Electronic Supplementary Information for

Theoretical Insights into the Separation of Am(III)/Eu(III): Designing Ligands Based on a Preorganization Strategy

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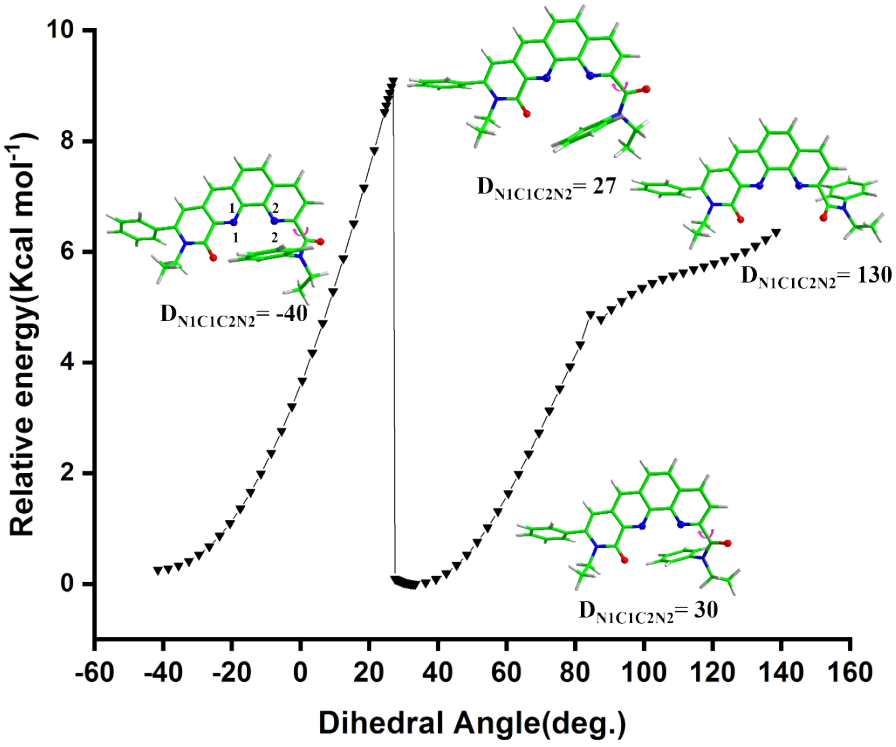

Fig. S1 PES scans of $D_{N1C1C2N2}$ dihedral angle for $\mathbf{L^1}$.

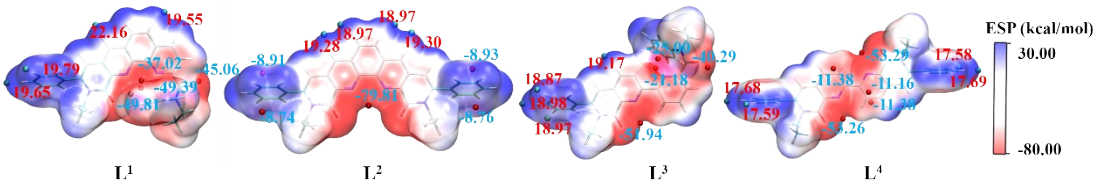

Fig. S2 ESP of $\mathbf{L^1}$-$\mathbf{L^4}$. The values (kcal/mol) of the negative and positive ESP are presented as blue and red spheres, respectively.

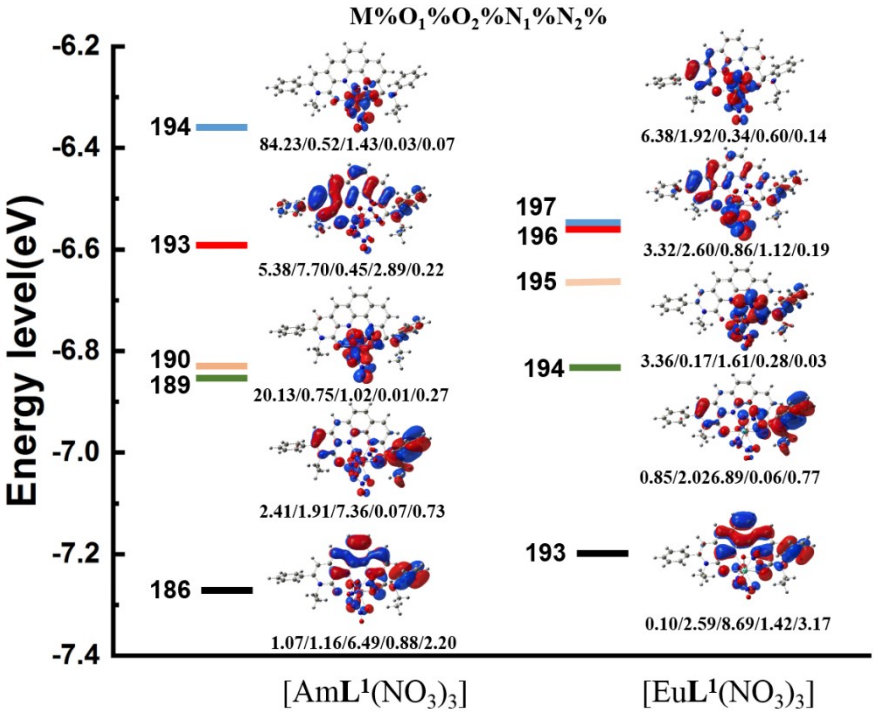

Fig. S3 Energy level (eV) and diagrams of the α-spin MOs of M$\mathbf{L^1}(NO_3)_3$ complexes at the B3LYP/6-31G(d)/RECP level of theory in the gas phase (the isosurface value is set as 0.02 au).

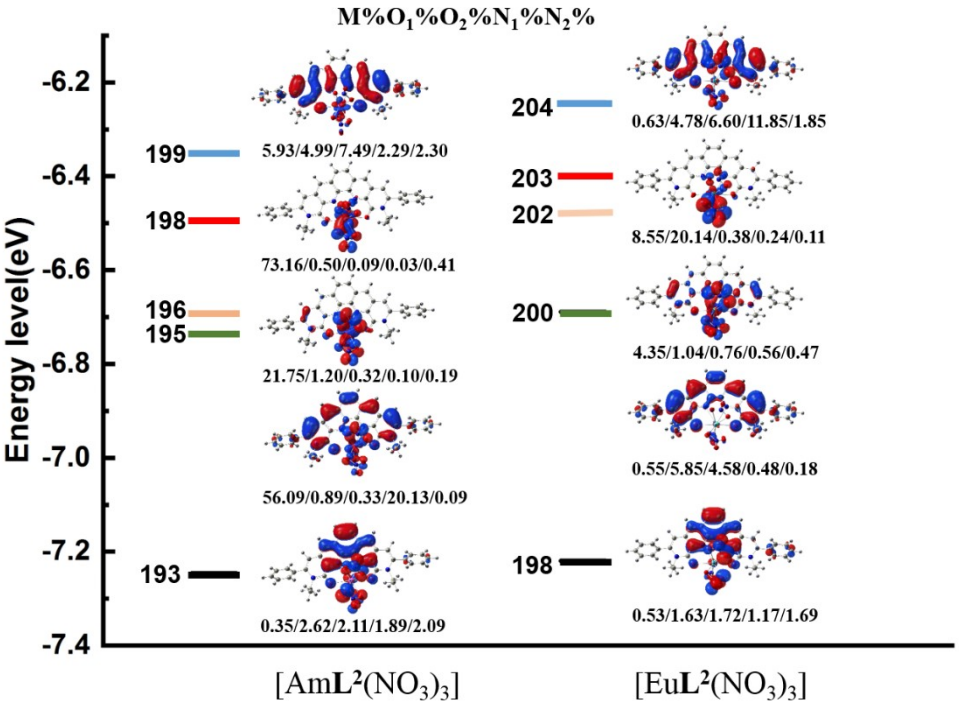

Fig. S4 Energy level (eV) and diagrams of the α-spin MOs of M$\mathbf{L^2}(NO_3)_3$ complexes at the B3LYP/6-31G(d)/RECP level of theory in the gas phase. (the isosurface value is set as 0.02 a.u.)

