374157	-0.07000085
H	1.35899806	0.72252244	-1.08882117
H	2.55351973	0.64735174	-0.00514300
N	-1.89977348	-1.67499602	2.95814466
O	-1.04007232	-2.37093663	2.28369308
O	-1.68646669	-0.39280641	2.95726824
O	-2.83952522	-2.17861605	3.54155588
H	1.12455750	-5.06317234	-2.81134272
H	-0.97099668	4.95023918	0.32423425
N	1.34539294	-0.59186047	-2.90276575
O	0.73273206	-1.22632539	-3.79287291
O	0.84656221	0.53411585	-2.48818970

O 2.40599656 -1.01974976 -2.38124871

**L4\*Sm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13133.355047, E0 = -13132.942414, G= 212.7990 at T=298.150 K

Cl -4.53173161 3.82072735 -1.06843984

Cl -3.33768463 -3.13381648 -3.91324568

N -1.07170045 1.20604539 0.19160460

N 0.07226521 3.96590137 2.19086051

N -0.65084833 -1.24810410 -0.81146318

N 1.46092284 -4.14163113 -1.11893678

O 0.40346375 1.74142194 2.27932262

O 1.15038013 -2.60946298 0.49979737

C -1.23197079 2.42852426 0.70937639

C -2.30369711 3.25835872 0.33667919

H -2.46937108 4.22637367 0.80389029

C -3.19867682 2.80919814 -0.62309468

C -3.02995539 1.53493464 -1.22294116

C -3.89019799 0.98977721 -2.22421670

H -4.72967243 1.59210634 -2.57480359

C -3.67569256 -0.25981107 -2.73530984

H -4.34219360 -0.66527832 -3.49806786

C -2.58404899 -1.06342304 -2.28552437

C -2.30861044 -2.37713027 -2.74406028

C -1.21674979 -3.07829118 -2.25403738

H -1.04221177 -4.09493637 -2.59867573

C -0.39219800 -2.46888518 -1.29231775

C -1.69918454 -0.55546421 -1.29408550

C -1.92660820 0.77012360 -0.75214946

C -0.20471129 2.72529745 1.77707553

C 0.79444164 -3.10323715 -0.60456002

C -0.32930359 5.26834440 1.60741448

H -1.30213606 5.58479118 2.02428961

C	0.78197092	6.21650362	2.07576704
H	1.64745784	6.14171076	1.39751577
H	0.44167879	7.26159525	2.09210205
C	1.13556969	5.66566610	3.46440983
H	0.37944183	5.97394562	4.20459223
H	2.12008381	5.99888420	3.82125401
C	1.09298444	4.14927721	3.25971317
H	2.05560160	3.74596357	2.90121293
H	0.80164450	3.57719731	4.15324068
C	2.60826015	-4.70157957	-0.35198119
H	2.27132487	-5.00629187	0.65016985
H	3.36762643	-3.91096854	-0.22524068
C	3.10521698	-5.85214424	-1.23099780
C	2.76539516	-5.37944508	-2.65153813
C	1.38345122	-4.73748732	-2.47430873
H	2.74170661	-6.19284153	-3.39052868
H	3.48915100	-4.62062407	-2.99071074
H	2.55942035	-6.77955914	-0.99313247
H	4.17826223	-6.03919601	-1.08535492
H	1.16691875	-3.96587801	-3.22693634
Sm	0.61205018	-0.42715171	1.30317318
N	-1.29821670	-1.50754631	3.14818144
O	-0.01623247	-1.38351095	3.38208842
O	-1.66839647	-1.09187114	1.97490227
O	-2.06244040	-1.96917462	3.95815015
N	2.97460151	0.52396387	-0.02060761
O	1.81611335	0.56717247	-0.60593951
O	2.95171404	0.02110916	1.18572462
O	3.99235964	0.91380399	-0.54055315
H	0.59625912	-5.51202154	-2.50151491
H	-0.40329701	5.19804382	0.51276672

**L4\*Eu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)****(H<sub>2</sub>O in outer coordination sphere)**

E= -13907.519099, E0 = -13907.068405, G= 230.0721 at T=298.150 K

Cl -4.84747505 3.68764496 -0.75023586

Cl -3.74979830 -3.30239868 -3.60663986

N -1.23715436 1.14456260 0.23302105

N 0.12730131 3.97706914 1.91676891

N -0.86075240 -1.30368686 -0.75269419

N 1.33845043 -4.03953886 -1.18053079

O 0.30591160 1.75901484 2.29258227

O 0.73070353 -2.89871597 0.68462116

C -1.36876428 2.37031746 0.73677206

C -2.48102522 3.18319249 0.45136127

H -2.60664535 4.16104126 0.91419673

C -3.45237947 2.69891715 -0.40954930

C -3.32115746 1.41926253 -1.00017416

C -4.25841522 0.83296192 -1.90395355

H -5.14413786 1.40774512 -2.17883825

C -4.06416035 -0.42117324 -2.41143394

H -4.79251814 -0.85705352 -3.09712577

C -2.91730094 -1.19490767 -2.05580807

C -2.64685822 -2.50735617 -2.51388121

C -1.51557755 -3.18649745 -2.08927727

H -1.32898164 -4.20742273 -2.42305660

C -0.64221352 -2.54083395 -1.19712162

C -1.95969033 -0.64664561 -1.15721142

C -2.16433072 0.68369538 -0.62044847

C -0.25448161 2.70354104 1.70231712

C 0.54225498 -3.18712330 -0.51192623

C -0.17475653 5.17313623 1.10449195

H -1.03184891 5.72590256 1.53132999

C	1.10967040	6.00442457	1.22471976
H	1.85509729	5.63665724	0.50064689
H	0.92777777	7.07187510	1.03181863
C	1.57031512	5.70824480	2.66013408
H	0.97405654	6.29310083	3.38021398
H	2.63241601	5.93814325	2.82714152
C	1.28531361	4.21067905	2.81745601
H	2.12574005	3.57822514	2.48298717
H	1.03140664	3.90818906	3.84491467
C	2.56261802	-4.52500439	-0.49116036
H	2.29759574	-5.27136517	0.27365756
H	3.03298879	-3.66927576	0.02274871
C	3.42713284	-5.08122349	-1.62967682
C	2.99081469	-4.24610472	-2.84357691
C	1.47297692	-4.14339209	-2.64864278
H	3.25457191	-4.70177174	-3.80934691
H	3.42822361	-3.23583436	-2.78958082
H	3.20738769	-6.14858198	-1.80021429
H	4.49903965	-4.98290396	-1.40458417
H	1.03857100	-3.26199150	-3.14093995
Eu	0.82010388	-0.37698114	1.10089898
N	-0.80332655	-1.32360983	3.35360336
O	0.47373655	-1.21753943	3.40538335
O	-1.33638513	-0.98594868	2.20824265
O	-1.48239040	-1.70932937	4.28708029
N	3.60346627	-0.29236925	1.95187664
O	2.93785977	0.77352613	1.63455033
O	2.94201159	-1.39458239	1.87084234
O	4.77043009	-0.24953765	2.29970670
N	2.04210567	0.25154626	-1.51106811
O	2.53614473	0.52829611	-2.59239531

O 2.16685081 -0.91601276 -0.97121567  
O 1.34631217 1.10557652 -0.83431691  
H 0.96657526 -5.05377340 -3.01987934  
H -0.40868476 4.89199591 0.06773264  
O -3.98104477 -0.94690740 1.27649915  
H -3.13346314 -1.00438845 1.77798223  
H -4.40821457 -1.79670274 1.47820473

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -13907.516763, E0 = -13907.065825, G= 231.1364 at T=298.150 K

Cl -5.23319340 3.23908448 -0.64997387  
Cl -3.35647488 -3.55817938 -3.54132462  
N -1.43028057 1.05322754 0.44276121  
N -0.44572860 4.04500532 2.17025638  
N -0.74596083 -1.31372392 -0.60661757  
N 1.72012818 -3.83818722 -1.16064751  
O 0.10531761 1.87796926 2.44680595  
O 1.25228989 -2.53617287 0.62975401  
C -1.68466008 2.26665807 0.93371636  
C -2.86355162 2.96590376 0.61323684  
H -3.10367775 3.92309856 1.07195175  
C -3.75659871 2.39297462 -0.27694905  
C -3.47924590 1.14051461 -0.87783211  
C -4.31879377 0.48492169 -1.82845926  
H -5.24155426 0.97836125 -2.13687921  
C -3.98005080 -0.73586273 -2.34258127  
H -4.63027191 -1.22871125 -3.06714225  
C -2.77413797 -1.39552939 -1.95507693  
C -2.35838318 -2.66606140 -2.42772579  
C -1.16052306 -3.21399474 -2.00937724  
H -0.85611373 -4.19395304 -2.37193632  
C -0.36542356 -2.48937154 -1.10143578

C -1.90552306 -0.77304345 -1.01885033  
 C -2.27101016 0.51328689 -0.45890459  
 C -0.61677688 2.73234391 1.90175438  
 C 0.93874842 -2.96792412 -0.50346988  
 C -0.93383574 5.22032738 1.41922653  
 H -1.89010489 5.58199978 1.84068072  
 C 0.17007145 6.26208973 1.64617205  
 H 0.99085498 6.09523630 0.92947143  
 H -0.20350341 7.28838062 1.51740360  
 C 0.63748497 5.95072317 3.07557702  
 H -0.08064063 6.35489559 3.80821037  
 H 1.63042450 6.36329746 3.30472565  
 C 0.63614374 4.41937256 3.11439133  
 H 1.58755136 3.98773146 2.75878024  
 H 0.43174803 3.99318290 4.10851526  
 C 3.01548839 -4.20603609 -0.53771847  
 H 2.84174919 -4.77462626 0.38902205  
 H 3.54913616 -3.27838778 -0.26887941  
 C 3.74019003 -4.98846960 -1.63657343  
 C 3.20100594 -4.34875870 -2.92387795  
 C 1.71387625 -4.14270782 -2.61399150  
 H 3.34889674 -4.97083092 -3.81878924  
 H 3.65684915 -3.35958958 -3.08940291  
 H 3.46872330 -6.05669832 -1.59205830  
 H 4.83230400 -4.90676546 -1.53530049  
 H 1.29207599 -3.29910302 -3.18449950  
 Eu 0.39192316 -0.46163613 1.64393318  
 N 2.75061989 -0.88659567 3.25299644  
 O 3.76822543 -1.10172176 3.88153243  
 O 2.70519328 -0.01376663 2.28648591  
 O 1.63861620 -1.49586701 3.48786569



O 1.57626498 0.77216142 -0.10326542  
 H 1.39347780 0.69166261 -1.11558509  
 H 2.54046965 0.66836423 0.00929093  
 N -1.93640125 -1.40419626 3.12165809  
 O -1.59438694 -1.90954304 1.97442806  
 O -1.20703316 -0.41573966 3.52226162  
 O -2.88027167 -1.82698846 3.76179433  
 H 1.14524257 -5.07214689 -2.80075216  
 H -1.07958794 4.97488832 0.35741767  
 N 1.43866122 -0.61377221 -2.97575760  
 O 0.86671537 -1.25799692 -3.88754034  
 O 0.92715943 0.50640881 -2.58872032  
 O 2.48007226 -1.04141259 -2.41418171

**L4\*Eu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13550.552946, E0 = -13550.140636, G= 212.4587 at T=298.150 K

Cl -4.54089928 3.81096601 -1.05873406  
 Cl -3.33832788 -3.13675690 -3.91055226  
 N -1.08157527 1.19856584 0.20480029  
 N 0.06425181 3.96224022 2.19006443  
 N -0.65292984 -1.25666761 -0.80354452  
 N 1.45546389 -4.15107298 -1.12481654  
 O 0.35464430 1.73222756 2.33855343  
 O 1.12875974 -2.65111589 0.52373165  
 C -1.24855900 2.41536903 0.73093224  
 C -2.32005358 3.24510336 0.35707939  
 H -2.49010348 4.20986176 0.83012468  
 C -3.20782590 2.80000925 -0.61112159  
 C -3.03217220 1.52978170 -1.21826780  
 C -3.88785386 0.98700619 -2.22467780  
 H -4.72772789 1.58870006 -2.57543421  
 C -3.67129493 -0.26167783 -2.73683572

H -4.33649397 -0.66717678 -3.50068879  
 C -2.58188844 -1.06656599 -2.28362656  
 C -2.31043243 -2.38248777 -2.73883057  
 C -1.22366071 -3.08763647 -2.24324226  
 H -1.05140686 -4.10590267 -2.58475757  
 C -0.39967969 -2.48068118 -1.27995849  
 C -1.69892561 -0.56022924 -1.28944254  
 C -1.92961645 0.76494068 -0.74567842  
 C -0.22677217 2.71386981 1.80676413  
 C 0.78508449 -3.12297535 -0.59008968  
 C -0.30477634 5.25247717 1.55975413  
 H -1.27347851 5.60447454 1.95725369  
 C 0.82281131 6.19199562 2.00600553  
 H 1.69288349 6.07453537 1.33975160  
 H 0.50586176 7.24428892 1.98299086  
 C 1.15026283 5.68160057 3.41645527  
 H 0.39232969 6.03027439 4.13662100  
 H 2.13739395 6.00667620 3.77363396  
 C 1.07822132 4.16025352 3.26186872  
 H 2.03640079 3.72765779 2.92624545  
 H 0.76810199 3.62415123 4.17121887  
 C 2.60129356 -4.72197723 -0.36465845  
 H 2.26082015 -5.05313635 0.62775898  
 H 3.35497952 -3.93014336 -0.21365494  
 C 3.11094832 -5.84739399 -1.26842129  
 C 2.77897954 -5.34050322 -2.67902589  
 C 1.39140189 -4.71235514 -2.49538112  
 H 2.76647377 -6.13473320 -3.43888950  
 H 3.50041461 -4.56861925 -2.99286509  
 H 2.56771398 -6.78321600 -1.05902815  
 H 4.18370104 -6.03333235 -1.11916482

