

Outer-Sphere Water Clusters Tune the Lanthanide Selectivity of Diglycolamides

Anna G. Baldwin,[†] Alexander S. Ivanov,[‡] Neil J. Williams,[‡] Ross J. Ellis,[‡] Bruce A. Moyer,[‡]
Vyacheslav S. Bryantsev,^{*,‡} Jenifer C. Shafer^{*,†}

[†]Department of Chemistry, Colorado School of Mines, Golden, CO

[‡]Oak Ridge National Laboratory, Oak Ridge, TN

E-mail: bryantsevv@ornl.gov; jshafer@mines.edu

Phone: (865)576-4272; (303)273-3996

SUPPORTING INFORMATION

Table of Contents

Methods	S2
Safety Statement	S2
Materials	S2
Solvent Extraction Studies	S2
Maximum Organic Phase Lanthanide Concentration	S5
Waters per Nitrate Calculation	S6
Organic Phase Water Concentration Data Table	S7
Density Functional Theory Calculations	S8
Classical Molecular Dynamics Simulations	S9
Additional Figures	S11
Sample Gaussian 09 Input File	S12
References	S29

Methods

Safety Statement

While no unexpected or unusually high safety hazards were encountered, it should be noted that ^{22}Na is radioactive and when working with radioactive materials, care should be taken to keep exposure to radiation as low as reasonably achievable.

Materials

Stock solutions of approximately 0.5 M $\text{La}(\text{NO}_3)_3$, $\text{Pr}(\text{NO}_3)_3$, $\text{Sm}(\text{NO}_3)_3$, $\text{Gd}(\text{NO}_3)_3$, $\text{Dy}(\text{NO}_3)_3$, and $\text{Tm}(\text{NO}_3)_3$ were prepared by dissolving 99.9% pure solid lanthanide(III) nitrate hydrates from Sigma Aldrich in 0.001 M HNO_3 , to prevent hydrolysis. A stock solution of 3 M NaNO_3 was prepared by dissolving ACS grade NaNO_3 in water. All non-radioactive solutions were standardized by inductively coupled plasma optical emission spectroscopy (ICP-OES) prior to use. For radiotracer experiments, radioactive ^{22}Na was purchased from PerkinElmer as a 1 mCi/mL solution of $^{22}\text{NaCl}$ and used as received. TODGA was used as received from Marshallton Research Laboratories, and dissolved in 99+% *n*-dodecane from Alfa Aesar to make a 0.25 M stock solution.

Solvent Extraction Studies

The 0.25 M TODGA solution was pre-equilibrated with water prior to all distribution experiments. Aqueous solutions at the desired lanthanide concentrations were prepared from the stock solutions for all samples such that the initial aqueous concentration of HNO_3 was 0.001 M and the equilibrium aqueous phase concentration of NO_3^- remained constant at 0.5 M NO_3^- . Tables of initial aqueous phase compositions for radioactive and non-radioactive experiments are provided in Tables S1 and S2.

Table S1. Initial aqueous phase compositions for all non-radioactive solvent extraction experiments.

Sample ID	Lanthanide	Ln Conc.	NaNO₃ Conc.	HNO₃ Conc.
		<i>mol/L</i>	<i>mol/L</i>	<i>mol/L</i>
1122Na05	None	0	0.5	0.001
1121La005	La	0.005	0.5	0.001
1121La015	La	0.015	0.49	0.001
1107La04	La	0.04	0.45	0.001
1107La09	La	0.09	0.35	0.001
1107La15	La	0.15	0.22	0.001
1107La28	La	0.28	0	0.001
1121Pr005	Pr	0.005	0.5	0.001
1121Pr015	Pr	0.015	0.49	0.001
1107Pr03	Pr	0.03	0.48	0.001
1107Pr06	Pr	0.06	0.44	0.001
1107Pr09	Pr	0.09	0.4	0.001
1107Pr14	Pr	0.14	0.33	0.001
1107Sm007	Sm	0.007	0.5	0.001
1107Sm014	Sm	0.014	0.5	0.001
1107Sm02	Sm	0.02	0.5	0.001
1114Sm027	Sm	0.027	0.5	0.001
1109Gd005	Gd	0.005	0.5	0.001
1109Gd01	Gd	0.01	0.5	0.001
1109Gd015	Gd	0.015	0.5	0.001
1114Gd019	Gd	0.019	0.5	0.001
1114Dy005	Dy	0.005	0.5	0.001
1114Dy009	Dy	0.009	0.5	0.001
1114Dy014	Dy	0.014	0.5	0.001
1114Dy018	Dy	0.018	0.5	0.001
1216Tm005	Tm	0.005	0.5	0.001
1216Tm009	Tm	0.009	0.5	0.001
1216Tm012	Tm	0.012	0.5	0.001
1216Tm014	Tm	0.014	0.5	0.001
1216Tm016	Tm	0.016	0.5	0.001

Table S2. Initial aqueous phase compositions for all ^{22}Na radiotracer solvent extraction experiments.

Sample ID	Lanthanide	Ln Conc.	NaNO₃ Conc.	HNO₃ Conc.
		<i>mol/L</i>	<i>mol/L</i>	<i>mol/L</i>
NaNO ₃ 0.5	None	0	0.5	0.001
La 0.2 M	La	0.2	0.5	0.001
La 0.05	La	0.05	0.5	0.001
La 0.01	La	0.01	0.5	0.001
La 0.005	La	0.005	0.5	0.001
Sm 0.01	Sm	0.01	0.5	0.001
Sm 0.005	Sm	0.005	0.5	0.001
Tm 0.01	Tm	0.01	0.5	0.001
Tm 0.005	Tm	0.005	0.5	0.001

For each non-radioactive extraction sample, 1 mL each of an aqueous phase and a pre-equilibrated 0.25 M TODGA organic phase were combined in a plastic centrifuge tube and contacted on a vertical rotating wheel in a thermostated incubator maintained at 21 °C. Samples were allowed to rotate until equilibrium was reached, at least one hour. Samples were centrifuged for five minutes at 3000 rpm to separate the phases, and aliquots taken from each phase for analysis. Metal concentrations in both phases were determined using ICP-OES. Aqueous phase samples were prepared for analysis by adding a small sample of the separated aqueous phase aliquot directly to a 4% HNO₃ solution. Organic phase samples were prepared by stripping the metal from the organic phase aliquot three times with equal volumes of 0.01 M HNO₃. These solutions were combined and the HNO₃ concentration adjusted to 4% HNO₃ for analysis by ICP-OES.

In radiotracer experiments to determine the extraction of Na for a subset of the conditions explored in non-radioactive experiments, 0.6 mL each of an aqueous phase and a pre-equilibrated 0.25 M TODGA organic phase were combined in a plastic centrifuge tube. Each centrifuge tube was then spiked with 10 µL of the 0.1 mCi/mL ^{22}Na stock solution and contacted on a vertical rotating wheel in a thermostated incubator maintained at 22 °C for one hour. Samples were centrifuged for five minutes at 3000 rpm in a temperature-controlled centrifuge set at 22 °C to separate the phases. Aliquots of 0.3 mL were taken from each phase and pipetted into individual polypropylene tubes for counting on a Canberra Gamma Analyst Integrated Gamma Spectrometer. Aqueous samples were counted for sixty minutes and organic samples were

counted for five minutes. The distribution ratios for each sample were calculated by dividing the organic phase count rate by the aqueous phase count rate. The final organic phase Na concentrations were calculated from the distribution ratio and initial concentration of Na in each sample. The results of all radiotracer experiments are provided in Table S3.

Table S3. Distribution ratios (D_{Na}) and final organic phase concentrations ($[\text{Na}^+]_{\text{org}}$) for ^{22}Na radiotracer solvent extraction experiments. The ratio of extracted Na to unextracted Na is approximately 1 to 10,000.

Sample ID	Lanthanide	D_{Na}	$[\text{Na}^+]_{\text{org}}$ Conc. $\mu\text{mol/L}$
NaNO3 0.5	None	1.13E-04	57
La 0.2 M	La	7.30E-05	37
La 0.05	La	1.03E-04	52
La 0.01	La	9.10E-05	46
La 0.005	La	8.82E-05	44
Sm 0.01	Sm	1.10E-04	55
Sm 0.005	Sm	1.08E-04	54
Tm 0.01	Tm	1.12E-04	56
Tm 0.005	Tm	1.11E-04	55

Organic phase water concentrations were determined using a Metrohm 831 Karl-Fischer coulometer.

All metal (radioactive and non-radioactive) and water analyses were performed in duplicate. The estimated uncertainty in the metal concentrations measured by ICP-OES is 2%. The estimated uncertainty in the organic phase Na concentrations determined from ^{22}Na radiotracer experiments is 7%. The estimated uncertainty in the measured water concentrations is 2%.

Maximum Organic Phase Lanthanide Concentration

To determine the maximum amount of each lanthanide that could be dissolved in the organic phase before the appearance of a third phase, referred to as the limiting organic concentration (LOC), solvent extraction studies were performed as described in the previous section. A range of initial aqueous phase lanthanide concentrations was used such that a third phase was observed for at least one of the concentrations. For La, the third phase appeared as a thin liquid phase located above the aqueous phase and below the larger organic phase. For the other lanthanides, the third phase appeared as a pale white gel or waxy solid in the upper organic

phase. The initial aqueous phase concentrations were refined until the organic phase limit was determined to within an initial aqueous phase concentration of 2 mM. Once the conditions under which the LOC was reached were determined, ICP-OES was used to find the organic phase lanthanide concentrations.

Waters per Nitrate Calculation

The number of water molecules co-extracted into the organic phase with each lanthanide was calculated by subtracting the concentration of water associated with free TODGA from the total water concentration in each sample. This value was then divided by three times the concentration of each lanthanide to give the number of water molecules per nitrate. Free TODGA refers to TODGA molecules in the organic phase which are not directly coordinated to a central lanthanide cation.

