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ESI

Enhanced Free Energy of Extraction of Eu^{3+} and Am^{3+} Ion Towards Diglycolamide Appended Calix[4]arene: Insights from DFT-D3 and COSMO-RS solvation model

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Computational methods for free energy calculation

The following complexation reaction between the ligands and the Eu^{3+}/Am3+ cations was used in the computation:

$$M^{3+}(H_2O)_9 + 3NO_3^- + nL \quad <===> M(NO_3)_3{\cdot}L_n + 9H_2O \quad \text{(n=3 or 4 for DGA and 1 for CAL4DGA} \qquad \text{(S1)}$$

Here, the stoichiometry of the complex was taken as 1:3 and 1:4 for DGA and 1:1 for CAL4DGA as obtained from the slope analysis in solvent extraction experiments. The aqueous environment was taken care by performing single point energy calculations employing the COSMO and COSMO-RS solvation model using the optimized gas phase geometry obtained from the BP level of theory. The binding energy is calculated using the following equation

$$\Delta E = [M(NO_3)_3{\cdot}L_n + 9H_2O] - [E_{M3+(H2O)9} + 3E_{NO3-} + nE_L] \qquad \text{(S2)}$$

Where E represents the total electronic energy of the respective chemical species. where E is the total electronic energy of the respective chemical species in the aqueous and organic (*n*-dodecane and methanol) phases. Next, we use the following standard thermodynamic relation for evaluating the free energy of complexation, ΔG:

$$\Delta G = \Delta H - T\Delta S \qquad \text{(S3)}$$

$$\Delta H = \Delta U + \Delta nRT \qquad \text{(S4)}$$

Here, ΔH is the enthalpy of complexation; T is the temperature ΔS is the difference in the entropy between the product and reactant species. The value of ΔH is obtained using ΔU = ΔE, when zero point energy corrected total electronic energy of the chemical species are used.

The strength of M – L interaction can also be evaluated by the amount of change transfer (ΔN)[1] which can be calculated by equation Eq. (4) as,

$$\Delta N = \frac{(\chi_M - \chi_L)}{\{2(\eta_M + \eta_L)\}} \qquad \text{(S5)}$$

The χ and η, represent absolute electronegativity and absolute hardness of M or L, respectively, estimated as.

$$\chi = \frac{I + A}{2} \quad \text{and} \quad \eta = \frac{I - A}{2} \qquad \text{(S6)}$$

I and A correspond to ionization potential and electron affinity respectively and can be obtained using Koopmans' theorem [2] as,

$$I = -E_{HOMO} \qquad A = -E_{LUMO} \qquad \text{(S7)}$$

E_{HOMO} and E_{LUMO} are the energy of highest occupied and lowest unoccupied molecular orbital of the M or L respectively and can be determined from the DFT calculation.

Table.S1: Calculated structural parameters in Å for the complexes of Eu^{3+} and Am^{3+} with CAL4DGA at the BP86 level of theory using SVP basis set.

System	Bond length (M-O)			
	Carbonyl O		Ether O	
	Eu	Am	Eu	Am
Without nitrate	2.57, 2.62, 2.66, 2.54, 2.76, 2.60, 2.56, 3.07	2.49, 2.51, 2.37, 2.47, 2.42, 2.35, 4.90, 5.29	2.94, 2.99, 3.00, 3.14	2.67, 2.79, 4.04, 4.04
With nitrate	2.48, 2.52, 2.55, 2.50, 2.46, 2.48, 3.58, 4.22	2.46, 2.32, 2.47, 2.48, 2.42, 2.45, 5.33, 5.40	2.67, 2.62, 3.11, 3.62	2.61, 2.70, 4.19, 4.19

Table S2: Calculated structural parameters in Å for Eu^{3+} and Am^{3+} with DGA (1:4) at the BP86 level of theory using SVP basis set.

System	Bond length (M-O)			
	Carbonyl O		Ether O	
	Eu	Am	Eu	Am
Without nitrate	2.613	2.592	2.877	2.900
With nitrate	2.678	2.672	2.807	2.761

Table S3: Calculated structural parameters in Å for the complexes of Eu^{3+} and Am^{3+} with DGA (1:4) at the BP86 level of theory using SVP basis set.

System	Bond length (M-O)			
	Carbonyl O		Ether O	
	Eu	Am	Eu	Am
Without nitrate	2.58, 2.55, 2.65, 2.64, 2.56, 2.64, 2.64, 2.58	2.61, 2.58, 2.61, 2.58, 2.60, 2.57, 2.59, 2.61	2.71, 2.72, 3.03, 3.04	2.75, 2.76, 3.05, 3.05
With nitrate	2.88, 2.66, 2.85, 2.60, 2.63, 2.64, 2.57, 2.60	2.61, 2.54, 2.56, 2.53, 2.63, 2.56, 2.90, 3.06	2.61, 2.87, 2.76, 2.99	2.57, 2.71, 2.83, 2.93

Table S4: Calculated value of free energy of extraction (kcal/mol) for Eu^{3+} and Am^{3+} with DGA (1:4) at the B3LYP level of theory using TZVP basis set (explicit monomer water).

System	ΔG Gas phase		ΔS (cal/mol/K) Gas phase		ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase
	Eu	Am	Eu	Am	Eu	Am	
Without nitrate	-182.97	-179.25	99.75	80.81	-20.35	-18.42	-1.93
With nitrate	-511.59	-506.85	-27.16	-43.96	-5.05	-0.43	-4.62

Table S5: Calculated value of free energy of extraction (kcal/mol) for Eu^{3+} and Am^{3+} with CAL4DGA at the PBE0 level of theory using TZVP basis set (explicit monomer water model).

System	ΔG Gas phase		ΔS (cal/mol/K) Gas phase		ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase	$\Delta\Delta\Delta G_{CAL4DGA-4DGA}=\Delta\Delta G_{CAL4DGA}-\Delta\Delta G_{4DGA}$ Solution phase
	Eu	Am	Eu	Am	Eu	Am		
Without nitrate	-199.09	-198.58	215.06	225.39	-34.18	-43.85	9.66	10.54
With nitrate	-547.13	-537.07	152.74	131.78	-53.54	-41.13	-12.40	-10.07

Table S6: Calculated value of free energy of extraction (kcal/mol) for Eu^{3+} and Am^{3+} with DGA (1:3) at the PBE0/TZVP level of theory using COSMO (explicit monomer water model).

System	ΔG Gas phase		ΔS (cal/mol/K) Gas phase		ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase
	Eu	Am	Eu	Am	Eu	Am	
Without nitrate	-193.29	-188.39	162	152	-57.06	-53.89	-3.17
With nitrate	-533.56	-531.10	14.03	18.22	-29.32	-29.07	-0.25

Table S7: Calculated value of free energy of extraction (kcal/mol) for Eu^{3+} and Am^{3+} with DGA (1:4) at the PBE0 level of theory using TZVP basis set (explicit monomer water model).

System	ΔG Gas phase		ΔS (cal/mol/K) Gas phase		ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase
	Eu	Am	Eu	Am	Eu	Am	
Without nitrate	-192.35	-189.72	99.75	80.81	-24.91	-24.03	-0.88
With nitrate	-517.08	-515.92	-27.16	-43.96	-12.73	-10.4	-2.33

Table S8 : Calculated value of reaction energy for Eu^{3+} ion in gas and solution phase at the B3LYP and PBE0 level of theory using TZVP basis set.

Reaction	ΔE (kcal/mol)			
	Gas phase		Solution phase	
	B3LYP	PBE0	B3LYP	PBE0
$Eu^{3+} + 4DGA = Eu^{3+}\text{-}(DGA)_4$	-696.09	-706.93	-56.26	-66.74
$Eu^{3+} + CAL4DGA = Eu^{3+}\text{-}CAL4DGA$	-681.34	-683.02	-37.38	-39.20
$Eu^{3+}\text{-}(H_2O)_9 + 4DGA = Eu^{3+}\text{-}(DGA)_4 + 9H_2O$	-147.65	-149.06	14.96	12.18
$Eu^{3+}\text{-}(H_2O)_9 + CAL4DGA = Eu^{3+}\text{-}CAL4DGA + 9H_2O$	-132.90	-125.18	33.84	39.71
$Eu^{3+} + 3NO_3^- + 4DGA = Eu^{3+}\text{-}(NO_3)_3(DGA)_4$	-1059.65	-1075.05	-76.40	-91.78
$Eu^{3+} + 3NO_3^- + CAL4DGA = Eu^{3+}\text{-}(NO_3)_3CAL4DGA$	-1043.37	-1053.33	-70.97	-80.82
$Eu^{3+}\text{-}(H_2O)_9 + 3NO_3^- + 4DGA = Eu^{3+}\text{-}(NO_3)_3(DGA)_4 + 9H_2O$	-511.71	-517.20	-5.17	-12.85
$Eu^{3+}\text{-}(H_2O)_9 + 3NO_3^- + CAL4DGA = Eu^{3+}\text{-}(NO_3)_3CAL4DGA + 9H_2O$	-495.12	-495.48	0.24	-1.89

Table S9: Calculated value of gas phase reaction energy for Am^{3+} ion in gas and solution phase at the B3LYP and PBE0 level of theory using TZVP basis set.

