

Electronic Supplementary Information

Ligand Architectural Effect on Coordination, Bonding, Interaction and Selectivity of Am(III) and Ln(III) Ions with Bitopic Ligands: Synthesis, Solvent Extraction and DFT Studies

P. Sinharoy^{a,d}, A.K. Singha Deb^{b,d}, Sk. M. Ali^{b,d*}, J.N. Sharma^{a*}, C.P. Kaushik^c

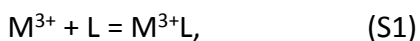
^aProcess Development Division, ^bHomi Bhabha National Institute, Mumbai

^cChemical Engineering Division, ^dWaste Management Division

Bhabha Atomic Research Centre, India, Mumbai 400085

Calculations of Gibbs free energy

The gas phase interaction energy (ΔE) between the M^{3+} ion and ligand (L) was calculated from energy of the optimized geometrics of individual reactant and products as in equation 1.



$$\Delta E = E_{M^{3+}L} - (E_{M^{3+}} + E_L) \quad (S2)$$

where, $E_{M^{3+}L}$, $E_{M^{3+}}$ and E_L refer to the energy of optimized geometric structures of $M^{3+}L$, M^{3+} , and L respectively. The thermal correction to the electronic energy (E_{el}), enthalpy (H) and free energy (G) of the optimized structures has been performed to predict the thermodynamic parameters. The zero point energy (ZPE) corrected binding energy is,

$$\Delta U = U_{Hg^{2+}-L} - (U_{Hg^{2+}} + U_L) \quad (S3)$$

Where U represents the internal energy of the molecular system i.e. $U = E + ZPE$. The binding enthalpy (ΔH) and binding free energy (ΔG) for the metal ion-L complexation reaction in equation (1) are calculated using the following standard thermodynamic relation

$$\Delta H = \Delta U + \Delta nRT. \quad (S4)$$

$$\Delta G = \Delta H - T\Delta S. \quad (S5)$$

Where Δn is the change in the number of moles in reaction in equation (1), R is the universal gas constant (8.314 J/(mol.K), and T is temperature in Kelvin. Entropy, S of individual molecular structure is calculated from the partition functions which is evaluated using the Turbomole software package.

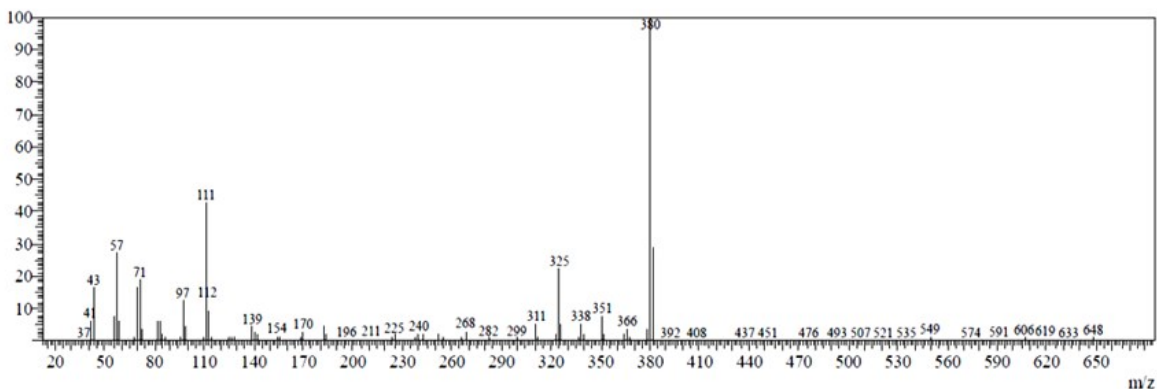


Fig. S1. MS spectrum of PIPDA (2-ethylhexyl)

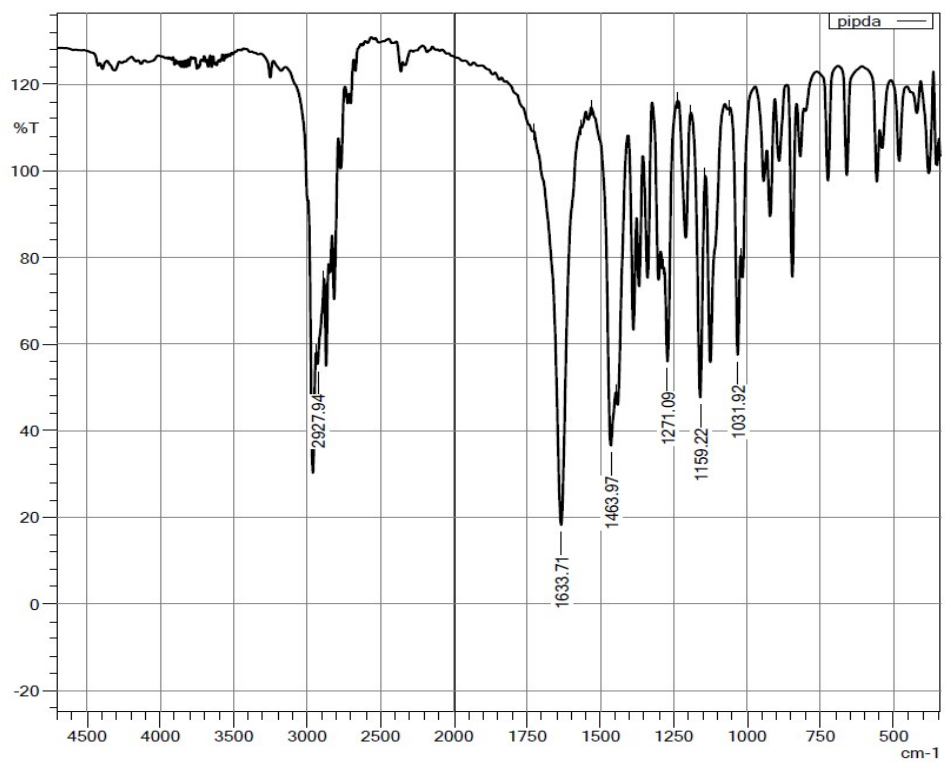


Fig. S2. FTIR spectrum of PIPDA (2-ethylhexyl)

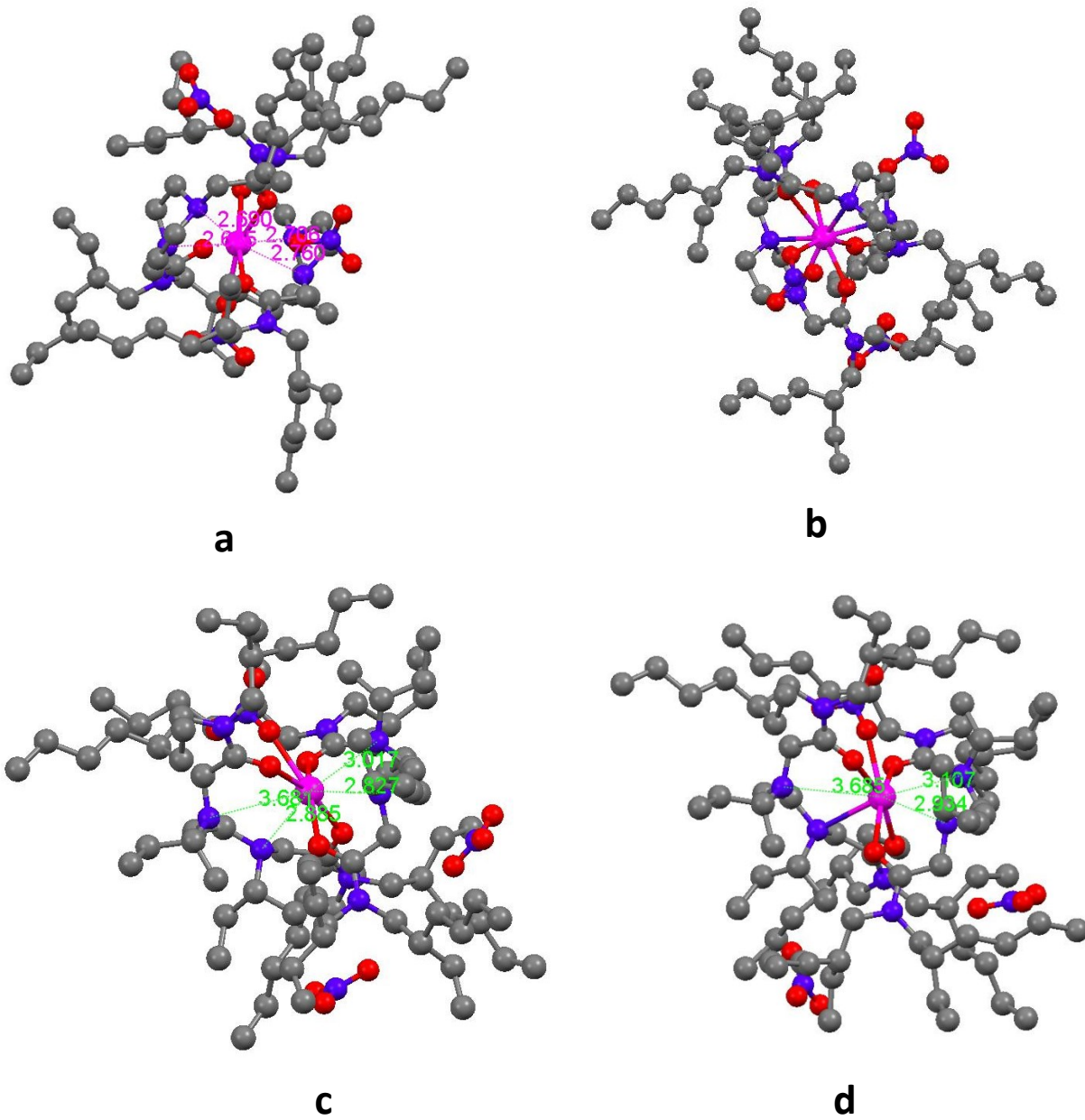
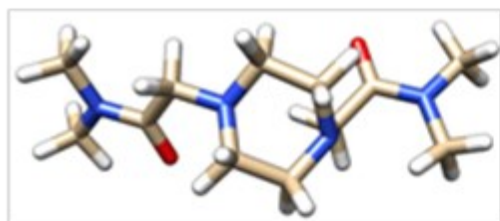
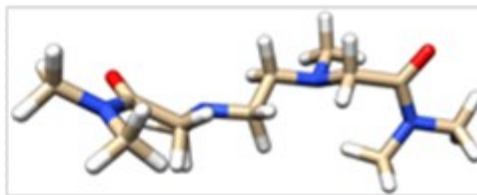


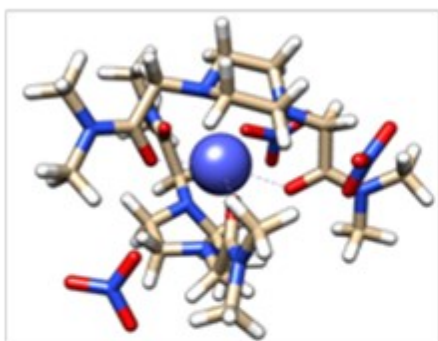
Figure S3. Optimized complexes PIPDA with (a) Am(III) and (b) Eu(III) and DADA with (c) Am(III) and (d) Eu(III) ions (H atoms were removed for better view of coordination).



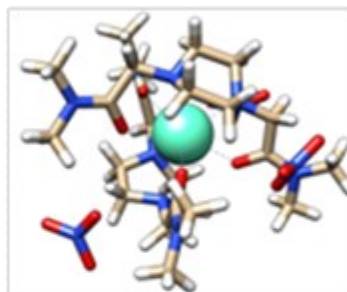
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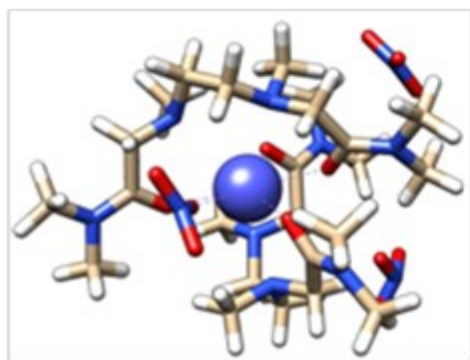
b



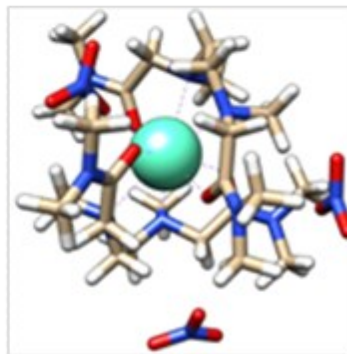
c



d



e



f

Figure S4. Optimized geometries of (a) methyl-PIPDA and (b) methyl-DADA and their complexes with (c) Am(III) and (d) Eu(III) and (e) Am(III) and (f) Eu(III) ions respectively.

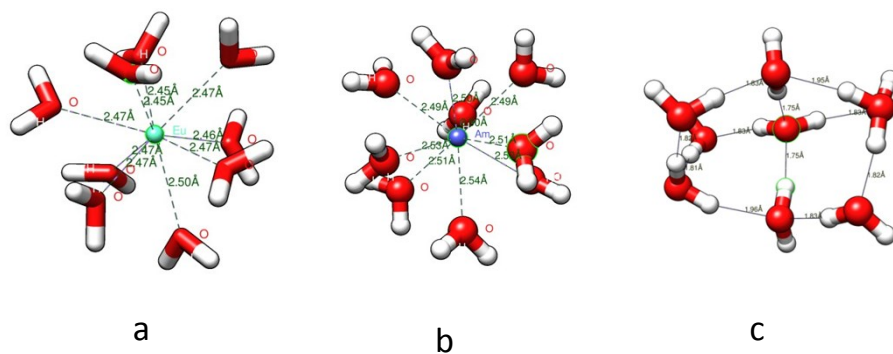


Figure S5. Optimized hydrated cluster of (a) $\text{Eu}^{3+}(\text{H}_2\text{O})_9$ and (b) $\text{Am}^{3+}(\text{H}_2\text{O})_9$ (c) 9-water cluster using COSMO approach.