This calculation relies on the following assumptions:

1. The average amount of water associated with each free TODGA molecule is constant and independent of free TODGA concentration
2. All metal-TODGA species are mononuclear, neutral lanthanide complexes
3. The amount of water co-extracted with each lanthanide changes with changing lanthanide concentration
4. The solubility of water in *n*-dodecane is very low (at 25° Celsius the solubility of water in *n*-dodecane is approximately 3 mM)¹
5. Consistent with our experimental results the background electrolyte, NaNO₃, is not extracted

The number of water molecules co-extracted into the organic phase with each lanthanide is then calculated using the following equation (SE1), where the concentrations of each component are indicated by square brackets, and initial concentrations are denoted by the subscript “i”:

$$\text{waters per nitrate} = \frac{[\text{H}_2\text{O}] - [\text{H}_2\text{O}]_i / [\text{TODGA}]_i ([\text{TODGA}]_i - 3[\text{Ln}])}{[\text{NO}_3^-]} \quad (\text{SE1})$$

Organic Phase Water Concentration Data Table

Table S4. The experimental water and lanthanide concentrations, and calculated nitrate concentrations and water per nitrate values that are the basis for Figure 3.

Sample ID	Water Conc.	Ln Conc.	Nitrate Conc.	Water/Nitrate
	<i>mol/L</i>	<i>mol/L</i>	<i>mol/L</i>	
0.25 M TODGA	0.046	0		
1122Na05	0.047	0		
1121La005	0.058	0.004	0.012	1.23
1121La015	0.079	0.011	0.034	1.15
1107La04	0.104	0.025	0.074	0.96
1107La09	0.143	0.044	0.132	0.91
1107La15	0.163	0.058	0.175	0.86
1107La28	0.173	0.077	0.231	0.73
1121Pr005	0.059	0.004	0.013	1.17
1121Pr015	0.087	0.013	0.038	1.25
1107Pr03	0.118	0.024	0.072	1.18
1107Pr06	0.168	0.042	0.126	1.16
1107Pr09	0.193	0.056	0.168	1.06
1107Pr14	0.215	0.070	0.211	0.98
1107Sm007	0.071	0.007	0.021	1.36
1107Sm014	0.101	0.014	0.042	1.49
1107Sm02	0.128	0.020	0.059	1.58
1114Sm027	0.161	0.025	0.076	1.71
1109Gd005	0.067	0.005	0.014	1.62
1109Gd01	0.089	0.010	0.029	1.68
1109Gd015	0.114	0.015	0.046	1.66
1114Gd019	0.137	0.018	0.054	1.88
1114Dy005	0.067	0.005	0.014	1.67
1114Dy009	0.085	0.009	0.026	1.69
1114Dy014	0.107	0.014	0.041	1.69
1114Dy018	0.130	0.018	0.054	1.74
1216Tm005	0.068	0.005	0.015	1.65
1216Tm009	0.085	0.009	0.027	1.64
1216Tm012	0.099	0.012	0.036	1.67
1216Tm014	0.109	0.014	0.042	1.70
1216Tm016	0.119	0.016	0.048	1.70

Density Functional Theory Calculations

Calculations were carried out with the Gaussian 09, revision D.01 program package.² The computational method was density functional theory (DFT) using the gradient-corrected exchange-correlation hybrid density functional B3LYP.^{3,4} Standard 6-31+G(d) basis set was adopted for the main group elements and hydrogen for geometry optimization. 4f-Elements (La, Pr, Sm, Gd, Dy, Tm, Yb) were modeled using the large-core (LC) relativistic effective core potentials (RECP) and the corresponding basis sets.⁵ The 4f shell was treated as a part of the core, leading to modeling lanthanide ion complexes in a pseudo singlet state configuration. Frequency calculations were performed to ensure real vibrational modes for the minimum ground state structures and to provide zero-point energies (ZPE). ZPE and thermal corrections (T = 298.15 K) were added to the total energy to obtain the Gibbs free energy. Thermal contributions to the gas-phase Gibbs free energies were calculated using standard molecular thermodynamic approximations.⁶ To correct for the well-known breakdown of the harmonic oscillator model for the free energies of low-frequency vibrational modes, frequencies lower than 60 cm⁻¹ were raised to 60 cm⁻¹ following the so-called quasiharmonic approximation.⁷ Computations taking into account bulk solvent effects were carried out using the IEF-PCM (IEF) implicit solvation model with default settings.⁸ All DFT calculations were conducted on the 1:3 lanthanide ion:ligand complexes with NO₃⁻ counterions. The hydrophobic *n*-octyl substituents present in experimental extractants (TODGA) were replaced by the ethyl groups, giving the corresponding *N,N,N',N'*-tetraethyldiglycolamide (TEDGA) model ligands. This shortening of the ligand enabled us to significantly reduce the computational resources, because finding the most stable configuration of the complexes containing TODGA would be computationally prohibitively expensive. In addition, recent theoretical study shows that the chain length of hydrocarbon substituents has a little impact on the relative stability of actinide and lanthanide complexes.⁹ The Gibbs free energy change for the competitive complexation of La(III) over Ln(III) was calculated using the approach described in our previous work on predicting stability trends along the Ln(III) series that was capable of reproducing aqueous selectivities arising from the variation in the size of the trivalent *f*-block metal ions.¹⁰ The UCSF Chimera package was used for graphical visualization of the DFT optimized structures.¹¹

Classical Molecular Dynamics Simulations

Classical molecular dynamics simulations were performed with the Medea modeling suite¹² using the Medea LAMMPS10 interface module.¹³ We employed the non-polarizable enhanced PCFF forcefield¹⁴ (PCFF+) with refined nonbonded parameters to reproduce densities and cohesive energies of molecular liquids in a fashion similar to that used in the development of the COMPASS forcefield.⁶ The PCFF+ forcefield is able to accurately reproduce experimental densities (0.23%) and heats of vaporization (0.28%) (the mean absolute error is shown in parentheses) for a range of hydrocarbons.¹⁵ Following our previous work,¹⁶ a formal charge of 3+ was assigned to the trivalent La, Gd, and Yb ions that was counterbalanced by a negative charge on each nitrate counterion. Since inner-sphere M-O bond distances change only slightly (<0.03 Å) after adding nitrate or chloride anions and we are interested in the outer-sphere coordination of homoleptic $\text{Ln}(\text{TODGA})^{3+}$ complexes that persist in organic solvents,¹⁶ the metal ion and nine O donor atoms of three DGA ligands were kept frozen in the DFT optimized geometry of $\text{Ln}(\text{TODGA})_3(\text{NO}_3)_3$ during the MD simulations, while all the other degrees of freedom were allowed to change. We note that there is no validated force field for trivalent lanthanides that is capable of reproducing structural features beyond water and simple counterions without imposing some constraints on the inner-sphere bond distances. For example, keeping a formal charge of 3+ on the metal center and a negative charge on the nitrate counterion would most likely result in the displacement of neutral DGA ligands with nitrates, leading to complex geometries in the organic phase inconsistent with the recent EXAFS data.¹⁶ A part of the problem is electron transfer effects that are very important for tripositive metal ions, but difficult to account for in the traditional polarizable and non-polarizable force fields. Therefore, these effects were not explicitly included in the majority of the published force fields for lanthanides,^{17–19} with few exceptions²⁰ that were limited to $\text{Ln}^{3+}/\text{An}^{3+}$ -water systems. The non-bonded Lennard-Jones (L-J) 9-6 parameters for all metal cations were selected to be the same as for a potassium cation K^+ ($r_o = 3.292$ Å and $\epsilon = 0.4691$ kcal/mol), which had no noticeable impact on the radial distribution functions presented in this paper. The Waldman and Hagler 6th order combination rules were used for the off-diagonal L-J-9-6 parameters.

Nine systems were considered in our MD simulations in dodecane: $\text{Ln}(\text{TODGA})_3(\text{NO}_3)_3 + n(\text{H}_2\text{O})$, where Ln = La, Gd, and Yb, and $n = 0, 6, 12$. The selected ions represent early, middle, and late lanthanides and the number of added water molecules is 6 and 12, with the

former roughly corresponding to the amount of water in experiment. A periodic cubic box of 40 Å length containing one metal ion complex, three randomly placed NO_3^- anions and from 0 to 12 water molecules was used to accommodate 160 dodecane molecules, corresponding to an initial density of 0.761-0.767 g/cm³, which closely matches the experimental density of pure dodecane (0.750 g/cm³) at $T = 298.15$ K. The initial configurations for MD simulations were generated using the Medea Amorphous Cell Builder¹² by randomly placing NO_3^- and H_2O in the simulation box and sampling energetically reasonable dihedral angles of flexible organic solvent molecules.

The dispersion interactions were evaluated using a non-bonded cutoff of 9.5 Å with an added long-range Van der Waals tail correction. The long-range electrostatic interaction was calculated by means of the Particle-Particle-Particle-Mesh (P3M) Ewald summation method²¹ with long-range precision smaller than 10^{-5} for the electrostatic energy. The initial structure of each system was first minimized with 500 steps using the conjugate gradient method, followed by 1 ns of equilibration ($T = 298$ K) in an NVT ensemble and 2 ns in an NPT ensemble, followed by 5-8 ns (8 ns in the presence of water) of production run in an NVT ensemble with a time step of 1 fs. The data for the last 4 ns were used for analysis. The temperature was controlled by the Nosé-Hoover thermostat and barostat with a temperature (T_{damp}) and pressure damping (P_{damp}) of 100 fs and a friction coefficient (drag) of 1.0 (NVT) and 0 (NPT). Graphical visualization of the complexes and the analysis of the trajectory were performed with VMD.²²

Additional Figures

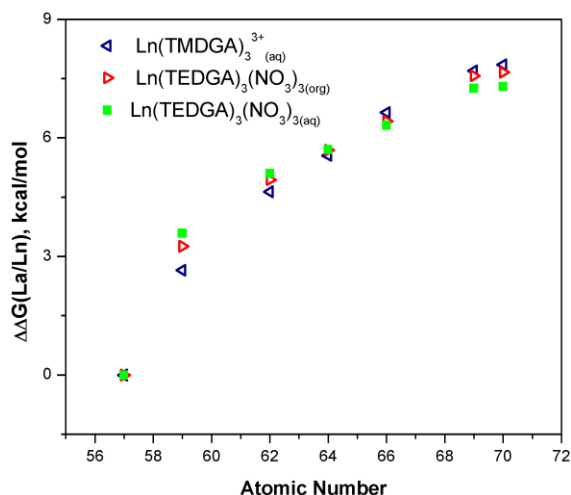


Figure S1. Plots of predicted selectivities, $\Delta\Delta G(\text{La/Ln})$ in kcal/mol ($\text{Ln} = \text{La}, \text{Pr}, \text{Sm}, \text{Gd}, \text{Dy}, \text{Tm}, \text{Yb}$), for the DGA complexes with and without inclusion of nitrate counterions in aqueous and organic media.