Reaction	ΔE (kcal/mol)			
	Gas phase		Solution phase	
	B3LYP	PBE0	B3LYP	PBE0
$Am^{3+} + 4DGA = Am^{3+}\text{-}(DGA)_4$	-685.83	-699.62	-73.84	-89.43
$Am^{3+} + CAL4DGA = Am^{3+}\text{-}CAL4DGA$	-663.21	-668.37	-56.39	-63.00
$Am^{3+}\text{-}(H_2O)_9 + 4DGA = Am^{3+}\text{-}(DGA)_4 + 9H_2O$	-150.30	-152.87	10.53	6.70
$Am^{3+}\text{-}(H_2O)_9 + CAL4DGA = Am^{3+}\text{-}CAL4DGA + 9H_2O$	-127.68	-121.59	27.98	33.13
$Am^{3+} + 3NO_3^- + 4DGA = Am^{3+}\text{-}(NO_3)_3(DGA)_4$	-1048.71	-1069.04	-91.14	-112.86
$Am^{3+} + 3NO_3^- + CAL4DGA = Am^{3+}\text{-}(NO_3)_3CAL4DGA$	-1026.19	-1039.42	-78.75	-92.83
$Am^{3+}\text{-}(H_2O)_9 + 3NO_3^- + 4DGA = Am^{3+}\text{-}(NO_3)_3(DGA)_4 + 9H_2O$	-513.17	-522.25	-6.75	-16.72
$Am^{3+}\text{-}(H_2O)_9 + 3NO_3^- + CAL4DGA = Am^{3+}\text{-}(NO_3)_3CAL4DGA + 9H_2O$	-490.66	-492.63	5.62	3.30

Table S10: Calculated value of gas phase reaction energy for Eu^{3+} ion using Grimme's dispersion correction (DFT-D3) at the B3LYP and PBE0 level of theory using TZVP basis set.

Reaction	ΔE (kcal/mol)			
	Gas phase		Solution phase	
	B3LYP	PBE0	B3LYP	PBE0
Eu^{3+} + 4DGA = Eu^{3+}-$(DGA)_4$	-753.71	-748.73	-98.86	-93.54
Eu^{3+} + CAL4DGA=Eu^{3+}-CAL4DGA	-711.14	-707.66	-61.97	-56.33
Eu^{3+}-$(H_2O)_9$ + 4DGA = Eu^{3+}-$(DGA)_4$ +9H_2O	-179.67	-173.05	-6.07	0.37
Eu^{3+}-$(H_2O)_9$ + CAL4DGA=Eu^{3+}-CAL4DGA +9H_2O	-137.19	-131.98	30.81	37.58
Eu^{3+} + 3NO_3^- + 4DGA = Eu^{3+}-$(NO_3)_3(DGA)_4$	-1143.37	-1137.49	-144.60	-140.02
Eu^{3+} + 3NO_3^- + CAL4DGA=Eu^{3+}-$(NO_3)_3$CAL4DGA	-1097.28	-1097.84	-119.60	-118.69
Eu^{3+}-$(H_2O)_9$ + 3NO_3^- + 4DGA = Eu^{3+}-$(NO_3)_3(DGA)_4$ +9H_2O	-569.42	-561.80	-51.81	-46.10
Eu^{3+}-$(H_2O)_9$ + 3NO_3^- + CAL4DGA=Eu^{3+}-$(NO_3)_3$CAL4DGA+9H_2O	-523.33	-522.15	-48.37	-39.76

Table S11 : Calculated value of gas phase interaction energy and partial charge population at the B3LYP level of theory using TZVP basis set.

Reaction	ΔE kcal/mol	ΔS (cal/mol/K)	ΔG kcal/mol	Partial charge population		
				metal ion	Carbonyl O	Ether O
Eu^{3+} + 4DGA = Eu^{3+}-(DGA)4	-696.07	-183.00	-638.86	1.851	-0.644	-0.473
Am^{3+} + 4DGA=Am^{3+}-(DGA)4	-685.03	-200.00	-615.86	1.851	-0.649	-0.473
Eu^{3+} + CAL4DGA=Eu^{3+}-CAL4DGA	-681.34	-68.00	-662.69	1.695	-0.635	-0.462
Am^{3+} + CAL4DGA=Am^{3+}-CAL4DGA	-663.21	-55.70	-641.36	2.058	-0.677	-0.484

Table S12: Calculated value of orbital population at the B3LYP level of theory using TZVP basis set.

Reaction	s	p	d	f	g
Eu^{3+} + 4DGA = Eu^{3+}-(DGA)4	4.16	11.99	10.87	6.11	0.00055
Am^{3+} + 4DGA=Am^{3+}-(DGA)4	4.17	11.99	10.85	6.12	0.00078
Eu^{3+} + CAL4DGA=Eu^{3+}-CAL4DGA	4.13	11.99	10.63	6.54	0.00035
Am^{3+} + CAL4DGA=Am^{3+}-CAL4DGA	4.14	11.98	10.67	6.13	0.00100

Table S13: Calculated free energy of extraction (kcal/mol) for Eu^{3+} and Am^{3+} with DGA (1:3 and 1:4) at the PBE0/TZVP level of theory using COSMO-RS.

System	ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase	$\Delta\Delta\Delta G_{CAL4DGA-nDGA}= \Delta\Delta G_{CAL4DGA}-\Delta\Delta G_{nDGA}$	
	Eu	Am			
DGA (1:3)	-5.61	-5.21	-0.39	1:3	1:4
DGA (1:4)	17.49	20.20	-2.71	-12.81	-10.50
CAL4DGA	-42.48	-29.26	-13.21		

Table S14: Calculated free energy of extraction (kcal/mol) for Eu^{3+} with DGA (1:3 and 1:4) at the B3LYP and PBE0 level of theory employing TZVP basis set with dispersion correction using COSMO.

System	ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase	
	B3LYP	PBE0	B3LYP	PBE0
DGA (1:3)	-19.88	-16.13	-29.52	-29.83
DGA (1:4)	-11.06	-5.13	-38.35	-40.84
CAL4DGA	-49.41	-45.97		

Table S15: Calculated free energy of extraction (kcal/mol) for Eu^{3+} with DGA (1:3 and 1:4) at the B3LYP and PBE0 level of theory employing TZVP basis set with dispersion correction using COSMO-RS.

System	ΔG Solution phase		$\Delta\Delta G=\Delta G_{Eu}-\Delta G_{Am}$ Solution phase	
	B3LYP	PBE0	B3LYP	PBE0
DGA (1:3)	-52.09	-41.25	-50.16	-47.92
DGA (1:4)	-51.70	-45.98	-48.32	-45.43
CAL4DGA	-100.02	-91.41		

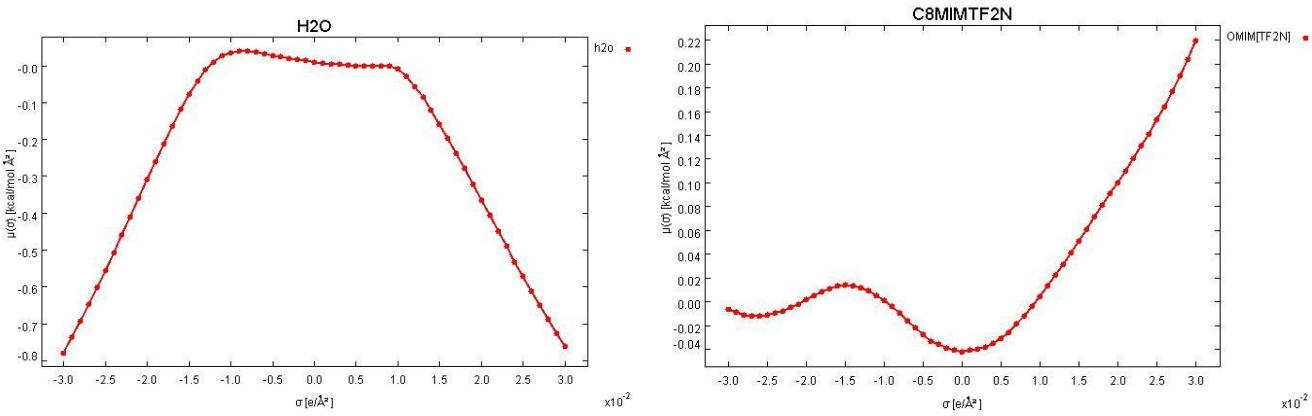

Figure S1: Sigma potential of H_2O and C_8mimntf2 ionic liquid used for the calculation of single point energy using COSMO-RS solvation model.

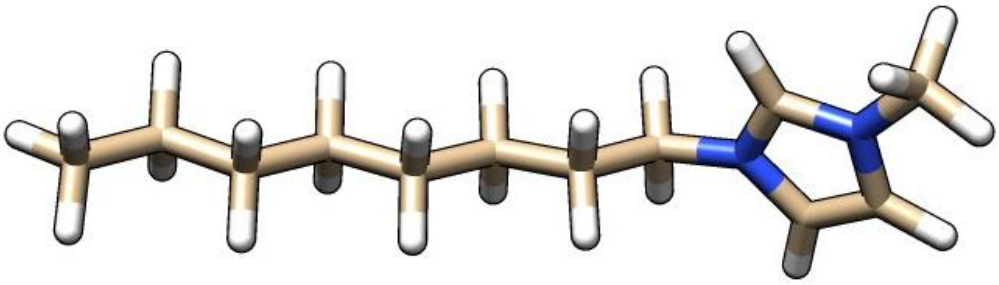

Figure S2: Optimized structure of c8mim cation at the BP/SVP level of theory.