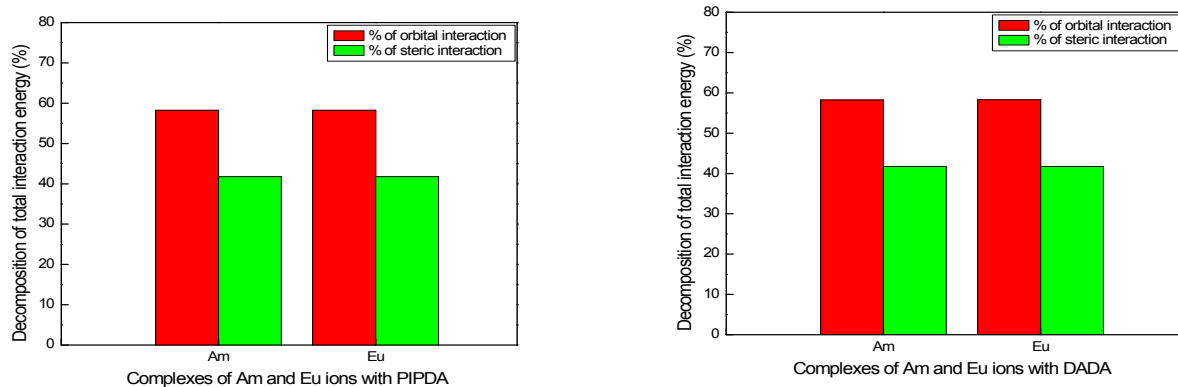


Fig. S6. Decomposition of total interaction energy in terms of orbital and steric contribution.

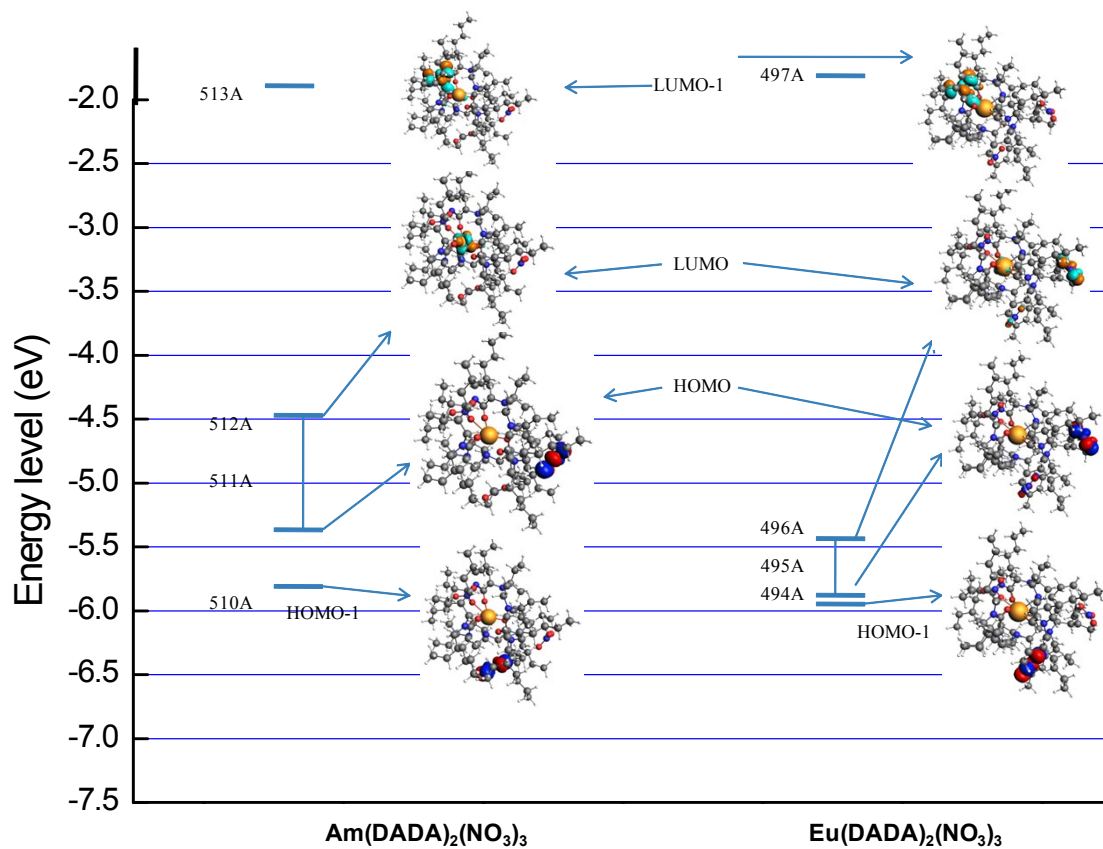


Fig. S7. The calculated energy levels (eV) of the α -spin valence MOs of the $[\text{M}(\text{DADA})_2(\text{NO}_3)_3]$ complexes using B3LYP/TZP/ZORA level of theory.

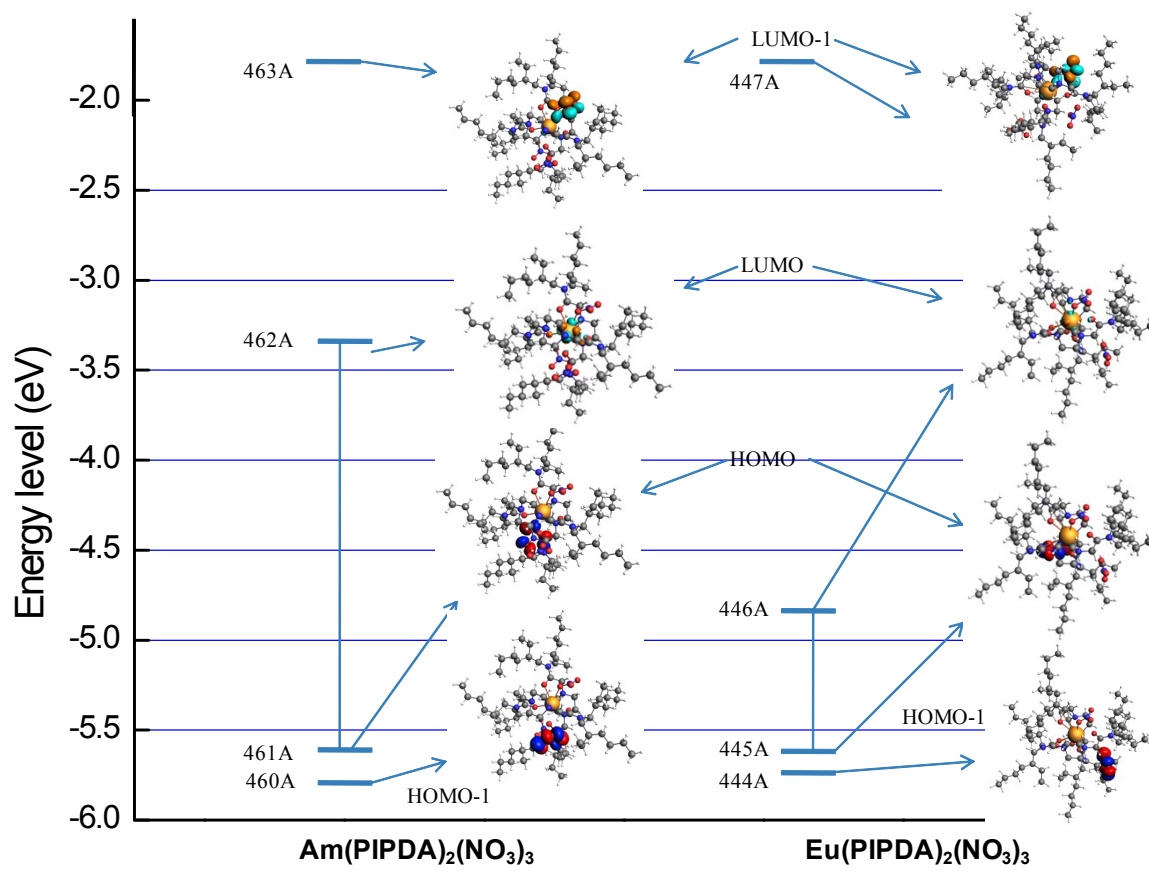


Fig. S8. The calculated energy levels (eV) of the α -spin valence MOs of the $[\text{M}(\text{PIPDA})_2(\text{NO}_3)_3]$ complexes using B3LYP/TZP/ZORA level of theory.

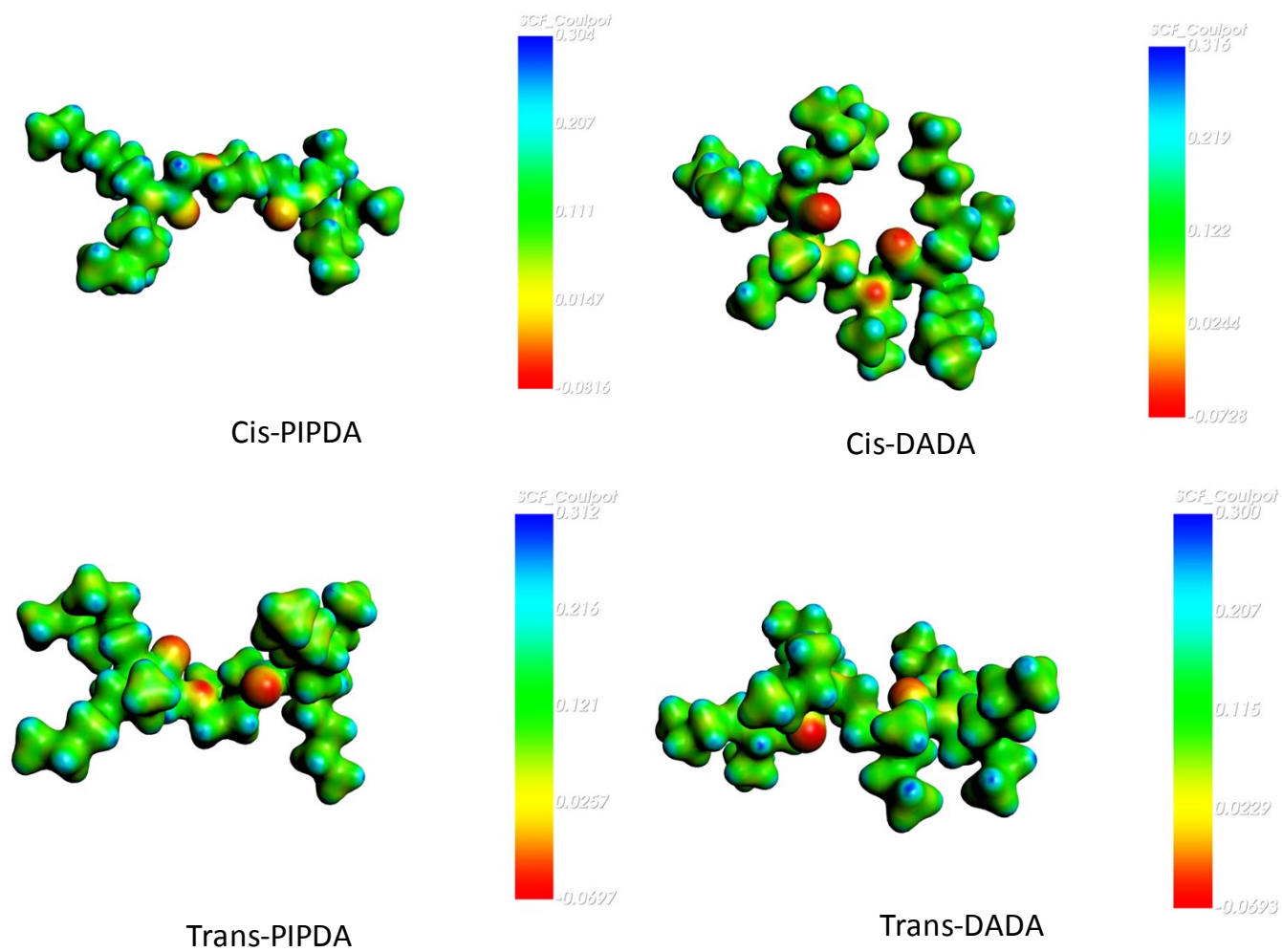


Fig S9 Molecular electrostatic potential of (a) cis-PIPDA (b) trans-PIPDA, (c) cis-DADA and (d)trans-DADA at the B3LYP/TZP level of theory. Colour bar displays the electron density distribution. Red is the high electron density site.

Table S1. Calculated structural parameters (Å) of complexes of Eu^{3+} and Am^{3+} ions at the B3LYP/TZVP level of theory.