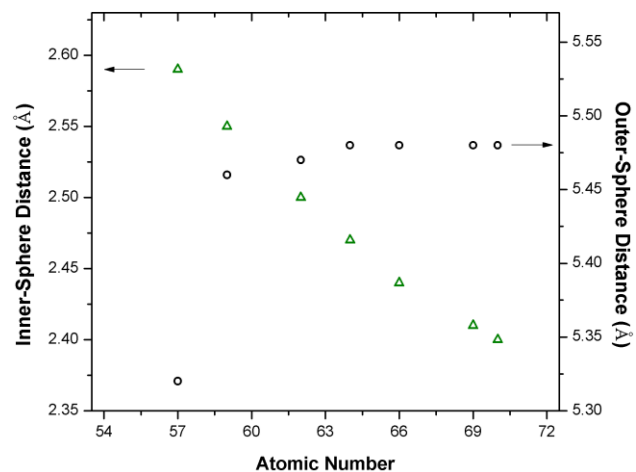


Figure S2. Inner- ($\text{Ln}-\text{O}_{\text{inner}}$) and outer-sphere ($\text{Ln}-\text{N}(\text{nitrate})$) average distances (Å) plotted against atomic number.

Sample Gaussian 09 Input File

Cartesian coordinates for La(TMDGA)₃(NO₃)₃, E = -3293.6584227 Hartree {B3LYP/SSC/6-31+G(d) level of theory}:

```
#N B3LYP/gen ginput pseudo=read scf=(MaxCycle=2000) opt freq nosymm integral=(grid=199302)
```

```
UO2_oxalate_3W
```

```
0 1
57      0.031868000      -0.029205000      0.041375000
8       0.846588000      -2.463789000      0.083314000
7      -1.515227000      -3.614064000      -2.420008000
6       0.216775000      -3.505989000      -0.665895000
1      -0.275575000      -4.203169000      0.029362000
1       0.975100000      -4.030415000      -1.265616000
8      -1.004070000      -1.613634000      -1.492718000
7       3.033828000      -1.983400000      2.928692000
6      -0.821610000      -2.854077000      -1.561479000
8       1.653970000      -0.652176000      1.713415000
6      -1.452981000      -5.085322000      -2.429932000
1      -2.460434000      -5.454017000      -2.208077000
6      -2.579907000      -2.972923000      -3.213657000
1      -3.117731000      -2.283757000      -2.556282000
6       1.697240000      -2.968779000      1.105785000
1       2.555684000      -3.481083000      0.652195000
1       1.138501000      -3.684340000      1.724821000
6       2.151612000      -1.778816000      1.946931000
6       3.710394000      -3.274070000      3.150896000
1       3.025394000      -4.089783000      2.900944000
6       3.447202000      -0.855341000      3.788587000
1       3.293450000      0.065731000      3.227810000
1       4.522457000      -0.949268000      3.956255000
8      -2.458563000      0.550328000      0.066356000
8       1.739796000      1.866909000      -0.078639000
7      -2.303569000      2.820189000      -2.757556000
7       3.592803000      0.456742000      -2.859306000
6      -3.061332000      1.499888000      -0.813118000
6       2.828917000      1.893186000      -1.000738000
1      -3.444428000      2.346070000      -0.225270000
1       3.775764000      1.884676000      -0.442870000
1      -3.880439000      1.007557000      -1.358238000
1       2.752353000      2.802181000      -1.616044000
8      -0.814992000      1.518456000      -1.653100000
8       1.779469000      -0.163235000      -1.655000000
7      -3.194938000      -1.453704000      2.986650000
7       0.480045000      3.569095000      2.857713000
6      -1.982146000      1.962366000      -1.776910000
6       2.710692000      0.650144000      -1.866949000
8      -1.342302000      -1.041209000      1.743432000
8      -0.122620000      1.725600000      1.680483000
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6       4.738112000      1.344536000      -3.129517000
1      -4.366509000      2.809502000      -2.377660000
1       4.548403000      2.313846000      -2.665236000
6      -1.254795000      3.245853000      -3.699673000
6       3.461608000      -0.748406000      -3.696443000
1      -0.312391000      3.300870000      -3.151154000
1       3.120153000      -1.566306000      -3.058463000
6      -3.323112000      0.162891000      1.130261000
6       1.844499000      2.871078000      0.927366000
1      -4.232144000      -0.292905000      0.716749000
1       1.830253000      3.863928000      0.458787000
1      -3.599396000      1.052143000      1.713193000
1       2.790914000      2.738779000      1.468661000
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6       0.649608000      2.697847000      1.859825000
6      -4.639254000      -1.298092000      3.240700000
6       1.311990000      4.773899000      3.028926000
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1	-4.944589000	-0.278577000	2.986463000
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1	-4.775299000	-1.393799000	4.322832000
1	1.371474000	4.960227000	4.106282000
6	-2.461417000	-2.404960000	3.848426000
6	-0.648620000	3.394838000	3.795348000
1	-1.646394000	-2.830775000	3.264017000
1	-1.439311000	2.857715000	3.272828000
1	-3.145156000	-3.224490000	4.080854000
1	-1.038224000	4.389400000	4.023416000
1	3.890394000	-3.349892000	4.228223000
1	-0.830209000	-5.421283000	-1.602002000
1	-3.276168000	-3.765742000	-3.502400000
1	-3.904553000	3.311820000	-3.993572000
1	-1.507476000	4.256990000	-4.030281000
1	4.763884000	1.517780000	-4.213135000
1	4.462638000	-1.001683000	-4.056147000
6	5.030552000	-3.399036000	2.381485000
1	5.527216000	-4.337269000	2.657117000
1	4.865171000	-3.397273000	1.299081000
1	5.700023000	-2.561560000	2.598862000
6	2.671334000	-0.826126000	5.107737000
1	3.030774000	0.003913000	5.727071000
1	1.599816000	-0.683957000	4.930468000
1	2.804438000	-1.751641000	5.680827000
6	-5.491525000	-2.338051000	2.504401000
1	-6.538451000	-2.241602000	2.816447000
1	-5.441484000	-2.201094000	1.418821000
1	-5.147658000	-3.355914000	2.711940000
6	-1.931548000	-1.735898000	5.118935000
1	-1.423065000	-2.481265000	5.741587000
1	-1.214737000	-0.944461000	4.874841000
1	-2.739010000	-1.295834000	5.716830000
6	0.743211000	6.001380000	2.307945000
1	1.349410000	6.882352000	2.551401000
1	0.748058000	5.865796000	1.221394000
1	-0.294862000	6.189121000	2.597810000
6	-0.231016000	2.648910000	5.064857000
1	-1.087518000	2.573747000	5.745018000
1	0.110872000	1.635526000	4.828966000
1	0.574578000	3.168140000	5.598131000
6	-0.936294000	-5.656879000	-3.752942000
1	-0.912763000	-6.751210000	-3.694403000
1	-1.580990000	-5.383924000	-4.595778000
1	0.078212000	-5.303278000	-3.971476000
6	-2.064262000	-2.232415000	-4.450691000
1	-2.907085000	-1.786212000	-4.992907000
1	-1.379107000	-1.430540000	-4.161295000
1	-1.540722000	-2.908866000	-5.135221000
6	6.076416000	0.784528000	-2.635856000
1	6.867036000	1.521793000	-2.818725000
1	6.029464000	0.561767000	-1.566231000
1	6.350321000	-0.134497000	-3.166107000
6	2.501780000	-0.547854000	-4.872581000
1	2.463378000	-1.457246000	-5.484339000
1	1.491123000	-0.332653000	-4.512658000
1	2.825801000	0.277484000	-5.517831000
6	-3.733844000	4.872582000	-2.482456000
1	-4.769194000	5.218083000	-2.586486000
1	-3.422180000	4.974727000	-1.438943000
1	-3.104094000	5.525703000	-3.097066000
6	-1.124016000	2.303641000	-4.899897000
1	-0.356141000	2.677037000	-5.588078000
1	-0.834622000	1.300042000	-4.573162000
1	-2.065813000	2.229869000	-5.456599000
7	-2.433144000	-4.803287000	1.436515000
8	-2.773720000	-4.232896000	0.356960000
8	-3.290464000	-5.124968000	2.287231000
8	-1.198796000	-5.034489000	1.651550000
7	-2.879243000	4.369574000	1.415678000
8	-2.781305000	5.264210000	2.282257000

8	-3.739852000	3.440316000	1.545367000
8	-2.120595000	4.367435000	0.398376000
7	5.305567000	0.497096000	1.271709000
8	6.063965000	0.038340000	2.152765000
8	4.887928000	-0.241855000	0.328597000
8	4.936019000	1.714545000	1.312116000

C,H,N,O 0
6-31+G(d)

La 0
S 3 1.00
5.0873990 -0.4172430
4.2709780 0.8860100
1.9154580 -1.4197520
S 1 1.00
0.5255960 1.0
S 1 1.00
0.2634740 1.0
S 1 1.00
0.0488200 1.0
S 1 1.00
0.0228360 1.0
P 3 1.00
3.0251610 0.5381960
2.3820950 -0.9816400
0.5844260 1.2395900
P 1 1.00
0.2603600 1.0
P 1 1.00
0.0833340 1.0
P 1 1.00
0.0302750 1.0
D 3 1.00
1.5768240 -0.0969440
0.5923900 0.4074660
0.2495000 0.7043630
D 1 1.00
0.1065130 1.0
D 1 1.00
0.0458310 1.0

La 0
ECP46MWB 4 46
G-Komponente
1
2 1.000000 0.000000
S-G
2
2 3.309900 91.932177
2 1.655000 -3.788764
P-G
2
2 2.836800 63.759486
2 1.418400 -0.647958
D-G
2
2 2.021300 36.116173
2 1.010700 0.219114
F-G
1
2 4.028600 -36.010016

Cartesian coordinates of optimized complexes (B3LYP/SSC/6-31+G(d)) discussed in the main text.