1 A. Szabo and N. S. Ostlund, Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, Dover Publications, 1996.

2 T. Koopmans, Über die Zuordnung von Wellenfunktionen und Eigenwerten zu den einzelnen Elektronen eines Atoms, Physica, 1933, 1, 104.

XYZ coordinates of the optimized chemical species

TMDGA

H	-5.8730060	-3.4417116	0.4741802
C	-5.5264742	-2.3909504	0.3524592
N	-5.1895310	-1.7964973	1.6366005
C	-4.1498604	-2.4659893	2.3959194
H	-4.4783070	-3.4674860	2.7599071
C	-5.9373258	-0.7135170	2.0785967
O	-6.8356878	-0.2130324	1.4142872
C	-5.5709925	-0.1671526	3.4746140
O	-6.3898212	0.9315894	3.7593572
C	-6.1321162	1.4632396	5.0281918
C	-7.0618489	2.6730106	5.2601995
N	-6.9360105	3.3060428	6.4895806
C	-6.0551005	2.8860165	7.5638079
H	-6.6141351	2.4054690	8.4006063
O	-7.8537679	3.0420139	4.4025721
C	-7.8254702	4.4179922	6.7883512
H	-8.4943376	4.1790849	7.6452567
H	-5.0618282	1.7874305	5.1261863
H	-6.2986450	0.6995367	5.8332230
H	-4.4857396	0.1169358	3.4996116
H	-5.6946536	-0.9807039	4.2378968
H	-4.6454346	-2.3941921	-0.3262634
H	-6.3370472	-1.7897840	-0.0974112
H	-3.8343628	-1.8704257	3.2704088
H	-3.2498174	-2.6230204	1.7614602
H	-8.4395932	4.6116531	5.8904265
H	-7.2457149	5.3314054	7.0463613
H	-5.5184015	3.7642491	7.9850486
H	-5.2896643	2.1731182	7.2101861

CAL4DGA

C	1.9273086	2.6132419	-0.5678653
C	1.9661784	2.1828558	0.7702793
C	0.7571729	2.1655174	1.5171175
C	-0.4788287	2.4659457	0.8865836
C	-0.4569728	2.8995375	-0.4533553
C	0.7319096	3.0089535	-1.1951513
C	3.2863718	1.6764110	1.3550296
C	3.7352587	0.3772182	0.6858481
C	4.6383657	0.4295164	-0.3972354
C	4.9436636	-0.6974163	-1.1814163
C	4.2620021	-1.8979866	-0.8953901
C	3.3571075	-2.0112175	0.1753178
C	3.1714629	-0.8831800	1.0164418
C	2.5290694	-3.2710822	0.3843017
C	1.1898989	-3.1737815	-0.3528887
C	1.1680119	-3.0251017	-1.7519907
C	-0.0259825	-2.8274308	-2.4699588
C	-1.2184728	-2.7164232	-1.7330073
C	-1.2536957	-2.8635770	-0.3339271
C	-0.0439833	-3.1519324	0.3490851

C	-2.5662555	-2.6272010	0.4111139
C	-3.0291395	-1.1809953	0.2801273
C	-4.0236091	-0.7873221	-0.6357894
C	-4.3781821	0.5656629	-0.8159234
C	-3.6748180	1.5433436	-0.0815455
C	-2.6701555	1.1987910	0.8427751
C	-2.3904672	-0.1740882	1.0389481
O	-1.4468695	-0.5368163	1.9711039
C	-1.8324847	2.2484134	1.5658555
O	-0.0536081	-3.3758882	1.7144991
O	2.4074066	-1.0577571	2.1503501
O	0.8151281	1.7717173	2.8452283
H	2.1230161	-3.0451736	-2.3012695
H	-2.1589657	-2.4906708	-2.2625663
H	-3.9220594	2.6082746	-0.2307665
H	5.1152970	1.3947564	-0.6378060
H	4.4555017	-2.7868037	-1.5191833
H	2.8658611	2.6218623	-1.1459102
H	-1.4163833	3.1295307	-0.9447149
H	-2.4219688	-2.8878903	1.4759289
H	-3.3535889	-3.2950132	0.0030563
H	2.3308017	-3.4162139	1.4611979
H	3.0982816	-4.1493216	0.0147188
H	4.0724927	2.4410895	1.1847698
H	3.1713042	1.5664752	2.4468448
H	-2.3954844	3.2052865	1.5853653
H	-1.6695404	1.9411995	2.6145972
H	-4.5431456	-1.5625304	-1.2240996
C	0.6559515	2.7668432	3.8677691
C	1.2775016	2.1601689	5.1367280
H	-0.4209752	2.9866873	4.0458724
H	1.1582666	3.7159290	3.5722903
H	2.3813329	2.1553693	5.0542661
H	0.9506719	1.1028234	5.2025557
N	0.9347875	2.8299331	6.3825251
H	1.7204441	3.1967502	6.9444589
C	-0.2298936	2.5405936	7.0275760
O	-1.1340703	1.8439921	6.5548638
C	-0.3714192	3.2366303	8.3895615
H	-0.8525506	4.2348645	8.2144999
H	0.6401362	3.4409170	8.8192805
O	-1.1540003	2.4417461	9.2504085
C	-1.3517446	3.0634823	10.4855458
H	-1.8397355	4.0662282	10.3644868
H	-0.3757679	3.2599928	11.0059810
C	-2.2346756	2.1716742	11.3807857
O	-2.6205719	1.0665791	11.0076754
N	-2.5689192	2.7015617	12.6157189
C	-3.4779636	1.9603738	13.4769441
H	-4.3469567	2.5927774	13.7620079
H	-3.8364952	1.0743946	12.9236922
H	-2.9715008	1.6281684	14.4104056
C	-2.1205010	3.9845734	13.1293757
H	-1.3190357	4.4171671	12.5064018
H	-2.9537710	4.7224152	13.1844416
H	-1.7142100	3.8647089	14.1578500

C	3.0209125	-0.7102051	3.3886095
C	2.9954680	-1.8802614	4.3889016
H	2.4768489	0.1463240	3.8332730
H	4.0784589	-0.4053179	3.2197565
H	1.9531391	-2.1607893	4.6313992
H	3.5100860	-2.7708389	3.9766559
N	3.6560738	-1.4676052	5.6239636
H	4.6774311	-1.4701212	5.6426852
C	2.9921748	-0.8052246	6.6214735
O	1.7745154	-0.6446365	6.6501162
C	3.8841762	-0.2382603	7.7383978
H	4.9672386	-0.4693142	7.5748997
H	3.5820352	-0.7176544	8.7018503
O	3.6635387	1.1626849	7.7754905
C	4.3950638	1.7928240	8.7870031
H	5.4979700	1.6710424	8.6288529
H	4.1729949	1.3465203	9.7916444
C	4.0363545	3.2902410	8.8136260
O	3.1456878	3.7544901	8.0924479
N	4.7496441	4.0793955	9.6847519
C	4.4431927	5.5025672	9.7636647
H	5.3493350	6.1082564	9.5482364
H	3.6610056	5.7328732	9.0194532
H	4.0790631	5.7720931	10.7789560
C	5.7785513	3.6054014	10.5973151
H	5.9915654	2.5327749	10.4549602
H	6.7263675	4.1650076	10.4406449
H	5.4703932	3.7561883	11.6558457
C	-0.1733806	-4.7492632	2.1075641
C	0.2701395	-4.8556385	3.5710788
H	0.4581257	-5.4000692	1.4609658
H	-1.2306203	-5.0934117	1.9933988
H	1.3602727	-4.6692313	3.6373436
H	-0.2591824	-4.1036618	4.1950490
N	0.0341964	-6.1770518	4.1281407
H	-0.8947723	-6.3688662	4.5086442
C	1.0576492	-7.0468774	4.4192704
C	0.5993329	-8.2720242	5.2307487
H	0.6927646	-8.0122226	6.3183503
O	1.3948520	-9.3812384	4.8986723
C	-1.9890971	-0.7259318	3.2833102
C	-0.8210285	-0.9891858	4.2261547
H	-2.7158106	-1.5719544	3.2965263
H	-2.5449366	0.1856928	3.6078951
H	-0.3939089	-1.9858206	4.0127472
H	-0.0457575	-0.2295976	4.0020251
N	-1.2135355	-0.9225866	5.6164901
H	-1.2716675	0.0178560	6.0386429
C	-1.2470244	-2.0211803	6.4253810
O	-1.1171075	-3.1828853	6.0303968
C	-1.3966116	-1.6640079	7.9087760
H	-0.3581614	-1.5692896	8.3217409
H	-1.8675429	-0.6579218	8.0299004
O	-2.1277500	-2.6696897	8.5713312
C	-2.3319965	-2.3501673	9.9183648
H	-1.3572058	-2.2010715	10.4580115