System	M-O _{C=O}	M-N _{pip}	M-O _{NO₃}
[Am-(PIPDA) ₂ -NO ₃](NO ₃) ₂	2.388, 2.493 2.376, 2.683	2.685, 2.690 2.706, 2.760	2.463
[Eu-(PIPDA) ₂ -NO ₃](NO ₃) ₂	2.360, 2.465 2.347, 2.659	2.680, 2.747 2.655, 2.675	2.430
[Am-(DADA) ₂ -NO ₃](NO ₃) ₂	2.467, 2.601 2.373, 2.556	2.827, 3.017 2.855	2.446
[Eu-(DADA) ₂ -NO ₃](NO ₃) ₂	2.521, 2.735 2.499, 2.709	2.934, 3.107 2.903	2.412

System	M-O _{C=O}	M-N _{pip}	M-O _{NO₃}
[Am-(Me-PIPDA) ₂ -NO ₃](NO ₃) ₂	2.381, 2.631 2.468, 2.390	2.7134, 2.706, 2.718, 2.712	2.465
[Eu-(Me-PIPDA) ₂ -NO ₃](NO ₃) ₂	2.457, 2.362, 2.608, 2.351	2.679, 2.683, 2.687, 2.684	2.405
[Am-(Me-DADA) ₂ -NO ₃](NO ₃) ₂	2.411, 2.388, 2.527, 2.563	2.757, 2.839, 2.930, 2.744	2.429
[Eu-(Me-DADA) ₂ -NO ₃](NO ₃) ₂	2.444, 2.591, 2.410, 2.529	2.747, 2.799, 2.714, 2.899	2.453

Table S2. Calculated structural parameters (Å) of hydrated cluster of Eu^{3+} and Am^{3+} ions at the B3LYP/TZVP level of theory using COSMO phase.

System	M-O		deviation
	COSMO	Experiments	
$\text{Eu}^{3+}\text{-(H}_2\text{O)}_9$	2.467	2.457 ¹	0.40%
$\text{Am}^{3+}\text{-(H}_2\text{O)}_9$	2.515	2.503 ²	0.47%

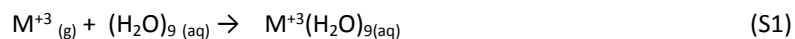
¹ R. Gerkin, W. Reppart, *Acta. Crystallogr. Sect. C: Cryst. Struct. Commun.* 1984, **40**, 781.

² P. Lindqvist-Reis, C. Apostolidis, J. Rebizant, A. Morgenstern, R. Klenze, O. Walter, T. Fanghänel, R. Haire, *Angew. Chem. Int. Ed.*, 2007, **46**, 919.

Table S3 Calculated values of binding energy using optimized geometry in solution phase.

Chemical reaction	BE(kcal/mol)
$Am^{3+} + 2L_I + 3NO_3^- \rightarrow [Am(L_I)_2(NO_3)](NO_3)_2$	-93.4
$Eu^{3+} + 2L_I + 3NO_3^- \rightarrow [Eu(L_I)_2(NO_3)](NO_3)_2$	-79.9
$Am^{3+} + 2L_{II} + 3NO_3^- \rightarrow [Am(L_{II})_2(NO_3)](NO_3)_2$	-50.8
$Eu^{3+} + 2L_{II} + 3NO_3^- \rightarrow [Eu(L_{II})_2(NO_3)](NO_3)_2$	-35.75

The metal ion solvation energy was determined by placing bare gas phase metal ion in cluster of water molecules (9 water units) as:

**Table S4** Calculated free energy of hydration (kcal/mol) for the Ln/An ions at the B3LYP/TZVP level of theory using COSMO solvation model.

Metal ion	COSMO	Exp	Deviation	CCSD	Deviation
Eu ³	-801.08	-803.82 ⁵¹	0.34%	-804.78 ⁵²	0.45%
Am ³⁺	-782.35	-	-	-786.60 ⁵³	0.54%

Table S5 Quantum chemical descriptors of L_I and L_{II} using the value of HOMO and LUMO at the B3LYP/TZVP level of theory.

S.No	Complex	E _{HOMO} (eV)	E _{LUMO} (eV)	ΔE (eV)	χ (eV)	η (eV)	ΔN Am/Eu
Gas Phase							
1	L _I	-5.26	0.55	5.82	2.34	2.91	1.51/1.78
2	L _{II}	-4.78	0.34	5.13	2.22	2.56	1.60/1.89
Solvent Phase							
1	L _I	-5.36	0.24	5.61	2.56	2.80	0.39/0.59
2	L _{II}	-4.89	0.31	5.21	2.28	2.60	0.44/0.66

Table S6 Partial atomic charge on nitrogen and oxygen atoms of free conformers of PIPDA and DADA and their complexes with Am and Eu ions.

Molecular system	N	O	Dipole moment (Debye)
Cis -PIPDA	-0.42, -0.42, -0.43, -0.41	-0.61, -0.61	3.69
Trans-PIPDA	-0.42, -0.42, -0.42, -0.41	-0.61, -0.63	2.60
Cis-DADA	-0.43, -0.43, -0.44, -0.42	-0.61, -0.62	3.46
Trans-DADA	-0.44, -0.44, -0.42, -0.42	-0.63, -0.62	2.28
[Am(PIPDA) ₂ -NO ₃](NO ₃) ₂	-0.437, -0.444, -0.443, -0.445	-0.657, -0.728, -0.648, -0.719	
[Eu(PIPDA) ₂ -NO ₃](NO ₃) ₂	-0.427, -0.430, -0.426, -0.435	-0.656, -0.720, -0.645, -0.709	
[Am(DADA) ₂ -NO ₃](NO ₃) ₂	-0.471, -0.455, -0.432, -0.475	-0.743, -0.688, -0.690, -0.755	
[Eu(DADA) ₂ -NO ₃](NO ₃) ₂	-0.462, -0.449, -0.435, -0.462	-0.719, -0.685, -0.679, -0.731	

Table S7 Contribution (%) of metal, oxygen atoms and nitrogen atoms to the delocalized canonical MOs for complexes [Am(PIPDA)₂-(NO₃)₃] and [Eu(PIPDA)₂-(NO₃)₃].

Atoms	463A	462 A	461 A	460 A	459 A	458 A	457 A	456 A
Am	-	100(f)	-	-	48.96(f)	53.58(f)	18.91(f)	7.46
O	50.70(p)	-	100(p)	100(p)	13.59(p)	17.71(p)	68.75(p)	76.56(p)
N	49.3(p)	-	-	-	37.45(p)	28.71(p)	-	1.29(d)
	447 A	446 A	445 A	444 A	443 A	442 A	441 A	440 A
Eu	3.86(d)	90.58(f)	-	-	-	-	-	-
O	57.37(p)	9.42(p)	100(p)	100(p)	87.58(p)	92.76(p)	79.8(p)	92.74(p)
N	36.67(p)	-	-	-	12.42(p)	1.34(p)	3.15(p)	1.46(p)

Table S8 Contribution (%) of metal, oxygen, and nitrogen atoms to the delocalized canonical MOs for complexes [Am(DADA)₂-(NO₃)₃] and [Eu(DADA)₂-(NO₃)₃].

Atoms	513A	512 A	511 A	510 A	509 A	508 A	507 A	506 A
Am		98.83(f)		-	-	-	-	-
O	50.48(p)	1.17(p)	100(p)	100(p)	100(p)	98.52(p)	77.74(p)	80.84(p)
N	36.62(p)	-	-	-		1.47(d)	5.66(p) 1.08(d)	4.46(p) 1.37(d)
	497 A	496 A	495 A	494 A	493 A	492 A		
Eu		56.69(f)	27.12(f)	10.75(f)	-	-		
O	35.51(p)	36.49(p)	72.88(p)	89.25(p)	-	45.1(p)		
N	64.49(p)	-	-	-	61.33(p)	26.91(p)		

Table S9. Calculated electron density (ρ_c), Laplacian ($\nabla^2 \rho_c$), total energy density (H) and Mayer bond orders of complexes of Am(III)/Eu(III) with DADA at the B3LYP/TZP/ZORA level of theory.

System	Bonds	ρ_c (e/au ³)	$\nabla^2 \rho_c$ (e/au ⁵)	H	Mayer bond order
PIPDA	M-O _{C=O}	0.047/0.032	0.19/0.13	-0.0023 /0.0011	0.25/0.15
	M-O _{NO3}	0.048/0.044	0.21/0.20	-0.0002 /0.001	0.26/0.21
	M-N	0.027/0.020	0.07/0.05	-0.0007 /0.005	0.14/0.09

Table S10. Calculated values total electronic energy, E, zero point energy (ZPE), entropy (S) and RT in gas phase.

Species	E (Hartree)	ZPE(kJ/mol)	S(kJ/mol.K)	RT(kcal/mol)
Am ³⁺	-593.8398269	0	0.1713	0.593
Eu ³⁺	-708.7741891	0	0.1777	
NO ₃ ⁻	-280.3477601	38.08	0.26063	
H ₂ O	-76.42314431	55.23	0.1949	
[Am(H ₂ O) ₉] ³⁺	-1282.503924	577.4	0.72206	
[Eu(H ₂ O) ₉] ³⁺	-1397.458676	580.8	0.69683	
L1	-1941.24725	3021	1.40129	
LII	-2178.208831	3509	1.5824	
[Am(L ₁) ₂ (NO ₃)](NO ₃) ₂	-5319.016943	6190	2.90891	
[Eu(L ₁) ₂ (NO ₃)](NO ₃) ₂	-5433.972966	6184.76	2.8933	
[Am(L _{II}) ₂ (NO ₃)](NO ₃) ₂	-5792.860582	7172	3.27203	
[Eu(L _{II}) ₂ (NO ₃)](NO ₃) ₂	-5907.823673	7168	3.25453	

Coordinates:

[Eu-(H₂O)₉]³⁺

O	-1.4238689	1.9565707	0.4543462
Eu	0.0084031	-0.0135609	0.0191154
O	1.3959326	1.9490752	-0.5440374
O	-0.7444411	1.0416165	-2.1171583
O	2.3993523	-0.5350602	0.3367843
O	-1.5929777	-0.5451866	1.8251677
O	0.7673254	0.8993288	2.1641626
O	-1.9425757	-1.2047325	-0.8954465
O	0.2896807	-2.3384166	0.7473606
O	0.8746059	-1.2579393	-1.9327736
H	-1.2022970	2.8843477	0.2993877
H	-2.2309501	1.9479132	0.9861434
H	-0.5072924	0.7704047	-3.0135742
H	3.1438933	0.0424649	0.1224264
H	2.7645505	-1.3483722	0.7095718
H	-1.3655306	1.7772796	-2.1999454
H	-2.4686708	-0.9433198	1.7345807
H	-1.4573936	-0.3628929	2.7643342
H	0.3882085	1.6560376	2.6305065
H	-2.2108206	-2.1172797	-0.7247955
H	1.6268236	0.7190238	2.5681561
H	-2.4884979	-0.8847748	-1.6261161
H	0.6356705	-3.0717215	0.2213122
H	-0.1376417	-2.7225302	1.5244599
H	1.8103646	-1.4444388	-2.0853735
H	0.3785172	-1.7511872	-2.5994713
H	1.3650674	2.3852471	-1.4060289
H	1.9245626	2.5121034	0.0369052

[Am-(H₂O)₉]³⁺

O	-1.4591333	1.9898220	0.4679395
Am	0.0083235	-0.0185675	0.0256063
O	0.9077510	-1.2696377	-1.9738771
O	1.4209344	1.9748513	-0.5629398
O	-0.7616648	1.0538183	-2.1467204
O	2.4173620	-0.5621541	0.3934891
O	-1.5681151	-0.5787220	1.8824013
O	0.7720257	0.9670302	2.1836073
O	-1.9847261	-1.2174544	-0.9064986
O	0.2726610	-2.4014285	0.7064729

H	-1.2445313	2.9163456	0.2961889
H	-2.2756026	1.9877146	0.9854289
H	-0.5207294	0.7876067	-3.0436945
H	3.1753726	0.0032720	0.1940620
H	2.7643783	-1.3877075	0.7568579
H	-1.3807279	1.7911815	-2.2300381
H	-2.4435750	-0.9827373	1.8183716
H	-1.4223547	-0.3594217	2.8121929
H	0.3851390	1.7298690	2.6333943
H	-2.2601088	-2.1272549	-0.7324264
H	1.6227540	0.7897546	2.6070419
H	-2.5292354	-0.8963984	-1.6378714
H	0.6190958	-3.1264687	0.1695920
H	-0.1340397	-2.7954825	1.4896351
H	1.8442521	-1.4552727	-2.1236939
H	0.4179905	-1.7531145	-2.6524136
H	1.3972711	2.4081789	-1.4266703
H	1.9592342	2.5323768	0.0145592

[(H₂O)₉]

O	-2.5441743	2.1432899	-0.4957474
O	1.7221857	1.0568523	0.3825589
O	-0.4693809	0.4719097	-1.1257226
O	2.5243666	-1.3975120	-0.9218577
O	-2.1646397	0.8760474	1.9527358
O	0.4188006	1.4803091	2.8265108
O	-1.4266760	-1.5088584	0.4841914
O	0.8862669	-3.0869095	0.5867468
O	0.9649258	-0.7225829	-3.1256301
H	-2.4140718	3.0981873	-0.4455995
H	-2.4689198	1.8092680	0.4287723
H	-0.1438133	0.2131891	-2.0159001
H	2.4522371	-0.5725831	-0.4053262
H	2.0017341	-2.0538222	-0.4095681
H	-1.1772754	1.1499885	-1.1900211
H	-2.0238366	-0.0295635	1.6173118
H	-1.2908887	1.1388891	2.3183997
H	0.5585007	2.3902754	3.1167287
H	-2.1775472	-1.9846516	0.1057420
H	0.9690966	1.3720470	2.0202416
H	-1.1312740	-0.8652679	-0.2055947
H	0.7097010	-3.9447442	0.1807620
H	0.0232337	-2.6183785	0.6012397
H	1.6032960	-1.0064634	-2.4299390
H	1.4804305	-0.2193867	-3.7678419
H	0.9239773	0.9831956	-0.1962976