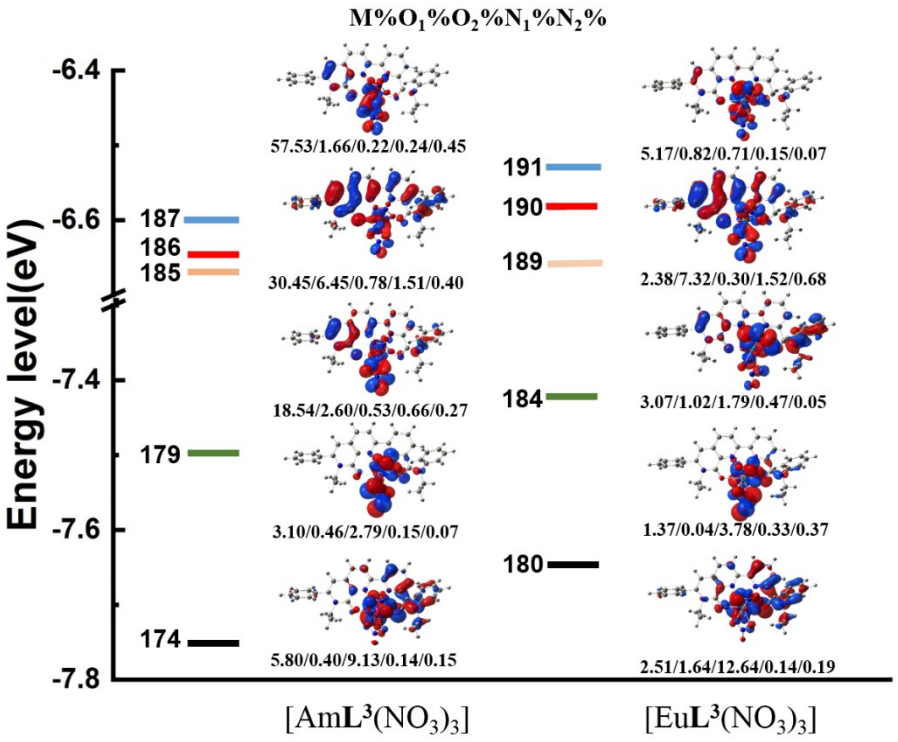

Fig. S5 Energy level (eV) and diagrams of the α-spin MOs of $ML^3(NO_3)_3$ complexes at the B3LYP/6-31G(d)/RECP level of theory in the gas phase. (the isosurface value is set as 0.02 a.u.)

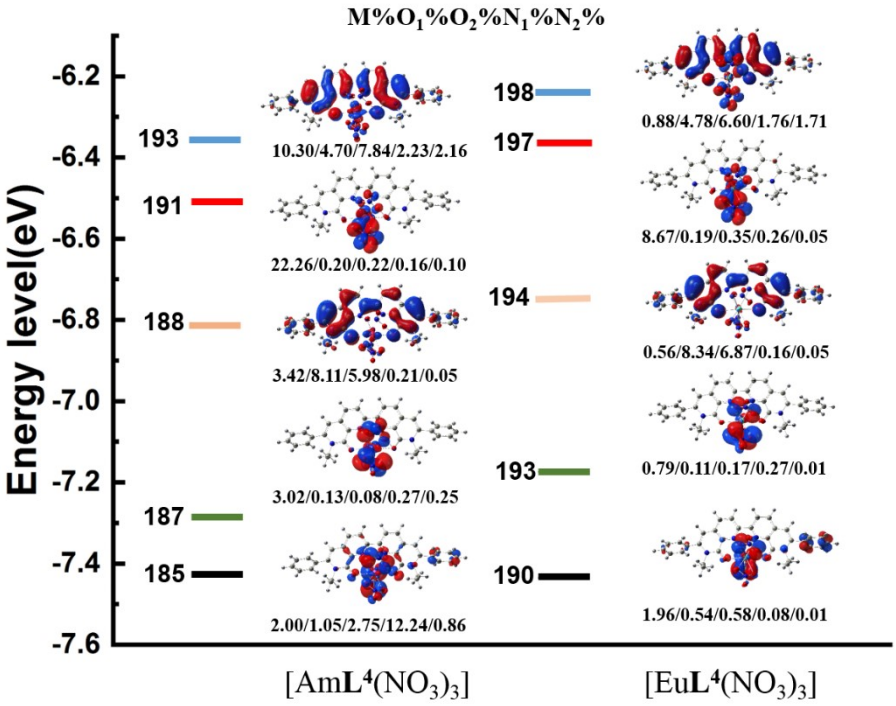

Fig. S6 Energy level (eV) and diagrams of the α-spin MOs of M$\mathbf{L^4}(NO_3)_3$ complexes at the B3LYP/6-31G(d)/RECP level of theory in the gas phase. (the isosurface value is set as 0.02 a.u.)

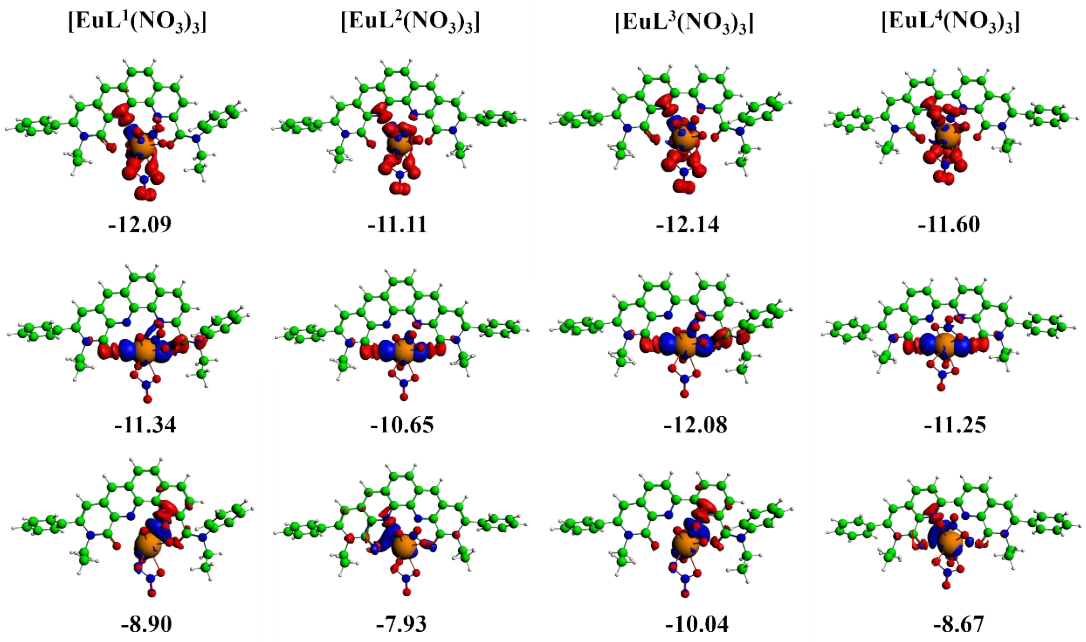

Fig. S7 Natural orbitals for the chemical valence (NOCV) with the larger contribution to the orbital interaction energy for the [Eu**L**$(NO_3)_3$] complexes. The corresponding orbital interaction energy (kcal/mol) contribution for each NOCV pair is also presented.

Table S1. The relative electronic energies (kcal/mol) to each ground state for the [Am**L**^{2}$(NO_3)_3$] and [Eu**L**^{2}$(NO_3)_3$] complexes at the B3LYP/6-31G(d)/RECP level of theory.

Spin state	**singlet**	**triplet**	**quintet**	**septet**
[Am**L**^{2}$(NO_3)_3$]	100.57	64.09	40.07	0.00
[Eu**L**^{2}$(NO_3)_3$]	145.33	90.60	57.20	0.00

Table S2. Properties of the **L**^{1}-**L**^{4} Ligands

	IP	**EA**	**η**
L^{1}	17.29	-9.72	13.50
L^{2}	17.16	-10.16	13.66
L^{3}	16.93	-9.70	13.31
L^{4}	16.73	-9.74	13.23

Table S3. WBIs of the M−N and M−O Bonds in the M**L**$(NO_3)_3$ Complexes at the B3LYP/6-31G(d)/RECP Level of Theory in the Gas Phas

complexes	M-N_1	M-N_2	M-O_1	M-O_2
[M(**L**^{1})$(NO_3)_3$]	0.206/0.163	0.189/0.164	0.238/0.210	0.223/0.203
[M(**L**^{2})$(NO_3)_3$]	0.199/0.155	0.192/0.159	0.229/0.202	0.221/0.199
[M(**L**^{3})$(NO_3)_3$]	0.200/0.160	0.188/0.164	0.228/0.219	0.241/0.211
[M(**L**^{4})$(NO_3)_3$]	0.201/0.154	0.194/0.158	0.236/0.212	0.227/0.208

Table S4. Second-order perturbative estimates (E(2), kcal/mol) of donor-acceptor interactions between O/N-ligands and Am(III)/Eu(III) in the [M**L**$(NO_3)_3$] complexes.