H	-2.8800261	-1.3813898	10.0297245
C	-3.1007411	-3.4970173	10.5955540
O	-3.3736035	-4.5345546	10.0013335
N	-3.4472545	-3.2913342	11.9270860
C	-4.1153600	-4.3650460	12.6408450
H	-3.5164258	-4.6992518	13.5183288
H	-5.1140922	-4.0411513	13.0108192
H	-4.2414442	-5.2095628	11.9387390
C	-3.1525724	-2.0968789	12.6944116
H	-4.0733470	-1.7318836	13.2038991
H	-2.3944029	-2.2940557	13.4889429
H	-2.7847835	-1.2742445	12.0557514
C	-5.4957744	0.9589122	-1.7569574
H	-5.2929149	1.9299515	-2.2528796
H	-5.6512014	0.1985518	-2.5479155
H	-6.4611193	1.0679578	-1.2153791
C	0.7284068	3.5156678	-2.6198179
H	1.0548548	4.5774091	-2.6740867
H	1.4198605	2.9323292	-3.2614051
H	-0.2823750	3.4601266	-3.0702803
C	-0.0249998	-2.7341671	-3.9793029
H	0.9147166	-2.2867691	-4.3612132
H	-0.1187076	-3.7391188	-4.4468889
H	-0.8710727	-2.1223707	-4.3516277
C	5.9317990	-0.6212533	-2.3239831
H	6.4986779	0.3304669	-2.3117841
H	6.6661393	-1.4528627	-2.2851636
H	5.4222044	-0.6911003	-3.3093067
O	2.2288484	-6.8536870	4.1131594
H	-0.4874085	-8.4788168	5.0489880
C	1.0565134	-10.5137557	5.6462733
H	1.1612067	-10.3232055	6.7474987
H	-0.0152710	-10.8041761	5.4848597
C	1.9785801	-11.6794972	5.2338794
O	2.8664806	-11.5282774	4.4040539
N	1.7403798	-12.8960770	5.8608723
C	0.7038813	-13.1517677	6.8433833
H	-0.0308688	-13.9030598	6.4721668
H	1.1410349	-13.5538357	7.7852867
H	0.1477017	-12.2338484	7.0997567
C	2.5704409	-14.0338343	5.4997956
H	3.0991644	-14.4405212	6.3904275
H	1.9590245	-14.8523401	5.0580657
H	3.3120570	-13.6898937	4.7561480

Eu^{3+}-$(DGA)_4$

H	-3.6136575	8.0884448	13.2482820
C	-3.4386075	7.4635545	12.3482443
N	-4.0879191	6.1609203	12.4907941
C	-5.5542732	6.1915852	12.5350917
H	-5.8756502	7.0883610	13.0995519
C	-3.3515295	5.0223588	12.5213498
O	-2.1010019	5.0173060	12.5031633
C	-4.1070322	3.6845550	12.6091333
O	-3.2737834	2.5897091	12.2670897

C	-3.4070811	2.1335982	10.9321011
C	-2.3210949	2.7235272	10.0164120
N	-2.4875852	2.6269800	8.6733155
C	-3.6492893	2.0338289	8.0043385
H	-3.3826981	1.0587889	7.5442774
O	-1.3026581	3.2317144	10.5384439
C	-1.4414369	3.0938867	7.7637237
H	-1.1925167	2.2946759	7.0364409
Eu	-0.3713071	3.0836949	13.0094653
H	-4.4287211	2.3477219	10.5546978
H	-3.2799052	1.0312658	10.9388576
H	-5.0169798	3.6913712	11.9730863
H	-4.4351401	3.5426324	13.6603452
H	-3.8512513	7.9987774	11.4685169
H	-2.3555592	7.3129675	12.2112922
H	-5.9716235	5.3131505	13.0568801
H	-5.9956763	6.2551775	11.5172310
H	-0.5417498	3.3544019	8.3448217
H	-1.7881279	3.9816568	7.1942276
H	-3.9963075	2.7086596	7.1958715
H	-4.4925932	1.8716802	8.6950911
H	3.0266520	-1.8002432	14.2087003
C	2.8037261	-1.2245870	13.2860222
N	3.4306054	0.0962367	13.3431808
C	4.8941679	0.0737832	13.2723391
H	5.2942656	-0.6365920	14.0240811
C	2.6666384	1.2150992	13.4200301
O	1.4159778	1.1787497	13.4587391
C	3.3725250	2.5834190	13.4096501
O	2.5033057	3.6258106	13.8167599
C	2.6108641	3.9893224	15.1837343
C	1.5420125	3.2903068	16.0400608
N	1.7418207	3.2240839	17.3799227
C	2.9010538	3.8036055	18.0684726
H	3.6917346	3.0444149	18.2496629
O	0.5221254	2.8302090	15.4800208
C	0.7899627	2.5196152	18.2376001
H	1.3246247	1.7700273	18.8558922
H	3.2022721	-1.7931075	12.4210663
H	1.7133818	-1.1067963	13.1772725
H	5.3382977	1.0630131	13.4684348
H	5.2305066	-0.2655117	12.2700602
H	0.0448642	2.0102875	17.6051518
H	0.2743715	3.2278382	18.9191128
H	2.5745243	4.1938665	19.0517695
H	3.3329205	4.6524910	17.5105201
H	-1.2868123	-1.9554029	9.8211361
C	-0.4582462	-1.4968404	10.4004941
N	-0.7794412	-1.4831582	11.8286964
C	-1.0050721	-2.7947629	12.4419698
H	-1.9711884	-3.2314337	12.1101583
C	-0.9676818	-0.3042252	12.4676996
O	-0.8596545	0.8057145	11.8994269
C	-1.3502905	-0.3378366	13.9494289
O	-1.5184161	1.0060453	14.3479330
C	-2.1757936	1.1551089	15.5873213

C	-2.4631073	2.6499565	15.7540559
N	-3.1113705	3.0600855	16.8690895
C	-3.6046317	2.1686571	17.9205538
H	-4.7098567	2.2369494	17.9970982
O	-2.1056475	3.4354648	14.8481042
C	-3.4001384	4.4816819	17.0660118
H	-4.4963117	4.6532302	17.0928895
H	-1.5511148	0.7720916	16.4282291
H	-3.1313435	0.5793784	15.5922675
H	-0.5625628	-0.8428902	14.5558089
H	-2.2984450	-0.9095104	14.0846469
H	0.4561691	-2.0986356	10.2249037
H	-0.2948591	-0.4604309	10.0606128
H	-1.0001316	-2.7404269	13.5441668
H	-0.1965252	-3.4875986	12.1356154
H	-2.9519638	5.0570052	16.2385288
H	-2.9766409	4.8234950	18.0323891
H	-3.1780442	2.4634034	18.9014343
H	-3.3370060	1.1156296	17.7314710
O	0.7385450	5.1719482	11.6773720
N	0.1528202	7.6109070	14.2850972
C	0.6404032	6.5074250	12.1222080
H	-0.1274007	7.0723481	11.5434654
H	1.6138864	7.0364899	11.9899371
O	0.1248150	5.3251617	14.1442875
N	2.2224067	3.1841491	9.0476008
C	0.2752822	6.4460986	13.6073455
O	1.3854346	2.7709510	11.1414953
C	0.4184513	8.9307870	13.7074661
H	-0.3614993	9.6429610	14.0424695
H	0.4011018	8.9093993	12.6042043
H	1.4029605	9.3224949	14.0408114
C	-0.1548180	7.5955697	15.7162404
H	0.6864498	8.0276177	16.2974886
H	-0.3316949	6.5541839	16.0335434
H	-1.0584268	8.2065809	15.9159367
C	1.2610530	5.0396966	10.3726980
H	2.1685821	5.6756759	10.2482721
H	0.5167176	5.3567401	9.6056534
C	1.6285587	3.5634203	10.2044402
C	2.6115875	4.1183891	7.9871413
H	2.0034751	5.0391969	8.0085118
H	2.4534741	3.6363695	7.0027297
H	3.6853813	4.3937526	8.0627914
C	2.6533088	1.7968715	8.8662509
H	2.3064949	1.1988439	9.7258365
H	3.7598974	1.7420764	8.7950319
H	2.2280071	1.3865084	7.9282565
H	3.6349846	3.7811813	15.5586550
H	2.4427282	5.0842593	15.2522649
H	4.2871654	2.5797260	14.0384973
H	3.6851592	2.7953667	12.3662549