H 2.2015078 1.8403997 0.0828776

Cis-DADA

C -2.0415070 -0.9780954 3.5848906
C -2.4045437 0.4340250 3.0844792
N -0.6100691 -1.2535585 3.6788270
H -2.4843588 -1.0906127 4.5858359
H -2.5624752 -1.7238042 2.9432651
N -3.8417084 0.6647399 3.1917688
H -1.8437926 1.1725096 3.6821504
H -2.0505299 0.5913693 2.0562970
C -4.3091875 1.4166133 4.3613212
H -3.6029183 1.1493305 5.1683265
C -4.2490200 2.9471463 4.1944833
C -5.6948213 0.9286310 4.8363401
C -0.1640999 -2.0111186 4.8588521
H 0.9205398 -2.1624853 4.7234203
C -0.3226123 -1.1860312 6.1432873
C -0.8007217 -3.4188394 4.9667504
C -4.6282119 0.6512498 1.9892625
C 0.0550138 -1.5943054 2.4281856
H 0.5924253 -2.5517690 2.5138064
H -0.6960765 -1.7463599 1.6332066
C -4.4270268 1.8419837 1.0136477
O -3.4624618 2.5841485 1.1294212
N -5.3190284 1.9976505 -0.0292536
C -5.0199580 3.0581174 -1.0007395
C -6.5466402 1.2276022 -0.2122224
C 0.9396574 -0.4569880 1.8658489
O 0.3757462 0.5385363 1.4293461
N 2.3149215 -0.5838391 1.8018908
C 3.0555298 0.5132849 1.1503939
C 3.0949238 -1.6320716 2.4673048
H -5.9521012 3.2861858 -1.5391177
H -4.7295273 3.9609575 -0.4418819
H -6.5708380 0.8452846 -1.2467467
H -6.5154523 0.3375065 0.4295101
C -7.8736089 1.9896441 0.0462142
H 2.3962297 -2.3323367 2.9359136
H 3.6537153 -2.2126466 1.7134569
H 3.9921168 0.6643575 1.7068256
H 2.4504063 1.4216068 1.2739452
H -6.4721656 1.2506981 4.1201739
H -5.6833871 -0.1744858 4.8077149
C -6.0949455 1.4000616 6.2371388
H -3.2625593 3.2600798 3.8241277
H -4.4436702 3.4636056 5.1488075

H	-4.9944896	3.2994134	3.4632833
H	-5.3512028	1.0953630	6.9933351
H	-7.0642983	0.9681416	6.5350590
H	-6.1948904	2.4957569	6.2948378
H	-1.8814450	-3.3140217	5.1668928
C	-0.1723780	-4.3341971	6.0213430
H	-0.7231590	-3.9065035	3.9783618
H	0.1398814	-0.1959269	6.0136697
H	0.1591596	-1.6840263	6.9990916
H	-1.3817763	-1.0344745	6.4074290
H	-0.3220350	-3.9536922	7.0445356
H	0.9151241	-4.4413681	5.8653453
H	-0.6114634	-5.3443328	5.9830312
C	-7.9491569	2.5757117	1.4749313
H	-7.9069784	2.8351947	-0.6664291
C	-9.0352098	1.0373717	-0.3099892
C	-10.4469324	1.6353798	-0.2836667
H	-9.0043895	0.1707560	0.3788780
H	-8.8402543	0.6238902	-1.3155318
C	-11.5573364	0.6611897	-0.7106372
H	-10.6752528	1.9910280	0.7348669
H	-10.4793572	2.5302252	-0.9332323
H	-12.5329086	1.1337572	-0.4997462
C	-11.5225053	0.2387400	-2.1821917
H	-11.5166061	-0.2378616	-0.0680568
H	-8.4286770	1.8406246	2.1479452
H	-6.9240241	2.7078050	1.8559340
C	-8.6558790	3.9308827	1.5924448
H	-9.7045218	3.8925299	1.2609587
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H	-12.3780053	-0.4107983	-2.4289074
H	-11.5689534	1.1161909	-2.8500762
H	-10.6072810	-0.3209657	-2.4354632
C	-3.8930650	2.7259766	-2.0057679
C	-4.2664411	1.5294536	-2.9070662
H	-3.0258055	2.4204617	-1.3969287
C	-3.1439320	0.9734295	-3.8100524
H	-4.5849715	0.7152266	-2.2364726
H	-5.1579848	1.7738898	-3.5136307
H	-3.2695719	-0.1214850	-3.8928137
H	-2.1750867	1.1164302	-3.2992220
C	-3.0473022	1.5321477	-5.2409645
C	-4.2244672	1.1627549	-6.1484257
H	-2.1171369	1.1469885	-5.6959039
H	-2.9327813	2.6290292	-5.2183358
H	-4.0782400	1.5497651	-7.1701873
H	-4.3446426	0.0680564	-6.2218719

H	-5.1790349	1.5730259	-5.7788972
C	-3.4572437	4.0046364	-2.7546263
C	-4.5153579	4.6795905	-3.6348363
H	-2.5714518	3.7698334	-3.3682159
H	-3.1030655	4.7308668	-2.0015628
H	-4.0930804	5.5613755	-4.1438690
H	-4.8999590	4.0057256	-4.4178740
H	-5.3806842	5.0313735	-3.0493377
C	3.4075882	0.3537868	-0.3493786
C	2.1760185	0.4524933	-1.2906073
H	4.0423330	1.2387558	-0.5519279
C	2.3574709	1.4304484	-2.4601219
H	1.9275015	-0.5492664	-1.6879902
H	1.2967940	0.7669856	-0.7087135
C	1.1400904	1.5159791	-3.3847968
H	2.5699202	2.4370242	-2.0525616
H	3.2472493	1.1585404	-3.0568089
C	1.3097171	2.5166170	-4.5296816
H	0.9260989	0.5133467	-3.7994858
H	0.2523076	1.7863123	-2.7848232
H	2.1691758	2.2538200	-5.1700651
H	1.4861023	3.5364848	-4.1472048
H	0.4152542	2.5534661	-5.1728531
C	4.2821544	-0.8872616	-0.6229119
C	4.9103998	-0.9514322	-2.0175643
H	3.6726503	-1.7950405	-0.4641606
H	5.0926132	-0.9255043	0.1279652
H	5.5538466	-1.8407240	-2.1187025
H	4.1488862	-1.0089539	-2.8117414
H	5.5350233	-0.0648715	-2.2196667
C	4.1068994	-1.1544429	3.5397493
C	3.4542493	-0.2726062	4.6182990
H	4.8635628	-0.5319857	3.0288344
C	4.4315512	0.3784352	5.6031810
H	2.8777191	0.5231030	4.1161338
H	2.7071418	-0.8599993	5.1808242
C	3.7575436	1.3592945	6.5687998
H	4.9569386	-0.3964070	6.1909955
H	5.2203033	0.9112695	5.0382702
C	4.7252847	2.0048378	7.5618183
H	3.2460140	2.1468224	5.9859160
H	2.9583988	0.8316406	7.1210932
H	5.5170745	2.5699345	7.0409695
H	5.2232911	1.2467215	8.1904010
H	4.2060120	2.7054734	8.2355560
C	4.8947213	-2.3654696	4.0938385
C	4.1188163	-3.3550876	4.9701925
H	5.7571755	-1.9866689	4.6677889

H	5.3326240	-2.9099785	3.2378269
H	4.7766836	-4.1756805	5.2991892
H	3.7166990	-2.8773877	5.8782175
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H	-4.3896982	-0.2593421	1.4050052

Trans DADA

C	-2.1960487	-0.7744329	3.5040084
C	-2.4899051	0.7275802	3.3008139
N	-0.7716675	-1.0729273	3.6396778
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H	-2.6572625	-1.3343075	2.6697077
N	-3.8984861	1.0381256	3.1632044
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H	-1.9414672	1.0726458	2.4100312
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H	-4.1325860	0.7381045	5.1809052
C	-4.8280074	2.7207719	4.7511030
C	-6.0604938	0.5108520	4.2961929
C	-0.3253504	-1.8003509	4.8321285
H	0.7650204	-1.9266794	4.7160742
C	-0.5275152	-0.9622388	6.1022521
C	-0.9286776	-3.2225339	4.9504518
C	-4.4200808	1.3943857	1.8809385
H	-5.2457970	2.1213026	1.9875492
H	-3.6460318	1.9152920	1.2877354
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H	0.4715821	-2.3088465	2.4523244
H	-0.7544086	-1.4106449	1.5716827
C	-4.9526955	0.1984514	1.0389915
O	-4.9002981	-0.9473331	1.4657307
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C	-6.0390194	-0.6742808	-0.9488362
C	-5.5137515	1.7775869	-0.8376877
C	0.8857894	-0.1700905	1.9928072
O	0.3556860	0.8816088	1.6487492
N	2.2593108	-0.3124868	1.9698819
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H	-6.1473932	-0.3533390	-1.9953082
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H	-6.5433265	1.9999556	-1.1686905
H	-5.2668467	2.5446637	-0.0926500
C	-4.5692476	1.9446039	-2.0569346
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H	3.4599015	-2.0086795	1.5840006

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H	-6.7057571	1.0206297	3.5562218
H	-5.8753631	-0.4966118	3.8923246
C	-6.8078231	0.4133176	5.6284412
H	-3.8332554	3.1884805	4.8244188
H	-5.3369330	2.8566089	5.7190531
H	-5.4070386	3.2772873	3.9938138
H	-6.1956069	-0.0927217	6.3951519
H	-7.7376086	-0.1678299	5.5162719
H	-7.0882115	1.4011383	6.0291702
H	-2.0085644	-3.1419095	5.1660410
C	-0.2627874	-4.1220222	5.9956728
H	-0.8552469	-3.7084600	3.9610944
H	-0.0520377	0.0233786	5.9841277
H	-0.0883533	-1.4544511	6.9842319
H	-1.5968585	-0.7994401	6.3153328
H	-0.3762370	-3.7277784	7.0184952
H	0.8186753	-4.2304474	5.8024017
H	-0.7016954	-5.1329238	5.9871343
C	-3.0976099	1.6186614	-1.7134957
H	-4.9015382	1.2251574	-2.8287675
C	-4.7905046	3.3629516	-2.6235031
C	-4.0551854	3.7066142	-3.9244486
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H	-5.8756364	3.5030274	-2.7774074
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C	-5.8071790	5.2807842	-5.0014879
H	-4.1703627	5.8599140	-3.7036950
H	-2.5782074	2.5424887	-1.3989071
H	-3.0739367	0.9534693	-0.8358004
C	-2.3057026	0.9266368	-2.8286314
H	-2.2343063	1.5385877	-3.7405365
H	-1.2790286	0.7032650	-2.4976639
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H	-5.9515535	6.2853943	-5.4312968
H	-6.0385305	4.5458312	-5.7915880
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C	-7.3795903	-1.2391199	-0.4282721
C	-8.5071679	-0.1877409	-0.4860348
H	-7.2132794	-1.4801927	0.6346828
C	-9.8308930	-0.5737522	0.2108909
H	-8.1196916	0.7190421	0.0061296
H	-8.6993218	0.1087767	-1.5336268
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C	-11.5363215	-0.2786726	-1.7029337
H	-11.7244943	-1.5832893	0.0023655
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H	-12.3296791	-0.7829925	-2.2783441
H	-11.9856568	0.6080197	-1.2233285
H	-10.7889588	0.0841591	-2.4281218
C	-7.6916649	-2.5816951	-1.1261836
C	-7.9023635	-2.5369579	-2.6443130
H	-8.5801615	-3.0290535	-0.6500818
H	-6.8637503	-3.2779836	-0.9018901
H	-8.1435173	-3.5399594	-3.0327816
H	-8.7311411	-1.8694599	-2.9316719
H	-7.0018722	-2.1935476	-3.1796867
C	3.4436521	0.9233318	0.0141554
C	2.2618845	1.2613683	-0.9354408
H	4.1348661	1.7892603	-0.0119607
C	2.5534448	2.4114415	-1.9104894
H	1.9725110	0.3610770	-1.5091345
H	1.3785894	1.5252367	-0.3353967
C	1.3826899	2.7475941	-2.8390363
H	2.8193012	3.3140576	-1.3278551
H	3.4449163	2.1809869	-2.5214310
C	1.6733567	3.9059612	-3.7958080
H	1.1104332	1.8483227	-3.4218817
H	0.4939367	2.9860328	-2.2266931
H	2.5327046	3.6797000	-4.4499037
H	1.9161830	4.8305735	-3.2444631
H	0.8101730	4.1240860	-4.4457615
C	4.2601999	-0.3027752	-0.4430230
C	4.9426189	-0.1636495	-1.8063385
H	3.5967926	-1.1861668	-0.4645835
H	5.0344803	-0.5189417	0.3151356
H	5.5430901	-1.0582694	-2.0388586
H	4.2134460	-0.0389428	-2.6224062
H	5.6198087	0.7068348	-1.8311351
C	4.0835680	-1.2536177	3.5068803
C	3.5442747	-0.5322458	4.7546770
H	4.8496559	-0.5973200	3.0572052
C	4.6161557	-0.0745007	5.7499439
H	2.9658002	0.3482022	4.4269940
H	2.8153271	-1.1795699	5.2741916
C	4.0530930	0.7187454	6.9348810
H	5.1735141	-0.9461503	6.1380367
H	5.3639429	0.5465102	5.2205029
C	5.1252550	1.1937404	7.9169605
H	3.4894659	1.5897525	6.5536218