H 1.17379594 -3.92415452 -3.23033738  
 Eu 0.58688891 -0.43554407 1.31864500  
 N -1.30327415 -1.52324784 3.17652678  
 O -0.00952540 -1.52516925 3.34622836  
 O -1.69521916 -0.98452312 2.06290841  
 O -2.06467462 -1.98595345 3.98986459  
 N 2.97102857 0.57481939 0.08429389  
 O 1.80750299 0.75283998 -0.46120319  
 O 2.94714236 -0.10661073 1.19633996  
 O 3.99584794 1.00182199 -0.39193940  
 H 0.61052448 -5.49200344 -2.54907775  
 H -0.37278131 5.14705467 0.46752992

**L4\*Gd(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14335.078043, E0 = -14334.626358, G= 231.0576 at T=298.150 K

Cl -4.86625290 3.68129373 -0.77335769  
 Cl -3.74760628 -3.31149602 -3.63813806  
 N -1.25097203 1.13975179 0.19497979  
 N 0.12274052 3.96192980 1.89133704  
 N -0.86806297 -1.29574323 -0.78496581  
 N 1.34933817 -4.02077627 -1.19418979  
 O 0.33028767 1.74117911 2.20707512  
 O 0.73656750 -2.84896970 0.64444596  
 C -1.37794912 2.36598587 0.69634199  
 C -2.49190593 3.17904401 0.41619751  
 H -2.61564684 4.15800667 0.87704152  
 C -3.46904039 2.69340777 -0.43840963  
 C -3.34102631 1.41316974 -1.02810812  
 C -4.27968550 0.82108492 -1.92703617  
 H -5.16917753 1.39126027 -2.19962835  
 C -4.08129072 -0.43285933 -2.43456149

H -4.80993938 -0.87218624 -3.11778140  
 C -2.92856407 -1.20114207 -2.08446169  
 C -2.64867210 -2.50974369 -2.54687119  
 C -1.50905740 -3.17934966 -2.12852216  
 H -1.31401610 -4.19709444 -2.46709561  
 C -0.63948506 -2.52826047 -1.23641455  
 C -1.97263479 -0.64859545 -1.18690550  
 C -2.18205762 0.68079382 -0.65120935  
 C -0.25149772 2.69261575 1.64880407  
 C 0.54632622 -3.16247582 -0.54760569  
 C -0.20610048 5.17890358 1.12255383  
 H -1.06574786 5.70524025 1.57756364  
 C 1.06874835 6.02355003 1.25345385  
 H 1.80833960 5.69059420 0.50696850  
 H 0.86957628 7.09421635 1.09934449  
 C 1.55443060 5.68543577 2.67134500  
 H 0.96162313 6.23805428 3.41920710  
 H 2.61586952 5.92376518 2.83034134  
 C 1.29126775 4.17998838 2.78271651  
 H 2.13374782 3.56823850 2.41654801  
 H 1.05589652 3.83900428 3.80243182  
 C 2.56840158 -4.49886560 -0.48929983  
 H 2.29182720 -5.20880270 0.30538723  
 H 3.05393767 -3.63197780 -0.00882056  
 C 3.41592550 -5.11737823 -1.60816324  
 C 2.98483181 -4.32995462 -2.85558033  
 C 1.47014618 -4.18986988 -2.65660143  
 H 3.23283458 -4.83331251 -3.80162358  
 H 3.44261694 -3.32727599 -2.85133004  
 H 3.17845964 -6.18745089 -1.73078728  
 H 4.49080181 -5.02649355 -1.39479280

H 1.04787612 -3.32175827 -3.18215156  
 Gd 0.85053831 -0.39062530 1.08262777  
 N -0.70170289 -1.19784284 3.38777542  
 O 0.56694162 -1.02962828 3.43789840  
 O -1.23268962 -0.98382896 2.20231700  
 O -1.38135457 -1.52836716 4.33856583  
 N 3.56194878 -0.47879311 2.01743627  
 O 2.89139986 0.62716579 1.85704815  
 O 2.90108657 -1.55249000 1.72882330  
 O 4.71407843 -0.49260336 2.40379453  
 N 2.03246474 0.44939709 -1.43551838  
 O 2.52102470 0.78793609 -2.49819183  
 O 2.08783650 -0.77690935 -1.00551045  
 O 1.41379046 1.27375138 -0.65590465  
 H 0.94499457 -5.10611963 -2.98474383  
 H -0.44810569 4.92771721 0.07996369  
 O -3.88948488 -0.93566567 1.30336881  
 H -3.03313446 -0.99445671 1.79001892  
 H -4.33566236 -1.76331878 1.55055988

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14335.077658, E0 = -14334.625583, G= 232.9019 at T=298.150 K

Cl -5.16535187 3.28397584 -0.70312601  
 Cl -3.38708711 -3.61521840 -3.45822239  
 N -1.38985288 1.05986536 0.39928472  
 N -0.36730883 4.01834011 2.15550184  
 N -0.76592731 -1.33929014 -0.56697583  
 N 1.73221850 -3.82459354 -1.15680265  
 O 0.14142996 1.83918905 2.40696716  
 O 1.32001173 -2.45270944 0.59541160  
 C -1.62723088 2.27710581 0.88566226  
 C -2.79850769 2.98800087 0.56138396

H	-3.02449179	3.95349312	1.00945103
C	-3.70418620	2.41786933	-0.31860986
C	-3.45434523	1.14840996	-0.89595324
C	-4.30785227	0.48090100	-1.82628119
H	-5.22593451	0.97892338	-2.14144516
C	-3.98754430	-0.75564039	-2.31681895
H	-4.64733076	-1.25330687	-3.02939224
C	-2.78903747	-1.42432249	-1.92073476
C	-2.37886834	-2.70562530	-2.37033248
C	-1.17296696	-3.24364090	-1.95950520
H	-0.86575413	-4.22306013	-2.32065725
C	-0.37153307	-2.50983953	-1.06495070
C	-1.91644382	-0.79297978	-0.99741429
C	-2.25326800	0.51357108	-0.47464925
C	-0.56046653	2.71613932	1.86554229
C	0.96361369	-2.94255829	-0.50236052
C	-0.84623706	5.21393061	1.43157685
H	-1.80343306	5.56816435	1.85693252
C	0.26116431	6.24438715	1.69147301
H	1.08440113	6.09310484	0.97421640
H	-0.10740594	7.27542925	1.58887672
C	0.72058862	5.89417982	3.11461782
H	0.00145286	6.28356171	3.85418558
H	1.71471190	6.29527998	3.35827756
C	0.71058512	4.36243486	3.11574793
H	1.66127908	3.93392825	2.75451207
H	0.49718335	3.91274691	4.09746790
C	3.05951762	-4.14162159	-0.57394397
H	2.93459415	-4.69695568	0.36860284
H	3.57318091	-3.19296098	-0.34222901
C	3.76819205	-4.92346096	-1.68308473

C 3.17199039 -4.31620693 -2.96059895  
 C 1.68978000 -4.14462137 -2.60790777  
 H 3.30867696 -4.94588232 -3.85197139  
 H 3.59392476 -3.31666422 -3.15135241  
 H 3.52570009 -5.99735641 -1.61399615  
 H 4.86057091 -4.81275129 -1.61863029  
 H 1.23397338 -3.31248498 -3.17073655  
 Gd 0.38026372 -0.45255741 1.57995200  
 N 2.48237419 -0.61726761 3.48375273  
 O 3.38630176 -0.67901981 4.28833771  
 O 2.64910603 -0.14661609 2.27734184  
 O 1.27350509 -1.00642657 3.74506211  
 O 1.54367590 0.75464427 -0.12204624  
 H 1.28952658 0.67206419 -1.14877212  
 H 2.50287795 0.57646865 -0.07650857  
 N -1.88286448 -1.62156427 2.91529942  
 O -1.05662584 -2.31983662 2.19868994  
 O -1.64344406 -0.34260133 2.92422271  
 O -2.80956054 -2.11728358 3.52264071  
 H 1.13836598 -5.08896303 -2.76861596  
 H -0.98582339 4.99557114 0.36301377  
 N 1.29456401 -0.63632452 -2.93052411  
 O 0.69102943 -1.28372920 -3.81638575  
 O 0.76701963 0.47941232 -2.50768781  
 O 2.36933327 -1.03515017 -2.41478133

**L4\*Gd(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -13978.112398, E0 = -13977.699292, G= 212.9570 at T=298.150 K

Cl -4.56790638 3.83238745 -1.10777736  
 Cl -3.37647390 -3.12951422 -3.94821429  
 N -1.10102069 1.22069502 0.13418517  
 N 0.04267312 3.96548510 2.15325737

N -0.68176556 -1.22816896 -0.86509079  
 N 1.42775059 -4.12475300 -1.14780283  
 O 0.37475610 1.74003029 2.21943927  
 O 1.11547840 -2.57673764 0.45632502  
 C -1.26402462 2.43946242 0.66138482  
 C -2.33829594 3.26746154 0.29341888  
 H -2.50476718 4.23295259 0.76583624  
 C -3.23384643 2.82185602 -0.66833377  
 C -3.06405640 1.55004990 -1.27453268  
 C -3.92462158 1.00402820 -2.27540660  
 H -4.76522636 1.60527086 -2.62520337  
 C -3.71060443 -0.24638541 -2.78558230  
 H -4.37878275 -0.65270948 -3.54642630  
 C -2.61900544 -1.05030119 -2.33546400  
 C -2.34564281 -2.36798000 -2.78574634  
 C -1.25410295 -3.06769872 -2.29127598  
 H -1.08097029 -4.08712101 -2.62865210  
 C -0.42631474 -2.45434976 -1.33542442  
 C -1.73235273 -0.53857940 -1.34914470  
 C -1.95919061 0.78656489 -0.80845886  
 C -0.23286013 2.72850442 1.72954321  
 C 0.76240683 -3.08210182 -0.64196551  
 C -0.36389601 5.27285862 1.58428359  
 H -1.33772802 5.58076429 2.00529504  
 C 0.74410903 6.21984816 2.06318331  
 H 1.60879362 6.15761995 1.38270462  
 H 0.39910010 7.26306295 2.09346962  
 C 1.10281265 5.65304661 3.44421029  
 H 0.34670126 5.94820118 4.18970203  
 H 2.08647490 5.98625088 3.80329204  
 C 1.06745434 4.13948727 3.22022486



H 2.03011513 3.74557710 2.85183072  
 H 0.78348261 3.55174589 4.10571194  
 C 2.57693338 -4.67641926 -0.37704217  
 H 2.24231386 -4.96798706 0.62960464  
 H 3.33670092 -3.88452005 -0.26177922  
 C 3.06999111 -5.83744478 -1.24398303  
 C 2.72865176 -5.38017130 -2.66922402  
 C 1.34790432 -4.73384905 -2.49720001  
 H 2.70237017 -6.20186853 -3.39886737  
 H 3.45311642 -4.62646914 -3.01807475  
 H 2.52296090 -6.76116514 -0.99480230  
 H 4.14292383 -6.02463436 -1.09792328  
 H 1.13200259 -3.96945930 -3.25736380  
 Gd 0.56676060 -0.39847997 1.21419907  
 N -0.97977823 -1.50587249 3.28256869  
 O 0.30854276 -1.32123148 3.37220192  
 O -1.49986935 -1.12856424 2.13595724  
 O -1.64036965 -1.98022830 4.16967773  
 N 3.10929871 0.41002169 0.31221536  
 O 2.02592206 0.52690363 -0.42212453  
 O 2.90767813 -0.11056521 1.48885620  
 O 4.19602203 0.75774264 -0.07704235  
 H 0.55925512 -5.50721931 -2.51554322  
 H -0.43798462 5.21467066 0.48889333

**L4\*Tb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -14773.021627, E0 = -14772.570072, G= 231.3208 at T=298.150 K

Cl -4.85855055 3.68776083 -0.78173250  
 Cl -3.69813824 -3.28768873 -3.68006110  
 N -1.22728789 1.16343069 0.16734809  
 N 0.10304678 3.97558451 1.93253398

N -0.83103406 -1.26635599 -0.81244075  
 N 1.34440565 -4.05377483 -1.16857648  
 O 0.39949176 1.75219691 2.12017035  
 O 0.79434001 -2.76632714 0.60903811  
 C -1.36067545 2.38591886 0.67905176  
 C -2.48305297 3.19129467 0.40608719  
 H -2.61822724 4.16371250 0.87651348  
 C -3.45477295 2.70639753 -0.45378193  
 C -3.31895351 1.43181551 -1.05525064  
 C -4.24998856 0.84128815 -1.95918286  
 H -5.14179611 1.40740490 -2.23238301  
 C -4.04125881 -0.41092053 -2.47259593  
 H -4.76512909 -0.85089475 -3.16044450  
 C -2.88841200 -1.17533660 -2.12164378  
 C -2.60402203 -2.48475790 -2.58415079  
 C -1.46713388 -3.15317416 -2.15789723  
 H -1.27696025 -4.17347908 -2.49030972  
 C -0.60004234 -2.50386333 -1.26341522  
 C -1.93640745 -0.62228531 -1.21981943  
 C -2.15481377 0.70356017 -0.68126100  
 C -0.23050150 2.70877743 1.62311959  
 C 0.57553440 -3.13345385 -0.56588602  
 C -0.28111047 5.22315454 1.24261796  
 H -1.16342509 5.68015671 1.72807729  
 C 0.95398974 6.11545324 1.42834294  
 H 1.70400274 5.87100506 0.65842944  
 H 0.70379746 7.18357229 1.34912574  
 C 1.46405268 5.70428705 2.81782818  
 H 0.85059589 6.17526960 3.60389948  
 H 2.51410055 5.98090601 2.98979974  
 C 1.27154231 4.18439245 2.82557726

H	2.13722348	3.64009166	2.41037416
H	1.06491339	3.76245022	3.82092190
C	2.54341650	-4.54538441	-0.44060209
H	2.23865461	-5.17519426	0.40931311
H	3.08526182	-3.67479110	-0.03245790
C	3.33769870	-5.29477978	-1.51708794
C	2.94501185	-4.57040977	-2.81430054
C	1.44425058	-4.31879330	-2.61785841
H	3.15026188	-5.15381241	-3.72389627
H	3.46841192	-3.60292268	-2.88466930
H	3.02887321	-6.35261965	-1.56236184
H	4.41838074	-5.26078033	-1.31708157
H	1.07509661	-3.45813990	-3.19367886
Tb	0.87737256	-0.34222609	0.97534132
N	-0.58389175	-1.15079010	3.31517124
O	0.68491447	-0.96409702	3.31689644
O	-1.15656555	-0.94410133	2.15136433
O	-1.22079861	-1.49224663	4.29087305
N	3.60295272	-0.38230103	1.84554589
O	2.92127562	0.71302849	1.67739964
O	2.94190836	-1.46366739	1.58804834
O	4.76189184	-0.38375783	2.21044421
N	2.00719619	0.48230034	-1.54862535
O	2.48101640	0.82635862	-2.61469960
O	2.09176493	-0.73701721	-1.10754228
O	1.37338722	1.29632807	-0.76788753
H	0.85879201	-5.21688843	-2.88947320
H	-0.51204073	5.02854347	0.18544316
O	-3.84539199	-0.90471649	1.31615174
H	-2.97814393	-0.96498644	1.78096759
H	-4.27030182	-1.74970484	1.54123902