Am^{3+}-$(DGA)_4$

H	-3.7206841	8.0321421	13.3485892

C	-3.4421384	7.4067242	12.4757614
N	-4.0880279	6.0974530	12.5613085
C	-5.5561491	6.1120804	12.5531102
H	-5.9044564	7.0407112	13.0435458
C	-3.3497502	4.9597163	12.5638714
O	-2.0980411	4.9573113	12.5591583
C	-4.1106116	3.6241627	12.6058569
O	-3.2761027	2.5342839	12.2490871
C	-3.3959509	2.1064297	10.9023809
C	-2.2902021	2.7067425	10.0177235
N	-2.4340454	2.6306650	8.6707840
C	-3.5849755	2.0472897	7.9754392
H	-3.2514710	1.2120274	7.3255023
O	-1.2846788	3.2159568	10.5642377
C	-1.4012192	3.1619225	7.7829387
H	-1.1028620	2.3882953	7.0465346
Am	-0.3727694	3.0661898	13.0028302
H	-4.4078042	2.3471053	10.5150362
H	-3.2867314	1.0023262	10.8891896
H	-5.0114266	3.6486214	11.9575840
H	-4.4555420	3.4568043	13.6479974
H	-3.7632082	7.9348673	11.5537914
H	-2.3492794	7.2679589	12.4583911
H	-5.9813665	5.2660973	13.1216946
H	-5.9658672	6.1018608	11.5200836
H	-0.5243920	3.4589623	8.3805869
H	-1.7851842	4.0401268	7.2223718
H	-4.0693766	2.8078929	7.3282220
H	-4.3403678	1.6527695	8.6733806
H	2.8871969	-1.8080166	14.1973085
C	2.7283265	-1.2456630	13.2532232
N	3.3807392	0.0619242	13.3167915
C	4.8448948	0.0067409	13.2816111
H	5.2161443	-0.6723529	14.0763004
C	2.6403114	1.1968415	13.3913479
O	1.3884100	1.1861744	13.4214761
C	3.3799634	2.5459996	13.3922594
O	2.5263066	3.6102979	13.7777303
C	2.6379854	4.0049508	15.1351214
C	1.5298282	3.3839146	16.0001943
N	1.6877825	3.4333725	17.3463579
C	2.8797900	3.9836944	18.0040025
H	3.6585663	3.2079381	18.1665703
O	0.5239783	2.8852785	15.4462359
C	0.6961522	2.8323531	18.2367747
H	1.1413749	1.9838560	18.7973601
H	3.1611106	-1.8390934	12.4225690
H	1.6486458	-1.1079075	13.0811474
H	5.3055591	0.9959544	13.4332569
H	5.1930317	-0.3898578	12.3049960
H	-0.1542416	2.4699460	17.6368990
H	0.3373472	3.5820474	18.9710738
H	2.5873704	4.3800461	18.9947151
H	3.3156652	4.8239409	17.4349750
H	-1.4374671	-1.9941009	9.8174909
C	-0.5915517	-1.5172868	10.3551731

N	-0.8448951	-1.5118819	11.7970796
C	-1.0543655	-2.8270404	12.4095933
H	-2.0562447	-3.2344531	12.1554828
C	-0.9904132	-0.3391253	12.4578134
O	-0.8916575	0.7774674	11.8991679
C	-1.3110530	-0.3902132	13.9531012
O	-1.4724899	0.9489760	14.3703884
C	-2.0778540	1.0928052	15.6372655
C	-2.4311860	2.5751432	15.7809246
N	-3.0755888	2.9751206	16.9016934
C	-3.5290217	2.0697757	17.9603617
H	-4.6323493	1.9466882	17.9301190
O	-2.1281523	3.3599779	14.8531442
C	-3.4575870	4.3786944	17.0676103
H	-4.5628466	4.4767458	17.0984771
H	-1.3927247	0.7636081	16.4531772
H	-3.0013603	0.4707954	15.6998833
H	-0.4945196	-0.8944970	14.5204928
H	-2.2491121	-0.9689826	14.1232519
H	0.3264714	-2.0984075	10.1334579
H	-0.4669873	-0.4782456	10.0071295
H	-0.9526121	-2.7906004	13.5080121
H	-0.2929336	-3.5342141	12.0260456
H	-3.0552691	4.9645078	16.2241571
H	-3.0520590	4.7703588	18.0223948
H	-3.2611689	2.4926943	18.9490611
H	-3.0604779	1.0745151	17.8815525
O	0.7433215	5.1944120	11.6501079
N	0.1586400	7.6165581	14.2733624
C	0.6447222	6.5278758	12.1024350
H	-0.1259962	7.0938880	11.5287244
H	1.6173179	7.0583578	11.9704689
O	0.1403632	5.3314600	14.1201177
N	2.2852416	3.1829711	9.0700196
C	0.2849759	6.4564223	13.5884680
O	1.3844822	2.7852156	11.1383442
C	0.4111782	8.9423597	13.7031130
H	-0.3962931	9.6369673	14.0093338
H	0.4359895	8.9204510	12.6002366
H	1.3738415	9.3557696	14.0717281
C	-0.1520072	7.5955085	15.7038132
H	0.6783403	8.0484784	16.2845387
H	-0.3059857	6.5516386	16.0244296
H	-1.0697174	8.1861209	15.9009218
C	1.3251877	5.0582140	10.3714134
H	2.2513942	5.6747923	10.2961868
H	0.6269514	5.3980075	9.5711120
C	1.6687691	3.5755685	10.2096012
C	2.7241235	4.1011985	8.0156789
H	2.2102765	5.0753423	8.0776481
H	2.4925629	3.6609112	7.0257812
H	3.8207607	4.2712415	8.0647531
C	2.6713588	1.7823572	8.8895714
H	2.2762670	1.1881939	9.7306453
H	3.7768525	1.6881235	8.8517837
H	2.2616315	1.3977187	7.9339205

H	3.6462020	3.7552447	15.5276191
H	2.5300732	5.1092644	15.1753438
H	4.2777053	2.5228437	14.0442844
H	3.7269515	2.7480162	12.3574862

Eu^{3+}-CAL4DGA

C	2.2348825	2.6179442	-1.2578949
C	2.2431968	2.0429421	0.0178895
C	1.1261192	2.2693927	0.8809545
C	-0.0194561	2.9812268	0.4188787
C	0.0531641	3.5649952	-0.8602936
C	1.1645290	3.4189839	-1.7143708
C	3.4381445	1.2032077	0.4620677
C	3.4808133	-0.1647390	-0.2154137
C	4.3024891	-0.3483328	-1.3460511
C	4.2924189	-1.5332041	-2.1095698
C	3.3873501	-2.5502433	-1.7317011
C	2.5498411	-2.4228978	-0.6105888
C	2.6434898	-1.2440841	0.1742696
C	1.5190365	-3.4904968	-0.2656094
C	0.1310368	-3.1400276	-0.8075275
C	-0.0468729	-3.1132259	-2.2024069
C	-1.2387305	-2.6719730	-2.8110673
C	-2.2578064	-2.1915508	-1.9652914
C	-2.1443398	-2.2089389	-0.5655895
C	-0.9602890	-2.7437394	0.0135726
C	-3.2716012	-1.6312704	0.2909219
C	-3.3561648	-0.1123242	0.1452131
C	-4.1642098	0.4289384	-0.8723298
C	-4.1424880	1.7963271	-1.2180477
C	-3.2181927	2.6268684	-0.5450685
C	-2.4028167	2.1507227	0.4926044
C	-2.5421796	0.7917871	0.8877343
O	-1.8409429	0.3960088	2.0100885
C	-1.3654076	3.0541079	1.1504042
O	-0.9150966	-2.8242588	1.4016432
O	1.8332864	-1.1638480	1.2976223
O	1.2428848	1.7304093	2.1425749
H	0.7887629	-3.4319344	-2.8456598
H	-3.1820127	-1.7998363	-2.4180529
H	-3.1601629	3.6913952	-0.8227730
H	4.9775212	0.4698170	-1.6451825
H	3.3470703	-3.4781140	-2.3250139
H	3.1033018	2.4589095	-1.9162782
H	-0.8103144	4.1448968	-1.2206749
H	-3.1190777	-1.9498107	1.3352105
H	-4.2354730	-2.0647883	-0.0440214
H	1.4803839	-3.6129742	0.8288616
H	1.8467078	-4.4577700	-0.6978589
H	4.3670866	1.7462703	0.1959073
H	3.4213418	1.1188564	1.5626328
H	-1.7318078	4.0999151	1.1158300
H	-1.2699041	2.7758966	2.2119024
H	-4.8357920	-0.2458285	-1.4273507
C	0.8723067	2.4490162	3.3111530

C	1.9222868	2.1339041	4.3967684
H	-0.1218510	2.1088706	3.6736602
H	0.8131398	3.5403821	3.1040341
H	2.8606874	2.6977118	4.2119175
H	2.1570931	1.0548995	4.3553032
N	1.4304596	2.4001766	5.7431040
H	1.2070286	3.3672180	5.9933835
C	1.2384272	1.4386892	6.6857361
O	1.4835493	0.2364927	6.5105945
C	0.7317406	1.9498313	8.0372759
H	0.0556044	2.8283618	7.9049219
H	1.6158878	2.2978393	8.6278795
O	0.0818909	0.8806322	8.6797037
C	-0.1948580	1.1230600	10.0382262
H	-1.0435469	1.8393312	10.1541246
H	0.6899739	1.5681919	10.5516754
C	-0.5325382	-0.2259178	10.6834661
O	-0.4856510	-1.2655708	9.9945961
N	-0.8607228	-0.2346014	12.0017789
C	-1.1699600	-1.5006528	12.6640672
H	-2.2427257	-1.5417783	12.9487033
H	-0.9348345	-2.3305075	11.9764440
H	-0.5665490	-1.5989999	13.5892481
C	-1.0047141	0.9602865	12.8337380
H	-0.7095538	1.8767323	12.2965335
H	-2.0571196	1.0778613	13.1685757
H	-0.3688642	0.8727060	13.7386223
C	2.4766935	-1.1657840	2.5598383
C	2.9931010	-2.5555476	2.9948837
H	1.7233919	-0.8131507	3.2895551
H	3.3396069	-0.4628252	2.5838467
H	2.1472226	-3.2333128	3.2187696
H	3.6040226	-3.0100253	2.1898490
N	3.8229996	-2.4421508	4.1932831
H	4.8268831	-2.2909912	4.0651243
C	3.3174720	-2.3609955	5.4461871
O	2.1076638	-2.4631498	5.7045759
C	4.3347221	-2.1647973	6.5709177
H	5.1549898	-1.4789241	6.2486530
H	4.8065450	-3.1493626	6.8168957
O	3.6236906	-1.6392355	7.6663966
C	4.4393711	-1.3517186	8.7772224
H	5.2558943	-0.6452788	8.4922040
H	4.9248850	-2.2753357	9.1746676
C	3.5436661	-0.7220336	9.8502479
O	2.3243072	-0.5902732	9.6332186
N	4.1388253	-0.3397529	11.0136398
C	3.3358032	0.2415502	12.0862307
H	3.5091142	1.3362700	12.1673565
H	2.2683061	0.0515053	11.8821586
H	3.6141774	-0.2206575	13.0550012
C	5.5761601	-0.4027733	11.2781947
H	6.1375163	-0.8127300	10.4223362
H	5.9732964	0.6114802	11.4938187
H	5.7797092	-1.0419893	12.1625992
C	-0.7352517	-4.1063587	2.0003928