H	3.3124558	0.0954294	7.4689065
H	5.8548780	1.8585085	7.4235154
H	5.6884846	0.3439351	8.3388356
H	4.6852112	1.7513971	8.7595274
C	4.8206382	-2.5808755	3.8085978
C	4.0329568	-3.6544161	4.5681858
H	5.7384375	-2.3490299	4.3750015
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H	4.6471776	-4.5592628	4.7021978
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C	-5.9017339	0.7375850	-2.2911043
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O	1.2200733	-2.4528883	0.7519223
N	3.3742088	-2.1343908	1.4070379
C	3.7077169	-3.5195764	1.0334308
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H	-5.7320715	2.7140834	0.4985454
C	-6.3696438	3.7535490	-1.2978898
H	4.0500861	-0.3742775	2.3232182
H	5.0372135	-1.7887666	2.6197495
H	4.7230862	-3.5129865	0.6046477
H	3.0153470	-3.8072281	0.2296152
C	-5.0258166	4.4136458	-1.6843425
H	-6.8876419	3.4696652	-2.2335149
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C	-7.8141313	5.9349375	-1.2192714
H	-6.8208456	4.9689234	0.4392712
H	-8.1973216	4.0718122	-0.1967228
C	-8.8054057	6.7819758	-0.4044538
H	-6.9513936	6.5710170	-1.4777891
H	-8.2829655	5.6514396	-2.1806278
H	-8.9790247	7.7282921	-0.9467168
C	-10.1569232	6.1177461	-0.1264498
H	-8.3329801	7.0702428	0.5531345

H	-4.7392156	5.1427642	-0.9040028
H	-4.2381834	3.6425479	-1.6798686
C	-4.9954281	5.0838944	-3.0630947
H	-5.7294310	5.8987406	-3.1561002
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H	-5.2134720	4.3526400	-3.8594343
H	-10.8357050	6.8066739	0.4020600
H	-10.6547993	5.8166615	-1.0643162
H	-10.0592146	5.2159585	0.4995979
C	-6.3181664	-0.7341155	-2.0673619
C	-7.4750314	-0.8503978	-1.0527157
H	-5.4409955	-1.2316715	-1.6219746
C	-7.8263286	-2.2775599	-0.5777590
H	-7.1776095	-0.2673049	-0.1655835
H	-8.3769873	-0.3453740	-1.4447653
H	-8.1440598	-2.2279864	0.4796419
H	-6.9042796	-2.8862013	-0.5766230
C	-8.9252898	-3.0276308	-1.3516885
C	-10.3270630	-2.4309331	-1.1992783
H	-8.9453709	-4.0718767	-0.9920103
H	-8.6675876	-3.0895535	-2.4224221
H	-11.0781229	-3.0318626	-1.7376397
H	-10.6309668	-2.3908302	-0.1390399
H	-10.3872028	-1.4039077	-1.5963499
C	-6.5557716	-1.4308049	-3.4252240
C	-7.6980807	-0.8840362	-4.2890451
H	-6.7195092	-2.5067159	-3.2462548
H	-5.6142954	-1.3746551	-3.9998440
H	-7.7948563	-1.4677255	-5.2189623
H	-8.6713336	-0.9303801	-3.7735699
H	-7.5314075	0.1649794	-4.5843516
C	3.6527574	-4.6071173	2.1355297
C	2.2205784	-4.8691718	2.6782462
H	3.9732671	-5.5213117	1.5971061
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H	2.1463481	-4.5113433	3.7221230
H	1.4982831	-4.2721842	2.1028003
C	0.3849674	-6.5849517	3.1961735
H	1.7994064	-6.6728055	1.5627706
H	2.5115830	-6.9805090	3.1453922
C	-0.0818301	-8.0370432	3.0782558
H	0.3740195	-6.2791475	4.2589939
H	-0.3382228	-5.9219776	2.6872230
H	0.6049527	-8.7250759	3.6008401
H	-0.1280643	-8.3582056	2.0236770
H	-1.0855541	-8.1776878	3.5117331
C	4.6865060	-4.3807868	3.2577130
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H	5.1973419	-6.4734749	3.6471253
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H	5.8107494	-1.7574033	0.2292383
C	5.7157775	0.3630121	-1.5570917
H	3.9129556	-0.4455079	-0.7066261
H	4.4937171	1.0069372	0.1056435
C	5.0043818	1.1862379	-2.6375972
H	6.6226954	0.9071575	-1.2364761
H	6.0751101	-0.5858273	-1.9985691
C	5.8884485	1.5078841	-3.8436101
H	4.1025014	0.6433976	-2.9747614
H	4.6358015	2.1277522	-2.1898520
H	6.2394037	0.5878143	-4.3411518
H	6.7827557	2.0810605	-3.5445041
H	5.3469498	2.1054439	-4.5947624
C	6.7404872	-0.2232285	1.3788997
C	6.5591570	1.1108267	2.1114366
H	7.5105398	-0.0998775	0.5991607
H	7.1568972	-0.9652762	2.0840402
H	7.5157551	1.4484999	2.5416893
H	6.2072466	1.9094007	1.4383680
H	5.8398099	1.0385813	2.9440453
C	-2.0178647	-0.1441603	1.3073738
C	-0.6619445	-0.3603586	1.9749565
N	0.4105621	0.1315529	1.1216318
C	0.2371224	1.5398239	0.8077177
C	-1.1072858	1.7618508	0.1144270
N	-2.1888793	1.2625033	0.9528097
H	-2.0912883	-0.8068416	0.4250493
H	-0.6499170	0.1570248	2.9649315
H	0.2842207	2.1827663	1.7196677
H	-1.2546710	2.8445192	-0.0468037
H	-1.0859470	1.2692299	-0.8777648
H	1.0468725	1.8614617	0.1314801
H	-2.8168187	-0.4281117	2.0144425
H	-0.5143184	-1.4356897	2.1431089
C	1.7377601	-0.2394292	1.5429184
H	2.4551251	0.4278466	1.0450511
H	1.9019622	-0.0972823	2.6391862

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C	-3.8322553	1.3904716	1.4656912
H	-4.6814060	1.5376840	2.1778306
H	-3.6909427	2.3584983	0.9675827
C	0.0995485	-0.2783826	1.6026717
H	0.0828268	-1.3759196	1.6901510
H	-0.6500018	-0.0016115	0.8431585
C	-4.2661933	0.3316800	0.4311926
O	-3.8106665	-0.8038039	0.4610371
N	-5.2074509	0.6919538	-0.5061352
C	-5.6175639	-0.3455939	-1.4614568
C	-5.7459832	2.0376571	-0.6870447
C	1.4485373	0.1977899	1.0395621
O	1.4499105	1.0863464	0.1915279
N	2.6157183	-0.3930671	1.4717004
C	3.8741366	0.0554169	0.8539596
C	2.6790043	-1.3223092	2.6040511
H	-6.0696410	0.1651728	-2.3247279
H	-4.7112009	-0.8594398	-1.8172822
H	-6.8401009	1.9562076	-0.7978976
H	-5.5897379	2.6181109	0.2324094
C	-5.1990316	2.8388747	-1.8993236
H	1.6549739	-1.5114971	2.9381353
H	3.0917053	-2.2875426	2.2656930
H	4.6458550	0.0865857	1.6385648
H	3.7086506	1.0869716	0.5144138
C	-3.6604968	2.9840554	-1.8703169
H	-5.4643341	2.2706863	-2.8110438
C	-5.9671068	4.1779465	-1.9439087
C	-5.6901629	5.1009391	-3.1366098
H	-5.7539818	4.7350475	-1.0109267
H	-7.0474980	3.9499770	-1.9115915
C	-6.5411454	6.3819098	-3.1544195
H	-4.6276986	5.3947350	-3.1319797
H	-5.8491933	4.5453418	-4.0798481
H	-6.1453783	7.0501164	-3.9394072
C	-8.0378024	6.1680800	-3.3990502
H	-6.3971399	6.9240567	-2.2013690
H	-3.3889444	3.8916993	-1.2987481
H	-3.2334795	2.1368275	-1.3106942
C	-2.9710232	3.0045339	-3.2401871
H	-3.2944797	3.8467062	-3.8700812
H	-1.8778193	3.0769135	-3.1235293
H	-3.1800542	2.0762347	-3.7984308
H	-8.5722484	7.1304558	-3.4515257
H	-8.2147862	5.6379879	-4.3507359
H	-8.5133938	5.5773725	-2.5989672
C	-6.5901965	-1.4094467	-0.9045569
C	-7.9276559	-0.7862319	-0.4518749

H	-6.1025573	-1.8241077	-0.0065774
C	-8.8928948	-1.7240198	0.3066223
H	-7.6764943	0.0509771	0.2196622
H	-8.4442286	-0.3255298	-1.3136908
H	-9.4216605	-1.1362711	1.0785946
H	-8.2970394	-2.4681726	0.8650660
C	-9.9611857	-2.4544351	-0.5269057
C	-11.0325729	-1.5385011	-1.1249534
H	-10.4557753	-3.1979640	0.1234035
H	-9.4857352	-3.0375726	-1.3334204
H	-11.7864138	-2.1167343	-1.6836670
H	-11.5622277	-0.9759349	-0.3368894
H	-10.6059264	-0.8001905	-1.8245079
C	-6.7131564	-2.5824609	-1.9024934
C	-7.3067838	-2.2554002	-3.2777210
H	-7.3059766	-3.3853340	-1.4329746
H	-5.7052565	-3.0125500	-2.0421355
H	-7.3690389	-3.1631652	-3.8996594
H	-8.3251785	-1.8402168	-3.2054694
H	-6.6928923	-1.5277326	-3.8332404
C	4.4198676	-0.7716752	-0.3373030
C	3.5147606	-0.7033340	-1.5974047
H	5.3709341	-0.2598926	-0.5867794
C	4.2606969	-0.3961412	-2.9038107
H	2.9613324	-1.6546841	-1.7089842
H	2.7472172	0.0709558	-1.4514583
C	3.3478448	-0.3577815	-4.1334910
H	4.7706789	0.5811282	-2.8033847
H	5.0646742	-1.1347982	-3.0736582
C	4.0813784	-0.0154026	-5.4317917
H	2.8440696	-1.3363790	-4.2415095
H	2.5391897	0.3753589	-3.9600406
H	4.8757805	-0.7496633	-5.6501431
H	4.5595614	0.9774716	-5.3728685
H	3.3959786	-0.0020477	-6.2951066
C	4.7878181	-2.2139441	0.0679404
C	5.6045491	-2.9983898	-0.9621461
H	3.8592736	-2.7725587	0.2838268
H	5.3549961	-2.1831690	1.0162120
H	5.8695971	-3.9961944	-0.5757603
H	5.0489950	-3.1494665	-1.9011106
H	6.5451271	-2.4790476	-1.2130002
C	3.5050286	-0.8527984	3.8265581
C	3.0486481	0.5213733	4.3469214
H	4.5570224	-0.7483193	3.5033369
C	3.8720252	1.0859239	5.5095582
H	3.0904082	1.2377533	3.5079686
H	1.9822018	0.4714555	4.6242812

C	3.4753028	2.5158459	5.8940065
H	3.7716198	0.4390469	6.4000648
H	4.9473254	1.0669658	5.2466519
C	4.2697621	3.0782961	7.0739783
H	3.6008026	3.1754281	5.0157049
H	2.3955136	2.5386503	6.1312466
H	5.3514141	3.0987658	6.8564265
H	4.1296216	2.4656787	7.9809162
H	3.9610470	4.1079724	7.3177839
C	3.5191994	-1.9666172	4.9009657
C	2.1946680	-2.2465698	5.6196350
H	4.2848275	-1.7149151	5.6536336
H	3.8752941	-2.8991910	4.4263434
H	2.3229754	-3.0475589	6.3656829
H	1.8191728	-1.3588535	6.1529704
H	1.4012409	-2.5722671	4.9279383
C	-2.6949085	0.0205096	3.1468176
C	-1.2699318	-0.3686589	3.6507239
N	-0.1919738	0.2848811	2.9231306
C	-0.3671688	1.7333882	2.9542419
C	-1.8118749	2.1920401	2.5729125
N	-2.5953668	1.0530002	2.1261671
H	-3.2002807	-0.8449378	2.7019709
H	-1.1667762	-0.0968073	4.7167598
H	-0.1257135	2.0898120	3.9715289
H	-2.2878015	2.7100468	3.4410787
H	-1.7656126	2.9279924	1.7543744
H	0.3614542	2.1900292	2.2706201
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H	-0.2144446	-5.4240586	14.2040924
C	-0.4473689	0.8456005	12.1275485
O	-0.8667206	0.6079424	13.2717040
N	-0.7478370	2.0018809	11.4897644
C	-1.5623643	2.9965422	12.2056609
C	-0.3395452	2.3226279	10.1139787
C	0.1087873	-4.2142304	15.9708547
O	0.1182762	-2.9779163	16.2266984
N	-0.1448404	-5.1287855	16.9096041
C	-0.2856569	-4.7056205	18.3160064
C	-0.2686344	-6.5703445	16.6355276