La(TEDGA)₃(NO₃)₃, E = -3293.6584227 Hartree

La 0.030904000 0.007598000 0.116536000

O	0.846111000	-2.555175000	0.147585000
N	-1.491657000	-3.727120000	-2.381968000
C	0.230425000	-3.592726000	-0.621914000
H	-0.259430000	-4.299972000	0.063996000
H	0.998408000	-4.104402000	-1.220931000
O	-0.998379000	-1.712977000	-1.475269000
N	3.067562000	-2.181552000	2.994010000
C	-0.808844000	-2.951413000	-1.525805000
O	1.627375000	-0.812468000	1.897931000
C	-1.431644000	-5.197745000	-2.367547000
H	-2.443593000	-5.562126000	-2.157277000
C	-2.548060000	-3.098159000	-3.195778000
H	-3.096723000	-2.403682000	-2.552968000
C	1.729429000	-3.083177000	1.131961000
H	2.596983000	-3.541075000	0.639558000
H	1.202450000	-3.849264000	1.717691000
C	2.162366000	-1.935204000	2.041354000
C	3.779719000	-3.464848000	3.123716000
H	3.110332000	-4.281919000	2.838222000
C	3.469014000	-1.097177000	3.911789000
H	3.315730000	-0.150356000	3.396072000
H	4.543814000	-1.195587000	4.080329000
O	-2.593795000	0.566985000	0.053644000
O	1.794991000	1.989068000	-0.105164000
N	-2.449097000	2.825485000	-2.787714000
N	3.634010000	0.576101000	-2.901322000
C	-3.200339000	1.448217000	-0.892716000
C	2.809120000	2.045573000	-1.108626000
H	-3.658093000	2.290502000	-0.355388000
H	3.789737000	2.121462000	-0.620131000
H	-3.958537000	0.890662000	-1.463503000
H	2.625920000	2.919365000	-1.752397000
O	-0.931981000	1.555174000	-1.683374000
O	1.840249000	-0.080036000	-1.682678000
N	-3.452105000	-1.421863000	2.960536000
N	0.763824000	3.735264000	2.905147000
C	-2.109595000	1.960494000	-1.818119000
C	2.737134000	0.762021000	-1.919596000
O	-1.522780000	-0.909759000	1.884912000
O	0.100886000	1.839990000	1.849292000
C	-3.812844000	3.347707000	-2.985274000
C	4.714898000	1.526242000	-3.218030000
H	-4.532701000	2.609011000	-2.624359000
H	4.392950000	2.534764000	-2.946614000
C	-1.390842000	3.371809000	-3.652469000
C	3.608317000	-0.688160000	-3.655029000
H	-0.481908000	3.459285000	-3.053995000
H	3.283196000	-1.477053000	-2.973911000
C	-3.509611000	0.155608000	1.064410000
C	1.932193000	3.034413000	0.854874000
H	-4.361427000	-0.358075000	0.600066000
H	1.811720000	4.006838000	0.359583000
H	-3.874594000	1.040950000	1.604073000
H	2.933349000	2.973269000	1.302614000
C	-2.763446000	-0.783917000	2.010047000
C	0.850924000	2.841471000	1.914857000
C	-4.918829000	-1.350952000	3.087895000
C	1.587600000	4.954719000	2.972411000
H	-5.260073000	-0.354675000	2.790224000
H	2.573283000	4.749757000	2.544649000
H	-5.141870000	-1.439403000	4.156326000
H	1.756724000	5.158370000	4.035300000
C	-2.738699000	-2.321790000	3.891555000
C	-0.264051000	3.561257000	3.949902000
H	-1.857742000	-2.705562000	3.377510000
H	-1.110202000	3.039733000	3.504857000

H	-3.393131000	-3.175552000	4.081551000
H	-0.615962000	4.558465000	4.224614000
H	3.983561000	-3.601201000	4.190962000
H	-0.822099000	-5.522431000	-1.525295000
H	-3.237970000	-3.896269000	-3.485555000
H	-3.966296000	3.419770000	-4.068998000
H	-1.698903000	4.382155000	-3.938954000
H	4.823819000	1.523692000	-4.309420000
H	4.639107000	-0.907059000	-3.950813000
C	5.086404000	-3.510224000	2.323376000
H	5.614512000	-4.447879000	2.535552000
H	4.898888000	-3.450673000	1.246310000
H	5.735033000	-2.666580000	2.575376000
C	2.684022000	-1.137520000	5.225353000
H	3.034331000	-0.338366000	5.889271000
H	1.613696000	-0.990084000	5.045495000
H	2.816173000	-2.090759000	5.751766000
C	-5.643825000	-2.449153000	2.301627000
H	-6.717540000	-2.409658000	2.521979000
H	-5.507115000	-2.325923000	1.221993000
H	-5.260183000	-3.441707000	2.556150000
C	-2.344890000	-1.611624000	5.188938000
H	-1.847655000	-2.321846000	5.859965000
H	-1.653680000	-0.785903000	4.988733000
H	-3.219046000	-1.209897000	5.715911000
C	0.933003000	6.165218000	2.297227000
H	1.559558000	7.052336000	2.450671000
H	0.808613000	6.005230000	1.221537000
H	-0.064423000	6.355897000	2.702468000
C	0.272652000	2.800708000	5.165110000
H	-0.510343000	2.725393000	5.929129000
H	0.578683000	1.787006000	4.886047000
H	1.133427000	3.308972000	5.616983000
C	-0.895973000	-5.792167000	-3.673045000
H	-0.876077000	-6.885562000	-3.597328000
H	-1.526434000	-5.530224000	-4.530039000
H	0.122623000	-5.443987000	-3.880863000
C	-2.019143000	-2.368767000	-4.434027000
H	-2.856598000	-1.931582000	-4.991828000
H	-1.340802000	-1.561020000	-4.144901000
H	-1.484632000	-3.050862000	-5.104479000
C	6.050580000	1.197450000	-2.543311000
H	6.808652000	1.919038000	-2.871175000
H	5.965480000	1.245964000	-1.455142000
H	6.399027000	0.194838000	-2.814149000
C	2.695179000	-0.626611000	-4.882886000
H	2.736214000	-1.576640000	-5.429278000
H	1.658300000	-0.446926000	-4.582163000
H	3.001364000	0.170317000	-5.571285000
C	-4.064428000	4.702324000	-2.314783000
H	-5.078369000	5.042643000	-2.557675000
H	-3.967519000	4.629508000	-1.228931000
H	-3.359227000	5.461365000	-2.670617000
C	-1.138132000	2.512445000	-4.894569000
H	-0.368747000	2.977553000	-5.522780000
H	-0.792358000	1.514242000	-4.608535000
H	-2.046147000	2.405605000	-5.500233000
N	-2.446295000	-4.800889000	1.486440000
O	-2.764812000	-4.154287000	0.442612000
O	-3.314327000	-5.120404000	2.327839000
O	-1.226729000	-5.113147000	1.673420000
N	-2.650246000	4.266616000	1.225046000
O	-2.397873000	5.075440000	2.143765000
O	-3.756339000	3.635891000	1.212520000
O	-1.812595000	4.060710000	0.295125000
N	5.154015000	0.475685000	1.105665000

O	5.828578000	-0.031916000	2.027767000
O	4.540093000	-0.256971000	0.272902000
O	5.075154000	1.742023000	0.991965000

Pr(TEDGA)₃(NO₃)₃, E = -3294.9451968 Hartree

Pr	0.031368000	-0.022517000	0.054118000
O	0.858457000	-2.536450000	0.097592000
N	-1.481580000	-3.713650000	-2.423534000
C	0.231172000	-3.580677000	-0.653510000
H	-0.268862000	-4.270479000	0.043292000
H	0.993971000	-4.111223000	-1.242103000
O	-0.987609000	-1.699593000	-1.517271000
N	3.063042000	-2.103633000	2.946051000
C	-0.800233000	-2.939728000	-1.566674000
O	1.659706000	-0.750878000	1.784647000
C	-1.418743000	-5.184573000	-2.412093000
H	-2.428945000	-5.550695000	-2.198056000
C	-2.538319000	-3.084981000	-3.237682000
H	-3.085386000	-2.388949000	-2.595359000
C	1.718043000	-3.051219000	1.109679000
H	2.578153000	-3.548846000	0.643255000
H	1.166458000	-3.782013000	1.717363000
C	2.169422000	-1.878868000	1.978311000
C	3.754917000	-3.392239000	3.126852000
H	3.076479000	-4.208713000	2.861828000
C	3.471712000	-0.994593000	3.832364000
H	3.316951000	-0.061484000	3.292306000
H	4.546825000	-1.090088000	3.999665000
O	-2.538150000	0.574567000	0.073083000
O	1.796008000	1.927823000	-0.082220000
N	-2.417153000	2.843626000	-2.761526000
N	3.658716000	0.541004000	-2.876737000
C	-3.146533000	1.514568000	-0.814515000
C	2.878265000	1.959633000	-1.014069000
H	-3.535082000	2.360390000	-0.230381000
H	3.827859000	1.953340000	-0.461182000
H	-3.962236000	1.012646000	-1.356310000
H	2.793864000	2.870715000	-1.625531000
O	-0.906197000	1.549209000	-1.680361000
O	1.837361000	-0.096861000	-1.694533000
N	-3.321516000	-1.428501000	2.990094000
N	0.585808000	3.666000000	2.862535000
C	-2.077250000	1.985861000	-1.786473000
C	2.767804000	0.721081000	-1.889003000
O	-1.437786000	-0.993086000	1.805081000
O	-0.023416000	1.789189000	1.745477000
C	-3.759923000	3.432851000	-2.912250000
C	4.806499000	1.431320000	-3.125397000
H	-4.477881000	2.816535000	-2.368552000
H	4.604028000	2.402938000	-2.671158000
C	-1.380720000	3.281961000	-3.711631000
C	3.539704000	-0.658150000	-3.724329000
H	-0.435845000	3.354883000	-3.169297000
H	3.198772000	-1.483209000	-3.095334000
C	-3.415998000	0.184281000	1.127293000
C	1.909403000	2.943956000	0.912892000
H	-4.314876000	-0.279488000	0.700786000
H	1.876623000	3.931125000	0.433546000
H	-3.707075000	1.075186000	1.700748000