C	-1.3637433	-4.0554168	3.4040988
H	0.3462049	-4.3534492	2.1119995
H	-1.1931855	-4.8990594	1.3675839
H	-1.2488202	-3.0284919	3.8000270
H	-2.4496394	-4.2872187	3.3669040
N	-0.6806486	-4.9256527	4.3564985
H	-0.5103760	-5.9010041	4.0973305
C	-0.2653052	-4.4990364	5.5770465
C	0.4515120	-5.5380074	6.4403099
H	-0.3262349	-6.1479030	6.9628782
O	1.2474590	-4.8374917	7.3668658
C	-2.5628782	-0.2677145	3.0423937
C	-2.4607693	0.5384783	4.3503795
H	-2.1258509	-1.2757123	3.1939292
H	-3.6317244	-0.3848537	2.7608615
H	-1.3975341	0.6770396	4.6217280
H	-2.9296527	1.5368434	4.2248478
N	-3.0905466	-0.1685202	5.4592988
H	-4.1079960	-0.2779140	5.4466209
C	-2.3906978	-0.7720250	6.4529144
O	-1.1556999	-0.7181518	6.5427058
C	-3.2226936	-1.5073949	7.5039024
H	-3.5952496	-0.7603122	8.2515703
H	-4.1246887	-1.9737049	7.0372509
O	-2.3860398	-2.4659517	8.0961492
C	-3.0211519	-3.2062166	9.1089280
H	-3.3971554	-2.5388626	9.9239438
H	-3.9068519	-3.7537837	8.7043578
C	-1.9969125	-4.1985263	9.6786044
O	-0.8223586	-4.1782245	9.2755534
N	-2.4487776	-5.0635619	10.6345689
C	-1.5387971	-6.0586152	11.1944418
H	-1.6548155	-6.0990000	12.2963068
H	-1.7514115	-7.0724907	10.7903086
H	-0.5020649	-5.7749553	10.9439926
C	-3.8459583	-5.1790169	11.0524097
H	-4.3425077	-6.0547257	10.5804456
H	-3.8931986	-5.3158007	12.1514812
H	-4.4257499	-4.2722964	10.8086231
C	-5.0737384	2.3567605	-2.2606059
H	-4.5874028	3.1502767	-2.8617886
H	-5.4428956	1.5733476	-2.9500321
H	-5.9662737	2.8189050	-1.7844781
C	1.2207669	4.0978380	-3.0572596
H	1.8712111	4.9988095	-3.0167638
H	1.6503827	3.4324618	-3.8328340
H	0.2212063	4.4301951	-3.3965692
C	-1.4177028	-2.7196373	-4.3072129
H	-0.4595273	-2.5654047	-4.8410081
H	-1.8072945	-3.7107452	-4.6267649
H	-2.1401282	-1.9584444	-4.6604418
C	5.1865542	-1.7012037	-3.3133499
H	6.0008013	-0.9517145	-3.3321525
H	5.6453950	-2.7099278	-3.3433492
H	4.6089508	-1.5861199	-4.2558268
O	-0.4674547	-3.3543056	6.0052826

H	1.0578867	-6.2340065	5.8128769
C	1.6962306	-5.6356434	8.4374206
H	0.8722941	-6.2816851	8.8195472
H	2.5311361	-6.3041962	8.1176551
C	2.1538063	-4.6909131	9.5525101
O	2.0582182	-3.4565751	9.3934400
N	2.6468471	-5.2474849	10.6894220
C	2.8375738	-6.6824933	10.9007342
H	3.9125645	-6.9110238	11.0595542
H	2.2840553	-7.0138656	11.8039353
H	2.4833698	-7.2781906	10.0432729
C	3.0703044	-4.3931878	11.7966051
H	2.5465450	-4.6914366	12.7279847
H	4.1625785	-4.4935950	11.9705835
H	2.8254311	-3.3454630	11.5537022
Eu	0.7012557	-1.9327273	7.8459192

Am^{3+}-CAL4DGA

C	1.7242316	2.3237708	-1.2091475
C	1.6370286	2.1802483	0.1888932
C	0.3940505	2.4320533	0.8218744
C	-0.7579922	2.7207191	0.0499929
C	-0.6140366	2.8551013	-1.3462050
C	0.6213329	2.7012538	-1.9981473
C	2.8645795	1.7005130	0.9646718
C	3.2721344	0.3067697	0.4984424
C	4.3074190	0.1581295	-0.4443679
C	4.5667876	-1.0646825	-1.0969106
C	3.6959445	-2.1455425	-0.8337840
C	2.6562421	-2.0586448	0.1083705
C	2.5187030	-0.8502610	0.8423253
C	1.6529883	-3.1888821	0.2825343
C	0.3938894	-2.9758058	-0.5634913
C	0.5122696	-2.8699085	-1.9638325
C	-0.5844363	-2.5787896	-2.7948817
C	-1.8225051	-2.3256033	-2.1725804
C	-1.9996035	-2.4291587	-0.7811722
C	-0.8912189	-2.8141104	0.0111334
C	-3.3424147	-2.0472143	-0.1614968
C	-3.6542494	-0.5726531	-0.3892153
C	-4.5693042	-0.1564753	-1.3736256
C	-4.7879827	1.2084744	-1.6680791
C	-4.0168428	2.1709947	-0.9791420
C	-3.0875585	1.8071769	0.0116095
C	-2.9559964	0.4316820	0.3212439
O	-2.1029556	0.0724365	1.3606615
C	-2.1560626	2.8234723	0.6584958
O	-1.0722355	-2.9752662	1.3893826
O	1.5835236	-0.8122641	1.8665460
O	0.3243764	2.4211387	2.2234825
H	1.5039562	-3.0022373	-2.4245919
H	-2.6829584	-2.0278614	-2.7937283
H	-4.1467636	3.2375228	-1.2253853
H	4.9222384	1.0374264	-0.6970358
H	3.8420514	-3.0937158	-1.3767523

H	2.6901285	2.1278014	-1.7017848
H	-1.5089361	3.0813751	-1.9473600
H	-3.3177876	-2.2845124	0.9190486
H	-4.1522345	-2.6550641	-0.6141215
H	1.3594548	-3.2456244	1.3446748
H	2.1373824	-4.1483708	0.0042673
H	3.7138053	2.3926727	0.7914626
H	2.6338433	1.7351705	2.0437715
H	-2.5677849	3.8416770	0.4992895
H	-2.0842506	2.6650161	1.7517993
H	-5.1359275	-0.9204066	-1.9308834
C	0.6147373	3.6983079	2.8105879
C	1.4589791	3.5829137	4.0804371
H	-0.3343363	4.2491739	3.0204246
H	1.1886169	4.3196754	2.0897886
H	1.9121825	4.5821199	4.2679852
H	2.2886704	2.8666714	3.9280828
N	0.7543698	3.1566452	5.2905327
H	0.0137570	3.7743472	5.6346546
C	1.2432788	2.2136679	6.1513240
O	2.1604479	1.4351236	5.8772527
C	0.6312423	2.2862064	7.5614684
H	-0.3791894	2.7638008	7.5435434
H	1.2995234	2.9730613	8.1369611
O	0.5762834	1.0061325	8.1632167
C	0.6204712	1.0757351	9.5667040
H	-0.1041407	1.8308031	9.9637252
H	1.6314434	1.3884144	9.9252490
C	0.2767888	-0.2805045	10.1848589
O	-0.0373355	-1.2537816	9.4477024
N	0.2886571	-0.3680619	11.5270291
C	0.0906529	-1.6567088	12.1903976
H	-0.6811280	-1.5565677	12.9799671
H	-0.2207585	-2.4084361	11.4476644
H	1.0489898	-1.9799366	12.6421297
C	0.7323659	0.7281524	12.3914210
H	0.4073458	1.7114963	12.0070909
H	0.2805945	0.5975989	13.3921569
H	1.8365576	0.7145836	12.4999593
C	2.0873672	-0.5376074	3.1676978
C	2.5924072	-1.8160467	3.8775458
H	1.2742141	-0.0690047	3.7510034
H	2.9269288	0.1893048	3.1309450
H	1.7563345	-2.4691249	4.1848225
H	3.2487332	-2.3836274	3.1837221
N	3.3490773	-1.4683299	5.0747618
H	4.1668290	-0.8681301	4.9282019
C	2.9698221	-1.6499707	6.3524882
O	1.9814636	-2.3548246	6.6784415
C	3.8288435	-0.8973270	7.3645066
H	3.5581592	0.1811413	7.2376380
H	4.8980443	-1.0179066	7.0599492
O	3.6124119	-1.3430043	8.6809874
C	4.6726261	-0.9381935	9.5260848
H	4.9111199	0.1453101	9.3804775
H	5.6033283	-1.5031719	9.2764915