H	-1.9752158	3.6828503	11.4502767
H	-2.4141119	2.4712449	12.6624484
H	0.0472801	3.3503409	10.1244714
H	0.5105790	1.6891423	9.8274113
H	-0.3367625	-6.7310452	15.5546180
H	-0.3372211	-3.6116307	18.3094289
H	0.6440446	-4.9801320	18.8416155
C	-2.0685298	0.6775756	16.4274094
C	3.1550831	-0.7229236	17.2290651
H	3.8044466	0.1234580	17.4995024
H	3.2723201	-1.4846106	18.0250677
C	-2.7190072	-0.5256680	15.7239654
O	-1.9693725	-1.2786897	15.0761262
N	-4.0508988	-0.7113808	15.7634225
C	-4.6342209	-1.8470219	15.0075967
C	-4.9913061	0.1341762	16.5129668
C	3.6555422	-1.3410994	15.9300561
O	2.8410720	-1.5567030	14.9951017
N	4.9641466	-1.6030773	15.7904301
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H	-3.9666639	-2.7178626	15.0988163
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H	6.1190271	-1.1355008	14.1114029
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N	2.9636153	1.1262111	13.7184489
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N	-3.0084140	-5.6322343	14.1851142
O	-4.1761947	-5.8368061	13.8372416
O	-2.7279597	-4.6361415	14.9258101
O	-2.0813662	-6.3867400	13.8043105
N	3.2410665	-3.9362308	18.6737822
O	2.9031088	-4.9622879	19.2815259
O	3.6919982	-2.9449483	19.3016494
O	3.1206611	-3.8646284	17.4158558
C	-0.5580645	-0.4508562	17.9654944
C	0.9225652	-0.8133026	18.2324842
N	1.7530178	-0.2775053	17.1397804
C	1.6286690	1.1936886	17.1445370
C	0.1521879	1.5967921	16.9023604
N	-0.6723948	0.3856575	16.7502246
H	-0.9957666	0.0895382	18.8287394
H	1.2567133	-0.4042480	19.2054980

H	1.9791550	1.5937568	18.1172120
H	-0.2279156	2.2234138	17.7352541
C	1.6564999	-3.5387218	12.7069548
C	1.6730553	-2.2440429	11.8524246
N	0.4763845	-1.4355803	12.1566244
C	-0.7343859	-2.2369625	11.8968321
C	-0.7466794	-3.4712582	12.8223703
N	0.5025544	-3.5100853	13.6211686
H	1.6129686	-4.4351625	12.0575962
H	2.5578087	-1.6328585	12.0793348
H	-1.6169978	-1.6104155	12.0835421
H	-1.5934085	-3.4498884	13.5213171
H	2.5730473	-3.6009826	13.3076585
H	-0.8442508	-4.4042119	12.2384909
H	-0.7594297	-2.5358690	10.8290627
H	1.7023784	-2.4917356	10.7721180
H	2.2686710	1.6065708	16.3551786
H	0.0682177	2.1862376	15.9788134
H	1.0519777	-1.9000039	18.2664151
H	-1.1457983	-1.3656155	17.8089224
H	-2.0925814	1.5058237	15.6995715
H	-2.6216113	1.0054202	17.3231736
H	-1.2502576	-6.8808154	17.0219793
H	-5.8270141	0.3613801	15.8367150
H	-5.5746386	-2.1037339	15.5152863
Am	0.5037098	-1.1015655	14.8202214
C	6.3253878	-3.2739191	14.4170749
H	7.1439591	-3.1834844	15.1542777
C	7.0355313	-0.4927004	16.7730351
H	7.6075849	-0.7380551	15.8586362
C	7.0322563	-3.3901613	13.0455371
H	7.7544792	-4.2233280	13.0943479
H	7.6448483	-2.4825359	12.8930529
C	6.1385379	-3.5903866	11.8143877
H	5.5405337	-4.5123966	11.9298790
H	5.4099265	-2.7626925	11.7313425
C	6.9329842	-3.6774062	10.5059785
H	7.5373157	-2.7594692	10.3872604
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C	6.0564627	-3.8745811	9.2679162
H	5.4677000	-4.8054340	9.3361776
H	5.3434930	-3.0411511	9.1443837
H	6.6605120	-3.9318668	8.3479141
C	5.4943420	-4.5078338	14.8132488
H	4.9703076	-4.2998882	15.7614747
H	4.6928379	-4.6622326	14.0681464
C	6.3067809	-5.7959800	14.9628990
H	6.7655701	-6.1216303	14.0146326

H	7.1208047	-5.6713619	15.6978021
H	5.6691224	-6.6200395	15.3183479
C	-5.5757587	-0.4762786	17.8096680
H	-6.0729711	-1.4225954	17.5284572
C	-6.6610512	0.4851290	18.3617810
H	-6.2296073	1.0975124	19.1755215
H	-6.9458338	1.2094614	17.5765083
C	-7.9460652	-0.1912164	18.8578556
H	-7.7056833	-0.9331349	19.6382287
H	-8.3937836	-0.7673465	18.0262891
C	-8.9826221	0.7965164	19.4019065
H	-8.5348750	1.3708302	20.2342259
H	-9.2195407	1.5405510	18.6191174
C	-4.4783066	-0.8156087	18.8342176
H	-3.7118435	-1.4321900	18.3349125
H	-3.9751940	0.1225001	19.1377756
C	-4.9502268	-1.5573791	20.0864825
H	-5.6383548	-0.9505470	20.6964557
H	-5.4685396	-2.4948242	19.8252260
H	-4.0940786	-1.8232805	20.7266642
C	-10.2730483	0.1280262	19.8795522
H	-10.0745794	-0.5938346	20.6896295
H	-10.9939208	0.8680781	20.2626282
H	-10.7662637	-0.4236892	19.0613602
C	-4.9054503	-1.5818389	13.5087774
H	-3.9208969	-1.3989620	13.0406763
C	-5.7710974	-0.3312507	13.2545384
H	-6.7326445	-0.4289139	13.7920659
H	-5.2667436	0.5481825	13.6940682
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H	-4.7960542	-3.7118631	13.0990006
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H	-6.9546028	-3.4964377	14.3548041
H	-7.6436184	-2.5169875	13.0337173
H	-7.1718581	-4.2082940	12.7569791
C	-6.0649586	-0.0166849	11.7833093
H	-6.6382473	-0.8425915	11.3278204
H	-5.1138465	0.0335929	11.2196728
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H	-7.7674468	1.2521888	12.1924909
H	-6.2532817	2.1318711	12.0016577
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H	-7.8308300	0.7855674	9.7051880
H	-7.7554231	2.5323519	10.0320785
H	-6.2984220	1.6594680	9.5018437
C	-0.8374621	3.8147995	13.3010612
H	-0.4240781	3.0856526	14.0182904

C	-1.9209635	4.6514640	14.0156038
H	-2.4064447	5.3102186	13.2693151
H	-2.7175327	3.9613003	14.3535764
C	-1.4938065	5.5068515	15.2135529
H	-0.9320323	4.8861333	15.9360132
H	-0.7951820	6.2951887	14.8862283
C	-2.6792839	6.1669138	15.9279738
H	-3.2534762	6.7659126	15.1972956
H	-3.3746900	5.3821722	16.2798904
C	0.3415964	4.6420736	12.7396633
H	-0.0456254	5.5931931	12.3271368
H	0.7769698	4.0999316	11.8859706
C	1.4920106	4.9147886	13.7169731
H	2.2895879	5.4922114	13.2220634
H	1.1760153	5.4870697	14.6011210
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C	-1.4482612	2.2182950	9.0408964
H	-2.2940337	2.8537181	9.3683790
C	-0.9302770	2.7875314	7.7021053
H	-1.6589150	2.5394114	6.9128670
H	-0.0017827	2.2534496	7.4273438
C	-0.7001708	4.3057358	7.6664649
H	0.1077997	4.5943533	8.3634116
H	-1.6128808	4.8080860	8.0357180
C	-0.3635696	4.8625875	6.2737315
H	-0.3575538	5.9650785	6.3325007
H	-1.1801320	4.6045622	5.5741884
C	0.9730888	4.3886863	5.6965395
H	0.9913386	3.2994048	5.5294586
H	1.1790518	4.8693403	4.7265236
H	1.8100568	4.6345340	6.3723423
C	-1.9820398	0.7803393	8.8931403
H	-1.1863027	0.1439939	8.4621441
H	-2.1890275	0.3761093	9.8987628
C	-3.2544324	0.6418804	8.0529073
H	-4.0697581	1.2644678	8.4580172
H	-3.1008006	0.9377078	7.0032188
H	-3.6075179	-0.4013165	8.0479887
C	-1.5116825	-5.2566005	19.0724967
H	-1.4296784	-6.3579123	19.1148097
C	-1.3962233	-4.7456145	20.5255106
H	-1.4696822	-3.6404444	20.5177872
H	-0.3775620	-4.9693396	20.8906541
C	-2.4045019	-5.2993213	21.5371257

H	-2.3882986	-6.4047428	21.5068499
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H	-2.1484837	-3.7254190	23.0012582
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C	-3.1348245	-5.3795771	23.9921553
H	-2.9161064	-5.0183202	25.0103341
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H	-3.1143453	-6.4822981	24.0200104
C	-2.8401264	-4.8942346	18.3664275
H	-3.1763502	-3.9052018	18.7318415
H	-2.6592833	-4.7693565	17.2863708
C	-3.9745353	-5.9146395	18.5176493
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H	-4.8542635	-5.6060301	17.9299873
H	-3.6683332	-6.9027871	18.1339691
C	0.8207771	-7.4669451	17.2592023
H	0.8540926	-7.2523971	18.3423657
C	0.4043631	-8.9513019	17.0806599
H	-0.6593896	-9.0094907	16.7858707
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C	0.5978742	-9.8293052	18.3239553
H	1.6449503	-9.7677150	18.6682337
H	-0.0108248	-9.4193651	19.1522639
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H	-0.8234119	-11.3582174	17.7525797
H	0.8371678	-11.7091179	17.2803312
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H	1.4404601	-12.1572927	19.7053146
H	-0.2354550	-11.8077868	20.1809014
H	0.1211260	-13.2176647	19.1555908
C	2.2159830	-7.1485728	16.6915795
H	2.2087296	-7.3674599	15.6055440
H	2.4098507	-6.0713013	16.8130468
C	3.3692269	-7.8998807	17.3588149
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H	3.2994914	-8.9926397	17.2288097
H	4.3346810	-7.5805157	16.9346503
C	6.4610491	0.9262623	16.5999942
H	5.6800750	0.9033313	15.8210117
H	5.9468347	1.2139181	17.5373433
C	8.0004118	-0.6448824	17.9769380
H	7.6810768	0.0403477	18.7827354
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C	9.4841818	-0.4265334	17.6631072
H	9.6872824	0.5828123	17.2743630
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H	9.8396564	-1.1477201	16.9075176

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[Eu-(PIPDA)₂NO₃](NO₃)₂

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N	-0.7402988	2.0081972	11.5409838
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C	0.0805880	-4.2025561	15.9837649
O	0.0950509	-2.9641495	16.2243925
N	-0.1752513	-5.1075689	16.9315866
C	-0.3039651	-4.6700685	18.3342177
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H	-0.4208202	-6.7243710	15.6007628
H	-0.3627069	-3.5769644	18.3154983
H	0.6313304	-4.9356399	18.8543460
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C	3.1185645	-0.7925148	17.2230264
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H	3.2324464	-1.5635910	18.0096240
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C	-4.6378036	-1.8558462	14.9465541
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C	-0.5899675	-0.4898942	17.9492917
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[Am-(DADA)₂NO₃](NO₃)₂

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H	1.9569225	-1.8941795	4.0862256
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[Eu-(DADA)₂NO₃](NO₃)₂

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H	-5.7352597	-2.5734086	2.9262649
C	-7.0743884	-2.5454497	1.2325345
H	-7.0652516	-2.3512202	0.1463462
H	-7.4749433	-3.5612033	1.3792007
H	-7.7885554	-1.8426436	1.6888772
C	0.9466585	6.0675180	-1.7692806
H	1.6621480	6.2885504	-0.9596564
H	0.0823232	6.7315337	-1.5920923
C	1.5914531	6.4332040	-3.1094879
H	0.9362008	6.1795800	-3.9596832
H	1.8001848	7.5137315	-3.1639290
H	2.5483153	5.9099874	-3.2625501
C	1.6414494	3.6072565	-1.8167100
H	2.0567548	3.6577477	-2.8354623
H	2.4701942	3.8191671	-1.1223386
H	1.2819717	2.5850796	-1.6394794
C	2.8018492	3.7083786	2.4925490
H	2.9768307	3.3646433	3.5241191
H	2.2835603	4.6766407	2.5700356
C	4.1689854	3.9383103	1.8378606
H	4.8217936	3.0613998	1.9472746
H	4.0741776	4.1786700	0.7641681
H	4.6851449	4.7846504	2.3184401
C	2.5349520	1.2986292	1.7629864
H	3.5416925	1.3469446	1.3372384