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -14773.021904, E0 = -14772.570032, G= 232.9343 at T=298.150 K

Cl -5.16410971 3.29988408 -0.70445418  
Cl -3.37726426 -3.59304762 -3.49165273  
N -1.38438606 1.07031560 0.38003451  
N -0.37050369 4.01538324 2.17642665  
N -0.77141464 -1.32668519 -0.58039773  
N 1.72337174 -3.82933831 -1.13196647  
O 0.19120221 1.84203660 2.33438087  
O 1.32140851 -2.39912176 0.57340086  
C -1.61942148 2.28975058 0.87200212  
C -2.79389787 2.99841642 0.55366051  
H -3.02091050 3.96132541 1.00620270  
C -3.70114374 2.43320155 -0.32712430  
C -3.45286918 1.16449535 -0.91165668  
C -4.30442953 0.50050992 -1.84360874  
H -5.22240448 0.99958873 -2.15750527  
C -3.98435068 -0.73634821 -2.33971286  
H -4.64436722 -1.23063612 -3.05431724  
C -2.78893089 -1.40696597 -1.94371355  
C -2.37513232 -2.68800139 -2.39443612  
C -1.17187643 -3.22791219 -1.97856390  
H -0.86458945 -4.20640373 -2.34176803  
C -0.37401414 -2.49887490 -1.07675970  
C -1.91900063 -0.77879339 -1.01510859  
C -2.25240183 0.52780968 -0.49168941  
C -0.54512566 2.72180390 1.83940959  
C 0.95790780 -2.92314434 -0.50865453  
C -0.88373989 5.22883320 1.50821805  
H -1.84492135 5.54181147 1.95628071  
C 0.20164061 6.27390146 1.80104089

H	1.01888299	6.17575407	1.06788194
H	-0.19355257	7.29887486	1.74936712
C	0.68841964	5.87242842	3.20123577
H	-0.02970703	6.21054411	3.96651578
H	1.67580128	6.28668308	3.45023465
C	0.71515125	4.34253311	3.13365364
H	1.67000973	3.95450187	2.73912334
H	0.52846831	3.84441805	4.09728622
C	3.04757214	-4.13466311	-0.53533399
H	2.91642070	-4.65366411	0.42683038
H	3.56828094	-3.18204808	-0.33845982
C	3.75162029	-4.96196890	-1.61373413
C	3.16519141	-4.39360428	-2.91334963
C	1.68352079	-4.19564772	-2.57211161
H	3.29832578	-5.05468559	-3.78219986
H	3.59754634	-3.40534258	-3.13680696
H	3.49844766	-6.03039169	-1.50788498
H	4.84478760	-4.85924721	-1.54965258
H	1.23979843	-3.37740541	-3.16415668
Tb	0.37826040	-0.41626182	1.50779951
N	2.50915527	-0.55764997	3.35737514
O	3.42270374	-0.61595106	4.15045023
O	2.65297794	-0.09112274	2.14990830
O	1.30312157	-0.94967121	3.63604379
O	1.51913643	0.73742735	-0.21461193
H	1.26327538	0.63076985	-1.24321771
H	2.47675014	0.54882991	-0.17165783
N	-1.81593907	-1.57480085	2.93107557
O	-1.01154411	-2.27282810	2.18889332
O	-1.58448482	-0.29536253	2.91585040
O	-2.71274209	-2.07147861	3.57942414

H 1.12233984 -5.13856459 -2.70460796  
H -1.02820933 5.05187178 0.43262169  
N 1.32881737 -0.70448589 -2.99832702  
O 0.75904864 -1.36585677 -3.89492702  
O 0.77248472 0.40682524 -2.59727812  
O 2.39553690 -1.08255303 -2.45122004

**L4\*Tb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -14416.057306, E0 = -14415.644256, G= 213.2188 at T=298.150 K

Cl -4.56534338 3.83420801 -1.09588480  
Cl -3.36896515 -3.13460755 -3.94656801  
N -1.09624827 1.21595263 0.13152774  
N 0.05864719 3.94757438 2.16206503  
N -0.67984384 -1.22265685 -0.86244220  
N 1.43912458 -4.11356449 -1.12781358  
O 0.39471871 1.72207713 2.19562101  
O 1.12692785 -2.53908062 0.45061862  
C -1.25404572 2.43738055 0.65833086  
C -2.32814384 3.26599908 0.29401335  
H -2.49027586 4.23284912 0.76509494  
C -3.23160768 2.82032919 -0.66212326  
C -3.06881523 1.54703069 -1.26620436  
C -3.93389225 0.99750507 -2.26174688  
H -4.77768373 1.59656262 -2.60770202  
C -3.71908832 -0.25274870 -2.77314734  
H -4.38989973 -0.66049498 -3.53097749  
C -2.62239027 -1.05406463 -2.32969379  
C -2.34128523 -2.36840296 -2.78387237  
C -1.24270594 -3.06219697 -2.29315209  
H -1.06398892 -4.07939720 -2.63422894  
C -0.41731334 -2.44745207 -1.33721292  
C -1.73636365 -0.53844613 -1.34592819

C	-1.96266687	0.78292620	-0.80644852
C	-0.21949191	2.71726704	1.72197318
C	0.77149820	-3.06403732	-0.64031190
C	-0.35368487	5.26185369	1.61441338
H	-1.32454860	5.56276369	2.04718685
C	0.75862432	6.20231915	2.09619093
H	1.61700022	6.14678621	1.40714276
H	0.41489810	7.24536514	2.14204049
C	1.12853372	5.61824989	3.46700120
H	0.37917167	5.90529871	4.22241545
H	2.11553526	5.94614315	3.82177854
C	1.08952188	4.10736227	3.22535801
H	2.04940224	3.71602798	2.84706497
H	0.80912125	3.51125598	4.10647297
C	2.58919048	-4.65112305	-0.34866390
H	2.25569701	-4.92613840	0.66299474
H	3.34845018	-3.85682750	-0.24732724
C	3.08189249	-5.82659626	-1.19623375
C	2.73725939	-5.39508390	-2.62874699
C	1.35678983	-4.74584627	-2.46594644
H	2.70956373	-6.22975206	-3.34344411
H	3.46087503	-4.64771795	-2.99264812
H	2.53650689	-6.74644566	-0.92977440
H	4.15531683	-6.00999117	-1.04896474
H	1.13989854	-3.99445748	-3.23873425
Tb	0.54663843	-0.38073561	1.16576803
N	-1.02241230	-1.49046504	3.19285011
O	0.26641759	-1.30448902	3.29412365
O	-1.52897894	-1.10876036	2.04299498
O	-1.68964827	-1.96869266	4.07186604
N	3.03966498	0.46001789	0.20663667

O 1.94013727 0.57050389 -0.50118506  
O 2.86642838 -0.06972171 1.38544559  
O 4.11501789 0.81882048 -0.20148335  
H 0.56737965 -5.51863337 -2.46931815  
H -0.43651685 5.21819830 0.51893878

**L4\*Dy(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15221.630413, E0 = -15221.178712, G= 231.2105 at T=298.150 K

Cl -4.85850096 3.68810773 -0.78474092  
Cl -3.73904657 -3.30698276 -3.65299821  
N -1.24364650 1.14243424 0.17879541  
N 0.12104460 3.95766139 1.89980984  
N -0.86658877 -1.29026043 -0.79179788  
N 1.34148288 -4.02865696 -1.17803264  
O 0.34790999 1.73300922 2.17234564  
O 0.73113406 -2.82829547 0.64348781  
C -1.37009907 2.36829901 0.68197137  
C -2.48439169 3.18148255 0.40398586  
H -2.60843349 4.15921211 0.86713892  
C -3.46208024 2.69847035 -0.45165247  
C -3.33487129 1.41934073 -1.04321325  
C -4.27250481 0.82818848 -1.94397080  
H -5.16125965 1.39903092 -2.21771383  
C -4.07379436 -0.42554155 -2.45226240  
H -4.80139589 -0.86369550 -3.13736629  
C -2.92271137 -1.19533312 -2.09980249  
C -2.64281011 -2.50440311 -2.55969119  
C -1.50506318 -3.17444992 -2.13582325  
H -1.31167459 -4.19329262 -2.47162557  
C -0.63809597 -2.52384353 -1.24168813  
C -1.96876633 -0.64325047 -1.19996917



C	-2.17666340	0.68596524	-0.66644663
C	-0.24266550	2.68936634	1.63408995
C	0.54277951	-3.15621519	-0.54468650
C	-0.21936230	5.18616295	1.15501726
H	-1.08540213	5.69445276	1.61846614
C	1.04609334	6.04182053	1.30464625
H	1.78935909	5.73377371	0.55121404
H	0.83499056	7.11331558	1.17378485
C	1.53565848	5.67872524	2.71491146
H	0.93707359	6.20882750	3.47436452
H	2.59448504	5.92504501	2.87903094
C	1.28825533	4.16854000	2.79419255
H	2.13659430	3.57330298	2.41470313
H	1.05762112	3.80379033	3.80675387
C	2.55398035	-4.50800991	-0.46300158
H	2.26871037	-5.20482111	0.34019551
H	3.04597545	-3.63930082	0.00740356
C	3.39882421	-5.14969969	-1.57081723
C	2.97875309	-4.37570095	-2.83039355
C	1.46500659	-4.21761847	-2.63769555
H	3.22405195	-4.89500809	-3.76849508
H	3.44708967	-3.37796450	-2.83944893
H	3.15153122	-6.21903276	-1.67951667
H	4.47390842	-5.06611443	-1.35562062
H	1.05328298	-3.35206938	-3.17567325
Dy	0.84448487	-0.37952891	1.03751338
N	-0.63478893	-1.17508137	3.36197424
O	0.63135463	-1.00417113	3.39251256
O	-1.18151510	-0.95909983	2.18163800
O	-1.30363321	-1.50809658	4.31937885
N	3.53571320	-0.45987719	1.95443058

O 2.85634971 0.64136392 1.81013691  
 O 2.87927175 -1.53187060 1.65112388  
 O 4.68795300 -0.47253272 2.33985853  
 N 2.00614810 0.46821347 -1.45629454  
 O 2.49321270 0.80994946 -2.51837230  
 O 2.04986000 -0.76256490 -1.03550065  
 O 1.40238118 1.28991914 -0.66427076  
 H 0.93179727 -5.13263750 -2.95626116  
 H -0.45654088 4.95352602 0.10699231  
 O -3.84942269 -0.94513059 1.30800736  
 H -2.98795819 -0.99136758 1.78648329  
 H -4.28043556 -1.77977753 1.55848420

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15221.631164, E0 = -15221.179022, G= 233.2607 at T=298.150 K

Cl -5.15198374 3.29977083 -0.71237957  
 Cl -3.37211657 -3.60182929 -3.47458053  
 N -1.38124907 1.06791461 0.38896042  
 N -0.36117446 4.01461267 2.17714381  
 N -0.76363337 -1.33051050 -0.56902897  
 N 1.73159075 -3.83129072 -1.12811315  
 O 0.18877798 1.83836079 2.34880400  
 O 1.32993448 -2.40869260 0.58523667  
 C -1.61343718 2.28725386 0.87487775  
 C -2.78391242 2.99951744 0.55018872  
 H -3.00974131 3.96489167 0.99803275  
 C -3.69093585 2.43158698 -0.33029896  
 C -3.44441366 1.16168690 -0.90828705  
 C -4.29703856 0.49551985 -1.84057319  
 H -5.21322584 0.99539781 -2.15827966  
 C -3.97730112 -0.74159217 -2.33080816  
 H -4.63595390 -1.23752189 -3.04564095

C -2.78138232 -1.41308796 -1.93156695  
C -2.36919641 -2.69369578 -2.38051605  
C -1.16467786 -3.23257065 -1.96491563  
H -0.85682118 -4.21112394 -2.32742691  
C -0.36677858 -2.50187016 -1.06498730  
C -1.91180885 -0.78309077 -1.00501478  
C -2.24628067 0.52395070 -0.48514390  
C -0.53876156 2.71894765 1.84759545  
C 0.96758860 -2.92732668 -0.49728829  
C -0.87167084 5.22662497 1.50480390  
H -1.83423817 5.54141092 1.94883955  
C 0.21343127 6.27178860 1.79882503  
H 1.03267419 6.17177773 1.06817043  
H -0.18103121 7.29688883 1.74411702  
C 0.69621104 5.87267017 3.20109773  
H -0.02394242 6.21252871 3.96369934  
H 1.68307245 6.28695154 3.45207214  
C 0.72213125 4.34263229 3.13650799  
H 1.67776942 3.95307302 2.74521255  
H 0.53281242 3.84643197 4.10058260  
C 3.05719280 -4.13773966 -0.53613591  
H 2.92939901 -4.66305017 0.42310154  
H 3.57670379 -3.18553233 -0.33365101  
C 3.76077771 -4.95729876 -1.62089694  
C 3.16989017 -4.38321257 -2.91599131  
C 1.68863475 -4.19063711 -2.56973267  
H 3.30252171 -5.03905106 -3.78890681  
H 3.59926319 -3.39269471 -3.13534403  
H 3.50984550 -6.02678490 -1.52055073  
H 4.85391521 -4.85307741 -1.55873775  
H 1.24103749 -3.37173343 -3.15795016