Complexes	donor→acceptor	Character of empty metal orbita	E(2)
[Am**L**^{1}$(NO_3)_3$]	N_1→Am	p(0.03%),d(99.50%),f(0.46%)	7.20
	N_2→Am	s(0.11%),p(0.13%),d(99.27%),f(0.49%)	5.84
	O_1→Am	s(1.33%),p(0.09%),d(98.00%),f(0.58%)	10.16
	O_2→Am	s(0.11%),p(0.13%),d(99.27%),f(0.49%)	8.72
[Eu**L**^{1}$(NO_3)_3$]	N_1→Eu	s(1.08%),p(0.01%),d(98.47%),f(0.40%)	14.41
	N_2→Eu	s(0.04%),p(0.12%),d(99.36%),f(0.46%)	6.72
	O_1→Eu	s(4.63%),p(0.03%),d(94.90%),f(0.43%)	10.06
	O_2→Eu	s(0.04%),p(0.12%),d(99.36%),f(0.46%)	7.47
[Am**L**^{2}$(NO_3)_3$]	N_1→Am	s(0.01%),p (0.09%),d (99.39%),f (0.52%)	8.70
	N_2→Am	s(0.08%),p(0.12%),d(99.05%),f(0.75%)	6.22
	O_1→Am	s(0.96%),p(0.05%),d(98.38%),f(0.61%)	6.26
	O_2→Am	s(0.08%),p(0.12%),d(99.05%),f(0.75%)	7.41
[Eu**L**^{2}$(NO_3)_3$]	N_1→Eu	s(0.61%),p(0.01%),d(98.98%),f(0.37%)	13.31
	N_2→Eu	s(0.03%),p(0.09%),d(99.17%),f(0.70%)	6.60
	O_1→Eu	s(0.42%),p(0.05%),d(99.27%),f(0.24%)	8.01
	O_2→Eu	s(0.03%),p(0.09%),d(99.17%),f(0.70%)	6.22
[Am**L**^{3}$(NO_3)_3$]	N_1→Am	p(0.04%),d(99.48%),f(0.48%)	6.88
	N_2→Am	s(0.14%),p(0.14%),d(99.17%),f(0.54%)	6.11
	O_1→Am	s(1.66%),p(0.08%),d(97.65%),f(0.61%)	9.84
	O_2→Am	s(0.14%),p(0.14%),d(99.17%),f(0.54%)	9.60
[Eu**L**^{3}$(NO_3)_3$]	N_1→Eu	s(1.81%),p(0.02%),d(97.72%),f(0.42%)	13.21
	N_2→Eu	s(0.04%),p(0.12%),d(99.33%),f(0.50%)	7.35
	O_1→Eu	s(5.44%),p(0.22%),d(94.09%),f(0.43%)	9.48
	O_2→Eu	s(0.04%),p(0.12%),d(99.33%),f(0.50%)	8.11
[Am**L**^{4}$(NO_3)_3$]	N_1→Am	s(0.01%),p(0.08%),d(99.41%),f(0.50%)	9.40
	N_2→Am	s(0.10%),p(0.10%),d(99.12%),f(0.68%)	5.77
	O_1→Am	s(1.26%),p(0.05%),d(98.05%),f(0.64%)	7.69
	O_2→Am	s(0.10%),p0.10%),d(99.12%),f(0.68%)	8.59
[Eu**L**^{4}$(NO_3)_3$]	N_1→Eu	s(0.53%),p(0.01%),d(99.04%),f(0.39%)	12.90
	N_2→Eu	s(0.02%),p(0.07%),d(99.22%),f(0.67%)	6.70
	O_1→Eu	s(0.34%),p(0.04%),d(99.38%),f(0.23%)	7.91
	O_2→Eu	s(0.02%),p(0.07%),d(99.22%),f(0.67%)	7.18

Table S5. Total bonding energy (kcal/mol), Pauli, electrostatic and orbital

interactions obtained from energy decomposition analysis at the BP86/TZ2P level of theory.

complexes	ΔE_{int}	ΔE_{Pauli}	ΔE_{orb}	ΔE_{elstat}
[Am($\mathbf{L^1}$)$(NO_3)_3$]	-89.10	109.04	-80.20	-117.94
[Am ($\mathbf{L^2}$)$(NO_3)_3$]	-86.14	99.39	-74.45	-111.08
[Am ($\mathbf{L^3}$)$(NO_3)_3$]	-89.34	114.82	-82.43	-114.82
[Am ($\mathbf{L^4}$)$(NO_3)_3$]	-87.36	107.06	-77.77	-116.65
[Eu($\mathbf{L^1}$)$(NO_3)_3$]	-91.08	94.68	-78.96	-106.80
[Eu($\mathbf{L^2}$)$(NO_3)_3$]	-87.84	84.49	-72.81	-99.51
[Eu($\mathbf{L^3}$)$(NO_3)_3$]	-91.66	100.65	-81.69	-110.62
[Eu($\mathbf{L^4}$)$(NO_3)_3$]	-89.20	92.12	-76.29	-105.03

Table S6. Changes of the Energy (ΔE, kcal/mol) for the Reactions $[M(NO_3)(H_2O)_8]^{2+} + L^3 + 2NO_3^- = [ML^3(NO_3)_3] + 8H_2O$ (M = Am and Eu) and the difference (ΔΔE) of between ΔE_{Am} and ΔE_{Eu} in the Cyclohexanone Solution at the B3LYP/TZP/SO and B3LYP/TZP/SR level of theory, respectively.

Reaction	ΔE_{SO}	$\Delta\Delta E_{SO}$	ΔE_{SR}	$\Delta\Delta E_{SR}$
$[Am(NO_3)(H_2O)_8]^{2+} + L^3 + 2NO_3^- = [AmL^3(NO_3)_3] + 8H_2O$	-0.93	-68.52	-37.42	-7.46
$[Eu(NO_3)(H_2O)_8]^{2+} + L^3 + 2NO_3^- = [EuL^3(NO_3)_3] + 8H_2O$	67.59		-29.96	

Cartesian coordinates

L^1

Atoms	X	Y	Z
O	2.07237700	14.64517500	2.57592300
O	7.56098400	11.62064200	-1.17242700
N	2.51237400	11.96471900	2.05911200
N	4.46456600	11.22023000	0.26561900
N	0.51664300	14.16136800	4.18242700
C	1.44683000	13.78751100	3.18902800
C	1.58419100	12.32647600	2.93924900
C	0.72672900	11.40748300	3.61003500
N	5.89408300	13.16185400	-1.42504700
C	-0.20768500	11.90741300	4.57448800
C	-0.28603400	13.23751500	4.85570200
C	0.87043700	10.05507600	3.29114100
H	0.23559700	9.31290800	3.77082200
C	1.83212900	9.65055200	2.35947700
C	2.65559400	10.66502500	1.76684800
C	3.68302400	10.26568700	0.80837300
C	3.82593700	8.88900600	0.48119200
C	2.96745300	7.91102900	1.09034700
H	3.10048000	6.86651300	0.81852600
C	2.01560400	8.27300300	1.99167900
H	1.37518800	7.52479300	2.45218600
C	4.84027600	8.53956100	-0.43743600
H	4.98204000	7.49510500	-0.70539600
C	5.64735100	9.52164600	-0.96894700
C	5.40578200	10.86333000	-0.59486800
C	6.36754600	11.91815200	-1.09856400
C	-3.00350600	14.45456600	7.95957700