C	4.2901894	-1.1542130	11.0027096
O	3.1282085	-1.4600189	11.3127251
N	5.2879578	-0.9692289	11.9205962
C	5.0050133	-1.1612271	13.3411859
H	5.1125725	-0.2055119	13.8966342
H	3.9737884	-1.5359580	13.4539215
H	5.7151746	-1.8933388	13.7791258
C	6.6598732	-0.5703113	11.6136089
H	6.7877991	-0.2995268	10.5523878
H	6.9408625	0.3155302	12.2209485
H	7.3750007	-1.3855749	11.8562521
C	-1.1726318	-4.3077659	1.8928098
C	-0.3224185	-4.2812765	3.1687922
H	-0.7936511	-5.0472725	1.1533696
H	-2.2329056	-4.5679353	2.1217523
H	0.7350865	-4.1179749	2.8756560
H	-0.6383931	-3.4103348	3.7701542
N	-0.3551837	-5.4363619	4.0699456
H	-0.0019631	-6.3360948	3.7308102
C	-0.5035838	-5.2631171	5.3957002
C	-0.0946992	-6.3799662	6.3578403
H	-0.9950629	-6.9188848	6.7373428
O	0.5666627	-5.6738891	7.4057502
C	-2.7817437	-0.0376863	2.5941103
C	-1.7522232	-0.0691918	3.7224837
H	-3.4091445	-0.9620676	2.6334717
H	-3.4713712	0.8307529	2.7406328
H	-1.0568781	-0.9163513	3.5721644
H	-1.1535628	0.8664706	3.7207227
N	-2.4716611	-0.2590509	4.9865782
H	-3.4361919	0.0857425	5.0225730
C	-2.0101295	-0.9187658	6.0603148
O	-0.8510876	-1.3748114	6.1520288
C	-2.9986641	-1.1049492	7.2172149
H	-3.0072923	-0.1929428	7.8609194
H	-4.0316662	-1.2675597	6.8341116
O	-2.5490713	-2.2380071	7.9465956
C	-3.4674983	-2.7161416	8.9153710
H	-3.6966548	-1.9283392	9.6718761
H	-4.4275415	-3.0083062	8.4301560
C	-2.8107752	-3.9250726	9.5917915
O	-1.6217477	-4.2112955	9.2968529
N	-3.5394107	-4.6286104	10.4815431
C	-2.9721767	-5.8145136	11.1289629
H	-3.0168748	-5.7011966	12.2308682
H	-3.5512296	-6.7176208	10.8460241
H	-1.9230911	-5.9320732	10.8123170
C	-4.9427771	-4.3374691	10.7939287
H	-5.6292900	-4.9723618	10.1944644
H	-5.1247886	-4.5521739	11.8643172
H	-5.1901794	-3.2748055	10.6244876
C	-5.8210526	1.6260129	-2.6849222
H	-5.5448266	2.5731178	-3.1884205
H	-5.9723428	0.8506234	-3.4607320
H	-6.8070558	1.7943900	-2.1991963
C	0.7637055	2.9276902	-3.4840024

H	1.1337853	3.9543240	-3.6941715
H	1.4893563	2.2243842	-3.9384514
H	-0.2031192	2.8165313	-4.0116941
C	-0.4451963	-2.5222710	-4.2972084
H	0.6154288	-2.5303863	-4.6133485
H	-0.9411453	-3.3933376	-4.7756017
H	-0.9219180	-1.6133305	-4.7166495
C	5.7127698	-1.2125820	-2.0659372
H	6.1818758	-0.2387380	-2.3028473
H	6.5046150	-1.8718477	-1.6499047
H	5.3832586	-1.6758245	-3.0181974
O	-0.8852503	-4.1770178	5.8909414
H	0.5812311	-7.1229797	5.8777817
C	1.1555048	-6.4726086	8.4182049
H	0.4021042	-7.1561681	8.8783054
H	1.9733436	-7.1010523	7.9977619
C	1.6965363	-5.4911046	9.4696941
O	1.3984521	-4.2743977	9.3611109
N	2.4693789	-5.9581290	10.4669413
C	2.8093586	-7.3691434	10.6594795
H	3.9044061	-7.5196530	10.5612155
H	2.5088318	-7.6897000	11.6778032
H	2.2989405	-8.0227028	9.9322271
C	3.0260814	-5.0305394	11.4573082
H	2.5877963	-5.2337443	12.4565483
H	4.1219468	-5.1846523	11.5228740
H	2.8150387	-3.9876392	11.1605405
Am	0.0176158	-2.9792061	7.8497792

$Eu(NO_3)_3$-$(DGA)_4$

H	-3.9006467	8.2526606	12.5219761
C	-3.2716788	7.3982282	12.2039113
N	-4.0201534	6.1554413	12.4157964
C	-5.4631542	6.2228395	12.2228802
H	-5.8670249	7.1029588	12.7643474
C	-3.3199599	4.9926835	12.5459196
O	-2.0768183	4.9839137	12.5834662
C	-4.0944397	3.6747134	12.7051558
O	-3.2639883	2.5591563	12.4278481
C	-3.4343301	2.0199856	11.1277908
C	-2.4334818	2.6478165	10.1483440
N	-2.6925557	2.6228074	8.8105904
C	-3.9484408	2.2025068	8.2048837
H	-3.7646710	1.4245028	7.4327457
O	-1.3737842	3.1265898	10.5952775
C	-1.7099988	3.2190353	7.9020696
H	-1.8449862	2.7818530	6.8936125
Eu	-0.3836934	3.0706750	13.0416771
H	-4.4969010	2.1120425	10.8275954
H	-3.2331475	0.9322586	11.2040430
H	-5.0038585	3.6275875	12.0744107
H	-4.4402607	3.5738663	13.7560811
H	-2.9788653	7.5201620	11.1383805
H	-2.3489874	7.3758008	12.8109259
H	-5.9713941	5.3282780	12.6223323

H	-5.7286113	6.3360490	11.1478719
H	-0.6910235	2.9979051	8.2683743
H	-1.8114427	4.3247802	7.8538498
H	-4.4518167	3.0611134	7.7089911
H	-4.6404529	1.7793600	8.9516515
H	3.5735976	-1.8493076	13.6081881
C	3.1062848	-1.2027410	12.8321200
N	3.5951428	0.1634041	12.9243675
C	5.0153309	0.3497606	12.6677635
H	5.6361698	-0.1656958	13.4351472
C	2.7290281	1.1738516	13.2727997
O	1.5294388	0.9685569	13.5000882
C	3.3005704	2.5945262	13.3596582
O	2.3317321	3.4753901	13.8880258
C	2.5626715	3.9426288	15.2041245
C	1.4668544	3.4548052	16.1512181
N	1.5959454	3.8102881	17.4744775
C	2.7253629	4.5601835	18.0066269
H	3.4234682	3.9072529	18.5791304
O	0.5170785	2.7801679	15.7326372
C	0.6205636	3.3419039	18.4455985
H	1.0774365	2.6224322	19.1620627
H	3.3441168	-1.6363472	11.8362504
H	2.0115210	-1.1935200	12.9770514
H	5.2923724	1.4174371	12.6598129
H	5.2869334	-0.0749929	11.6765950
H	-0.2013861	2.8420171	17.9040698
H	0.2112408	4.1944749	19.0290781
H	2.3601143	5.3475999	18.7000001
H	3.2954635	5.0625112	17.2055752
H	-1.4291258	-1.8770783	9.8559134
C	-0.5541825	-1.5850661	10.4784209
N	-0.8981906	-1.5677746	11.8944725
C	-1.3492111	-2.8281664	12.4706037
H	-2.3956504	-3.0663464	12.1771464
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O	-0.8087477	0.7144862	11.9514409
C	-1.5145068	-0.3695630	13.9710546
O	-1.4805542	0.9607481	14.4399174
C	-2.2840136	1.1385524	15.5889821
C	-2.5188212	2.6291089	15.7693154
N	-3.2652914	3.0136505	16.8488997
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O	-2.0701845	3.4473240	14.9505366
C	-3.6220061	4.4194301	16.9939531
H	-4.6897865	4.5922628	16.7339836
H	-1.7911676	0.7046423	16.4928632
H	-3.2864157	0.6659321	15.4426913
H	-0.8744789	-1.0326050	14.6022776
H	-2.5673574	-0.7463425	13.9782501
H	0.2637099	-2.3121198	10.2902795
H	-0.2282403	-0.5704047	10.1891076
H	-1.2955765	-2.8071635	13.5736406
H	-0.6925351	-3.6495439	12.1184799
H	-2.9865301	5.0125453	16.3129684