Dy 0.37794918 -0.41946656 1.51331663  
 N 2.48297453 -0.55865335 3.36539268  
 O 3.39813375 -0.61028248 4.15692806  
 O 2.62662196 -0.09180484 2.15469813  
 O 1.28036034 -0.95568860 3.64338112  
 O 1.48991871 0.74733961 -0.22191057  
 H 1.23693538 0.63864219 -1.24579775  
 H 2.45064998 0.57722253 -0.17614856  
 N -1.82739556 -1.57380211 2.90017176  
 O -1.01376772 -2.27238393 2.17056131  
 O -1.59324527 -0.29419258 2.88752556  
 O -2.73566723 -2.06792498 3.53559017  
 H 1.13013601 -5.13486147 -2.70566916  
 H -1.01245165 5.04844093 0.42884621  
 N 1.28612697 -0.70223516 -3.00589705  
 O 0.71063417 -1.37198460 -3.89339781  
 O 0.73133236 0.40969098 -2.60754085  
 O 2.35828638 -1.07523131 -2.46517158

**L4\*Dy(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -14864.668600, E0 = -14864.255327, G= 213.6019 at T=298.150 K

Cl -4.55432320 3.83858466 -1.11452985  
 Cl -3.37698245 -3.13842559 -3.93859076  
 N -1.07926726 1.22866058 0.10801244  
 N 0.05317262 3.95422006 2.16303182  
 N -0.66692054 -1.21662939 -0.88247836  
 N 1.43235433 -4.12257862 -1.12636459  
 O 0.42598715 1.73540556 2.16101503  
 O 1.13598490 -2.53617024 0.44247928  
 C -1.24191523 2.44525933 0.64020073  
 C -2.31871295 3.27259946 0.27782026  
 H -2.48477912 4.23595381 0.75396007

C -3.21763420 2.82821321 -0.68200982  
 C -3.04984522 1.55756390 -1.29065609  
 C -3.91492009 1.00803292 -2.28605962  
 H -4.75777054 1.60819149 -2.63225937  
 C -3.70397282 -0.24459457 -2.79287839  
 H -4.37656260 -0.65446883 -3.54789472  
 C -2.61078548 -1.04793143 -2.34489846  
 C -2.34087873 -2.36950183 -2.78539038  
 C -1.24941325 -3.06811142 -2.28777480  
 H -1.08030856 -4.09063911 -2.61759734  
 C -0.41640404 -2.44801378 -1.34081304  
 C -1.71865511 -0.53054178 -1.36705351  
 C -1.94198036 0.79577905 -0.83022308  
 C -0.20455015 2.72603965 1.70415759  
 C 0.77447426 -3.06529140 -0.64238775  
 C -0.38392508 5.27150965 1.64209473  
 H -1.36325014 5.54214621 2.07579613  
 C 0.70451486 6.22523546 2.15175486  
 H 1.56773424 6.20683575 1.46687937  
 H 0.33629361 7.25864124 2.22036576  
 C 1.08094680 5.61767149 3.51044512  
 H 0.32154244 5.86977673 4.26826286  
 H 2.05850029 5.95923281 3.87820339  
 C 1.07734489 4.11248684 3.23291683  
 H 2.04727888 3.75243068 2.84911609  
 H 0.80820876 3.48898911 4.09840631  
 C 2.58357906 -4.66081572 -0.34956622  
 H 2.25616336 -4.91483831 0.66940075  
 H 3.35258102 -3.87363195 -0.26798347  
 C 3.05600882 -5.85361338 -1.18399465  
 C 2.70913768 -5.43542099 -2.61993074

C 1.33747983 -4.76722956 -2.45814681  
 H 2.66732645 -6.27840424 -3.32411408  
 H 3.44003654 -4.70171976 -2.99674416  
 H 2.49983454 -6.76259565 -0.90288591  
 H 4.12772799 -6.04928255 -1.04028082  
 H 1.12765813 -4.02103567 -3.23787284  
 Dy 0.58550560 -0.37013051 1.14668024  
 N -0.93996376 -1.45720041 3.20913458  
 O 0.35897657 -1.34923983 3.25376701  
 O -1.47244799 -1.01528382 2.09350872  
 O -1.59562325 -1.91794574 4.10674334  
 N 3.06409287 0.44003540 0.15210603  
 O 1.96577728 0.47307235 -0.56584120  
 O 2.89001179 0.01001787 1.36905241  
 O 4.13620949 0.77785021 -0.28231889  
 H 0.53876752 -5.53031206 -2.45120931  
 H -0.45942065 5.25116158 0.54543829

**L4\*Ho(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -15681.073845, E0 = -15680.622052, G= 231.3687 at T=298.150 K

Cl -4.85930777 3.68332815 -0.76703650  
 Cl -3.72827840 -3.30751681 -3.63921833  
 N -1.23368549 1.15009284 0.18252057  
 N 0.12598109 3.96494770 1.91060126  
 N -0.84796697 -1.27992952 -0.79291725  
 N 1.35005307 -4.03204775 -1.16956973  
 O 0.37666047 1.74011767 2.15638041  
 O 0.75664204 -2.81039095 0.64261514  
 C -1.36139429 2.37452793 0.68777299  
 C -2.47994947 3.18409514 0.41457587  
 H -2.60739923 4.16045332 0.87959641

C -3.45795012 2.69872379 -0.43937713  
 C -3.32783985 1.42119408 -1.03404009  
 C -4.26581621 0.82778907 -1.93286896  
 H -5.15726376 1.39566576 -2.20388818  
 C -4.06455660 -0.42526790 -2.44157600  
 H -4.79283953 -0.86604810 -3.12423539  
 C -2.91032720 -1.19177604 -2.09224796  
 C -2.62989187 -2.50115490 -2.55063367  
 C -1.49070168 -3.16915703 -2.12792659  
 H -1.29848754 -4.18923330 -2.46040726  
 C -0.62067884 -2.51519179 -1.23896539  
 C -1.95400023 -0.63629967 -1.19703245  
 C -2.16597104 0.69163460 -0.66170704  
 C -0.22835098 2.69625711 1.63346422  
 C 0.56061542 -3.14674973 -0.54154742  
 C -0.23233856 5.19879723 1.18328202  
 H -1.10097826 5.69166803 1.65833521  
 C 1.02459633 6.06658888 1.33536172  
 H 1.76566136 5.77719402 0.57241255  
 H 0.80057466 7.13730049 1.22055185  
 C 1.52860987 5.69033670 2.73699903  
 H 0.92955840 6.20336771 3.50772357  
 H 2.58571362 5.94653797 2.89694071  
 C 1.29858124 4.17659378 2.79755402  
 H 2.15014052 3.59628725 2.40238428  
 H 1.08114064 3.79536605 3.80690432  
 C 2.55993366 -4.51586390 -0.45351520  
 H 2.26994371 -5.19563818 0.36242157  
 H 3.06627393 -3.64652920 0.00023596  
 C 3.38943100 -5.18686581 -1.55548096  
 C 2.97493768 -4.42539120 -2.82443476

C 1.46473026 -4.24134636 -2.62708497  
 H 3.20697665 -4.96261311 -3.75586891  
 H 3.45940137 -3.43564892 -2.85125637  
 H 3.12478423 -6.25366402 -1.64692128  
 H 4.46676207 -5.11708784 -1.34694684  
 H 1.06396234 -3.37670088 -3.17473888  
 Ho 0.85178095 -0.36279488 1.02338970  
 N -0.66509473 -1.17850244 3.30302572  
 O 0.60421062 -1.00707746 3.33384132  
 O -1.21108365 -0.94404483 2.13097501  
 O -1.32738888 -1.52776754 4.25921822  
 N 3.54972219 -0.44238096 1.90533090  
 O 2.87421584 0.65762389 1.73085594  
 O 2.88217092 -1.51839161 1.65451741  
 O 4.70883465 -0.44640133 2.27086115  
 N 2.00460649 0.47516179 -1.46617866  
 O 2.50461173 0.81098461 -2.52397966  
 O 2.07214904 -0.74573916 -1.02096081  
 O 1.36080909 1.29195321 -0.70216328  
 H 0.91638881 -5.15214062 -2.93194032  
 H -0.47340289 4.97641468 0.13393241  
 O -3.88881350 -0.94778454 1.28257143  
 H -3.02305055 -0.98868215 1.75319326  
 H -4.30635738 -1.79118359 1.52631998

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -15681.076691, E0 = -15680.623914, G= 234.0345 at T=298.150 K

Cl -5.14383554 3.30037045 -0.73008555  
 Cl -3.38333440 -3.63159561 -3.44814229  
 N -1.39339626 1.04814351 0.39811853  
 N -0.34324303 3.99451804 2.15662241  
 N -0.77848762 -1.34575009 -0.55087024



N	1.73121941	-3.82116294	-1.11857390
O	0.16000991	1.81015551	2.37494159
O	1.30864489	-2.42265344	0.61372995
C	-1.61909330	2.27057433	0.87667477
C	-2.78301167	2.98998117	0.54375994
H	-3.00119185	3.96119046	0.98320365
C	-3.69233680	2.42256808	-0.33521628
C	-3.45328593	1.14717901	-0.90418845
C	-4.30596638	0.47786134	-1.83463085
H	-5.21987772	0.97857976	-2.15752912
C	-3.98924041	-0.76311201	-2.31782699
H	-4.64840031	-1.26039970	-3.03131652
C	-2.79500318	-1.43580580	-1.91443706
C	-2.38145876	-2.71823239	-2.35774469
C	-1.17548847	-3.25319290	-1.94061494
H	-0.86496198	-4.23295021	-2.29834509
C	-0.37846503	-2.51583242	-1.04496074
C	-1.92676020	-0.80265743	-0.98957700
C	-2.25950146	0.50616980	-0.47496146
C	-0.54404324	2.69684362	1.85190034
C	0.95775509	-2.93344116	-0.47641170
C	-0.82118845	5.19994354	1.44876099
H	-1.77554619	5.55227757	1.88202941
C	0.29103097	6.22376204	1.71475422
H	1.10910821	6.07926369	0.99026525
H	-0.07513532	7.25709152	1.62771046
C	0.75884318	5.85439396	3.13027287
H	0.04633353	6.23722887	3.87954092
H	1.75607407	6.24895430	3.37187147
C	0.74327630	4.32272434	3.11247492
H	1.68966711	3.89537096	2.73880792

H 0.53533989 3.86177492 4.09011221  
 C 3.05857825 -4.12936211 -0.53072119  
 H 2.93368673 -4.72736645 0.38584533  
 H 3.54254103 -3.18095851 -0.24324958  
 C 3.80457520 -4.85301208 -1.65670455  
 C 3.18608713 -4.24952078 -2.92613840  
 C 1.70026469 -4.13774776 -2.57079053  
 H 3.34549665 -4.86299610 -3.82511187  
 H 3.56874871 -3.23218942 -3.10465240  
 H 3.61377072 -5.93834162 -1.61041021  
 H 4.89034271 -4.69229460 -1.58588183  
 H 1.21356606 -3.32184935 -3.13289762  
 Ho 0.34226653 -0.44438794 1.54024458  
 N 2.42230225 -0.60937864 3.40972137  
 O 3.32699633 -0.67588079 4.21283579  
 O 2.58405924 -0.13599402 2.20570087  
 O 1.21271050 -0.99624068 3.67005229  
 O 1.47391796 0.72863352 -0.15215605  
 H 1.21028566 0.65162104 -1.17542160  
 H 2.43028808 0.53270584 -0.12026408  
 N -1.87290967 -1.59376371 2.89601755  
 O -1.05599821 -2.29243541 2.17085171  
 O -1.63378060 -0.31554550 2.89114141  
 O -2.78837848 -2.08708382 3.52164793  
 H 1.18508959 -5.10125923 -2.73415923  
 H -0.96564686 4.99426985 0.37830132  
 N 1.24810159 -0.64953673 -2.95709705  
 O 0.66559279 -1.31137311 -3.84563661  
 O 0.69502640 0.45581958 -2.53998828  
 O 2.32736945 -1.02466583 -2.43119836

**L4\*Ho(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15324.111885, E0 = -15323.698660, G= 212.8647 at T=298.150 K

Cl	-4.54983330	3.84354973	-1.11158204
Cl	-3.35619688	-3.12861609	-3.95722699
N	-1.08432412	1.22364938	0.11486546
N	0.05865136	3.93670750	2.17769146
N	-0.66658849	-1.21150064	-0.88008219
N	1.43759847	-4.11719036	-1.10927320
O	0.42890000	1.71732473	2.15554595
O	1.15343499	-2.50168848	0.43086368
C	-1.24477482	2.43948579	0.64960593
C	-2.31976652	3.26923633	0.28667921
H	-2.48594141	4.23276901	0.76273549
C	-3.21630478	2.82947206	-0.67781276
C	-3.04840159	1.56084025	-1.29068673
C	-3.90850234	1.01418197	-2.29223490
H	-4.75022793	1.61442089	-2.64122343
C	-3.69434237	-0.23668857	-2.80277967
H	-4.36375666	-0.64309496	-3.56258130
C	-2.60274005	-1.04155672	-2.35301161
C	-2.32755113	-2.36095548	-2.79646587
C	-1.23628116	-3.05829406	-2.29616308
H	-1.06312871	-4.07879972	-2.62979627
C	-0.40891853	-2.44018912	-1.34267402
C	-1.71724010	-0.52670318	-1.36861956
C	-1.94398642	0.79618108	-0.82835859
C	-0.20362251	2.71301579	1.71046793
C	0.78370774	-3.04982138	-0.64264029
C	-0.38099751	5.25789022	1.66890824
H	-1.35857844	5.52476263	2.10874963
C	0.70979673	6.20850563	2.17967343
H	1.56780839	6.19823360	1.48816538

H	0.34048268	7.24060059	2.26093817
C	1.09769678	5.58917189	3.52976251
H	0.34443101	5.83383417	4.29610729
H	2.07802773	5.92840624	3.89226007
C	1.09289753	4.08649921	3.23914242
H	2.05931687	3.73047948	2.84295344
H	0.83217376	3.45544004	4.10172272
C	2.58927369	-4.64404726	-0.32516220
H	2.26345992	-4.87898779	0.69897884
H	3.36078978	-3.85780287	-0.25979352
C	3.05523872	-5.85467434	-1.13704443
C	2.70448232	-5.46504927	-2.58002138
C	1.33629751	-4.78721046	-2.42783785
H	2.65622067	-6.32249594	-3.26608324
H	3.43713498	-4.74275684	-2.97498107
H	2.49775076	-6.75623369	-0.83544666
H	4.12695694	-6.05043364	-0.99341029
H	1.12940204	-4.05506659	-3.22156405
Ho	0.57640362	-0.35791999	1.11919844
N	-0.93637800	-1.45740640	3.16761327
O	0.35283682	-1.26123965	3.23812866
O	-1.47068465	-1.08584857	2.02971601
O	-1.57823122	-1.93629169	4.06572914
N	2.99047208	0.50692254	0.03604475
O	1.86386549	0.59223467	-0.62616634
O	2.87458134	-0.01243377	1.22765636
O	4.04460287	0.87693834	-0.41709784
H	0.53326362	-5.54543638	-2.40449595
H	-0.46065733	5.24567890	0.57241356