C	-1.62531300	14.58353200	8.15016500
C	-0.74016000	14.21136800	7.13986700
C	-1.22156500	13.70662500	5.92079900
C	-2.60545800	13.57282200	5.74249200
C	-3.49091900	13.94663500	6.75542900
H	-3.69205400	14.74528500	8.74815100
H	-1.23830500	14.96678700	9.09034700
H	0.33168800	14.29646900	7.29883000
H	-2.98391100	13.17600500	4.80470800
H	-4.56119000	13.84048300	6.60085100
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H	7.75892800	13.66541700	-2.19941900
C	0.32411000	15.62011200	4.33630500
C	-0.68780900	16.18297600	3.33705600
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H	0.00803100	15.82012800	5.35876600
H	-0.77766700	17.26678500	3.47207300
H	-0.36016100	15.99290000	2.31133200
H	-1.67856300	15.73887700	3.48216100
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H	2.21536800	13.67411000	-4.13006600
H	1.83330300	14.80063500	0.01625800
H	0.84418800	14.60852300	-2.27585500

L^2

Atoms	X	Y	Z
O	1.94508200	15.02107300	4.39190300

O	5.20831900	14.83381700	-0.09613600
N	1.76549300	12.89608200	2.62691400
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C	0.98412500	12.93603400	3.70305100
C	-0.00436100	11.95558800	4.00288200
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C	-0.77825400	12.08643300	5.20098600
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C	1.62964000	11.88046300	1.76560700
C	2.49268500	11.82982100	0.58234800
C	2.34209100	10.73772200	-0.33547300
C	1.35482800	9.71826900	-0.09002000
H	1.26549900	8.90480700	-0.80614400
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C	3.17810400	10.70344400	-1.45373100
H	3.09364600	9.88695200	-2.16815100
C	4.12432900	11.71247600	-1.65483800
C	4.17984100	12.74904100	-0.67981800
C	5.14495000	13.87282400	-0.84614000
C	5.94770500	12.74553200	-2.89298400
C	5.03342100	11.74369500	-2.76119400
C	-2.89209900	13.17923100	9.68378200
C	-1.51028400	12.97970800	9.74026500
C	-0.75300800	12.98413100	8.57010800

C	-1.36723400	13.19109300	7.32417300
C	-2.75504200	13.38184100	7.27715700
C	-3.51233500	13.37800300	8.45036000
H	-3.48089800	13.17591400	10.59696600
H	-1.02207700	12.81259100	10.69654100
H	0.31920900	12.81234900	8.61649600
H	-3.23701700	13.53555800	6.31582700
H	-4.58682400	13.53129200	8.39785400
C	8.69922200	12.49057200	-6.18988100
C	9.16728000	12.35896000	-4.87990900
C	8.28441500	12.46241500	-3.80634400
C	6.91828600	12.70215900	-4.02717800
C	6.45716300	12.82425400	-5.34520200
C	7.34292100	12.72109100	-6.41974900
H	9.38888500	12.41006000	-7.02563200
H	10.22058600	12.16749800	-4.69383200
H	8.64952200	12.34273200	-2.78964700
H	5.40050300	13.00302000	-5.52293600
H	6.97067800	12.82212100	-7.43562900
C	6.86262800	14.97445400	-2.17790800
H	7.15831000	15.31690700	-1.18595100
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C	-0.40372300	16.47860000	6.05844200
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H	0.21606900	15.10473600	7.61873500
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C	6.13116100	16.09281100	-2.92237700

H	6.79342800	16.95907100	-3.03291200
H	5.82455700	15.76890100	-3.92311600
H	5.24620500	16.40834700	-2.36326000
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H	5.03041400	10.93584500	-3.48437600

L^3

Atoms	X	Y	Z
O	1.79424200	14.57094400	2.26749200
O	7.49767100	11.07455100	-0.86490200
N	2.26472500	11.85901500	1.93157400

N	4.33147900	10.96781400	0.32821800
N	0.46492000	14.19841300	4.09224200
C	1.28549400	13.75571400	3.02917600
C	1.45485800	12.28593000	2.91100900
C	0.76447200	11.42180200	3.79216100
N	6.08689300	12.85501200	-1.17047100
C	-0.05953000	11.97713300	4.81983400
C	-0.18585400	13.32732700	4.96312200
C	0.96105300	10.03653600	3.60663100
H	0.46729200	9.32818700	4.26728400
C	1.79425800	9.60010500	2.59902100
C	2.43842700	10.54866500	1.76560900
C	3.35760100	10.11031700	0.67385000
C	3.20723900	8.86615000	0.04264100
C	4.12411500	8.49215700	-0.93888300
H	4.03117800	7.53162600	-1.43841800
C	5.15661200	9.36386000	-1.26619200
C	5.19696800	10.60654300	-0.62074000
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C	-2.56637700	14.76809800	8.24258000
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C	-1.00821700	13.87222100	6.08440600
C	-2.39607900	13.67635600	6.09074000
C	-3.17059400	14.12399300	7.16292600
H	-3.16856000	15.11591200	9.07735500
H	-0.70385700	15.45004600	9.09279300
H	0.67039600	14.65034400	7.19607800
H	-2.86533900	13.17268600	5.25034300
H	-4.24586900	13.96817300	7.15212200

C	7.22326600	13.78029400	-1.32882500
H	8.11628200	13.16332800	-1.44288200
C	0.22580100	15.65831200	4.12265500
C	-0.90957700	16.07965400	3.18854300
H	1.15992300	16.12781800	3.81381700
H	0.00992400	15.95024300	5.14892400
H	-1.03312400	17.16792600	3.22424900
H	-0.68249500	15.79510800	2.15761400
H	-1.85858600	15.61952400	3.48456200
H	7.07308700	14.34608400	-2.25529700
C	7.37187500	14.73378900	-0.14199700
H	8.21630200	15.41313500	-0.30885700
H	6.46996800	15.33907400	-0.00191500
H	7.55758300	14.17440600	0.78074900
H	-0.56028600	11.32381900	5.52548500
H	5.91776800	9.10746100	-1.99484100
C	4.78232300	13.35278300	-1.53375100
C	4.44209800	13.40472800	-2.89172700
C	3.88869100	13.83107500	-0.57232500
C	3.21338500	13.93393100	-3.28614100
H	5.14483200	13.02805800	-3.63076000
C	2.65691800	14.35406400	-0.97061800
H	4.12570800	13.75219700	0.48084900
C	2.32031800	14.41154700	-2.32395200
H	2.95438700	13.96894300	-4.34133000
H	1.97091100	14.69851800	-0.20379900
H	1.36089400	14.82106900	-2.63045200
H	1.97768200	8.53906700	2.46516600
H	2.38214600	8.20915100	0.29830200

L[4]

Atoms	X	Y	Z
O	2.54557100	14.32143200	4.90917900
O	4.40785000	15.19969000	-0.71288900
N	1.90800000	12.69364000	2.75841600
N	3.16203200	12.90793100	0.22690600
N	0.59897000	13.79639600	5.99692900

C	1.49850800	13.69229100	4.90341900
C	1.06351900	12.80359800	3.79427900
C	-0.18453300	12.14073300	3.86515400
N	5.65202400	14.00793000	-2.22288200
C	-1.01579100	12.32550500	5.01423600
C	-0.61930300	13.12646100	6.04451700
C	-0.52976000	11.31324600	2.77562200
H	-1.48181700	10.78797900	2.77709600
C	0.34493900	11.19129200	1.71650500
C	1.56713900	11.90651200	1.73971800
C	2.52505600	11.79972500	0.60096200
C	2.73693500	10.55570400	-0.04185300
C	3.64285900	10.47618000	-1.07866300
H	3.84094500	9.52967800	-1.57587000
C	4.33094100	11.63885900	-1.48554900
C	4.03456600	12.83391300	-0.78843100
C	4.67993500	14.11008700	-1.19357600
C	5.95116100	12.81170600	-2.86781200
C	5.30572400	11.65797700	-2.53211800
C	-3.22062000	13.40140400	9.45964100
C	-1.98697800	12.75536500	9.57393400
C	-1.13032800	12.68137200	8.47682800
C	-1.49441700	13.25581100	7.24818700
C	-2.73756600	13.89425500	7.14111500
C	-3.59439900	13.96830600	8.24123800
H	-3.88716600	13.45846900	10.31583300
H	-1.69432400	12.30157100	10.51689400
H	-0.17823900	12.16454400	8.56500300
H	-3.02807400	14.33408900	6.19126100
H	-4.55334300	14.46996400	8.14368900