H	2.6765483	0.9242624	2.7838080
H	1.9439573	0.5781830	1.1878253
C	-5.9299547	3.5089094	-2.3527870
H	-5.8821177	4.4666003	-1.8055501
C	-6.3099893	2.4439008	-1.2965036
H	-5.4731064	2.3582956	-0.5870310
H	-7.1501564	2.8343721	-0.6953998
C	-6.6852030	1.0436778	-1.8301271
H	-6.1507545	0.8372089	-2.7756833
H	-6.3129440	0.2869788	-1.1198557
C	-7.0267216	3.6689140	-3.4286814
H	-7.0062406	2.8022891	-4.1144027
H	-8.0019905	3.6200077	-2.9175053
C	-8.1850273	0.7798836	-2.0349585
H	-8.6161280	1.5231274	-2.7252821
H	-8.7055861	0.9309027	-1.0715103
C	-8.4817105	-0.6243203	-2.5638524
H	-8.1051728	-1.4016714	-1.8774789
H	-9.5637591	-0.7910172	-2.6898622
H	-8.0041234	-0.7939979	-3.5443359
C	-6.9935319	4.9622544	-4.2443585
H	-7.0515669	5.8501180	-3.5922822
H	-6.0825836	5.0554150	-4.8552445
H	-7.8473389	5.0096145	-4.9392392
C	-2.5164521	6.1379295	-3.7066424
H	-1.5678000	6.1391356	-3.1463476
C	-2.8572002	7.6139650	-3.9968398
H	-3.8221249	7.6747381	-4.5330330
H	-3.0267045	8.1260887	-3.0314491
C	-1.7940472	8.3933913	-4.7790211
H	-1.6695282	7.9577219	-5.7865871
H	-0.8136853	8.2800978	-4.2798146
C	-2.1162518	9.8854936	-4.9198888
H	-3.1127501	9.9999995	-5.3852481
H	-2.2035348	10.3336763	-3.9129831
C	-1.0798026	10.6591949	-5.7364411
H	-1.0144576	10.2760178	-6.7689752
H	-1.3291299	11.7308179	-5.7952724
H	-0.0738002	10.5761926	-5.2909612
C	-2.2513127	5.2865122	-4.9690804
H	-1.2788704	5.5964734	-5.3883591
H	-2.1070282	4.2379714	-4.6552521
C	-3.2955904	5.3435843	-6.0877192
H	-4.2957378	5.0366457	-5.7456628
H	-3.3925603	6.3540888	-6.5151815
H	-3.0144425	4.6672602	-6.9106270
C	-4.6837951	3.4253368	5.3711545
H	-4.7023663	3.5145107	4.2758621

C	-4.4618594	-1.0258217	6.8103637
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C	-4.0036189	4.7009649	5.9198998
H	-2.9153974	4.6341462	5.7396708
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C	-4.5013554	6.0090672	5.2944364
H	-4.3467188	5.9536373	4.2027084
H	-5.5914284	6.1140467	5.4449028
C	-3.8054043	7.2535924	5.8558101
H	-2.7131153	7.1546154	5.7134006
H	-3.9605504	7.2994052	6.9501257
C	-4.2840906	8.5593462	5.2182476
H	-3.7634920	9.4339649	5.6415745
H	-4.1077285	8.5596677	4.1291964
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H	-6.5104393	4.3253817	6.1122485
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C	-7.1370540	2.6993203	4.8742097
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H	-7.1569836	3.2825051	3.9409520
H	-6.8729626	1.6684972	4.5944115
C	-4.2883747	-0.4315100	8.2252824
H	-3.6110646	0.4376283	8.1613281
H	-5.2573352	-0.0229636	8.5670922
C	-3.7462500	-1.3893172	9.2914868
H	-4.4337185	-2.2435463	9.4183847
H	-2.7900681	-1.8233708	8.9455275
C	-3.5393047	-0.7233442	10.6571306
H	-4.4983810	-0.2905427	10.9969695
H	-2.8484768	0.1326256	10.5474459
C	-3.0021078	-1.6774020	11.7251921
H	-2.0202976	-2.0895916	11.4373664
H	-2.8779540	-1.1702991	12.6956671
H	-3.6839229	-2.5305978	11.8807520
C	-5.3367827	-2.3023437	6.7886113
H	-5.3507356	-2.6936265	5.7550543
H	-4.8374284	-3.0845101	7.3831050
C	-6.7794038	-2.1415427	7.2807470
H	-6.8242526	-1.8237431	8.3348311
H	-7.3443696	-1.4015364	6.6893045
H	-7.3221996	-3.0972204	7.2057828
C	1.2664404	1.6166480	6.5895005
H	1.1691992	2.5894953	6.0801200
C	-0.1378334	1.2886226	7.1463782
H	-0.5633078	2.2283582	7.5410512
H	-0.7959107	0.9937819	6.3112401
C	-0.2176024	0.2274175	8.2472675

H	-1.2660053	0.0441661	8.5261055
H	0.2075633	-0.7373687	7.9317726
H	0.3117735	0.5397459	9.1601581
C	2.2926819	1.8321090	7.7253016
H	1.8332945	2.5084327	8.4703922
H	2.4534639	0.8743316	8.2529072
C	3.6563766	2.3996852	7.3155583
H	4.1583423	1.7322207	6.5979062
H	3.5143109	3.3559620	6.7764661
C	4.5897156	2.6259609	8.5102995
H	4.6889568	1.6780853	9.0715997
H	4.1269707	3.3430593	9.2149367
C	5.9799294	3.1208137	8.1063931
H	5.9244397	4.0887619	7.5796777
H	6.6325129	3.2560930	8.9844829
H	6.4717185	2.4059431	7.4261876
C	0.8931681	-2.4113584	5.5348246
H	0.9838599	-1.8174852	6.4599558
C	1.9163812	-3.5596313	5.7012781
H	1.6892599	-4.0868702	6.6449444
H	2.9133717	-3.1058283	5.8580382
C	2.0055241	-4.5871708	4.5683246
H	1.0120094	-5.0225113	4.3689474
H	2.2846201	-4.0880251	3.6249737
C	3.0026319	-5.7127983	4.8623513
H	2.7136531	-6.2210393	5.8020544
H	4.0030730	-5.2809776	5.0539645
C	3.0974162	-6.7443758	3.7364360
H	3.8066512	-7.5519788	3.9822087
H	2.1160106	-7.2057470	3.5350170
H	3.4358331	-6.2785033	2.7953717
C	-0.5732385	-2.8738141	5.4380198
H	-0.7225888	-3.4229975	4.4934947
H	-1.2000733	-1.9644458	5.3801114
C	-1.0581416	-3.7322722	6.6076189
H	-0.8771768	-3.2436993	7.5813530
H	-2.1398405	-3.9299335	6.5303797
H	-0.5555094	-4.7115936	6.6294184
C	4.1999050	-0.2781186	-1.8913198
H	4.4310123	-1.2552232	-2.3452454
C	4.8243265	-0.2394456	-0.4815856
H	4.1654808	-0.7545590	0.2364758
H	4.8586748	0.8095544	-0.1437343
C	6.2260208	-0.8418402	-0.3731462
H	6.6029713	-0.7285706	0.6545136
H	6.2256538	-1.9169778	-0.6217975
H	6.9446252	-0.3478576	-1.0483753
C	4.8260485	0.8002588	-2.8086275

H	5.8808490	0.9403363	-2.5204841
H	4.3364953	1.7719809	-2.6072220
C	4.7748078	0.4969092	-4.3105498
H	5.3675717	-0.4150669	-4.5116925
H	3.7414225	0.2541018	-4.6210556
C	5.2976253	1.6421577	-5.1846529
H	4.6652039	2.5353820	-5.0262749
H	6.3084068	1.9284235	-4.8404977
C	5.3432946	1.3051145	-6.6759198
H	5.6981900	2.1600598	-7.2740789
H	6.0212209	0.4576465	-6.8741165
H	4.3462963	1.0237612	-7.0562227
C	2.6097659	-3.2201519	-2.6651767
H	2.8222681	-2.4202486	-3.3971476
C	1.4002112	-4.0091713	-3.2159912
H	0.5241749	-3.3380071	-3.2396063
H	1.5966176	-4.2508883	-4.2758497
C	1.0441739	-5.2988910	-2.4644047
H	1.9168989	-5.9756432	-2.4572126
H	0.8181854	-5.0841176	-1.4061167
C	-0.1442822	-6.0599067	-3.0642865
H	0.0818232	-6.3339829	-4.1123864
H	-1.0221195	-5.3901291	-3.1134823
C	-0.5127888	-7.3099739	-2.2621454
H	-1.3718187	-7.8382302	-2.7075659
H	0.3301820	-8.0215673	-2.2238568
H	-0.7703693	-7.0435808	-1.2243220
C	3.8884107	-4.0822360	-2.5638067
H	3.7549403	-4.8461928	-1.7781911
H	4.7121462	-3.4391821	-2.2081991
C	4.3226423	-4.7546830	-3.8674748
H	4.4470797	-4.0158994	-4.6779839
H	5.2883462	-5.2695617	-3.7386280
H	3.5958935	-5.5065454	-4.2131186

[Am-(me-PIPDA)₂NO₃](NO₃)₂

C	0.3885172	0.0305719	11.3614147
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C	-0.0294327	-4.3891800	14.5411129
H	-0.8829247	-5.0454582	14.2983015
C	-0.2805448	1.1730755	12.1252940
O	-0.6860162	0.9933833	13.2855378
N	-0.3964832	2.3671392	11.5008808
C	-1.0648543	3.4794214	12.1627420
C	0.0586278	2.6148920	10.1378041
C	-0.1401213	-3.8978596	15.9773093
O	0.0565634	-2.6809026	16.2361772

N	-0.3636606	-4.7866690	16.9404244
C	-0.3019293	-4.3419414	18.3382312
C	-0.7292329	-6.1715997	16.6346365
H	-2.0052006	3.7355204	11.6432280
H	-1.2923310	3.1994063	13.1961397
H	0.4081454	3.6554397	10.0635688
H	0.9024251	1.9684438	9.8696601
H	-1.4789031	-6.2061168	15.8301118
H	0.1534668	-6.7742105	16.3565675
H	-1.0572044	-3.5624160	18.5258560
H	0.6982678	-3.9545772	18.5857198
C	-1.9744271	1.1306849	16.3577554
C	3.2471994	-0.3895088	16.9169453
H	3.9146038	0.4210050	16.5850814
H	3.5384524	-0.6849216	17.9396767
C	-2.6831807	-0.0638176	15.7010870
O	-1.9856209	-0.8718078	15.0598981
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C	-4.6520729	-1.3894282	15.2022515
C	-4.9031680	0.7753485	16.4043307
C	3.4845152	-1.5370177	15.9485052
O	2.6478041	-1.7897750	15.0383952
N	4.6376069	-2.2039282	16.0054406
C	5.5977119	-2.0336876	17.1000487
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H	-4.8593564	-1.2331962	14.1305157
H	-4.0232000	-2.2860524	15.3141141
H	-5.2888055	0.4159279	17.3741268
H	-4.4120540	1.7434828	16.5560245
H	4.2750024	-4.1054359	15.1385830
H	4.6861689	-2.8048846	13.9814688
H	6.2228444	-2.9344559	17.1552463
H	5.0750422	-1.9319260	18.0629235
H	0.8844720	-5.0036327	14.4802635
N	3.2596005	0.7469095	13.4151129
O	3.5220791	0.3192226	12.2854585
O	2.0161609	0.7856600	13.7799767
O	4.1168863	1.1536502	14.1920365
N	-3.4738146	-4.7726741	14.4004599
O	-4.5133933	-4.3895253	13.8505698
O	-2.9977418	-4.1299877	15.3832000
O	-2.8536953	-5.7826195	13.9796926
N	2.8701572	-2.6239374	19.5328301
O	2.1016310	-3.0177391	20.4159750
O	3.7039111	-1.7071726	19.7682247
O	2.8126831	-3.1147699	18.3678361
C	-0.4070103	0.0481007	17.8819420
C	1.0628748	-0.4089463	18.0331483

N	1.8528774	0.0929117	16.8854678
C	1.7709866	1.5633597	16.8604151
C	0.2989310	1.9943731	16.6332560
N	-0.5747855	0.8068421	16.6225505
H	-0.7208334	0.6782457	18.7389181
H	1.4964125	-0.0444740	18.9819469
H	2.1535102	1.9850018	17.8106828
H	-0.0250318	2.7072375	17.4182836
C	1.1648941	-3.4574415	12.6153468
C	1.2928031	-2.2041262	11.7123553
N	0.2508559	-1.2293918	12.0808690
C	-1.0788854	-1.8464686	11.9126249
C	-1.2089240	-3.0727352	12.8457594
N	0.0635042	-3.2749190	13.5775899
H	0.9942873	-4.3632778	12.0010866
H	2.2703709	-1.7196810	11.8447530
H	-1.8467043	-1.1012695	12.1601481
H	-1.9980854	-2.9088810	13.5877246
H	2.0936416	-3.6023020	13.1833295
H	-1.4741420	-3.9820597	12.2763693
H	-1.2233784	-2.1360956	10.8514428
H	1.1970226	-2.4830299	10.6433976
H	2.4014900	1.9293070	16.0407146
H	0.1958795	2.4982789	15.6605185
H	1.1253055	-1.5020175	18.0366268
H	-1.0703323	-0.8279486	17.8505797
H	-2.0136178	1.9614892	15.6335132
H	-2.4864272	1.4693897	17.2766194
Am	0.4630271	-0.8625058	14.7535122
H	-0.4137631	4.3687255	12.1611712
H	-0.7514504	2.4731328	9.3995788
H	6.2542228	-1.1643810	16.9227288
H	5.9565705	-3.5010415	15.0293391
H	-1.1730921	-6.6177521	17.5329972
H	-0.5167265	-5.1999507	18.9860081
H	-5.7648712	0.9419685	15.7388095
H	-5.6053722	-1.5620558	15.7207677

[Eu-(me-PIPDA)₂NO₃](NO₃)₂

C	0.3417881	0.0578577	11.3866816
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C	0.0407998	-4.3484628	14.5741273
H	-0.7587449	-5.0646477	14.3165163