**L4\*Er(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16151.450460, E0 = -16150.998578, G= 231.5624 at T=298.150 K

Cl	-4.86028147	3.68116188	-0.78343624
Cl	-3.73447943	-3.31330514	-3.65819836
N	-1.23743701	1.14077687	0.16419402
N	0.11715614	3.94903779	1.90741861
N	-0.86143565	-1.28889906	-0.80376154
N	1.34489691	-4.03462267	-1.17765272
O	0.35436991	1.72289002	2.15643597
O	0.75343329	-2.79777193	0.62435639
C	-1.36553621	2.36436892	0.67247570
C	-2.48294449	3.17537069	0.39968228
H	-2.60842252	4.15118456	0.86648864
C	-3.46151042	2.69315457	-0.45534918
C	-3.33374286	1.41539395	-1.04973328
C	-4.27245140	0.82269692	-1.94852972
H	-5.16305542	1.39187217	-2.21980882
C	-4.07297230	-0.43058357	-2.45802283
H	-4.80167913	-0.86937243	-3.14154100
C	-2.91975594	-1.19863486	-2.10849071
C	-2.63753605	-2.50744152	-2.56800437
C	-1.49741280	-3.17463493	-2.14598751
H	-1.30340254	-4.19340515	-2.48143482
C	-0.63005185	-2.52152824	-1.25358617
C	-1.96497381	-0.64468497	-1.21108997
C	-2.17308617	0.68423009	-0.67749393
C	-0.23962678	2.68166327	1.62703979
C	0.55414009	-3.14630795	-0.55553359
C	-0.22608210	5.18279600	1.17311919
H	-1.09478593	5.68422318	1.63916707
C	1.03622115	6.04153013	1.33238816
H	1.78130460	5.74334383	0.57683837

H	0.82137775	7.11348915	1.21170664
C	1.52572381	5.66665030	2.73959374
H	0.92457378	6.18744516	3.50345874
H	2.58353043	5.91504812	2.90710974
C	1.28328502	4.15494156	2.80413961
H	2.13338661	3.56574869	2.41909814
H	1.05360663	3.77973986	3.81309080
C	2.55758834	-4.50903463	-0.45982021
H	2.27100825	-5.18338490	0.36184061
H	3.06144452	-3.63472438	-0.01308120
C	3.38750648	-5.18624640	-1.55777943
C	2.96569180	-4.43977547	-2.83331585
C	1.45528293	-4.25986767	-2.63293195
H	3.19755864	-4.98548222	-3.75977206
H	3.44578004	-3.44835973	-2.87196994
H	3.12851858	-6.25527859	-1.63807309
H	4.46499014	-5.10857916	-1.35286415
H	1.04878175	-3.40324020	-3.18891835
Er	0.84025681	-0.36038312	1.01139355
N	-0.60492015	-1.12778056	3.33914304
O	0.66219717	-0.95543540	3.34566140
O	-1.17071390	-0.91814619	2.16918421
O	-1.25442421	-1.45750284	4.31113482
N	3.51727486	-0.44454938	1.93484843
O	2.83956051	0.65414363	1.78233767
O	2.86227822	-1.51514030	1.63108325
O	4.66849756	-0.45630470	2.32604098
N	2.00977230	0.54338968	-1.43694961
O	2.50554705	0.90773994	-2.48727417
O	2.05011678	-0.69570482	-1.04103076
O	1.39939272	1.34696841	-0.63261330

H 0.90997112 -5.17644787 -2.92559505  
H -0.46022370 4.95872736 0.12253288  
O -3.84278679 -0.93466705 1.30893922  
H -2.97990274 -0.96714860 1.78581595  
H -4.26038933 -1.77535069 1.56188619

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16151.453010, E0 = -16151.000605, G= 233.6760 at T=298.150 K

Cl -5.14624262 3.30742264 -0.70808166  
Cl -3.38755178 -3.60349178 -3.48231387  
N -1.37714565 1.06156623 0.37180379  
N -0.35019848 3.99230170 2.18316841  
N -0.77176464 -1.33080983 -0.58726043  
N 1.72787571 -3.82863522 -1.13288188  
O 0.20655710 1.81629503 2.32265592  
O 1.32483947 -2.38456655 0.56143713  
C -1.60477209 2.27849889 0.86388612  
C -2.77549124 2.99422503 0.54655957  
H -2.99681687 3.95916176 0.99746668  
C -3.68818521 2.43156672 -0.33157489  
C -3.44855690 1.16217959 -0.91300148  
C -4.30648994 0.49680156 -1.84156084  
H -5.22383547 0.99800950 -2.15408063  
C -3.99169469 -0.74098706 -2.33406568  
H -4.65502453 -1.23531568 -3.04573035  
C -2.79441810 -1.41453612 -1.94104886  
C -2.38205433 -2.69481492 -2.39120674  
C -1.17575431 -3.23379946 -1.97909653  
H -0.86899209 -4.21190596 -2.34372950  
C -0.37493780 -2.50221515 -1.08224189  
C -1.92086089 -0.78488511 -1.01875031  
C -2.24947691 0.52247769 -0.49693745

C	-0.52490121	2.70073700	1.83606899
C	0.96264923	-2.91926146	-0.51392001
C	-0.86427081	5.21266651	1.52885854
H	-1.82712317	5.51863194	1.97846985
C	0.21835279	6.25650311	1.83688164
H	1.03635085	6.17055368	1.10307634
H	-0.17956425	7.28103304	1.79880786
C	0.70536655	5.83746958	3.23185754
H	-0.01406691	6.16355228	4.00110817
H	1.69160259	6.25074434	3.48687387
C	0.73560292	4.30876350	3.14368701
H	1.69101489	3.92801142	2.74329591
H	0.55116475	3.79680443	4.10041332
C	3.05545211	-4.12349224	-0.53908515
H	2.92997742	-4.63060379	0.43010604
H	3.57450294	-3.16707516	-0.35668343
C	3.75576735	-4.96302938	-1.61047113
C	3.16144252	-4.41299391	-2.91442609
C	1.68126416	-4.21162844	-2.56826949
H	3.29080653	-5.08567858	-3.77490258
H	3.59154677	-3.42749500	-3.15369368
H	3.50552297	-6.03048897	-1.48925996
H	4.84900618	-4.85711098	-1.55361164
H	1.23505533	-3.40002322	-3.16769862
Er	0.37518126	-0.42045668	1.47279942
N	2.42509031	-0.40747920	3.37493944
O	3.31678367	-0.37546474	4.19551420
O	2.59451628	-0.02965080	2.13854790
O	1.22597170	-0.81339723	3.64424872
O	1.47856545	0.74018741	-0.23531437
H	1.25244904	0.62135243	-1.26405048



H 2.44494772 0.62515247 -0.15680884  
 N -1.78240919 -1.58260882 2.89468646  
 O -0.93198436 -2.28070712 2.20827055  
 O -1.60547256 -0.29855165 2.81421232  
 O -2.67220426 -2.08347845 3.55104160  
 H 1.11966741 -5.15616751 -2.68727636  
 H -1.00552857 5.05035782 0.45046037  
 N 1.31060767 -0.72751963 -3.02297997  
 O 0.72750992 -1.40186512 -3.90293264  
 O 0.75922555 0.38720047 -2.62829971  
 O 2.38555312 -1.09803581 -2.48795605

**L4\*Er(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -15794.490674, E0 = -15794.077249, G= 213.9134 at T=298.150 K

Cl -4.54334450 3.83924365 -1.09693301  
 Cl -3.34867644 -3.13479376 -3.94249177  
 N -1.07641947 1.21940768 0.12551661  
 N 0.06854865 3.92903376 2.18958426  
 N -0.65929693 -1.21368766 -0.86765158  
 N 1.44655609 -4.11680841 -1.09366059  
 O 0.43463087 1.70849657 2.16872334  
 O 1.15750003 -2.50344372 0.44869435  
 C -1.23744035 2.43405223 0.66228431  
 C -2.31314874 3.26356149 0.30101430  
 H -2.47998834 4.22625113 0.77870959  
 C -3.20956302 2.82485175 -0.66418958  
 C -3.04137540 1.55701768 -1.27829158  
 C -3.90091324 1.01030838 -2.28042150  
 H -4.74224043 1.61071956 -2.63008428  
 C -3.68664098 -0.24068324 -2.79083347  
 H -4.35556078 -0.64689112 -3.55118275  
 C -2.59550476 -1.04594064 -2.34034705

C -2.32047725 -2.36579251 -2.78203988  
 C -1.22952056 -3.06264830 -2.28016090  
 H -1.05623162 -4.08386517 -2.61150455  
 C -0.40185043 -2.44304681 -1.32794940  
 C -1.71000838 -0.53013432 -1.35652924  
 C -1.93665469 0.79243815 -0.81679404  
 C -0.19610612 2.70523143 1.72387815  
 C 0.79045469 -3.05139279 -0.62563699  
 C -0.36878026 5.25028181 1.67877078  
 H -1.34511781 5.51999617 2.11956978  
 C 0.72472781 6.19947529 2.18625402  
 H 1.58186018 6.18605804 1.49370134  
 H 0.35777876 7.23254776 2.26588154  
 C 1.11297143 5.58183908 3.53705931  
 H 0.36136168 5.82975054 4.30397034  
 H 2.09458923 5.91954041 3.89750934  
 C 1.10444534 4.07860661 3.24943137  
 H 2.06947279 3.71987081 2.85235906  
 H 0.84352297 3.44975567 4.11352730  
 C 2.59854484 -4.64404011 -0.31028968  
 H 2.27192068 -4.88409472 0.71239376  
 H 3.36785007 -3.85602903 -0.24072376  
 C 3.06887150 -5.85012817 -1.12678409  
 C 2.71820593 -5.45606089 -2.56852770  
 C 1.34802330 -4.78292942 -2.41446495  
 H 2.67308354 -6.31090450 -3.25804830  
 H 3.44905639 -4.73016119 -2.96020532  
 H 2.51390123 -6.75450993 -0.82906806  
 H 4.14107275 -6.04313231 -0.98302221  
 H 1.13875151 -4.04888630 -3.20573926  
 Er 0.57827908 -0.35449848 1.11205840

N -1.00731099 -1.43985438 3.10614204  
 O 0.28156990 -1.26179218 3.21142888  
 O -1.50254464 -1.05570006 1.95623755  
 O -1.68037522 -1.91351628 3.98439980  
 N 2.93502688 0.52805048 -0.05491454  
 O 1.78469396 0.58637655 -0.67674476  
 O 2.86359715 0.02252885 1.14558315  
 O 3.96713281 0.90779603 -0.54829228  
 H 0.54745495 -5.54380083 -2.39363313  
 H -0.45036542 5.23608065 0.58247811

**L4\*Tm(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -16632.950468, E0 = -16632.498789, G= 231.3732 at T=298.150 K

Cl -4.84146404 3.70217729 -0.80293179  
 Cl -3.73665309 -3.31151891 -3.63208032  
 N -1.21708703 1.16695440 0.14742374  
 N 0.11507273 3.96765614 1.92843509  
 N -0.84776628 -1.27356732 -0.80244714  
 N 1.33207154 -4.04464769 -1.13960981  
 O 0.38765958 1.73995543 2.12091208  
 O 0.74280846 -2.79015398 0.65343982  
 C -1.34770381 2.38883018 0.65842605  
 C -2.46681023 3.19787145 0.38555065  
 H -2.59707808 4.17221594 0.85375053  
 C -3.44220901 2.71511292 -0.47268197  
 C -3.31335449 1.43702269 -1.06636596  
 C -4.25270891 0.84239006 -1.96307051  
 H -5.14222050 1.41181743 -2.23724747  
 C -4.05591536 -0.41449106 -2.46433115  
 H -4.78568745 -0.85654467 -3.14459085  
 C -2.90629101 -1.18452311 -2.10741949

C -2.63432932 -2.50101852 -2.55045319  
 C -1.50154924 -3.17297554 -2.11690450  
 H -1.31597841 -4.19816017 -2.43737984  
 C -0.62852073 -2.51568532 -1.23341751  
 C -1.94748282 -0.62609738 -1.21706378  
 C -2.15206385 0.70713156 -0.69314337  
 C -0.22280686 2.70178127 1.61625540  
 C 0.54742438 -3.14531565 -0.52449507  
 C -0.24583499 5.21547270 1.22713482  
 H -1.12579906 5.68833017 1.70183587  
 C 0.99985218 6.09190559 1.41806304  
 H 1.75429547 5.82985258 0.65836698  
 H 0.76615793 7.16282558 1.32701492  
 C 1.48889637 5.68565035 2.81664729  
 H 0.87478095 6.17381525 3.59160280  
 H 2.54121637 5.94787359 2.99704766  
 C 1.27268350 4.16872597 2.83698869  
 H 2.13550735 3.60561991 2.44152308  
 H 1.04411900 3.76160622 3.83375931  
 C 2.54110432 -4.52012396 -0.41675076  
 H 2.25037527 -5.18854570 0.40823525  
 H 3.04891157 -3.64501286 0.02412495  
 C 3.37042284 -5.20616388 -1.50931096  
 C 2.96128178 -4.45586109 -2.78656960  
 C 1.45083869 -4.26622915 -2.59507442  
 H 3.19537568 -5.00199223 -3.71222734  
 H 3.44728994 -3.46722269 -2.82061744  
 H 3.10179734 -6.27282286 -1.59045303  
 H 4.44755936 -5.13833761 -1.29895651  
 H 1.05503464 -3.40450811 -3.15093970  
 Tm 0.85355222 -0.33665755 0.96106732