C	9.00042200	12.57049300	-5.89227800
C	9.35065600	12.86128400	-4.57123500
C	8.36518900	12.96232900	-3.59072300
C	7.01214800	12.77641300	-3.91813300
C	6.67171900	12.47661700	-5.24437700
C	7.66001300	12.37640800	-6.22573300
H	9.76989900	12.49239000	-6.65542600
H	10.39393500	13.00189300	-4.30197000
H	8.64304700	13.17181200	-2.56106900
H	5.62750500	12.32483500	-5.50264300
H	7.37983200	12.14728700	-7.25032500
C	6.20056600	15.30347200	-2.67791900
H	6.29035300	15.92618900	-1.78748900
C	0.99144800	14.78864200	7.02065800
C	0.58365500	16.21147900	6.63456800
H	2.07600200	14.72215100	7.11104000
H	0.54228200	14.50192000	7.97008200
H	0.91626000	16.91432000	7.40696000
H	1.04900900	16.49828700	5.68781000
H	-0.50415000	16.30018200	6.53903500
H	7.19460400	15.13337100	-3.08826800
C	5.29861000	15.98709100	-3.70700000
H	5.73073100	16.95222300	-3.99508200
H	5.19484600	15.37721200	-4.61124300
H	4.30718900	16.16888500	-3.28363200
H	-1.95898300	11.79631000	5.09133800
H	5.57542300	10.73749500	-3.03768600
H	2.21329500	9.66811100	0.30025900
H	0.08831900	10.57633800	0.85915300

[AmL^1(NO$_3$)$_3$]

Atoms	X	Y	Z
Am	3.55984900	14.41824300	1.96176200
O	2.02958000	14.73081300	3.98744000
O	5.60418800	13.72834600	0.55659300
N	1.86233700	12.40510600	2.66191200
N	3.56618000	12.05252600	0.59741300
N	0.33380000	14.16403500	5.41459700
C	1.18169300	13.89957200	4.35673700

C	1.03087500	12.60628400	3.68013300
O	4.59564400	12.72561000	3.52292300
C	0.05110500	11.67163600	4.09922500
O	5.22231700	14.79165400	3.76894400
N	6.02643400	13.38347800	-1.64790300
C	-0.78099000	12.03841600	5.20527300
O	6.03210400	13.24533100	5.09384600
N	3.78389900	17.28932700	1.51565400
C	-0.63383000	13.24089300	5.83428500
O	4.77294600	16.48074500	1.35939400
N	1.84699500	14.52107500	-0.51615600
O	3.86859200	18.47566900	1.27582400
N	5.31648400	13.57489600	4.16814700
O	2.69934000	16.74565200	1.94413500
O	3.09555900	14.81169900	-0.55690900
O	1.16957000	14.45063400	-1.53088200
O	1.36528600	14.28224100	0.64419500
C	-0.00960000	10.45794300	3.40028200
H	-0.73535800	9.70051300	3.68620300
C	0.86896800	10.21805700	2.33708900
C	1.79732500	11.25041300	1.99402100
C	2.72058300	11.05061500	0.89479600
C	2.72009700	9.81822900	0.19614100
C	1.77423300	8.79847900	0.56782400
H	1.78096700	7.86243200	0.01590700
C	0.88727900	8.99063100	1.58307300
H	0.17824800	8.21128300	1.84836700
C	3.67453000	9.66938300	-0.83042300
H	3.72796000	8.73587900	-1.38435700
C	4.54297800	10.70548600	-1.12495700

C	4.44822800	11.90384000	-0.38734900
C	5.39315300	13.08776500	-0.48873600
C	-3.18011800	14.09005700	9.18904200
C	-1.82503700	13.81756300	9.39516300
C	-0.98914500	13.55991300	8.30937500
C	-1.50172300	13.57490100	7.00203400
C	-2.86372500	13.84023600	6.80356000
C	-3.69769000	14.09933400	7.89330400
H	-3.82930600	14.29118800	10.03650400
H	-1.41903500	13.79915600	10.40254500
H	0.06155600	13.33538800	8.47337100
H	-3.26552900	13.84596300	5.79430200
H	-4.75068200	14.30817300	7.72701700
C	7.03026500	14.48069000	-1.62123100
H	7.52927200	14.43153800	-0.65236300
C	0.44213300	15.52897400	5.99692900
C	-0.32441900	16.56735000	5.17700700
H	1.50547900	15.77004400	6.01964200
H	0.07267200	15.48308500	7.01921600
H	-0.20878100	17.55068600	5.64524200
H	0.06865500	16.63074200	4.15886600
H	-1.39339900	16.33167500	5.13829400
H	7.76045100	14.24675800	-2.40169000
C	6.41743600	15.86382600	-1.84206600
H	7.21933800	16.61024200	-1.87038800
H	5.87554300	15.91080800	-2.79257000
H	5.73674400	16.12558300	-1.02845300
H	-1.52819200	11.34575300	5.57470500
H	5.28180700	10.59894400	-1.90863300
C	5.54913200	12.96325200	-2.93846000

C	6.41618500	12.27989800	-3.80105000
C	4.24681400	13.27834700	-3.34523900
C	5.97234000	11.89373600	-5.06543400
H	7.42621500	12.04698700	-3.47492300
C	3.81030700	12.87633800	-4.60987800
H	3.59336000	13.84087800	-2.68433100
C	4.66653800	12.18676100	-5.46994800
H	6.64510000	11.36159100	-5.73226100
H	2.79893600	13.11985400	-4.92230200
H	4.32266800	11.88450300	-6.45521900

[AmL^2(NO$_3$)$_3$]

Atoms	X	Y	Z
Am	3.31022900	14.83830700	1.93015800
O	2.03311900	14.79728100	4.16948300
O	5.18335300	14.50930100	0.18027100
N	1.76713600	12.65556300	2.58250700
N	3.33774000	12.56660300	0.41384300
N	0.42232500	14.05950200	5.61856100
C	1.20363500	13.92775900	4.48574900
C	0.99565700	12.73066500	3.66291500
O	4.69536600	13.05884300	3.06976800

C	0.01583300	11.76590300	4.00422300
O	5.14448400	15.11788900	3.59872000
N	5.92918400	13.69991300	-1.82699800
C	-0.74061700	11.99041100	5.19839100
O	6.24240300	13.48449100	4.56226900
N	3.32038200	17.74867200	1.86063200
C	-0.53286100	13.09725300	5.97156900
O	4.32546500	17.04000600	1.48880700
N	1.30542700	15.13960000	-0.27296100
O	3.31874500	18.96094500	1.80204400
N	5.39771900	13.87311000	3.77797600
O	2.31227500	17.07771700	2.30092500
O	2.53845500	15.43679300	-0.44807200
O	0.47269200	15.25504900	-1.15499400
O	1.00205200	14.68827600	0.89285600
C	-0.12504400	10.66787800	3.14020900
H	-0.86050900	9.89666200	3.35598500
C	0.67651700	10.57138600	1.99808600
C	1.62201200	11.61480200	1.76054100
C	2.46889300	11.56798800	0.58562500
C	2.35972800	10.47764700	-0.32971900
C	1.39193400	9.44158300	-0.05352900
H	1.30988400	8.61493000	-0.75403000
C	0.59582000	9.48568500	1.04878200
H	-0.12577300	8.69448200	1.23340400
C	3.19676600	10.48492100	-1.45000500
H	3.13428700	9.68236100	-2.18097100
C	4.12113700	11.52760000	-1.63041800
C	4.15197200	12.53872300	-0.63828800
C	5.11158100	13.64937100	-0.71049800

C	5.89367200	12.70911100	-2.81396800
C	5.03108300	11.65267600	-2.72731100
C	-2.85288700	13.50220700	9.56496600
C	-1.48469000	13.22941300	9.64701400
C	-0.72193600	13.11645400	8.48547600
C	-1.32148600	13.27787100	7.22570800
C	-2.69598600	13.54268400	7.15107800
C	-3.45664100	13.65691500	8.31662100
H	-3.44499800	13.59085000	10.47142400
H	-1.01144900	13.09812900	10.61595800
H	0.33921700	12.89103200	8.55193300
H	-3.16454300	13.66314100	6.17847400
H	-4.52000900	13.86757900	8.24628800
C	8.56600700	12.83944000	-6.17545100
C	9.07073900	12.59954200	-4.89448000
C	8.21227100	12.57613800	-3.79628600
C	6.83561100	12.79468900	-3.96827300
C	6.33544500	13.02571500	-5.25725500
C	7.19855500	13.05083400	-6.35476500
H	9.23709600	12.85879500	-7.02951600
H	10.13313700	12.42447100	-4.75041800
H	8.60579100	12.37623900	-2.80308400
H	5.27076000	13.19140100	-5.39480100
H	6.80001100	13.23698100	-7.34804000
C	6.73214900	14.94502100	-1.96881000
H	7.07051200	15.20756300	-0.96635400
C	0.57293500	15.34577900	6.35160300
C	-0.22165200	16.47763700	5.69866800
H	1.63863800	15.57776100	6.34955800
H	0.25329300	15.18140700	7.37842300