H	2.868116000	2.825318000	1.435803000
C	-2.661653000	-0.808012000	2.008517000
C	0.739869000	2.774944000	1.879124000
C	-4.773817000	-1.292048000	3.203527000
C	1.405310000	4.884266000	2.988662000
H	-5.085863000	-0.277307000	2.938492000

H	2.422171000	4.674552000	2.643979000
H	-4.939117000	-1.387250000	4.281679000
H	1.486183000	5.094938000	4.060166000
C	-2.598016000	-2.367662000	3.873882000
C	-0.514784000	3.494168000	3.833307000
H	-1.764764000	-2.787243000	3.310860000
H	-1.319138000	2.952140000	3.337448000
H	-3.278217000	-3.193392000	4.094362000
H	-0.899580000	4.489346000	4.066730000
H	3.946517000	-3.495022000	4.199980000
H	-0.806047000	-5.509057000	-1.572162000
H	-3.229279000	-3.883031000	-3.524791000
H	-4.027580000	3.358987000	-3.974216000
H	-1.652160000	4.287425000	-4.044905000
H	4.855646000	1.599045000	-4.208957000
H	4.544590000	-0.902735000	-4.079640000
C	5.068494000	-3.480895000	2.341333000
H	5.580945000	-4.418810000	2.587672000
H	4.891648000	-3.453719000	1.261015000
H	5.728219000	-2.639695000	2.573269000
C	2.691670000	-0.996871000	5.149393000
H	3.047476000	-0.180569000	5.788863000
H	1.620707000	-0.851858000	4.970969000
H	2.824089000	-1.935252000	5.701529000
C	-5.590606000	-2.345406000	2.446289000
H	-6.647270000	-2.263658000	2.728300000
H	-5.511692000	-2.210095000	1.362169000
H	-5.237782000	-3.357614000	2.666051000
C	-2.104698000	-1.686089000	5.152480000
H	-1.602752000	-2.422656000	5.790755000
H	-1.390741000	-0.888500000	4.920350000
H	-2.930648000	-1.251695000	5.728965000
C	0.803713000	6.087968000	2.254136000
H	1.399183000	6.983719000	2.468433000
H	0.791013000	5.930353000	1.170582000
H	-0.232121000	6.263634000	2.559132000
C	-0.057853000	2.756306000	5.094100000
H	-0.893391000	2.682993000	5.800141000
H	0.278633000	1.742272000	4.853205000
H	0.762482000	3.280374000	5.599667000
C	-0.885399000	-5.774527000	-3.720431000
H	-0.862264000	-6.867964000	-3.646627000
H	-1.519398000	-5.513271000	-4.574983000
H	0.131615000	-5.423303000	-3.931028000
C	-2.009842000	-2.358658000	-4.477800000
H	-2.847410000	-1.921046000	-5.034970000
H	-1.329834000	-1.551516000	-4.190849000
H	-1.477228000	-3.042396000	-5.148025000
C	6.134974000	0.876550000	-2.600092000
H	6.929528000	1.611996000	-2.772851000
H	6.067277000	0.662236000	-1.530126000
H	6.418269000	-0.047532000	-3.116263000
C	2.586301000	-0.453222000	-4.904968000
H	2.555543000	-1.358349000	-5.523479000
H	1.572460000	-0.245030000	-4.549806000
H	2.910707000	0.378249000	-5.542181000
C	-3.849515000	4.884111000	-2.427954000
H	-4.886227000	5.230618000	-2.513137000
H	-3.526213000	4.963274000	-1.386156000
H	-3.225870000	5.551905000	-3.032939000
C	-1.242103000	2.336687000	-4.908584000
H	-0.484699000	2.719401000	-5.603274000
H	-0.934316000	1.339459000	-4.579175000
H	-2.186332000	2.245369000	-5.458646000
N	-2.451081000	-4.796867000	1.448073000
O	-2.767755000	-4.240753000	0.353693000

O	-3.326331000	-5.096628000	2.288644000
O	-1.223306000	-5.037218000	1.687599000
N	-2.844590000	4.357655000	1.411762000
O	-2.702154000	5.247019000	2.277757000
O	-3.744439000	3.467363000	1.546799000
O	-2.094399000	4.324162000	0.388667000
N	5.281134000	0.484167000	1.260878000
O	6.016173000	-0.005646000	2.145097000
O	4.825338000	-0.239916000	0.323881000
O	4.976230000	1.719731000	1.290738000

Sm(TEDGA)₃(NO₃)₃, E = -3296.7918352 Hartree

Sm	0.031314000	-0.027913000	0.045817000
O	0.850055000	-2.489990000	0.089487000
N	-1.501852000	-3.651897000	-2.421716000
C	0.221479000	-3.533355000	-0.660259000
H	-0.274209000	-4.227059000	0.035960000
H	0.981869000	-4.060550000	-1.254884000
O	-0.998753000	-1.645837000	-1.502404000
N	3.044180000	-2.027112000	2.936016000
C	-0.813816000	-2.886141000	-1.563519000
O	1.657279000	-0.687082000	1.739376000
C	-1.438120000	-5.123017000	-2.423674000
H	-2.446721000	-5.491554000	-2.206713000
C	-2.563424000	-3.016165000	-3.223905000
H	-3.105956000	-2.325107000	-2.572414000
C	1.703964000	-2.998468000	1.108340000
H	2.562639000	-3.506169000	0.650080000
H	1.147528000	-3.719038000	1.723671000
C	2.158178000	-1.814789000	1.959022000
C	3.725637000	-3.317485000	3.143626000
H	3.042799000	-4.133264000	2.888025000
C	3.455936000	-0.905963000	3.805685000
H	3.302236000	0.019602000	3.252394000
H	4.531038000	-1.000741000	3.973587000
O	-2.486345000	0.559440000	0.069099000
O	1.760172000	1.886222000	-0.078477000
N	-2.344662000	2.825800000	-2.761651000
N	3.616530000	0.487386000	-2.866022000
C	-3.091273000	1.504717000	-0.814205000
C	2.846671000	1.915361000	-1.004310000
H	-3.476421000	2.351164000	-0.228308000
H	3.794534000	1.907769000	-0.448297000
H	-3.909116000	1.008294000	-1.357593000
H	2.766790000	2.825427000	-1.617686000
O	-0.846918000	1.529912000	-1.663315000
O	1.801715000	-0.141614000	-1.668829000
N	-3.241308000	-1.441029000	2.990500000
N	0.516414000	3.604655000	2.858658000
C	-2.015914000	1.969979000	-1.781485000
C	2.731837000	0.674386000	-1.874468000
O	-1.377673000	-1.026268000	1.765574000
O	-0.090126000	1.749336000	1.703228000
C	-3.686088000	3.414396000	-2.928710000
C	4.762052000	1.377050000	-3.128526000
H	-4.406788000	2.808847000	-2.376791000
H	4.567612000	2.346513000	-2.666430000
C	-1.300547000	3.254691000	-3.707567000
C	3.489774000	-0.714885000	-3.708038000
H	-0.357670000	3.320288000	-3.160939000
H	3.150390000	-1.536468000	-3.073691000
C	-3.355834000	0.172320000	1.130042000
C	1.867386000	2.895526000	0.922988000
H	-4.262051000	-0.285190000	0.712279000
H	1.847865000	3.885962000	0.449563000

H	-3.636060000	1.062818000	1.709259000
H	2.817573000	2.767866000	1.458876000
C	-2.595120000	-0.827782000	1.995764000
C	0.680221000	2.725620000	1.866412000
C	-4.687994000	-1.288755000	3.231610000
C	1.344916000	4.813811000	3.013735000
H	-4.994160000	-0.270892000	2.971821000
H	2.364857000	4.599045000	2.681620000
H	-4.833284000	-1.381757000	4.312796000
H	1.411135000	5.009485000	4.089048000
C	-2.511983000	-2.387536000	3.861265000
C	-0.602818000	3.432181000	3.807894000
H	-1.693465000	-2.816167000	3.283745000
H	-1.399231000	2.894799000	3.294407000
H	-3.196717000	-3.206038000	4.094215000
H	-0.989279000	4.427345000	4.038561000
H	3.909399000	-3.403077000	4.219601000
H	-0.820531000	-5.454227000	-1.589970000
H	-3.256683000	-3.811494000	-3.512921000
H	-3.949433000	3.322143000	-3.990395000
H	-1.561971000	4.261959000	-4.043173000
H	4.795049000	1.549659000	-4.212015000
H	4.491907000	-0.963485000	-4.068026000
C	5.043663000	-3.429803000	2.368628000
H	5.545592000	-4.368329000	2.633524000
H	4.874436000	-3.418424000	1.286846000
H	5.709946000	-2.591291000	2.591626000
C	2.678039000	-0.888073000	5.123851000
H	3.036074000	-0.063027000	5.750662000
H	1.606808000	-0.744718000	4.945757000
H	2.810535000	-1.818350000	5.689382000
C	-5.530651000	-2.333385000	2.490833000
H	-6.580710000	-2.239250000	2.792889000
H	-5.470971000	-2.199567000	1.405322000
H	-5.185554000	-3.349523000	2.704653000
C	-1.989386000	-1.711189000	5.130958000
H	-1.483547000	-2.452771000	5.760269000
H	-1.271891000	-0.920576000	4.886226000
H	-2.800474000	-1.268592000	5.722077000
C	0.765954000	6.032752000	2.286328000
H	1.368593000	6.918933000	2.519492000
H	0.765750000	5.888622000	1.200845000
H	-0.271647000	6.216854000	2.580186000
C	-0.172323000	2.687561000	5.073921000
H	-1.021631000	2.613655000	5.763214000
H	0.166299000	1.673676000	4.835459000
H	0.639294000	3.207017000	5.597838000
C	-0.912081000	-5.700862000	-3.740296000
H	-0.887677000	-6.794867000	-3.676123000
H	-1.551429000	-5.432832000	-4.588758000
H	0.103416000	-5.347092000	-3.953920000
C	-2.042603000	-2.280091000	-4.461459000
H	-2.883472000	-1.837801000	-5.009876000
H	-1.360464000	-1.475621000	-4.172148000
H	-1.514394000	-2.958581000	-5.140398000
C	6.097602000	0.818923000	-2.625330000