N -0.57870907 -1.20013714 3.25916219  
 O 0.69804251 -1.10086167 3.22622204  
 O -1.17337394 -0.85349584 2.14284801  
 O -1.20507550 -1.58169615 4.22827816  
 N 3.55604911 -0.37362564 1.82886314  
 O 2.83648491 0.70472711 1.71162939  
 O 2.93704939 -1.45771372 1.52180314  
 O 4.71553898 -0.34533173 2.19757032  
 N 1.98188889 0.38654494 -1.56349921  
 O 2.45141315 0.70405287 -2.64143753  
 O 2.06075168 -0.81785852 -1.09389675  
 O 1.35744989 1.22369194 -0.80016029  
 H 0.90076971 -5.17766094 -2.89483070  
 H -0.47031945 5.01755142 0.16919750  
 O -3.84552670 -0.93635827 1.28686082  
 H -2.98239589 -0.94650722 1.76405430  
 H -4.23881197 -1.78973925 1.53626359

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -16632.953476, E0 = -16632.501303, G= 233.4576 at T=298.150 K

Cl -5.13874388 3.31361246 -0.73249751  
 Cl -3.39185023 -3.62100220 -3.45252657  
 N -1.37600064 1.06681347 0.36935732  
 N -0.34527993 3.99832416 2.17232466  
 N -0.77250469 -1.33321667 -0.56883836  
 N 1.72505486 -3.83150673 -1.13063467  
 O 0.19575065 1.81820917 2.32529902  
 O 1.33481932 -2.39510632 0.57305133  
 C -1.60448742 2.28491855 0.85632193  
 C -2.77289820 3.00190687 0.53264648  
 H -2.99389982 3.96924186 0.97880334  
 C -3.68352365 2.43696451 -0.34623864

C -3.44449854 1.16359627 -0.91957021  
 C -4.30153275 0.49395683 -1.84590411  
 H -5.21703053 0.99463356 -2.16460276  
 C -3.98783970 -0.74766523 -2.32896233  
 H -4.65022612 -1.24575317 -3.03884721  
 C -2.79309225 -1.42122126 -1.92804992  
 C -2.38439298 -2.70590353 -2.36823988  
 C -1.17826080 -3.24262428 -1.95353520  
 H -0.87173021 -4.22323465 -2.31181049  
 C -0.37614813 -2.50618052 -1.06188488  
 C -1.92011225 -0.78759146 -1.00746012  
 C -2.24770498 0.52430063 -0.49664664  
 C -0.52633995 2.70555425 1.83205831  
 C 0.96405977 -2.92363620 -0.50015080  
 C -0.85412884 5.21741819 1.51184797  
 H -1.81881595 5.52644920 1.95538056  
 C 0.22853981 6.26063395 1.82215750  
 H 1.04975867 6.17170238 1.09229898  
 H -0.16757643 7.28569221 1.77962768  
 C 0.70876849 5.84434986 3.22035551  
 H -0.01373964 6.17307663 3.98559666  
 H 1.69430196 6.25717306 3.47883415  
 C 0.73734760 4.31536627 3.13579559  
 H 1.69402599 3.93333268 2.73960042  
 H 0.54914886 3.80545521 4.09284401  
 C 3.05557418 -4.13060713 -0.54524595  
 H 2.93479371 -4.65406179 0.41588011  
 H 3.57169962 -3.17583776 -0.34716332  
 C 3.75657535 -4.95110416 -1.63113058  
 C 3.15423846 -4.38654709 -2.92514420  
 C 1.67423129 -4.19935369 -2.56958866

H 3.28408122 -5.04601955 -3.79577208  
 H 3.57737350 -3.39491820 -3.15123105  
 H 3.51334929 -6.02169180 -1.52415490  
 H 4.84939146 -4.83942461 -1.57706797  
 H 1.21915472 -3.38605857 -3.15881205  
 Tm 0.36089528 -0.43355149 1.49249542  
 N 2.41627216 -0.42011908 3.38348675  
 O 3.30266309 -0.38961160 4.21112394  
 O 2.62510252 -0.19736947 2.11979747  
 O 1.18006504 -0.67120987 3.68113256  
 O 1.49704492 0.74381751 -0.19085066  
 H 1.26429820 0.64557612 -1.20728636  
 H 2.45638847 0.57452714 -0.12234237  
 N -1.78732002 -1.63267434 2.88038993  
 O -0.89142352 -2.31241822 2.23462963  
 O -1.66630411 -0.34690276 2.76248121  
 O -2.66807246 -2.15457058 3.53281307  
 H 1.11881781 -5.14642572 -2.69761753  
 H -0.99005711 5.05193996 0.43322271  
 N 1.29923689 -0.69179380 -3.01211095  
 O 0.70258629 -1.36009824 -3.88821936  
 O 0.76035100 0.41988236 -2.60602522  
 O 2.37977505 -1.07141435 -2.49549079

**L4\*Tm(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -16275.992948, E0 = -16275.579604, G= 213.9323 at T=298.150 K

Cl -4.54130125 3.84079432 -1.09528112  
 Cl -3.34410429 -3.13462520 -3.94511771  
 N -1.06263566 1.22789800 0.10606498  
 N 0.07585930 3.92411447 2.19324136  
 N -0.64595324 -1.20218098 -0.88610119  
 N 1.45094800 -4.11526775 -1.08549786

O 0.47790384 1.71242154 2.11954784  
 O 1.19033396 -2.46300936 0.41843662  
 C -1.22437978 2.43965387 0.64746833  
 C -2.30455637 3.26719952 0.29350808  
 H -2.47346067 4.22815943 0.77369845  
 C -3.20310235 2.82853508 -0.67002523  
 C -3.03454375 1.56264722 -1.28792274  
 C -3.89693904 1.01373756 -2.28662038  
 H -4.74149895 1.61179149 -2.63260174  
 C -3.68229389 -0.23716511 -2.79758430  
 H -4.35425711 -0.64496279 -3.55443192  
 C -2.58789587 -1.04056919 -2.35122633  
 C -2.31262016 -2.36135602 -2.78997254  
 C -1.21989191 -3.05648518 -2.28912497  
 H -1.04851568 -4.07841396 -2.61901259  
 C -0.38909134 -2.43262172 -1.34176779  
 C -1.69876051 -0.52186865 -1.37248123  
 C -1.92565882 0.80084211 -0.83229220  
 C -0.17521437 2.70752883 1.70197213  
 C 0.80701166 -3.03318119 -0.63946176  
 C -0.39122552 5.24972439 1.72189987  
 H -1.37121379 5.48627281 2.17340612  
 C 0.68495888 6.20733118 2.25064254  
 H 1.53653073 6.23456097 1.55171788  
 H 0.29553354 7.22890520 2.36443639  
 C 1.09834659 5.55836725 3.57905912  
 H 0.34830746 5.76633596 4.35923338  
 H 2.07550216 5.90675879 3.94143128  
 C 1.11971295 4.06469822 3.24625230  
 H 2.08803582 3.73953390 2.82871127  
 H 0.88204902 3.40481949 4.09377384



C 2.60367036 -4.63323164 -0.29731253  
 H 2.28380275 -4.83863878 0.73500603  
 H 3.38352704 -3.85345578 -0.25846529  
 C 3.05106497 -5.86925077 -1.08114040  
 C 2.69353938 -5.51295710 -2.53093553  
 C 1.33415210 -4.81593990 -2.38666224  
 H 2.63061762 -6.38714266 -3.19430280  
 H 3.43131304 -4.80961800 -2.94977593  
 H 2.48646116 -6.75668383 -0.75219440  
 H 4.12176561 -6.07251978 -0.94035041  
 H 1.13175011 -4.10064316 -3.19663906  
 Tm 0.61099899 -0.33743834 1.08301616  
 N -0.98867846 -1.42082965 3.07089472  
 O 0.30044955 -1.24205494 3.17370939  
 O -1.48427594 -1.03926384 1.92617869  
 O -1.65701282 -1.89486969 3.95371413  
 N 2.92475843 0.56555325 -0.15584609  
 O 1.76520002 0.61113417 -0.75041431  
 O 2.88382459 0.06402140 1.04799402  
 O 3.94524717 0.95162910 -0.66992819  
 H 0.52239507 -5.56372595 -2.34043813  
 H -0.47649065 5.26500177 0.62591404

**L4\*Yb(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -17125.721365, E0 = -17125.269951, G= 231.1715 at T=298.150 K

Cl -4.84003782 3.69956136 -0.78223974  
 Cl -3.72434306 -3.30737281 -3.62596440  
 N -1.21503890 1.16624546 0.16597655  
 N 0.11821893 3.95658398 1.95554793  
 N -0.82870364 -1.26132584 -0.81021255  
 N 1.33860159 -4.04829788 -1.13118398

O 0.37508017 1.72591627 2.15397525  
 O 0.76766193 -2.77022719 0.65136766  
 C -1.34906232 2.38517475 0.68347770  
 C -2.46782136 3.19419909 0.41013300  
 H -2.60092998 4.16587448 0.88315004  
 C -3.43920732 2.71415854 -0.45435986  
 C -3.30548286 1.44008374 -1.05577660  
 C -4.24217510 0.84745842 -1.95663571  
 H -5.13234615 1.41639698 -2.22960567  
 C -4.04388666 -0.40805468 -2.46086001  
 H -4.77346134 -0.84966183 -3.14163327  
 C -2.89312387 -1.17738819 -2.10596752  
 C -2.62073708 -2.49460196 -2.54705381  
 C -1.48854291 -3.16656351 -2.11159515  
 H -1.30584657 -4.19354725 -2.42791724  
 C -0.61150151 -2.50641632 -1.23382747  
 C -1.93322170 -0.61779922 -1.21812558  
 C -2.14355230 0.71049184 -0.68476075  
 C -0.22705247 2.69232464 1.64641929  
 C 0.56380367 -3.13519502 -0.52165902  
 C -0.23749383 5.20401049 1.25041521  
 H -1.11469793 5.68217564 1.72477162  
 C 1.01252377 6.07496452 1.43715799  
 H 1.76492941 5.80697632 0.67752361  
 H 0.78377169 7.14668274 1.34319913  
 C 1.50130486 5.67067003 2.83644748  
 H 0.89003456 6.16350698 3.61068034  
 H 2.55495715 5.92879772 3.01494765  
 C 1.27862227 4.15473413 2.86115885  
 H 2.13824534 3.58812451 2.46357441  
 H 1.05054331 3.75107741 3.85943103

C 2.54643726 -4.52405787 -0.40795457  
 H 2.25549078 -5.18365145 0.42404625  
 H 3.06065059 -3.64790106 0.02318919  
 C 3.36964965 -5.22339439 -1.49670374  
 C 2.96323442 -4.47940159 -2.77849030  
 C 1.45441031 -4.27870178 -2.58555102  
 H 3.19197989 -5.03360701 -3.70069528  
 H 3.45576239 -3.49432230 -2.82052779  
 H 3.09337258 -6.28868961 -1.56951535  
 H 4.44756889 -5.16159058 -1.28852606  
 H 1.06384301 -3.41752791 -3.14596558  
 Yb 0.82680589 -0.31938326 0.95315403  
 N -0.62857038 -1.19359052 3.23603487  
 O 0.64391887 -1.04278874 3.22635150  
 O -1.21209741 -0.91988003 2.09610486  
 O -1.25847805 -1.56080174 4.20946503  
 N 3.56058931 -0.25765529 1.74387872  
 O 2.86923981 0.80601221 1.47879279  
 O 2.91333818 -1.36038983 1.61998665  
 O 4.73072577 -0.20776542 2.08163095  
 N 1.97354460 0.33887574 -1.58931863  
 O 2.45983768 0.62763387 -2.66959310  
 O 2.08928347 -0.83898628 -1.06558692  
 O 1.29410052 1.18209004 -0.88539511  
 H 0.89794743 -5.18797779 -2.88005686  
 H -0.46442053 5.00357008 0.19349580  
 O -3.88723326 -0.92952526 1.25943720  
 H -3.02200699 -0.96859968 1.73166287  
 H -4.28895617 -1.78773129 1.47667301

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -17125.725615, E0 = -17125.273655, G= 232.9416 at T=298.150 K

Cl -5.15610266 3.31237769 -0.71434826  
 Cl -3.40772104 -3.62601781 -3.42468476  
 N -1.37207603 1.08436406 0.35808715  
 N -0.34943479 4.00107622 2.17833686  
 N -0.77741897 -1.32292902 -0.56436557  
 N 1.72833180 -3.81493497 -1.13606727  
 O 0.15851793 1.81388187 2.35754991  
 O 1.36283743 -2.34515262 0.54283398  
 C -1.61001861 2.29547763 0.85617644  
 C -2.78458953 3.00754571 0.54294938  
 H -3.00858450 3.97149277 0.99553239  
 C -3.69533420 2.44143009 -0.33485684  
 C -3.45392609 1.16884518 -0.90965259  
 C -4.31558084 0.49395034 -1.82819986  
 H -5.23558760 0.99043876 -2.14047217  
 C -4.00190735 -0.74774402 -2.31122804  
 H -4.66838980 -1.24935603 -3.01478362  
 C -2.80340719 -1.41767514 -1.91523206  
 C -2.39511752 -2.70383453 -2.35086465  
 C -1.18547356 -3.23742557 -1.94077897  
 H -0.88184261 -4.22010469 -2.29578352  
 C -0.37939140 -2.49555635 -1.05683088  
 C -1.92628980 -0.77965325 -1.00102222  
 C -2.25080657 0.53590524 -0.49614987  
 C -0.54145515 2.70881510 1.84479773  
 C 0.97274369 -2.89790606 -0.50918365  
 C -0.83673114 5.21887541 1.49980533  
 H -1.80000043 5.54646158 1.93295848  
 C 0.25833476 6.24987030 1.80662155  
 H 1.08585393 6.13786840 1.08710444  
 H -0.12127254 7.28023148 1.74568880