H	-0.07936000	17.39574400	6.27881300
H	0.12691400	16.66579000	4.67975300
H	-1.29286700	16.24958400	5.67905000
H	7.60047800	14.71614200	-2.58310700
C	5.90617500	16.08222400	-2.57201900
H	6.52026700	16.98797300	-2.61761800
H	5.58044100	15.83770400	-3.58890800
H	5.02748600	16.29757300	-1.95797400
H	-1.47825100	11.26373300	5.51846800
H	5.05873700	10.89304800	-3.49973700

[AmL^3(NO$_3$)$_3$]

Atoms	X	Y	Z
Am	3.59339600	14.34982300	2.01825700
O	2.17300500	14.60716200	4.08635300
O	5.60682900	13.76198800	0.57962900
N	1.94377500	12.28523600	2.72401400
N	3.60319900	11.98600200	0.63722900
N	0.40159100	14.11630400	5.44211600
C	1.27337400	13.81180600	4.41135200
C	1.08045500	12.53627500	3.71975500
O	4.74814200	12.64830400	3.47935400
C	0.03278500	11.67241300	4.09140500
O	5.31203200	14.72675200	3.76928800

N	5.96991200	13.43976700	-1.63832200
C	-0.81917200	12.06515700	5.16684700
O	6.23633500	13.16798800	5.00134100
N	3.68669800	17.23944700	1.61229600
C	-0.62861200	13.25164500	5.81896800
O	4.70511500	16.47623600	1.42356600
N	1.79653400	14.42041200	-0.40565400
O	3.71780600	18.43315100	1.39567900
N	5.46708100	13.50150000	4.12097200
O	2.63271800	16.64300000	2.04705500
O	3.03592000	14.74185800	-0.48115700
O	1.09412900	14.33113100	-1.40221500
O	1.35174200	14.17216700	0.76664400
C	-0.08240300	10.47324900	3.35199800
H	-0.87577500	9.76784800	3.58276600
C	0.81229300	10.21493900	2.33546700
C	1.83540300	11.15002700	2.03698400
C	2.83189000	10.93273800	0.95353300
C	2.99303000	9.69765000	0.30895600
C	3.96276600	9.57560400	-0.68081600
H	4.11597100	8.62425000	-1.18136400
C	4.74213800	10.67962800	-1.01799600
C	4.52399800	11.87616900	-0.32920500
C	5.39274300	13.11216400	-0.45981900
C	-3.24825800	14.20144500	9.08819800
C	-1.91382300	13.87103400	9.33940500
C	-1.05287800	13.58093500	8.28183600
C	-1.51951500	13.62089000	6.95787000
C	-2.86148400	13.94415600	6.71389600
C	-3.72030700	14.23603300	7.77560700

H	-3.91692000	14.42805800	9.91378700
H	-1.54370500	13.83295300	10.35996000
H	-0.01888200	13.31165300	8.48083400
H	-3.22772100	13.97054900	5.69153500
H	-4.75699400	14.49049300	7.57427700
C	6.91475400	14.58856300	-1.64663800
H	7.44200600	14.57362500	-0.69172100
C	0.56437600	15.47297700	6.03415400
C	-0.08586100	16.55889400	5.17578200
H	1.63790700	15.64533600	6.11930500
H	0.13372200	15.44988100	7.03280900
H	0.05265900	17.52948400	5.66413200
H	0.37738200	16.61062800	4.18703500
H	-1.16153500	16.38437100	5.06456700
H	7.63468700	14.38716000	-2.44544900
C	6.22375200	15.93550000	-1.85960200
H	6.98410800	16.72259500	-1.91688800
H	5.65244500	15.94555000	-2.79379700
H	5.55422900	16.16819300	-1.02820300
H	-1.61836600	11.41109000	5.49542300
H	5.50176200	10.61172300	-1.78603000
C	5.48089400	12.98287300	-2.91261100
C	6.35994100	12.33941100	-3.79333100
C	4.15375700	13.22579400	-3.28650800
C	5.90426600	11.92008400	-5.04284600
H	7.38946800	12.16364700	-3.49319700
C	3.70625400	12.79138500	-4.53651200
H	3.48966400	13.75962600	-2.61263100
C	4.57477000	12.14071600	-5.41441700
H	6.58660900	11.41889600	-5.72376900

H	2.67577000	12.97932700	-4.82390300
H	4.22159300	11.81289200	-6.38815800
H	0.71418800	9.30449200	1.75589200
H	2.39472200	8.83848600	0.58824200

[AmL^4(NO$_3$)$_3$]

Atoms	X	Y	Z
Am	3.21988000	14.79015000	1.84897500
O	1.96156500	14.80380500	4.05009000
O	5.16443500	14.40977200	0.25155700
N	1.67002200	12.60640400	2.50248400
N	3.26703900	12.48104800	0.38418900
N	0.42036600	14.07271100	5.56883700
C	1.15849600	13.92458600	4.40644000
C	0.93567200	12.70984300	3.61796100
O	4.52423900	13.05840700	3.15693400
C	-0.01548900	11.75482700	4.02766400
O	5.04021900	15.13768800	3.52067300
N	5.93216200	13.66186600	-1.76664800
C	-0.73226800	11.98993300	5.23908000

O	6.05783100	13.55363000	4.64163900
N	3.20686500	17.70041500	1.68700200
C	-0.50865900	13.11534500	5.98265800
O	4.22470800	16.99054500	1.35472600
N	1.30232600	15.01152000	-0.44326200
O	3.19482600	18.91046600	1.58912700
N	5.24294500	13.90419600	3.80832400
O	2.19804800	17.03456900	2.13257300
O	2.54048200	15.30946900	-0.57923500
O	0.50678200	15.08801700	-1.36343100
O	0.95304500	14.60304000	0.72470000
C	-0.16945800	10.62615300	3.19124200
H	-0.88244000	9.84970800	3.45417400
C	0.59087900	10.52119400	2.04540900
C	1.51581500	11.54269000	1.71380300
C	2.37141500	11.49989800	0.50034800
C	2.27329600	10.48878300	-0.48817100
C	3.10872400	10.51799000	-1.58535500
H	3.03111100	9.75778000	-2.35766500
C	4.07313900	11.54537200	-1.70326400
C	4.10364800	12.49408600	-0.66288500
C	5.08613900	13.58365700	-0.67130800
C	5.89298400	12.72643300	-2.80082900
C	4.99906900	11.69123800	-2.77861900
C	-2.69732900	13.57525400	9.65043600
C	-1.32572900	13.30995100	9.68722000
C	-0.60528400	13.17942000	8.50074900
C	-1.25156700	13.31564100	7.26133300
C	-2.62924200	13.57267600	7.23209300
C	-3.34720500	13.70476100	8.42252100

H	-3.25635600	13.67759100	10.57624000
H	-0.81670100	13.19831200	10.64033600
H	0.45874900	12.96012300	8.53221100
H	-3.13390200	13.67311400	6.27539300
H	-4.41349700	13.90932600	8.38752100
C	8.61648000	12.95749000	-6.11491900
C	9.09258900	12.61611800	-4.84612700
C	8.21807300	12.55881500	-3.76184100
C	6.85431000	12.84490700	-3.93617000
C	6.38213100	13.17761300	-5.21338100
C	7.26148700	13.23653500	-6.29657900
H	9.30002600	13.00304600	-6.95803600
H	10.14486600	12.38865900	-4.70098800
H	8.58874700	12.28122500	-2.77857400
H	5.32711400	13.39538300	-5.35280300
H	6.88526000	13.50156300	-7.28058100
C	6.78228400	14.88327900	-1.82332100
H	7.12017400	15.07004300	-0.80378800
C	0.59588800	15.37302200	6.27229200
C	-0.22387600	16.49184900	5.62822900
H	1.66038300	15.60587900	6.22812200
H	0.31285800	15.22630100	7.31236400
H	-0.06273800	17.41991900	6.18715100
H	0.08786000	16.66294100	4.59459500
H	-1.29466100	16.26196800	5.65117700
H	7.64702700	14.65773200	-2.44386300
C	6.00870500	16.08790900	-2.36127400
H	6.66505300	16.96474800	-2.35806400
H	5.67306200	15.91496500	-3.38949800
H	5.14157700	16.31074500	-1.73424700