H	-3.4603311	4.7496925	18.0414373
H	-4.2302772	2.5214330	18.6480653
H	-3.4018198	1.1494513	17.8645775
O	0.7805785	5.0223234	11.7545025
N	0.2846624	7.5942447	14.2625067
C	0.8013770	6.3677297	12.2026784
H	0.1465805	6.9980779	11.5551090
H	1.8465558	6.7564463	12.1674600
O	0.1217874	5.3109079	14.2545733
N	2.0019571	3.0911534	8.9417134
C	0.3664284	6.3752967	13.6526388
O	1.3446810	2.5876697	11.0786664
C	0.7523423	8.8169944	13.6135791
H	0.2706046	9.6881185	14.0988673
H	0.4690449	8.8325863	12.5447446
H	1.8563663	8.9210466	13.6935288
C	0.0124168	7.6623285	15.6903974
H	0.9182814	7.9776253	16.2545027
H	-0.2966235	6.6587472	16.0325482
H	-0.7983671	8.3928322	15.8961970
C	1.3543707	4.9084677	10.4645310
H	2.3562813	5.4003100	10.4618818
H	0.7115509	5.3991436	9.6949612
C	1.5512332	3.4336366	10.1871098
C	2.3161779	4.0786427	7.9120184
H	1.6757598	4.9750376	8.0073316
H	2.1171955	3.6352676	6.9158331
H	3.3849547	4.3871505	7.9465532
C	2.3506239	1.7069698	8.6611273
H	2.0811307	1.0970279	9.5417553
H	3.4403044	1.6036305	8.4612601
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H	3.5614936	3.6126062	15.5586571
H	2.5990910	5.0543289	15.1763658
H	4.2267924	2.6371108	13.9689226
H	3.5819795	2.9617830	12.3499880
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O	5.0504395	5.0485969	13.9435489
O	3.5580244	6.6370611	13.8072886
O	4.1680959	5.5439833	12.0076404
N	-1.3802535	6.8605312	8.9589252
O	-0.5567686	6.2264650	8.2315225
O	-0.9562314	7.7240383	9.7743704
O	-2.6098932	6.6243980	8.8608332
N	-5.2535706	0.6554562	13.4987773
O	-5.9799992	1.2139153	12.6410185
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O	-4.5505524	-0.3483038	13.1814061

$Am(NO_3)_3$-$(DGA)_4$

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C	-3.3296774	5.0122866	12.5327168
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O	-3.2383379	2.5881727	12.4199349

Am	-0.4208786	3.1066005	13.0231188
O	0.7188340	5.0212698	11.7392590
C	1.3042685	4.8944175	10.4523533
C	1.5065832	3.4183916	10.2103348
O	1.2883859	2.5920032	11.1242934
C	-5.4694463	6.2375103	12.2124503
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C	-3.4243179	2.0172188	11.1324681
C	-2.4386969	2.6375968	10.1375582
O	-1.3774142	3.1307052	10.5749957
N	-2.7017305	2.5946270	8.8052383
C	-1.7260143	3.1885107	7.8860260
C	-3.9614514	2.1635762	8.2140983
O	1.5918840	0.8583577	13.5237671
C	2.7714131	1.1310758	13.2653261
C	3.2650026	2.5796545	13.3441084
O	2.2563856	3.4045524	13.8984418
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C	1.4235727	3.4256079	16.1675349
O	0.4588308	2.7630044	15.7608207
O	-0.7692858	0.7954594	11.9673278
C	-1.0030777	-0.2879021	12.5350596
C	-1.4717061	-0.3044415	13.9765535
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C	-2.2535548	1.2110857	15.5878598
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C	0.6129733	3.3175534	18.4743880
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N	0.3231061	7.5415643	14.3009516
C	0.0930497	7.5770321	15.7379184
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C	2.3332450	1.6568286	8.7380347
C	2.2855732	4.0125608	7.9338653
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O	4.9464848	5.0276309	13.9750333
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O	3.4186095	6.5919326	13.8856516

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H	5.3611182	0.0265721	11.6040640
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H	3.2777421	5.0227926	17.1876590
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H	-4.9490027	1.7763800	17.0856902
H	-4.7495703	4.6319866	16.6255905
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H	-3.2498739	0.7224582	15.4332045
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H	-2.5293957	-0.6732949	13.9848021
H	0.2328282	-2.2271231	10.2579416
H	-0.2349538	-0.4789319	10.1730370
H	-1.2829475	-2.7387630	13.5506188
H	-0.7444328	-3.5706932	12.0642023
H	-3.0516414	5.0878402	16.2219073
H	-3.5423370	4.8391821	17.9465070
H	-4.3126716	2.6153012	18.5613654
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H	0.0945923	7.0012221	11.5640522
H	1.8108770	6.7361007	12.1487177
H	0.4232187	9.6375876	14.2140123
H	0.5035996	8.8323404	12.6218066
H	1.9430461	8.7887320	13.7106152
H	1.0282045	7.8391440	16.2798527
H	-0.2459805	6.5782781	16.0644079
H	-0.6807854	8.3334368	15.9857599

H	2.3041056	5.3890627	10.4609539
H	0.6622249	5.3724081	9.6720323
H	1.6303697	4.9009998	8.0022132
H	2.1035089	3.5405820	6.9479433
H	3.3491415	4.3365524	7.9732582
H	2.0715648	1.0636557	9.6321243
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H	1.7836934	1.2625752	7.8566605
H	3.5088722	3.5561582	15.5512499
H	2.5637099	5.0057961	15.1638505
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C	-0.2053608	2.8875726	-0.8038272
C	0.8522347	2.6721336	-1.7047712
C	3.4127957	0.9627512	0.6107615
C	3.5177314	-0.4532553	0.0479280
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C	4.5058647	-1.9664854	-1.6386383
C	3.5115892	-2.9160792	-1.3290449
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C	2.6114986	-1.4845352	0.4155244
C	1.3780194	-3.6451974	-0.1374008
C	0.1240181	-3.1030711	-0.8273912
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C	-2.0785703	-1.8288968	-2.0380417
C	-2.1716782	-2.2196977	-0.6909660
C	-1.0804247	-2.9135482	-0.1104721
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C	-3.5186349	-0.3125441	0.2877419
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C	-3.5750438	2.5077394	0.1834366
C	-2.5348795	1.8699161	0.8845874
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O	-1.5397844	-0.1416873	1.7122848
C	-1.3610147	2.6560462	1.4484592
O	-1.1840516	-3.3805096	1.1928934
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O	1.2850884	1.6958089	2.3714077
H	1.1041625	-2.8300161	-2.7374713
H	-2.9240353	-1.2839400	-2.4900132
H	-3.5745002	3.6090184	0.1232437
H	5.1820461	0.0563699	-1.2380649
H	3.4828519	-3.8685555	-1.8846208
H	2.8329284	1.8005933	-1.9088086
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H	-4.3159919	-2.1955083	-0.3635631
H	1.1458199	-3.7836402	0.9353892
H	1.6485264	-4.6369822	-0.5583485
H	4.3073909	1.5279706	0.2763403
H	3.4253639	0.9690001	1.7157985
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H	-5.3038198	-0.2143230	-0.9297502
C	1.2309989	2.7323181	3.3524568
C	2.5114136	2.6837449	4.2229149
H	0.3585787	2.5604666	4.0211609
H	1.0974048	3.7224165	2.8639017
H	3.2966095	3.3659932	3.8393685
H	2.8932415	1.6459343	4.1649673
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H	2.2170786	3.9204324	5.9613179
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O	1.9164495	0.7541978	6.1188517
C	1.6648708	2.3455488	7.9234141
H	1.2043969	3.3645939	7.9365028
H	2.6169805	2.4078905	8.5100223
O	0.7808516	1.4016378	8.5115003
C	0.3780793	1.8560715	9.7879329
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H	1.2564811	2.1733717	10.4009525
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C	-1.7133066	0.0632823	12.4183734
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C	2.4944247	-2.5579980	3.4517778
H	1.5659583	-0.5835862	3.3509931
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O	1.6124428	-2.1148244	6.1420348
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O	3.1778154	-1.2285719	8.0725048
C	4.0623040	-1.0823886	9.1738615
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H	3.4052294	-1.4504821	13.6147378
C	5.3094299	-0.7433873	11.7269379
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H	5.5525419	0.3398668	11.7638296
H	5.6550992	-1.2270082	12.6620091
C	-1.8126343	-4.6625965	1.2990085
C	-2.0790955	-4.9931345	2.7616259
H	-1.1744709	-5.4447742	0.8203366
H	-2.7834455	-4.6623701	0.7504937
H	-2.5530836	-4.1257093	3.2602601
H	-2.8014062	-5.8375855	2.8193203
N	-0.8910760	-5.3141939	3.5350552
H	-0.4748088	-6.2323751	3.3603151
C	-0.6797769	-4.7859412	4.7873044
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C	-1.9015602	-0.8707204	2.8838987
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H	-2.7810664	0.8765597	3.8610353
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H	-3.5884962	-1.2430865	4.9793702
C	-2.0403864	-1.1812342	6.2949040
O	-0.9220797	-0.7534861	6.6186580
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C	-1.4068620	-3.9364129	10.0624228
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H	-0.3468106	-6.3158582	11.8416525
H	0.0674045	-4.5636809	11.9577308
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H	-2.9669138	-6.1589187	9.6895436
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H	-1.3781904	-2.4848084	-4.9067466
H	-1.3985310	-0.7550298	-4.4710443
C	5.5743346	-2.2614431	-2.6671101
H	6.0329986	-1.3320604	-3.0591481
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C	1.5746342	-5.7615965	7.5249019
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C	2.1438804	-4.9602476	8.6913904
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C	3.2673738	-7.0421193	9.4376407
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N	3.7160778	2.5076459	11.3014288
O	2.6553293	3.1914242	11.4145667
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$Am(NO_3)_3$-CAL4DGA

C	1.9294817	2.2083762	-1.2352283
C	1.8970670	2.1126282	0.1679723
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C	-0.4044721	2.7881714	-1.2978061
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