C	0.71698719	5.84603548	3.21591020
H	-0.00855739	6.19717550	3.96820140
H	1.70593858	6.24731541	3.47950411
C	0.72277099	4.31537867	3.15412331
H	1.67916524	3.91241097	2.77867365
H	0.51197731	3.82332015	4.11583853
C	3.06751394	-4.09939814	-0.56414104
H	2.96160054	-4.59218025	0.41467905
H	3.59011745	-3.14086270	-0.40475011
C	3.74770045	-4.95533419	-1.63556623
C	3.12928128	-4.42499781	-2.93653321
C	1.65589106	-4.21782303	-2.56387639
H	3.24116373	-5.11138105	-3.78863192
H	3.55813980	-3.44518375	-3.19995022
H	3.49937344	-6.02070189	-1.49410319
H	4.84181786	-4.84930325	-1.60127425
H	1.19686997	-3.41776443	-3.16648793
Yb	0.35695237	-0.41764045	1.50309408
N	2.38475466	-0.36739776	3.42190957
O	3.26414680	-0.29495135	4.25617790
O	2.60212731	-0.15438229	2.15647626
O	1.15944278	-0.65646982	3.71013641
O	1.51269090	0.76868850	-0.17396142
H	1.30437362	0.65989774	-1.18025792
H	2.46904516	0.59362328	-0.08035686
N	-1.77377272	-1.72764933	2.82081747
O	-0.77328730	-2.36304307	2.30339742
O	-1.76285708	-0.44535160	2.60890913
O	-2.65768147	-2.28030658	3.44560528
H	1.09197450	-5.16334820	-2.66277146
H	-0.96848637	5.04172039	0.42254928

N 1.35332453 -0.67865312 -3.04157114  
 O 0.75812674 -1.35026979 -3.91696501  
 O 0.81222075 0.42216107 -2.63070536  
 O 2.44099307 -1.05395055 -2.53803658

**L4\*Yb(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -16768.763641, E0 = -16768.350608, G= 213.6745 at T=298.150 K

Cl -4.53099203 3.84630418 -1.11160123  
 Cl -3.34964681 -3.14021778 -3.94074488  
 N -1.06805527 1.22383189 0.10889833  
 N 0.07599076 3.92548299 2.18744588  
 N -0.65259403 -1.21186543 -0.87860388  
 N 1.44653141 -4.12408495 -1.08973563  
 O 0.46410921 1.70921850 2.13647056  
 O 1.18072212 -2.48577666 0.42976043  
 C -1.22485805 2.43736148 0.64629239  
 C -2.29969740 3.26870036 0.28445768  
 H -2.46564198 4.23266649 0.75923812  
 C -3.19913292 2.82908154 -0.67773819  
 C -3.03674150 1.55871999 -1.28836489  
 C -3.90033722 1.00872993 -2.28533697  
 H -4.74337816 1.60759234 -2.63363743  
 C -3.68780994 -0.24403597 -2.79249573  
 H -4.35999203 -0.65268719 -3.54866290  
 C -2.59440541 -1.04797471 -2.34435129  
 C -2.31864047 -2.36831307 -2.78439617  
 C -1.22513330 -3.06348109 -2.28512406  
 H -1.05379403 -4.08525610 -2.61574054  
 C -0.39504191 -2.44197345 -1.33577776  
 C -1.70589960 -0.53003216 -1.36466765  
 C -1.93132687 0.79498911 -0.82799137  
 C -0.17843667 2.70432305 1.70692205

C	0.80092990	-3.04618549	-0.63184595
C	-0.37849894	5.24902344	1.69830477
H	-1.36100113	5.49687767	2.13824415
C	0.69842792	6.20538330	2.22765183
H	1.55750358	6.21907473	1.53751993
H	0.31505141	7.23080730	2.32633209
C	1.09332764	5.56762314	3.56701541
H	0.33489183	5.78680754	4.33604908
H	2.06793976	5.91455221	3.93762660
C	1.11064696	4.07086897	3.24837804
H	2.08170938	3.73844028	2.84294057
H	0.86248046	3.41992259	4.09971952
C	2.60171556	-4.64442158	-0.30701923
H	2.28189850	-4.86737776	0.72168541
H	3.37491536	-3.85886431	-0.25454000
C	3.06029963	-5.86536026	-1.10777414
C	2.70062542	-5.49212217	-2.55306554
C	1.33485365	-4.81033850	-2.39892936
H	2.64703727	-6.35857344	-3.22735882
H	3.43267155	-4.77640581	-2.96081018
H	2.50194526	-6.76175833	-0.79251701
H	4.13228321	-6.06295347	-0.96872067
H	1.12439835	-4.08776855	-3.20037770
Yb	0.58839869	-0.34300706	1.08370006
N	-0.98180532	-1.41309786	3.09515643
O	0.31662741	-1.32159185	3.14553189
O	-1.50048232	-0.96103531	1.98806643
O	-1.64204109	-1.87512457	3.99149108
N	2.92502427	0.57006305	-0.09085657
O	1.76684880	0.69973022	-0.67363328
O	2.87320948	-0.03041228	1.06347227

O 3.95541334 0.96880156 -0.57642132  
H 0.53061604 -5.56673908 -2.36095953  
H -0.45365980 5.25385714 0.60142905

**L4\*Lu(NO<sub>3</sub>)<sub>3</sub>(H<sub>2</sub>O)**

**(H<sub>2</sub>O in outer coordination sphere)**

E= -17629.924236, E0 = -17629.471678, G= 232.5959 at T=298.150 K

Cl -4.88080740 3.68029141 -0.74388206  
Cl -3.73431587 -3.30866647 -3.63720155  
N -1.23456323 1.16160321 0.15570208  
N 0.11664879 3.94874477 1.93816745  
N -0.84074765 -1.25390816 -0.82509768  
N 1.33719647 -4.03695440 -1.13914776  
O 0.41917241 1.72321844 2.07504606  
O 0.76879269 -2.73259020 0.62111336  
C -1.36413753 2.37940216 0.67422956  
C -2.49059391 3.18405175 0.41754213  
H -2.62352872 4.15430927 0.89340955  
C -3.47130895 2.70086980 -0.43539736  
C -3.33849978 1.42941511 -1.04260898  
C -4.27840662 0.83280092 -1.93761969  
H -5.17545080 1.39529037 -2.20140123  
C -4.07377100 -0.41908032 -2.44933128  
H -4.80568790 -0.86302412 -3.12609172  
C -2.91378832 -1.18132043 -2.10833311  
C -2.63181996 -2.49248362 -2.56047964  
C -1.48997617 -3.15624642 -2.13693404  
H -1.30178988 -4.18034124 -2.45901561  
C -0.61474383 -2.49372196 -1.25941396  
C -1.95302415 -0.61918116 -1.22307575  
C -2.16983438 0.70548254 -0.68367559  
C -0.21854834 2.68805718 1.60850167



C	0.56395841	-3.11402392	-0.54871863
C	-0.28066850	5.20846033	1.27882826
H	-1.15115774	5.65771866	1.79219663
C	0.96004057	6.09575701	1.45163739
H	1.69179654	5.86276388	0.66095436
H	0.71040696	7.16547489	1.39576948
C	1.50048912	5.66062593	2.82226396
H	0.90693057	6.12095642	3.62961721
H	2.55509734	5.93161869	2.97398639
C	1.30354536	4.14116764	2.81079578
H	2.15804887	3.59909773	2.37017441
H	1.11484420	3.70515084	3.80358195
C	2.54165888	-4.50789833	-0.40473536
H	2.24244261	-5.14502668	0.44158685
H	3.06311750	-3.62686777	0.00807493
C	3.35567307	-5.24197626	-1.47743750
C	2.95047379	-4.53120375	-2.77846622
C	1.44420910	-4.31047726	-2.58638477
H	3.16992736	-5.11390972	-3.68519545
H	3.45250845	-3.55273533	-2.85128617
H	3.07256818	-6.30706263	-1.52042663
H	4.43468380	-5.18138885	-1.27488995
H	1.05909228	-3.46177745	-3.16923809
Lu	0.87831533	-0.32634500	0.93057096
N	-0.50075781	-1.11508000	3.25792289
O	0.76573032	-0.92609149	3.22929335
O	-1.09653318	-0.90827888	2.10310721
O	-1.11854482	-1.45549262	4.24590063
N	3.57874537	-0.36974770	1.70592344
O	2.87516022	0.71627146	1.53757644
O	2.92079759	-1.45874500	1.49384165

O 4.74958134 -0.34536159 2.03107047  
 N 1.93522942 0.45735863 -1.57586753  
 O 2.39815855 0.77908587 -2.65359521  
 O 2.03368616 -0.75208431 -1.10521460  
 O 1.29913616 1.27825189 -0.80747908  
 H 0.87791145 -5.22267866 -2.85142541  
 H -0.53512436 5.03298187 0.22378550  
 O -3.79254603 -0.93982220 1.31568849  
 H -2.91515112 -0.97274625 1.76551902  
 H -4.20994711 -1.77193844 1.59568787

**(NO<sub>3</sub><sup>-</sup> in outer coordination sphere)**

E= -17629.931080, E0 = -17629.478036, G= 234.4627 at T=298.150 K

Cl -5.15501738 3.30927372 -0.70456171  
 Cl -3.36983562 -3.61042500 -3.46673083  
 N -1.38218987 1.07159865 0.36784342  
 N -0.34094384 3.99234796 2.18369150  
 N -0.77290672 -1.31411815 -0.57464904  
 N 1.74190533 -3.80320811 -1.09784186  
 O 0.22952224 1.81839895 2.28203344  
 O 1.34517908 -2.32124734 0.56367999  
 C -1.60666072 2.28944230 0.85837412  
 C -2.77998257 3.00241613 0.54402405  
 H -3.00124288 3.96874785 0.99191809  
 C -3.69556451 2.43628478 -0.33021313  
 C -3.45713973 1.16563177 -0.90992141  
 C -4.31279421 0.49352115 -1.83588803  
 H -5.23252916 0.98933530 -2.15003347  
 C -3.99268317 -0.74471843 -2.32561064  
 H -4.65458584 -1.24305904 -3.03587461  
 C -2.79281306 -1.41367531 -1.93159294  
 C -2.37177277 -2.69274950 -2.37704110

C -1.16137195 -3.22148299 -1.96250415  
 H -0.84767729 -4.19795227 -2.32535362  
 C -0.36582488 -2.48309803 -1.06613255  
 C -1.92427886 -0.77796805 -1.01041675  
 C -2.25724578 0.52919036 -0.49444959  
 C -0.51524693 2.70643687 1.82013595  
 C 0.97646618 -2.88197374 -0.49606058  
 C -0.87428248 5.21938038 1.55786455  
 H -1.83120084 5.51070976 2.02920461  
 C 0.20705219 6.26535559 1.86331391  
 H 1.01215613 6.19677210 1.11360967  
 H -0.19807161 7.28763485 1.84875512  
 C 0.72223175 5.82775021 3.24236250  
 H 0.01586807 6.13820314 4.02993059  
 H 1.71088374 6.24269342 3.48498011  
 C 0.75919318 4.30070400 3.13080573  
 H 1.70929897 3.92999864 2.70908904  
 H 0.59258294 3.77385831 4.08267784  
 C 3.07191634 -4.08092546 -0.50095862  
 H 2.95012212 -4.57024622 0.47777346  
 H 3.58707237 -3.11915946 -0.33688554  
 C 3.77398849 -4.93749666 -1.55748987  
 C 3.17618036 -4.41333961 -2.87045598  
 C 1.69554341 -4.21158218 -2.52621245  
 H 3.30707073 -5.10094786 -3.71881437  
 H 3.60281062 -3.43089080 -3.12794447  
 H 3.52769446 -6.00341320 -1.41647375  
 H 4.86688566 -4.82650900 -1.50388682  
 H 1.24640787 -3.41290784 -3.14044762  
 Lu 0.35726923 -0.39054769 1.44319630  
 N 2.42547154 -0.53427958 3.27412891

O 3.33673525 -0.59243393 4.07003164  
 O 2.56868887 -0.05319720 2.07050943  
 O 1.22183144 -0.93785810 3.53750849  
 O 1.43603957 0.72418338 -0.26531711  
 H 1.18817306 0.60636812 -1.29057097  
 H 2.39756989 0.56007820 -0.21310665  
 N -1.79567564 -1.53868949 2.84255624  
 O -0.99063778 -2.23291564 2.10063124  
 O -1.56807089 -0.25791067 2.81662989  
 O -2.68768501 -2.03476548 3.49894619  
 H 1.13743377 -5.16013241 -2.62845969  
 H -1.03255522 5.07290554 0.47964886  
 N 1.28317273 -0.73805147 -3.04379964  
 O 0.72520339 -1.42541564 -3.92922878  
 O 0.70094138 0.36298949 -2.65255499  
 O 2.36192417 -1.08292127 -2.49837232

**L4\*Lu(NO<sub>3</sub>)<sub>2</sub><sup>+</sup>**

E= -17272.970752, E0 = -17272.556767, G= 214.5861 at T=298.150 K

Cl -4.55833626 3.85447264 -1.13173532  
 Cl -3.37119889 -3.13185501 -3.96836996  
 N -1.07835853 1.24137175 0.06022176  
 N 0.05243400 3.92531061 2.17042637  
 N -0.66351610 -1.18562090 -0.92870164  
 N 1.42837465 -4.10544777 -1.10683870  
 O 0.46984917 1.71826923 2.06529212  
 O 1.18462813 -2.42744231 0.37001535  
 C -1.23909616 2.45237422 0.60538930  
 C -2.31958055 3.27937722 0.25243443  
 H -2.48642039 4.24077940 0.73234957  
 C -3.22100592 2.84155607 -0.70932400  
 C -3.05576849 1.57478893 -1.32705164

C -3.92206573 1.02306545 -2.32094908  
H -4.76854944 1.61971760 -2.66462302  
C -3.70908570 -0.22921650 -2.82973289  
H -4.38444138 -0.63930649 -3.58230138  
C -2.61226869 -1.03104866 -2.38615680  
C -2.33703089 -2.35364437 -2.82042885  
C -1.24197030 -3.04607415 -2.31977510  
H -1.07127583 -4.06929588 -2.64588380  
C -0.40729848 -2.41920877 -1.37831807  
C -1.71966207 -0.50841278 -1.41387749  
C -1.94523787 0.81445044 -0.87558919  
C -0.18920606 2.71393037 1.66240883  
C 0.79238564 -3.01345372 -0.67436564  
C -0.42185971 5.25507259 1.71857548  
H -1.40451956 5.47821379 2.17124796  
C 0.64669931 6.21096849 2.26574898  
H 1.50048029 6.25297785 1.57027459  
H 0.25114012 7.22851276 2.39337039  
C 1.05943084 5.54392195 3.58538818  
H 0.30491757 5.73404026 4.36585379  
H 2.03273535 5.89334202 3.95701671  
C 1.09309900 4.05634737 3.22821665  
H 2.06451535 3.74498415 2.80740809  
H 0.85869837 3.37888598 4.06253338  
C 2.58515620 -4.61207628 -0.31663373  
H 2.27228165 -4.79290247 0.72236413  
H 3.36812067 -3.83467531 -0.30001226  
C 3.02020264 -5.86677551 -1.07702684  
C 2.65200543 -5.54085827 -2.53138232  
C 1.29802835 -4.83211327 -2.39217091  
H 2.57823825 -6.42920923 -3.17449260