H	-1.44869700	11.26048000	5.59849700
H	5.01451500	10.96972400	-3.58706200
H	1.53555700	9.69972700	-0.40037500
H	0.47679200	9.65251800	1.40746000

[EuL^1(NO$_3$)$_3$]

Atoms	X	Y	Z
Eu	3.54963700	14.39062600	1.95585200
O	2.06282900	14.68935800	3.97693400
O	5.56450900	13.72105300	0.57888700
N	1.86442200	12.37454200	2.66064800
N	3.55311900	12.03247400	0.60387400
N	0.35483000	14.15368500	5.40195200
C	1.20236300	13.87360300	4.34838800
C	1.03472200	12.58098200	3.67649400
O	4.58080000	12.72835100	3.49031200
C	0.04531400	11.65622500	4.09440200
O	5.17677000	14.80368700	3.72687700
N	6.01680000	13.38602000	-1.62100400
C	-0.78367600	12.03765100	5.19836000
O	5.99752700	13.27806600	5.06642400
N	3.76128500	17.22964600	1.54195500

C	-0.62393300	13.24188800	5.82231300
O	4.74138400	16.43188100	1.32015500
N	1.82320300	14.50078800	-0.45994300
O	3.82765600	18.42252600	1.32460300
N	5.28321600	13.59122000	4.13295200
O	2.70067100	16.67422600	2.01276300
O	3.07648500	14.77059200	-0.51027700
O	1.13757300	14.44362000	-1.47046500
O	1.34703400	14.27170900	0.70207600
C	-0.02465200	10.44229900	3.39520200
H	-0.75702000	9.69074300	3.67986800
C	0.85336000	10.19662700	2.33164000
C	1.78797500	11.22328300	1.99178300
C	2.70913900	11.02751600	0.89210200
C	2.70591100	9.80048000	0.18550700
C	1.75608500	8.78257800	0.55436500
H	1.75856100	7.84879300	-0.00148500
C	0.86895500	8.97278100	1.57090500
H	0.15768500	8.19362800	1.83093700
C	3.65992100	9.65981100	-0.84293200
H	3.71362000	8.73115200	-1.40497200
C	4.52799900	10.69919300	-1.12978600
C	4.43373800	11.89190500	-0.38232500
C	5.37181000	13.08245400	-0.47026500
C	-3.16882000	14.13115600	9.16786700
C	-1.81533600	13.85338100	9.37751900
C	-0.97974500	13.58278100	8.29469200
C	-1.49087600	13.58970100	6.98665800
C	-2.85125100	13.86071000	6.78479000
C	-3.68496200	14.13283300	7.87153800

H	-3.81779300	14.34244600	10.01302900
H	-1.41040600	13.84102100	10.38543700
H	0.06966900	13.35442400	8.46155500
H	-3.25181200	13.86106300	5.77503700
H	-4.73663900	14.34605400	7.70244700
C	7.01553400	14.48740600	-1.57910000
H	7.49797900	14.44051800	-0.60180800
C	0.48060900	15.52089200	5.97576300
C	-0.23011800	16.57279400	5.12302200
H	1.54901400	15.73436000	6.03042900
H	0.07766700	15.49419000	6.98587200
H	-0.11517500	17.55393900	5.59614500
H	0.20775600	16.62774100	4.12296800
H	-1.30101700	16.35798000	5.03968700
H	7.75983300	14.25510500	-2.34677200
C	6.40264500	15.86873000	-1.81124600
H	7.20379600	16.61629300	-1.83116500
H	5.87372700	15.91250400	-2.76924400
H	5.71130100	16.13146900	-1.00690200
H	-1.53952300	11.35593800	5.57065000
H	5.26586200	10.59904100	-1.91527900
C	5.54704600	12.97603000	-2.91744000
C	6.41971200	12.30422500	-3.78323900
C	4.24503400	13.29082000	-3.32601600
C	5.98200200	11.92916000	-5.05314600
H	7.42922900	12.07146500	-3.45547200
C	3.81480800	12.89984600	-4.59618400
H	3.58695900	13.84341000	-2.66104200
C	4.67680100	12.22178300	-5.45974800
H	6.65905600	11.40584100	-5.72261100

H	2.80379700	13.14269700	-4.91034500
H	4.33772600	11.92813700	-6.44928100

[EuL^2(NO$_3$)$_3$]

Atoms	X	Y	Z
Eu	3.32161500	14.80282000	1.93022100
O	2.07573700	14.74812900	4.15427400
O	5.16793400	14.48082600	0.20883800
N	1.78240600	12.61299500	2.58284900
N	3.33954500	12.53340200	0.42583900
N	0.44349200	14.04853800	5.59876000
C	1.23075000	13.89612000	4.47302300
C	1.00808900	12.69740200	3.65783400
O	4.68609100	13.05807800	3.05984600
C	0.01532000	11.74540200	3.99719700
O	5.11827300	15.12539500	3.56767600
N	5.91320300	13.70059000	-1.81035700
C	-0.74358800	11.98901200	5.18653900
O	6.21966800	13.51101100	4.55564100
N	3.36281300	17.67468800	1.89924400
C	-0.52586500	13.10002200	5.95212500
O	4.32699500	16.97386300	1.43120700

N	1.30528100	15.11344100	-0.19813900
O	3.36473500	18.88922600	1.87777300
N	5.37666800	13.88474200	3.76111400
O	2.38491000	16.99929800	2.39752300
O	2.54228600	15.37667700	-0.39839200
O	0.46098500	15.24189000	-1.06807100
O	1.01055600	14.68572500	0.97614600
C	-0.13236300	10.64541300	3.13557100
H	-0.87633000	9.88195100	3.34991600
C	0.67297500	10.53979000	1.99571100
C	1.62677400	11.57529500	1.76191900
C	2.47384300	11.53138800	0.58893100
C	2.36383200	10.44705800	-0.33241100
C	1.39175300	9.41350100	-0.05878100
H	1.30718200	8.58875600	-0.76129600
C	0.59197400	9.45740500	1.04197400
H	-0.13302400	8.66783100	1.22044900
C	3.20104300	10.46257400	-1.45319600
H	3.13924700	9.66565700	-2.19040700
C	4.12240200	11.50980100	-1.62687400
C	4.15151900	12.51305700	-0.62690900
C	5.10209700	13.63059100	-0.69079900
C	5.88364800	12.71614600	-2.80453700
C	5.03046500	11.65105700	-2.72387400
C	-2.86153300	13.55784100	9.52914800
C	-1.49507700	13.27950600	9.62121100
C	-0.72709400	13.14955000	8.46494400
C	-1.31944600	13.29907500	7.20025400
C	-2.69221200	13.56986500	7.11579500
C	-3.45816700	13.70117100	8.27603600

H	-3.45773900	13.65981300	10.43152300
H	-1.02731100	13.15718800	10.59399300
H	0.33264000	12.92004700	8.53940800
H	-3.15506900	13.68205500	6.13949600
H	-4.52007500	13.91645000	8.19787200
C	8.55367600	12.88642400	-6.16600800
C	9.06358700	12.66931400	-4.88299300
C	8.20557100	12.63361900	-3.78486800
C	6.82382200	12.81658000	-3.95864700
C	6.31891700	13.02512500	-5.24966800
C	7.18151300	13.06271000	-6.34718300
H	9.22445000	12.91557100	-7.02004500
H	10.12990100	12.52150000	-4.73729300
H	8.60361400	12.45106100	-2.79014600
H	5.25064800	13.16440500	-5.38859600
H	6.77891200	13.23150100	-7.34193100
C	6.69030900	14.96262800	-1.94832100
H	7.04471300	15.21550200	-0.94880400
C	0.60829100	15.34020700	6.31955900
C	-0.13006500	16.48720800	5.62753100
H	1.68013200	15.54136300	6.34887400
H	0.25135700	15.19914300	7.33741600
H	0.00907000	17.40398100	6.21067900
H	0.26729400	16.66290900	4.62449100
H	-1.20469300	16.28455500	5.56306500
H	7.54934800	14.76056500	-2.58451000
C	5.82969600	16.09346700	-2.51454800
H	6.42653600	17.01065600	-2.56092100
H	5.48463500	15.85773100	-3.52719700
H	4.96224700	16.28407200	-1.87680800