H	6.889054000	1.556392000	-2.803704000
H	6.043887000	0.597090000	-1.555899000
H	6.375232000	-0.100752000	-3.152460000
C	2.530220000	-0.512540000	-4.884109000
H	2.494670000	-1.419767000	-5.499254000
H	1.518718000	-0.301385000	-4.524145000
H	2.852539000	0.316089000	-5.526014000
C	-3.776949000	4.873840000	-2.470073000
H	-4.813009000	5.218961000	-2.568069000
H	-3.461036000	4.970239000	-1.427334000

H	-3.149824000	5.531207000	-3.082853000
C	-1.164244000	2.307082000	-4.902921000
H	-0.400251000	2.682645000	-5.594255000
H	-0.866699000	1.307526000	-4.571188000
H	-2.106398000	2.223257000	-5.457640000
N	-2.441235000	-4.798344000	1.441846000
O	-2.771867000	-4.240138000	0.352833000
O	-3.306177000	-5.107920000	2.289358000
O	-1.209301000	-5.030163000	1.669289000
N	-2.866813000	4.367658000	1.411672000
O	-2.752476000	5.261018000	2.277616000
O	-3.738337000	3.449415000	1.546607000
O	-2.114903000	4.356590000	0.389440000
N	5.298313000	0.490956000	1.270045000
O	6.047563000	0.020781000	2.152955000
O	4.873375000	-0.241109000	0.324836000
O	4.946263000	1.713591000	1.310298000

Gd(TEDGA)₃(NO₃)₃, E = -3297.979839 Hartree

Gd	0.031868000	-0.029205000	0.041375000
O	0.846588000	-2.463789000	0.083314000
N	-1.515227000	-3.614064000	-2.420008000
C	0.216775000	-3.505989000	-0.665895000
H	-0.275575000	-4.203169000	0.029362000
H	0.975100000	-4.030415000	-1.265616000
O	-1.004070000	-1.613634000	-1.492718000
N	3.033828000	-1.983400000	2.928692000
C	-0.821610000	-2.854077000	-1.561479000
O	1.653970000	-0.652176000	1.713415000
C	-1.452981000	-5.085322000	-2.429932000
H	-2.460434000	-5.454017000	-2.208077000
C	-2.579907000	-2.972923000	-3.213657000
H	-3.117731000	-2.283757000	-2.556282000
C	1.697240000	-2.968779000	1.105785000
H	2.555684000	-3.481083000	0.652195000
H	1.138501000	-3.684340000	1.724821000
C	2.151612000	-1.778816000	1.946931000
C	3.710394000	-3.274070000	3.150896000
H	3.025394000	-4.089783000	2.900944000
C	3.447202000	-0.855341000	3.788587000
H	3.293450000	0.065731000	3.227810000
H	4.522457000	-0.949268000	3.956255000
O	-2.458563000	0.550328000	0.066356000
O	1.739796000	1.866909000	-0.078639000
N	-2.303569000	2.820189000	-2.757556000
N	3.592803000	0.456742000	-2.859306000
C	-3.061332000	1.499888000	-0.813118000
C	2.828917000	1.893186000	-1.000738000
H	-3.444428000	2.346070000	-0.225270000
H	3.775764000	1.884676000	-0.442870000
H	-3.880439000	1.007557000	-1.358238000
H	2.752353000	2.802181000	-1.616044000
O	-0.814992000	1.518456000	-1.653100000
O	1.779469000	-0.163235000	-1.655000000
N	-3.194938000	-1.453704000	2.986650000
N	0.480045000	3.569095000	2.857713000
C	-1.982146000	1.962366000	-1.776910000
C	2.710692000	0.650144000	-1.866949000
O	-1.342302000	-1.041209000	1.743432000
O	-0.122620000	1.725600000	1.680483000
C	-3.643587000	3.410245000	-2.931828000
C	4.738112000	1.344536000	-3.129517000
H	-4.366509000	2.809502000	-2.377660000
H	4.548403000	2.313846000	-2.665236000
C	-1.254795000	3.245853000	-3.699673000

C	3.461608000	-0.748406000	-3.696443000
H	-0.312391000	3.300870000	-3.151154000
H	3.120153000	-1.566306000	-3.058463000
C	-3.323112000	0.162891000	1.130261000
C	1.844499000	2.871078000	0.927366000
H	-4.232144000	-0.292905000	0.716749000
H	1.830253000	3.863928000	0.458787000
H	-3.599396000	1.052143000	1.713193000
H	2.790914000	2.738779000	1.468661000
C	-2.556975000	-0.840193000	1.987048000
C	0.649608000	2.697847000	1.859825000
C	-4.639254000	-1.298092000	3.240700000
C	1.311990000	4.773899000	3.028926000
H	-4.944589000	-0.278577000	2.986463000
H	2.333299000	4.557773000	2.702003000
H	-4.775299000	-1.393799000	4.322832000
H	1.371474000	4.960227000	4.106282000
C	-2.461417000	-2.404960000	3.848426000
C	-0.648620000	3.394838000	3.795348000
H	-1.646394000	-2.830775000	3.264017000
H	-1.439311000	2.857715000	3.272828000
H	-3.145156000	-3.224490000	4.080854000
H	-1.038224000	4.389400000	4.023416000
H	3.890394000	-3.349892000	4.228223000
H	-0.830209000	-5.421283000	-1.602002000
H	-3.276168000	-3.765742000	-3.502400000
H	-3.904553000	3.311820000	-3.993572000
H	-1.507476000	4.256990000	-4.030281000
H	4.763884000	1.517780000	-4.213135000
H	4.462638000	-1.001683000	-4.056147000
C	5.03052000	-3.399036000	2.381485000
H	5.527216000	-4.337269000	2.657117000
H	4.865171000	-3.397273000	1.299081000
H	5.700023000	-2.561560000	2.598862000
C	2.671334000	-0.826126000	5.107737000
H	3.030774000	0.003913000	5.727071000
H	1.599816000	-0.683957000	4.930468000
H	2.804438000	-1.751641000	5.680827000
C	-5.491525000	-2.338051000	2.504401000
H	-6.538451000	-2.241602000	2.816447000
H	-5.441484000	-2.201094000	1.418821000
H	-5.147658000	-3.355914000	2.711940000
C	-1.931548000	-1.735898000	5.118935000
H	-1.423065000	-2.481265000	5.741587000
H	-1.214737000	-0.944461000	4.874841000
H	-2.739010000	-1.295834000	5.716830000
C	0.743211000	6.001380000	2.307945000
H	1.349410000	6.882352000	2.551401000
H	0.748058000	5.865796000	1.221394000
H	-0.294862000	6.189121000	2.597810000
C	-0.231016000	2.648910000	5.064857000
H	-1.087518000	2.573747000	5.745018000
H	0.110872000	1.635526000	4.828966000
H	0.574578000	3.168140000	5.598131000
C	-0.936294000	-5.656879000	-3.752942000
H	-0.912763000	-6.751210000	-3.694403000
H	-1.580990000	-5.383924000	-4.595778000
H	0.078212000	-5.303278000	-3.971476000
C	-2.064262000	-2.232415000	-4.450691000
H	-2.907085000	-1.786212000	-4.992907000
H	-1.379107000	-1.430540000	-4.161295000
H	-1.540722000	-2.908866000	-5.135221000
C	6.076416000	0.784528000	-2.635856000
H	6.867036000	1.521793000	-2.818725000
H	6.029464000	0.561767000	-1.566231000
H	6.350321000	-0.134497000	-3.166107000

C	2.501780000	-0.547854000	-4.872581000
H	2.463378000	-1.457246000	-5.484339000
H	1.491123000	-0.332653000	-4.512658000
H	2.825801000	0.277484000	-5.517831000
C	-3.733844000	4.872582000	-2.482456000
H	-4.769194000	5.218083000	-2.586486000
H	-3.422180000	4.974727000	-1.438943000
H	-3.104094000	5.525703000	-3.097066000
C	-1.124016000	2.303641000	-4.899897000
H	-0.356141000	2.677037000	-5.588078000
H	-0.834622000	1.300042000	-4.573162000
H	-2.065813000	2.229869000	-5.456599000
N	-2.433144000	-4.803287000	1.436515000
O	-2.773720000	-4.232896000	0.356960000
O	-3.290464000	-5.124968000	2.287231000
O	-1.198796000	-5.034489000	1.651550000
N	-2.879243000	4.369574000	1.415678000
O	-2.781305000	5.264210000	2.282257000
O	-3.739852000	3.440316000	1.545367000
O	-2.120595000	4.367435000	0.398376000
N	5.305567000	0.497096000	1.271709000
O	6.063965000	0.038340000	2.152765000
O	4.887928000	-0.241855000	0.328597000
O	4.936019000	1.714545000	1.312116000

Dy(TEDGA)₃(NO₃)₃, E = -3299.1581062 Hartree

Dy	0.032257000	-0.030896000	0.037239000
O	0.843970000	-2.440714000	0.078713000
N	-1.526475000	-3.579667000	-2.417613000
C	0.212075000	-3.481917000	-0.668949000
H	-0.279212000	-4.180216000	0.026024000
H	0.968170000	-4.006276000	-1.271582000
O	-1.004220000	-1.584065000	-1.485764000
N	3.023190000	-1.942415000	2.923379000
C	-0.826760000	-2.825069000	-1.559588000
O	1.648743000	-0.620809000	1.690462000
C	-1.467752000	-5.051104000	-2.433215000
H	-2.474987000	-5.418233000	-2.208034000
C	-2.592772000	-2.932935000	-3.204481000
H	-3.125555000	-2.244156000	-2.542588000
C	1.690241000	-2.942037000	1.105621000
H	2.548664000	-3.459388000	0.657738000
H	1.128619000	-3.652200000	1.728268000
C	2.144182000	-1.745781000	1.937302000
C	3.696164000	-3.232761000	3.158959000
H	3.009468000	-4.048935000	2.915189000
C	3.438247000	-0.807747000	3.773693000
H	3.282653000	0.109052000	3.206408000
H	4.514010000	-0.899866000	3.939350000
O	-2.434161000	0.540428000	0.061238000
O	1.719783000	1.850441000	-0.079539000
N	-2.264181000	2.811073000	-2.757703000
N	3.569704000	0.429152000	-2.853043000