H	3.39026380	-4.85155678	-2.97205567
H	2.45500231	-6.74443102	-0.72382230
H	4.09128666	-6.07145023	-0.94145179
H	1.09516406	-4.13315201	-3.21624875
Lu	0.58216357	-0.31133303	1.00840914
N	-0.72805321	-1.40558422	3.13461041
O	0.55478150	-1.18194187	3.12435794
O	-1.33787763	-1.05341554	2.01930213
O	-1.31226110	-1.88768446	4.06849289
N	3.01416135	0.49425820	0.06329885
O	1.90158713	0.58914238	-0.63776636
O	2.84866500	-0.01831878	1.24737191
O	4.08145857	0.85277063	-0.36356395
H	0.48162901	-5.57322264	-2.32435155
H	-0.50363868	5.28782606	0.62262261

#### Nitrates

##### La(NO<sub>3</sub>)<sub>3</sub>

E= -9336.284233, E0 = -9336.240076, G= -1.6603 at T=298.150 K

La	0.00001769	-0.00003848	-0.00000325
N	-2.90586615	0.01336963	0.05776037
O	-2.20656466	0.68517798	-0.82677323
O	-4.10616684	0.01895838	0.08170674
O	-2.17813969	-0.66517508	0.91379160
N	1.41289687	-1.98400593	-1.58599830
O	1.08368850	-2.17620158	-0.32982165
O	1.04821169	-0.81732994	-2.06362891
O	1.99683034	-2.80388880	-2.24032688
N	1.49282134	1.97067058	1.52826393
O	1.11489129	2.16643786	0.28641924
O	2.10974574	2.78510880	2.15868187
O	1.13763368	0.80691624	2.01992869

**Ce(NO<sub>3</sub>)<sub>3</sub>**

E= -9703.698544, E0 = -9703.654621, G= -3.1254 at T=298.150 K

Ce 0.01325159 -0.00005793 -0.00031676

N -2.85419488 0.01306607 0.05679771

O -2.15112543 0.68750197 -0.82212991

O -4.05391550 0.01851519 0.08067576

O -2.12286687 -0.66788226 0.90718979

N 1.38688433 -1.96393526 -1.56819594

O 1.07031250 -2.14300060 -0.30613726

O 1.04337847 -0.78423816 -2.03209925

O 1.92896450 -2.80121565 -2.23577523

N 1.46596551 1.95087302 1.51144469

O 1.10103607 2.13311219 0.26296231

O 2.04162216 2.78310466 2.15686202

O 1.13068771 0.77415687 1.98872221

**Pr(NO<sub>3</sub>)<sub>3</sub>**

E= -10080.779371, E0 = -10080.735193, G= -2.1144 at T=298.150 K

Pr 0.01586251 0.00000078 -0.00031168

N -2.82815266 0.01285240 0.05620209

O -2.12219620 0.68811464 -0.82121718

O -4.02770329 0.01835372 0.08015907

O -2.09396267 -0.66901970 0.90489709

N 1.37120199 -1.95889008 -1.56366873

O 1.03669703 -2.14566994 -0.30869672

O 1.01051748 -0.78776538 -2.03282094

O 1.95495474 -2.77799606 -2.21763659

N 1.45025003 1.94604659 1.50757396

O 1.06751931 2.13635969 0.26701921

O 2.06728244 2.75945830 2.13766003

O 1.09772921 0.77815503 1.99084032

**Nd(NO<sub>3</sub>)<sub>3</sub>**

E= -10467.685921, E0 = -10467.641630, G= -2.0626 at T=298.150 K

Nd 0.00072433 0.00504316 -0.00696500

N -2.83198118 0.01291180 0.05764951

O -2.12624669 0.79934633 -0.72058380

O -4.03116798 0.01686896 0.08455694

O -2.09697580 -0.77782995 0.80304176

N 1.37683094 -1.93652308 -1.54500532

O 1.17032194 -2.05412650 -0.25478247

O 0.88404632 -0.83126140 -2.05267286

O 1.95899403 -2.75817943 -2.19672585

N 1.45471191 1.92182791 1.48990571

O 1.20102465 2.04891944 0.20865670

O 2.07016277 2.73366427 2.12308311

O 0.96955508 0.81933838 2.00984168

### **Pm(NO<sub>3</sub>)<sub>3</sub>**

E= -10864.548907, E0 = -10864.504658, G= -0.5963 at T=298.150 K

Pm -0.02315194 -0.00152896 0.00314578

N -2.84424090 -0.02219432 0.10059166

O -2.13659453 0.65779483 -0.77898616

O -4.04364967 -0.01119621 0.11704404

O -2.11465216 -0.70167094 0.94314265

N 1.38741612 -1.88944674 -1.54561615

O 0.84865528 -2.15826154 -0.37648380

O 1.21148396 -0.65132111 -1.92846835

O 1.98172879 -2.70513415 -2.19418263

N 1.46499348 1.91251624 1.44347525

O 1.26223552 1.99964273 0.15446903

O 2.09227204 2.71961355 2.07140279

O 0.91350412 0.85118693 1.99046576

### **Sm(NO<sub>3</sub>)<sub>3</sub>**

E= -11271.487493, E0 = -11271.443375, G= -1.7063 at T=298.150 K



Sm -0.11102058 0.00127051 0.00197510  
 N -2.92669868 0.02567798 0.06345502  
 O -2.23266435 0.23235433 -1.02981436  
 O -4.12645435 0.03640363 0.08975135  
 O -2.18924832 -0.19368589 1.12541103  
 N 1.43372667 -1.83199322 -1.46817291  
 O 0.73742867 -2.17122221 -0.41384146  
 O 1.34296644 -0.55980039 -1.77231610  
 O 2.09454870 -2.60973811 -2.09974933  
 N 1.52787316 1.80589199 1.40407479  
 O 0.79103631 2.15863061 0.38220060  
 O 2.22884321 2.57141423 2.00662827  
 O 1.42966318 0.53479666 1.71039796

### **Eu(NO<sub>3</sub>)<sub>3</sub>**

E= -11688.686686, E0 = -11688.642767, G= -1.6288 at T=298.150 K

Eu -0.00040956 0.00005385 0.00008606  
 N -2.81777573 0.01283353 0.05601045  
 O -2.10939622 1.01220977 -0.40208748  
 O -4.01907682 0.01823581 0.07981354  
 O -2.10082650 -0.99293768 0.48593813  
 N 1.37018275 -1.92394626 -1.53614879  
 O 1.48323298 -1.83753026 -0.23606995  
 O 0.56286407 -1.03771532 -2.05889511  
 O 1.95527649 -2.74380279 -2.19129682  
 N 1.44773650 1.91116858 1.48007619  
 O 1.50827849 1.82384074 0.17656264  
 O 2.06590962 2.72551823 2.11127162  
 O 0.65400380 1.03207183 2.03473973

### **Gd(NO<sub>3</sub>)<sub>3</sub>**

E= -12116.240312, E0 = -12116.195668, G= -1.6729 at T=298.150 K

Gd -0.00034861 0.00149084 -0.00177597

N -2.77423048 0.01277978 0.05502230  
 O -2.06638837 0.80802512 -0.71570069  
 O -3.97202015 0.01748536 0.07951467  
 O -2.04177594 -0.78816861 0.79631269  
 N 1.34883487 -1.89458323 -1.51259303  
 O 1.15525925 -2.01016402 -0.21777789  
 O 0.84183085 -0.79453140 -2.02290750  
 O 1.93178630 -2.71301770 -2.16501427  
 N 1.42537725 1.88122678 1.45822752  
 O 1.17897975 2.00278735 0.17277186  
 O 2.04149508 2.69297504 2.08813334  
 O 0.93120033 0.78369468 1.98578703

### **Tb(NO<sub>3</sub>)<sub>3</sub>**

E= -12554.185252, E0 = -12554.140565, G= -1.1803 at T=298.150 K

Tb 0.00022869 0.00008624 -0.00025795  
 N -2.75734234 0.01270564 0.05493535  
 O -2.04427004 0.93380946 -0.55440629  
 O -3.95488858 0.01821032 0.07876861  
 O -2.02904773 -0.91502607 0.63542390  
 N 1.34073031 -1.88379765 -1.50392771  
 O 1.31626105 -1.89500308 -0.18963613  
 O 0.66524190 -0.88740408 -2.03219819  
 O 1.92245948 -2.70218515 -2.15703583  
 N 1.41651845 1.87096119 1.44912195  
 O 1.33888316 1.88364744 0.13688448  
 O 2.03146839 2.68358541 2.07856154  
 O 0.75375700 0.88041043 2.00376630

### **Dy(NO<sub>3</sub>)<sub>3</sub>**

E= -13002.797004, E0 = -13002.752377, G= -1.3150 at T=298.150 K

Dy 0.01642095 -0.01882173 0.00158654  
 N -2.72606516 0.03294614 0.05116201

O -2.00636911 0.82482022 -0.71024448  
 O -3.92338967 0.04955097 0.07503923  
 O -2.00069284 -0.78169459 0.78757453  
 N 1.33424139 -1.89134765 -1.51141453  
 O 1.24541831 -1.95097136 -0.20029895  
 O 0.73277402 -0.84197813 -2.02541542  
 O 1.90803230 -2.71048784 -2.16981554  
 N 1.38598907 1.86375952 1.45873475  
 O 1.14482260 1.97613215 0.17088243  
 O 1.99149191 2.68346357 2.08799291  
 O 0.89732605 0.76462865 1.98421681

### **Ho(NO<sub>3</sub>)<sub>3</sub>**

E= -13462.241767, E0 = -13462.197053, G= -0.9266 at T=298.150 K

Ho 0.00281437 -0.11804630 0.15013550  
 N -2.72314405 0.02620037 0.03395709  
 O -1.93993187 0.85188919 -0.61232531  
 O -3.91885209 0.07421960 -0.00667118  
 O -2.06241083 -0.87069666 0.74226415  
 N 1.32492495 -1.84441030 -1.50425935  
 O 1.24710476 -1.99283671 -0.19481511  
 O 0.69869673 -0.78140330 -1.94091988  
 O 1.90977955 -2.61064291 -2.21454883  
 N 1.39715326 1.86370134 1.41251338  
 O 1.20178080 1.84617698 0.11854985  
 O 2.00395465 2.72456503 1.98205626  
 O 0.85812968 0.83128357 2.03406358

### **Er(NO<sub>3</sub>)<sub>3</sub>**

E= -13932.619529, E0 = -13932.574812, G= -1.3639 at T=298.150 K

Er -0.01323813 0.01545679 0.01511501  
 N -2.73721170 -0.02880375 0.06403738  
 O -2.02470183 0.85735059 -0.60282665

O -3.93460917 -0.02822050 0.07980536  
 O -2.00160885 -0.90401423 0.70253593  
 N 1.31173337 -1.84955382 -1.45855296  
 O 0.90599537 -2.06129837 -0.22872068  
 O 1.01267254 -0.64807713 -1.90241742  
 O 1.89516759 -2.66587043 -2.11239338  
 N 1.42944181 1.87323296 1.38941205  
 O 1.19666362 1.97164917 0.10606029  
 O 2.05178881 2.68035793 2.01808262  
 O 0.90790647 0.78779072 1.92986250

**Tm(NO<sub>3</sub>)<sub>3</sub>**

E= -14414.122148, E0 = -14414.077615, G= -1.1839 at T=298.150 K

Tm -0.06158710 0.00014260 0.00088560  
 N -2.77747059 0.01307720 0.05542854  
 O -2.06103277 0.99270809 -0.44849125  
 O -3.97501135 0.01877779 0.07950559  
 O -2.05071306 -0.97343326 0.53033495  
 N 1.36232030 -1.80947161 -1.43707752  
 O 1.31431973 -1.80446017 -0.12482589  
 O 0.65545577 -0.84974426 -1.98489296  
 O 1.99008846 -2.61049652 -2.06904101  
 N 1.43432212 1.79635060 1.38139117  
 O 1.33332145 1.79300046 0.07213638  
 O 2.09366560 2.59161592 1.98796666  
 O 0.74232137 0.84193325 1.95667970

**Yb(NO<sub>3</sub>)<sub>3</sub>**

E= -14906.893758, E0 = -14906.849325, G= -0.7877 at T=298.150 K

Yb -0.00056226 0.00007002 0.00003668  
 N -2.71518612 0.01231269 0.05396819  
 O -2.00053859 1.00079978 -0.42699859  
 O -3.91387081 0.01775904 0.07787323  
 O -1.99094391 -0.98272717 0.50622183  
 N 1.32025504 -1.85368240 -1.47983837

O	1.40966678	-1.77866948	-0.17383891
O	0.53043497	-0.94620472	-2.00129819
O	1.90390944	-2.67197704	-2.13340092
N	1.39508200	1.84132910	1.42586780
O	1.43151259	1.76596260	0.11734218
O	2.01197839	2.65392876	2.05557013
O	0.61826199	0.94109887	1.97849476

# **Lu(NO<sub>3</sub>)<sub>3</sub>**

E= -15411.094022, E0 = -15411.048970, G= -0.9794 at T=298.150 K

Lu	0.00038829	0.00028653	0.00002928
N	-2.68301368	0.01198070	0.05306493
O	-1.96719754	0.86947393	-0.64548492
O	-3.87848854	0.01708121	0.07664666
O	-1.94756734	-0.85176516	0.72300607
N	1.30441868	-1.83314216	-1.46325481
O	1.18484581	-1.90169585	-0.15306827
O	0.71929699	-0.77273554	-1.98193359
O	1.88447928	-2.65040088	-2.11545086
N	1.37856102	1.82110512	1.41021049
O	1.20604563	1.89202631	0.10601298
O	1.99333358	2.63179636	2.03836322
O	0.80489767	0.76598930	1.95185888