H	-1.49203000	11.27479700	5.50965500
H	5.06476000	10.89714800	-3.50164100

[EuL^3(NO$_3$)$_3$]

Atoms	X	Y	Z
Eu	3.56671400	14.32501800	2.00099400
O	2.18491800	14.57332600	4.04927800
O	5.55635700	13.75026800	0.60948200
N	1.93607400	12.24969800	2.71460600
N	3.58468300	11.95965800	0.64322200
N	0.41801900	14.10812100	5.41976700
C	1.28317200	13.78796000	4.38882800
C	1.08010200	12.50702700	3.71225800
O	4.70265900	12.67449400	3.47011600
C	0.03319900	11.64847200	4.09698300
O	5.24139300	14.76401500	3.71939300
N	5.96120100	13.44337800	-1.60301400
C	-0.81073300	12.05603500	5.17368700
O	6.16225400	13.24432400	4.99915500
N	3.64037600	17.18021500	1.60449300
C	-0.61257600	13.24970100	5.81129400
O	4.65202300	16.42898600	1.36396600
N	1.76659200	14.38461100	-0.36669800
O	3.65163100	18.37743000	1.39983200

N	5.40174700	13.54907600	4.09969500
O	2.61042600	16.57352800	2.07964900
O	3.01061700	14.68944900	-0.44741900
O	1.06046200	14.30429600	-1.36178400
O	1.32318800	14.14716600	0.80563800
C	-0.08550300	10.44305700	3.36771900
H	-0.87646400	9.73843900	3.60903200
C	0.80290700	10.17754900	2.34643100
C	1.82212500	11.11247900	2.03452600
C	2.81302900	10.90282400	0.94516500
C	2.96944100	9.67736800	0.28168700
C	3.93829400	9.56839900	-0.71063400
H	4.08888400	8.62466600	-1.22621500
C	4.72006400	10.67585100	-1.03178900
C	4.50350400	11.86262300	-0.32556400
C	5.36586200	13.10501600	-0.43655600
C	-3.20967500	14.24001900	9.08663400
C	-1.87220000	13.91773900	9.33223500
C	-1.01855800	13.61472500	8.27240300
C	-1.49551600	13.63320800	6.95159300
C	-2.84039300	13.94867200	6.71348900
C	-3.69193700	14.25357900	7.77738300
H	-3.87264400	14.47679900	9.91397000
H	-1.49400000	13.89611400	10.35031700
H	0.01785900	13.35188000	8.46732200
H	-3.21445800	13.95913000	5.69369100
H	-4.73094900	14.50189600	7.58035300
C	6.90149700	14.59599900	-1.58832500
H	7.40304000	14.58353100	-0.61971500
C	0.59052000	15.47176300	5.99312100

C	-0.03113200	16.55442200	5.10935400
H	1.66521500	15.63094200	6.09117800
H	0.14528900	15.46970700	6.98556000
H	0.10277900	17.52788200	5.59341400
H	0.45639300	16.59498800	4.13188700
H	-1.10525500	16.38671400	4.97458500
H	7.64317700	14.39593500	-2.36750700
C	6.21263700	15.94080200	-1.82094800
H	6.97305500	16.72882400	-1.86380600
H	5.66315000	15.94706600	-2.76824300
H	5.52478000	16.17521600	-1.00505800
H	-1.60979800	11.40858600	5.51551700
H	5.47893200	10.61746100	-1.80128700
C	5.48856900	12.99922700	-2.88778100
C	6.37964700	12.37054400	-3.76691000
C	4.16412300	13.24094000	-3.27252500
C	5.93891700	11.96465500	-5.02625300
H	7.40669700	12.19538400	-3.45813600
C	3.73178900	12.81996400	-4.53231900
H	3.49049100	13.76202300	-2.59790700
C	4.61245900	12.18404100	-5.40904500
H	6.63056300	11.47479700	-5.70603900
H	2.70349400	13.00653100	-4.82838500
H	4.27097300	11.86668500	-6.39039800
H	0.70289300	9.26174000	1.77530500
H	2.36721600	8.81653600	0.54766400

[EuL^4(NO$_3$)$_3$]

Atoms	X	Y	Z
Eu	3.23732800	14.74486600	1.86505600
O	2.05390300	14.71390000	4.06469100
O	5.12029500	14.40540600	0.26159100
N	1.70283000	12.54066800	2.51546900
N	3.26329600	12.44636300	0.39254400
N	0.46039400	14.04612000	5.55819700
C	1.21305900	13.86766500	4.41014300
C	0.95843400	12.66152300	3.61978400
O	4.57038800	13.03165800	3.08682000
C	-0.02968000	11.73811500	4.01290300
O	5.05396800	15.11457900	3.47089000
N	5.90025400	13.67864800	-1.75905000
C	-0.75537000	11.99958800	5.21397000
O	6.12579600	13.53465200	4.54330300
N	3.21614000	17.62196900	1.78226000
C	-0.50626400	13.11991800	5.95825800
O	4.20060300	16.93503100	1.33704500
N	1.26686600	14.98969700	-0.31893100
O	3.19072800	18.83602900	1.73830700
N	5.28474100	13.88124800	3.73342600
O	2.24878700	16.93417900	2.28373800

O	2.50595900	15.26160300	-0.49488300
O	0.44438000	15.08632600	-1.21393900
O	0.94622500	14.58882800	0.85725100
C	-0.20807800	10.61868400	3.16832100
H	-0.95064300	9.86520700	3.41586300
C	0.56291200	10.49579900	2.03027100
C	1.52353500	11.48991600	1.71741800
C	2.38893100	11.44670100	0.51121000
C	2.32009200	10.42344400	-0.46713400
C	3.15860100	10.46283600	-1.56196200
H	3.10362700	9.69304200	-2.32672000
C	4.09691400	11.51356200	-1.68621600
C	4.10294800	12.46814300	-0.65095600
C	5.06009300	13.57886900	-0.66123900
C	5.88701200	12.73662600	-2.78834000
C	5.02118900	11.67755500	-2.76069300
C	-2.73748400	13.65743700	9.58978700
C	-1.37280800	13.36208900	9.64899600
C	-0.63804800	13.20639000	8.47445300
C	-1.26263100	13.34696000	7.22437700
C	-2.63360800	13.63453000	7.17282300
C	-3.36597600	13.79185500	8.35132300
H	-3.30768700	13.77950300	10.50634900
H	-0.88051400	13.24670300	10.61043600
H	0.42027800	12.96398000	8.52353800
H	-3.12140700	13.73955300	6.20793000
H	-4.42671100	14.02022400	8.29880000
C	8.61417900	13.00991800	-6.09610600
C	9.09892300	12.72233100	-4.81724700
C	8.22266000	12.65256500	-3.73522500

C	6.84797100	12.87179000	-3.92161700
C	6.36784400	13.15071500	-5.20876400
C	7.24885700	13.22248400	-6.28980000
H	9.29915100	13.06549400	-6.93746300
H	10.15965300	12.54635700	-4.66242100
H	8.60082100	12.41601400	-2.74412600
H	5.30486900	13.31769200	-5.35741700
H	6.86588800	13.44591800	-7.28150300
C	6.70310600	14.93133900	-1.82589500
H	7.04489500	15.13192800	-0.81030200
C	0.66732200	15.34541800	6.25582400
C	-0.06765800	16.49639100	5.56669700
H	1.74295200	15.52699400	6.25625600
H	0.33271600	15.22411300	7.28367300
H	0.09840100	17.41629200	6.13776700
H	0.31054100	16.65661900	4.55377100
H	-1.14653700	16.31022800	5.52815900
H	7.56860400	14.73928800	-2.45635800
C	5.87630300	16.10429000	-2.35531600
H	6.49749500	17.00636400	-2.35969100
H	5.53668400	15.91721500	-3.37984800
H	5.00793700	16.29337500	-1.71884300
H	5.05903300	10.95070700	-3.56362000
H	-1.50108700	11.29577800	5.56491900
H	0.42455600	9.63809200	1.38196000
H	1.60496200	9.61461000	-0.37055700