C	-3.034605000	1.492030000	-0.816670000
C	2.809534000	1.875744000	-0.999980000
H	-3.417652000	2.338283000	-0.228805000
H	3.756414000	1.869836000	-0.442122000
H	-3.853512000	1.002098000	-1.364250000
H	2.732580000	2.782471000	-1.618575000
O	-0.785629000	1.504337000	-1.645111000
O	1.758650000	-0.182394000	-1.640858000
N	-3.152409000	-1.461247000	2.984162000
N	0.446437000	3.535066000	2.857423000
C	-1.950752000	1.951826000	-1.775870000
C	2.689945000	0.629091000	-1.860130000

O	-1.311338000	-1.054760000	1.720896000
O	-0.151958000	1.702876000	1.659204000
C	-3.602754000	3.402031000	-2.940737000
C	4.713028000	1.316655000	-3.132719000
H	-4.328480000	2.805178000	-2.386067000
H	4.526315000	2.286369000	-2.668108000
C	-1.209689000	3.234295000	-3.694431000
C	3.436202000	-0.780631000	-3.683012000
H	-0.269040000	3.281308000	-3.142252000
H	3.094506000	-1.594299000	-3.039794000
C	-3.293855000	0.155141000	1.128920000
C	1.822384000	2.849339000	0.930933000
H	-4.206049000	-0.299201000	0.720742000
H	1.811951000	3.844708000	0.467575000
H	-3.565510000	1.044404000	1.713895000
H	2.765777000	2.713042000	1.476382000
C	-2.522788000	-0.849878000	1.978142000
C	0.621231000	2.671667000	1.853754000
C	-4.593628000	-1.299601000	3.252583000
C	1.281310000	4.735773000	3.043856000
H	-4.897133000	-0.278795000	3.001355000
H	2.303816000	4.518771000	2.721308000
H	-4.719064000	-1.394720000	4.336036000
H	1.334865000	4.912850000	4.123083000
C	-2.415229000	-2.416590000	3.838025000
C	-0.690432000	3.358794000	3.784644000
H	-1.606099000	-2.843583000	3.246390000
H	-1.476096000	2.822221000	3.254023000
H	-3.099675000	-3.234592000	4.073781000
H	-1.082757000	4.352746000	4.010782000
H	3.873638000	-3.298917000	4.237312000
H	-0.842099000	-5.391442000	-1.609224000
H	-3.292707000	-3.722781000	-3.492422000
H	-3.859627000	3.298226000	-4.002989000
H	-1.454965000	4.248272000	-4.021817000
H	4.731144000	1.488549000	-4.216745000
H	4.436493000	-1.037233000	-4.042263000
C	5.017733000	-3.368960000	2.393891000
H	5.510202000	-4.306435000	2.679416000
H	4.855109000	-3.376619000	1.311123000
H	5.689842000	-2.532046000	2.605279000
C	2.666503000	-0.768859000	5.094994000
H	3.027633000	0.065975000	5.706831000
H	1.594332000	-0.628568000	4.920406000
H	2.801872000	-1.689831000	5.674763000
C	-5.458126000	-2.335645000	2.525064000
H	-6.501416000	-2.233391000	2.847271000
H	-5.417942000	-2.199542000	1.438997000
H	-5.117829000	-3.355263000	2.729790000
C	-1.873738000	-1.752637000	5.106277000
H	-1.363337000	-2.501370000	5.723292000
H	-1.155999000	-0.963070000	4.858989000
H	-2.675121000	-1.311270000	5.711297000
C	0.721620000	5.971427000	2.329803000
H	1.331559000	6.847224000	2.582394000
H	0.730005000	5.843984000	1.242312000
H	-0.316519000	6.162769000	2.616983000
C	-0.284302000	2.611272000	5.056857000
H	-1.147095000	2.534689000	5.728841000
H	0.060465000	1.598454000	4.822872000
H	0.515845000	3.130112000	5.598552000
C	-0.958255000	-5.618961000	-3.760583000
H	-0.936783000	-6.713529000	-3.705904000
H	-1.606189000	-5.341823000	-4.599571000
H	0.056027000	-5.266809000	-3.982485000
C	-2.080649000	-2.190228000	-4.441638000

H	-2.924658000	-1.740289000	-4.978896000
H	-1.392120000	-1.391042000	-4.152884000
H	-1.561862000	-2.866054000	-5.130364000
C	6.055117000	0.758203000	-2.647608000
H	6.843526000	1.496396000	-2.836244000
H	6.015320000	0.536422000	-1.577443000
H	6.327003000	-0.160654000	-3.179210000
C	2.475307000	-0.586059000	-4.859279000
H	2.435697000	-1.498846000	-5.465878000
H	1.465191000	-0.368175000	-4.499482000
H	2.799149000	0.235379000	-5.509547000
C	-3.693664000	4.866740000	-2.499309000
H	-4.728288000	5.212307000	-2.610228000
H	-3.387519000	4.973707000	-1.454615000
H	-3.060774000	5.516481000	-3.114253000
C	-1.080017000	2.296334000	-4.898085000
H	-0.307554000	2.668177000	-5.581947000
H	-0.797537000	1.289758000	-4.574517000
H	-2.020082000	2.230150000	-5.458606000
N	-2.430266000	-4.804442000	1.432232000
O	-2.778591000	-4.225255000	0.359857000
O	-3.281504000	-5.134751000	2.285672000
O	-1.194120000	-5.035094000	1.637578000
N	-2.887958000	4.366802000	1.415158000
O	-2.803634000	5.263008000	2.281477000
O	-3.738015000	3.427543000	1.542308000
O	-2.125243000	4.372537000	0.400901000
N	5.307199000	0.504086000	1.270526000
O	6.074628000	0.055048000	2.148729000
O	4.895041000	-0.240350000	0.329314000
O	4.922053000	1.716604000	1.312456000

Tm(TEDGA)₃(NO₃)₃, E = -3300.9078284 Hartree

Tm	0.034147000	-0.030979000	0.036141000
O	0.840643000	-2.411095000	0.075019000
N	-1.543060000	-3.529293000	-2.412147000
C	0.205656000	-3.449378000	-0.672079000
H	-0.283775000	-4.150848000	0.021214000
H	0.958153000	-3.972448000	-1.280391000
O	-1.003856000	-1.542222000	-1.471069000
N	3.008882000	-1.890574000	2.918383000
C	-0.834310000	-2.783824000	-1.553891000
O	1.639757000	-0.582380000	1.663949000
C	-1.490842000	-5.000998000	-2.436722000
H	-2.498199000	-5.365101000	-2.207342000
C	-2.610863000	-2.873132000	-3.188910000
H	-3.135440000	-2.184434000	-2.520385000
C	1.680914000	-2.908581000	1.107035000
H	2.539571000	-3.431842000	0.666457000
H	1.115838000	-3.612536000	1.733639000
C	2.133631000	-1.704550000	1.927275000
C	3.679173000	-3.179606000	3.169587000
H	2.991680000	-3.997030000	2.932390000
C	3.425233000	-0.747687000	3.756866000
H	3.264039000	0.163669000	3.182424000
H	4.502158000	-0.835120000	3.917741000
O	-2.403049000	0.528327000	0.055858000
O	1.697058000	1.830653000	-0.080165000
N	-2.210261000	2.795708000	-2.758947000
N	3.536788000	0.390523000	-2.845292000
C	-3.000633000	1.478221000	-0.824002000
C	2.784121000	1.854897000	-1.002081000
H	-3.388802000	2.324424000	-0.239370000
H	3.732943000	1.855405000	-0.447501000
H	-3.815279000	0.987497000	-1.377213000

H	2.703014000	2.756877000	-1.627069000
O	-0.745400000	1.487830000	-1.628881000
O	1.731408000	-0.207503000	-1.617553000
N	-3.098046000	-1.472725000	2.979257000
N	0.407012000	3.495285000	2.855278000
C	-1.908363000	1.936813000	-1.773445000
C	2.662022000	0.601015000	-1.850485000
O	-1.271072000	-1.067142000	1.694003000
O	-0.182596000	1.674241000	1.634291000
C	-3.547496000	3.385206000	-2.957293000
C	4.677099000	1.277078000	-3.140579000
H	-4.278271000	2.788465000	-2.409138000
H	4.492507000	2.249959000	-2.681789000
C	-1.145856000	3.219554000	-3.683951000
C	3.400422000	-0.827977000	-3.661782000
H	-0.210479000	3.261355000	-3.122537000
H	3.059606000	-1.634200000	-3.008816000
C	-3.257723000	0.144601000	1.126624000
C	1.796940000	2.825037000	0.933382000
H	-4.172245000	-0.310071000	0.723987000
H	1.788407000	3.822691000	0.474800000
H	-3.526553000	1.033399000	1.713459000
H	2.737765000	2.686981000	1.482681000
C	-2.479244000	-0.861249000	1.966984000
C	0.589456000	2.640779000	1.845725000
C	-4.535931000	-1.306888000	3.264080000
C	1.242920000	4.692905000	3.058210000
H	-4.838478000	-0.284565000	3.017989000
H	2.266928000	4.476728000	2.740018000
H	-4.649261000	-1.403442000	4.348731000
H	1.289971000	4.859881000	4.139353000
C	-2.355670000	-2.433408000	3.822133000
C	-0.738609000	3.315297000	3.770779000
H	-1.549243000	-2.854656000	3.222812000
H	-1.517163000	2.777037000	3.231488000
H	-3.037841000	-3.254144000	4.055214000
H	-1.136309000	4.307873000	3.993611000
H	3.853341000	-3.234558000	4.249067000
H	-0.861577000	-5.348759000	-1.618572000
H	-3.317115000	-3.657733000	-3.475760000
H	-3.792935000	3.278998000	-4.022006000
H	-1.384782000	4.235679000	-4.009406000
H	4.686611000	1.440693000	-4.226023000
H	4.399654000	-1.089358000	-4.020483000
C	5.002855000	-3.326833000	2.410260000
H	5.491483000	-4.262773000	2.707153000
H	4.843880000	-3.345189000	1.327127000
H	5.676941000	-2.489938000	2.615409000
C	2.661088000	-0.699081000	5.082215000
H	3.023401000	0.142469000	5.684030000
H	1.587442000	-0.563750000	4.913153000
H	2.802777000	-1.613992000	5.669950000
C	-5.412861000	-2.338226000	2.544862000
H	-6.451849000	-2.231530000	2.879302000
H	-5.384529000	-2.200791000	1.458650000
H	-5.075098000	-3.359743000	2.744121000
C	-1.807994000	-1.779302000	5.092786000
H	-1.294250000	-2.532723000	5.701240000
H	-1.091914000	-0.987403000	4.848314000
H	-2.606311000	-1.343177000	5.705540000
C	0.690768000	5.936402000	2.352038000
H	1.303350000	6.807460000	2.614408000
H	0.702953000	5.817779000	1.263625000
H	-0.347640000	6.130046000	2.636622000
C	-0.344004000	2.568141000	5.046723000
H	-1.213891000	2.488225000	5.709071000

H	0.006829000	1.556725000	4.815919000
H	0.448237000	3.089122000	5.597814000
C	-0.992265000	-5.563206000	-3.770583000
H	-0.974746000	-6.658126000	-3.722105000
H	-1.644663000	-5.278952000	-4.603733000
H	0.021938000	-5.213821000	-3.997190000
C	-2.102986000	-2.127504000	-4.426021000
H	-2.948150000	-1.671452000	-4.956256000
H	-1.409077000	-1.332746000	-4.138040000
H	-1.591436000	-2.802698000	-5.120714000
C	6.023764000	0.724391000	-2.661687000
H	6.809220000	1.462709000	-2.861785000
H	5.992548000	0.510632000	-1.589574000
H	6.293565000	-0.197635000	-3.188895000
C	2.436972000	-0.645730000	-4.837925000
H	2.395985000	-1.564816000	-5.434831000
H	1.427720000	-0.423920000	-4.478182000
H	2.759473000	0.168763000	-5.497497000
C	-3.644915000	4.850600000	-2.519785000
H	-4.678529000	5.194774000	-2.643691000
H	-3.351537000	4.959902000	-1.471663000
H	-3.005636000	5.499877000	-3.128583000
C	-1.007183000	2.286554000	-4.890389000
H	-0.227200000	2.659314000	-5.565141000
H	-0.730548000	1.277844000	-4.568624000
H	-1.941896000	2.225343000	-5.460306000
N	-2.426531000	-4.806159000	1.425013000
O	-2.784938000	-4.201226000	0.370258000
O	-3.268772000	-5.150119000	2.281957000
O	-1.189300000	-5.048416000	1.609333000
N	-2.901991000	4.357079000	1.412289000
O	-2.833841000	5.253055000	2.280253000
O	-3.743832000	3.409426000	1.530981000
O	-2.130158000	4.371038000	0.404998000
N	5.307761000	0.521881000	1.268867000
O	6.083185000	0.087129000	2.147263000
O	4.899176000	-0.233840000	0.335103000
O	4.910346000	1.730608000	1.303362000

Yb(TEDGA)₃(NO₃)₃, E = -3301.4918459 Hartree

Yb	0.034622000	-0.030730000	0.036103000
O	0.840622000	-2.401638000	0.072794000
N	-1.547634000	-3.513361000	-2.411035000
C	0.204993000	-3.438930000	-0.674481000
H	-0.282977000	-4.142216000	0.018006000
H	0.956350000	-3.960504000	-1.285502000
O	-1.004286000	-1.529222000	-1.465883000
N	3.004192000	-1.874924000	2.916745000
C	-0.836281000	-2.770787000	-1.552442000
O	1.636586000	-0.570739000	1.655955000
C	-1.496811000	-4.985092000	-2.439133000
H	-2.503843000	-5.348822000	-2.207757000
C	-2.616572000	-2.854485000	-3.183901000
H	-3.138821000	-2.166564000	-2.512757000
C	1.678702000	-2.898095000	1.106566000
H	2.537831000	-3.422641000	0.668419000
H	1.112483000	-3.600543000	1.733841000
C	2.130278000	-1.691981000	1.923937000
C	3.673764000	-3.163488000	3.172562000
H	2.986248000	-3.981322000	2.936881000
C	3.420597000	-0.729781000	3.752084000
H	3.257892000	0.180088000	3.175720000
H	4.497817000	-0.815860000	3.911823000
O	-2.393526000	0.524635000	0.055330000
O	1.690069000	1.824824000	-0.080857000

N	-2.194796000	2.792116000	-2.757316000
N	3.525814000	0.378598000	-2.843697000
C	-2.990790000	1.473749000	-0.825024000
C	2.776182000	1.848420000	-1.003371000
H	-3.381140000	2.319600000	-0.241334000
H	3.725737000	1.850611000	-0.450040000
H	-3.803745000	0.982305000	-1.380119000
H	2.694021000	2.749046000	-1.630205000
O	-0.733971000	1.482845000	-1.623272000
O	1.721589000	-0.214371000	-1.611546000
N	-3.080418000	-1.477687000	2.977993000
N	0.396193000	3.483424000	2.854547000
C	-1.896243000	1.932517000	-1.771452000
C	2.652518000	0.592661000	-1.848407000
O	-1.257810000	-1.070224000	1.686584000
O	-0.190659000	1.665264000	1.627394000
C	-3.531729000	3.381005000	-2.959842000
C	4.665925000	1.264080000	-3.143182000
H	-4.263720000	2.784444000	-2.413136000
H	4.482307000	2.238161000	-2.686557000
C	-1.127743000	3.216730000	-3.678851000
C	3.388076000	-0.842138000	-3.656543000
H	-0.193522000	3.254891000	-3.115303000
H	3.044901000	-1.645546000	-3.001377000
C	-3.246526000	0.140561000	1.126831000
C	1.789390000	2.818085000	0.933322000
H	-4.161359000	-0.314771000	0.725640000
H	1.780673000	3.816334000	0.476009000
H	-3.515112000	1.028854000	1.714512000
H	2.729804000	2.679979000	1.483277000
C	-2.465157000	-0.865190000	1.964224000
C	0.580689000	2.631498000	1.843229000
C	-4.517559000	-1.312265000	3.267119000
C	1.231994000	4.680474000	3.061753000
H	-4.820633000	-0.289510000	3.023469000
H	2.256417000	4.464917000	2.744490000
H	-4.627785000	-1.410437000	4.351933000
H	1.277483000	4.844662000	4.143384000
C	-2.336184000	-2.440219000	3.817042000
C	-0.751477000	3.302223000	3.767211000
H	-1.528351000	-2.856469000	3.216152000
H	-1.527972000	2.762953000	3.225974000
H	-3.016269000	-3.263890000	4.045993000
H	-1.151033000	4.294337000	3.988825000
H	3.846515000	-3.215339000	4.252412000
H	-0.865547000	-5.335288000	-1.623556000
H	-3.324393000	-3.637719000	-3.470639000
H	-3.774240000	3.273834000	-4.025126000
H	-1.363900000	4.234363000	-4.001620000
H	4.673683000	1.424881000	-4.229053000
H	4.387215000	-1.106652000	-4.013212000
C	4.998384000	-3.313691000	2.415469000
H	5.485737000	-4.249268000	2.715594000
H	4.840956000	-3.334784000	1.332182000
H	5.672990000	-2.476918000	2.619384000
C	2.658335000	-0.678638000	5.078409000
H	3.020605000	0.164883000	5.677481000
H	1.584291000	-0.544990000	4.910659000
H	2.801908000	-1.591790000	5.668396000
C	-5.396913000	-2.342288000	2.548958000
H	-6.434823000	-2.235645000	2.886750000
H	-5.371844000	-2.203286000	1.462887000
H	-5.059042000	-3.364257000	2.745670000
C	-1.790711000	-1.790745000	5.091007000
H	-1.275482000	-2.545813000	5.696147000
H	-1.076448000	-0.995920000	4.850755000

H	-2.590289000	-1.359495000	5.705531000
C	0.681226000	5.925984000	2.358045000
H	1.294289000	6.795932000	2.622969000
H	0.694132000	5.809925000	1.269381000
H	-0.357220000	6.119869000	2.642314000
C	-0.359491000	2.555858000	5.044381000
H	-1.231178000	2.474937000	5.704238000
H	-0.006623000	1.544886000	4.814816000
H	0.430431000	3.077930000	5.597744000
C	-1.002556000	-5.544738000	-3.775671000
H	-0.985944000	-6.639774000	-3.729647000
H	-1.657070000	-5.258061000	-4.606335000
H	0.011344000	-5.195842000	-4.004380000
C	-2.110854000	-2.106921000	-4.420712000
H	-2.956793000	-1.649170000	-4.948239000
H	-1.415624000	-1.313314000	-4.132753000
H	-1.601381000	-2.781218000	-5.117788000
C	6.013217000	0.712321000	-2.664984000
H	6.798408000	1.450219000	-2.867682000
H	5.983311000	0.500930000	-1.592343000
H	6.282369000	-0.210771000	-3.190664000
C	2.426270000	-0.661896000	-4.834334000
H	2.384401000	-1.582754000	-5.428438000
H	1.416984000	-0.437290000	-4.476400000
H	2.750758000	0.149981000	-5.496139000
C	-3.631108000	4.846673000	-2.523719000
H	-4.664568000	5.190129000	-2.650907000
H	-3.340991000	4.956807000	-1.474771000
H	-2.990529000	5.495940000	-3.131142000
C	-0.988167000	2.287327000	-4.887958000
H	-0.206228000	2.660988000	-5.559939000
H	-0.713771000	1.277161000	-4.568869000
H	-1.921747000	2.229339000	-5.460047000
N	-2.422525000	-4.808142000	1.422194000
O	-2.784747000	-4.196523000	0.372608000
O	-3.261587000	-5.156989000	2.280303000
O	-1.184699000	-5.051903000	1.600276000
N	-2.906245000	4.353665000	1.412182000
O	-2.843063000	5.249343000	2.280837000
O	-3.745445000	3.403380000	1.528083000
O	-2.131456000	4.370241000	0.407198000
N	5.307572000	0.528458000	1.268692000
O	6.084439000	0.098820000	2.148333000
O	4.900450000	-0.231723000	0.337880000
O	4.906749000	1.736119000	1.299220000

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