C	-0.3070518	1.1955752	12.1738650
O	-0.6665928	1.0145394	13.3480984
N	-0.4552088	2.3885096	11.5529506
C	-1.1068990	3.4975330	12.2355927
C	-0.0212581	2.6524579	10.1861264
C	-0.1497367	-3.8350625	15.9946037
O	-0.0238650	-2.6057899	16.2304652
N	-0.3692683	-4.7167199	16.9650954
C	-0.4266780	-4.2447942	18.3528438
C	-0.6166981	-6.1288404	16.6640528
H	-1.9838492	3.8400839	11.6597203
H	-1.4342032	3.1677191	13.2265458
H	0.3443445	3.6885541	10.1224962
H	0.8062721	1.9975258	9.8900129
H	-1.4154824	-6.2261048	15.9123095
H	0.2976518	-6.6343286	16.3085869
H	-1.0835554	-3.3658527	18.4210110
H	0.5752613	-3.9783081	18.7250329
C	-1.9453729	1.1299461	16.3124839
C	3.2578240	-0.4152140	16.8805222
H	3.9303610	0.3733362	16.5088251
H	3.5587418	-0.6810806	17.9085497
C	-2.6482313	-0.0753339	15.6680527
O	-1.9473719	-0.8826667	15.0348396
N	-3.9778108	-0.2254835	15.7610707
C	-4.5990920	-1.4181607	15.1617220
C	-4.8844980	0.7443607	16.3585572
C	3.4583401	-1.6014574	15.9516729
O	2.5983382	-1.8750414	15.0717678
N	4.6035532	-2.2823420	16.0146378
C	5.5843469	-2.0655250	17.0833261
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H	-3.9861167	-2.3186351	15.3206912
H	-5.3334441	0.3492593	17.2861536
H	-4.3828407	1.6913979	16.5877763
H	4.1661756	-4.2236007	15.2852030
H	4.5884001	-3.0164995	14.0345689
H	6.2725677	-2.9200007	17.1015175
H	5.0831930	-2.0090555	18.0618456
H	0.9965668	-4.8981940	14.5577427
N	3.2678485	0.7276410	13.3748660
O	3.5086804	0.3779735	12.2149860
O	2.0344738	0.7130749	13.7731567
O	4.1357674	1.1088900	14.1531669
N	-3.3829634	-4.8172619	14.3647466
O	-4.3479051	-4.3861116	13.7193627
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O	-2.7577815	-5.8386225	13.9848695
N	2.8435041	-2.6503123	19.5261786
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O	3.6897801	-1.7438004	19.7512298
O	2.7693708	-3.1474160	18.3668104
C	-0.3837158	0.0698737	17.8543099
C	1.0798106	-0.4022314	18.0045733
N	1.8701926	0.0836952	16.8505098
C	1.8011930	1.5544573	16.8120341
C	0.3326308	1.9920352	16.5746766
N	-0.5461052	0.8088510	16.5837445
H	-0.6865766	0.7173871	18.7021651
H	1.5225608	-0.0363050	18.9486320
H	2.1843719	1.9814865	17.7595238
H	0.0126219	2.7216514	17.3457329
C	1.1692361	-3.4299225	12.6032710
C	1.2671457	-2.1701985	11.7053619
N	0.2273295	-1.2047971	12.1042289
C	-1.1025489	-1.8289716	11.9686904
C	-1.1954267	-3.0599768	12.8994464
N	0.0983849	-3.2469675	13.5967443
H	0.9795968	-4.3323256	11.9895866
H	2.2440149	-1.6789115	11.8173048
H	-1.8665755	-1.0902060	12.2452196
H	-1.9680399	-2.9054025	13.6594942
H	2.1139644	-3.5781998	13.1430721
H	-1.4634254	-3.9716072	12.3353419
H	-1.2771106	-2.1136110	10.9108132
H	1.1494304	-2.4429146	10.6370773
H	2.4371929	1.9066673	15.9906978
H	0.2344459	2.4759419	15.5915114
H	1.1305654	-1.4958414	18.0142694
H	-1.0561359	-0.7989038	17.8374659
H	-1.9828689	1.9496543	15.5764981
H	-2.4575555	1.4804859	17.2266209
H	-0.4112238	4.3464036	12.3469899
H	-0.8481238	2.5365394	9.4622705
H	6.1739677	-1.1506395	16.9027089
H	5.8619376	-3.6803942	15.0982082
H	-0.9377348	-6.6283928	17.5858278
H	-0.8468114	-5.0430665	18.9765781
H	-5.7029297	0.9633079	15.6535157
H	-5.5803885	-1.5693261	15.6321236
Eu	0.4935608	-0.8531952	14.7514969

[Am-(me-DADA)₂NO₃](NO₃)₂

H	-1.6562327	-1.6903729	-2.9273915
C	-1.6173792	-0.6958277	-2.4407811
N	-1.7707968	-0.8189298	-0.9790104
C	-0.6441369	-1.5928240	-0.4045849
C	0.6331311	-0.7791870	-0.5901058
N	1.8139763	-1.3780491	-0.6638212
C	-3.0871177	-1.4386740	-0.7198353
C	-3.4878626	-1.4830629	0.7412273
N	-3.4651835	-0.1584769	1.4009976
C	-3.3534171	-0.3490018	2.8539284
C	-2.8476617	0.9099676	3.5357463
N	-3.0972577	1.0901773	4.8494909
C	-3.7043958	0.0775239	5.7055538
O	0.5053196	0.4769253	-0.7118580
C	3.0097602	-0.6352490	-1.0686506
C	-4.6809714	0.6119310	1.0795649
O	-2.1960127	1.7421856	2.8819108
C	-2.7178145	2.3458584	5.4865340
H	-3.1086222	-2.4785910	-1.1043260
H	-3.8202359	-0.8687902	-1.3128366
H	-4.4993599	-1.9323345	0.8071062
H	-2.8210300	-2.1586498	1.2891901
H	-5.5895830	0.0572421	1.3910552
H	-4.6629391	1.5903997	1.5758133
H	-4.7404334	0.7860196	-0.0041187
H	-0.6637526	-0.2166993	-2.6912590
H	-2.4257570	-0.0715625	-2.8421090
H	-4.3256374	-0.6649152	3.2769089
H	-2.6282351	-1.1662604	3.0439497
H	-0.8035104	-1.7772854	0.6791025
H	-0.5627107	-2.5903411	-0.8723864
H	-3.4772786	2.6136531	6.2365676
H	-1.7388146	2.2638422	5.9916804
H	-2.6735130	3.1394790	4.7316920
H	-4.7868209	0.2501788	5.8441989
H	-3.5493923	-0.9317646	5.3067778
H	-3.2232298	0.1130551	6.6948720
H	2.7115445	0.2987839	-1.5574572
H	3.5678935	-1.2604166	-1.7844144
H	3.6608676	-0.4055846	-0.2061508
C	2.0600000	-2.7526843	-0.2190375
H	2.3669414	-3.3840074	-1.0701372
H	2.8780622	-2.7105588	0.5180164
H	1.1855034	-3.1896018	0.2801660
Am	-1.3346472	1.4781310	0.4825065
H	0.5635111	4.1693549	-2.9481219
C	0.2614983	3.3211954	-2.3001563
N	-0.4687516	3.7821572	-1.1074581

C	-1.7308759	4.4037980	-1.5049760
C	-2.7974261	3.3589463	-1.8131722
N	-3.9806128	3.7966888	-2.2825612
C	0.3541664	4.7005627	-0.2767599
C	0.3174712	4.3841347	1.2204557
N	0.7186835	2.9924391	1.4924245
C	0.7138018	2.6666883	2.9281849
C	0.5800530	1.1448668	3.0947361
N	0.9334477	0.5545778	4.2316101
C	1.5908991	1.2620971	5.3272294
O	-2.5660375	2.1468774	-1.6209123
C	-5.0734949	2.8539850	-2.4983031
C	2.0711872	2.7140307	0.9525445
O	0.0907026	0.4996112	2.1297117
C	1.0300048	-0.9126563	4.2936012
H	0.0346512	5.7484651	-0.4163182
H	1.3915107	4.6538253	-0.6349510
H	0.9951384	5.1010038	1.7310011
H	-0.6958297	4.5583213	1.6133389
H	2.7582459	3.5496942	1.1861462
H	2.5037056	1.8246552	1.4170768
H	2.0460908	2.5523399	-0.1293215
H	-0.3764304	2.6452210	-2.8846430
H	1.1552912	2.7567038	-2.0075236
H	1.6305733	3.0360499	3.4165027
H	-0.1574693	3.1387437	3.4077776
H	-2.1147811	5.0185068	-0.6772784
H	-1.5886176	5.0717010	-2.3803013
H	2.0558719	-1.1996172	4.0044800
H	0.8196276	-1.2324535	5.3247871
H	0.3140758	-1.3894281	3.6121694
H	2.6823475	1.2069882	5.1911966
H	1.2702057	2.3097684	5.3827444
H	1.3092687	0.7750299	6.2724752
H	-4.6695417	1.8374625	-2.5472059
H	-5.5862157	3.0883922	-3.4439549
H	-5.8071341	2.9068216	-1.6751115
C	-4.3038499	5.2221319	-2.3509025
H	-5.2761398	5.3378712	-2.8465546
H	-4.3672586	5.6726110	-1.3462385
H	-3.5602405	5.7787573	-2.9397808
N	-3.4394624	4.1566216	1.6005071
O	-3.0435795	5.3230671	1.4810949
O	-2.9409080	3.2727523	0.7971338
O	-4.2940399	3.8154588	2.4090183
N	4.0303022	0.0867903	2.3183472
O	3.6401759	0.8832726	3.2116477
O	3.8255386	-1.1389821	2.4327553

O 4.5995476 0.5473028 1.3023117
N -1.1982502 -3.8349405 2.2868103
O -0.2203794 -4.3465646 1.5609505
O -1.1738896 -2.5772786 2.5845034
O -2.2842651 -4.3419317 1.7292053

[Eu-(me-DADA)₂NO₃](NO₃)₂

H -1.9868453 -1.8324122 -2.7506922
C -1.9441085 -0.8286152 -2.2842973
N -1.7926377 -0.9331743 -0.8214300
C -0.5139934 -1.5983082 -0.4976523
C 0.6562368 -0.6694347 -0.7847229
N 1.8868754 -1.1744583 -0.8701944
C -2.9424348 -1.6943397 -0.2755989
C -3.1061996 -1.5641075 1.2290227
N -3.2834992 -0.1645472 1.6782071
C -3.1291246 -0.1046563 3.1356328
C -2.7898151 1.3092923 3.6019272
N -3.2085508 1.7496546 4.8067164
C -3.9034795 0.9470351 5.8053455
O 0.4157444 0.5591140 -0.9369082
C 3.0171847 -0.3230708 -1.2358653
C -4.6109295 0.3571410 1.3001884
O -2.0868465 2.0225871 2.8684158
C -2.9249683 3.1331751 5.1856455
H -2.8520754 -2.7724888 -0.5052323
H -3.8425225 -1.3304646 -0.7947973
H -3.9707686 -2.1866346 1.5340247
H -2.2394641 -1.9999381 1.7448623
H -5.4152129 -0.3042693 1.6823476
H -4.7502267 1.3728065 1.6918856
H -4.7018963 0.4123936 0.2067499
H -1.1017552 -0.2715202 -2.7119374
H -2.8640411 -0.2805562 -2.5254380
H -4.0280287 -0.5083535 3.6336473
H -2.2795630 -0.7459261 3.4233490
H -0.4826875 -1.8581138 0.5722933
H -0.4161802 -2.5546571 -1.0414863
H -3.6828542 3.4611548 5.9110074
H -1.9285866 3.2287517 5.6520830
H -2.9821134 3.7816856 4.3042606
H -4.9549846 1.2662952 5.9107155
H -3.8817761 -0.1194226 5.5595672
H -3.4091151 1.0694684 6.7830543
H 2.6485436 0.6037639 -1.6875177

H	3.6398835	-0.8635798	-1.9671326
H	3.6177085	-0.0960070	-0.3413414
C	2.2578994	-2.5187563	-0.4152668
H	2.7680531	-3.0592109	-1.2295754
H	2.9488903	-2.4025345	0.4353684
H	1.3970785	-3.1109416	-0.0792595
Eu	-1.3881731	1.4771961	0.4335063
H	0.5345153	4.3257864	-2.8396185
C	0.2462712	3.4354205	-2.2433986
N	-0.5073096	3.8148060	-1.0370124
C	-1.7753510	4.4275231	-1.4303484
C	-2.7895823	3.3685734	-1.8582771
N	-3.9656411	3.7948290	-2.3639167
C	0.2870494	4.6837013	-0.1299825
C	0.3111062	4.2144877	1.3299865
N	0.7374966	2.8098542	1.4672575
C	0.8294569	2.3794309	2.8734282
C	0.5906805	0.8643592	2.9665329
N	0.9896517	0.1959843	4.0516657
C	1.6482811	0.8097998	5.2065143
O	-2.5265959	2.1584509	-1.7201434
C	-5.0272658	2.8320830	-2.6337832
C	2.0498483	2.5598051	0.8342854
O	-0.0130310	0.2969885	2.0229496
C	0.9239251	-1.2700199	4.0953177
H	-0.0966708	5.7184874	-0.1438855
H	1.3159004	4.7401519	-0.5128944
H	0.9877237	4.8969760	1.8871363
H	-0.6935944	4.3260529	1.7717067
H	2.8044820	3.2798258	1.2040641
H	2.4113862	1.5583435	1.0963793
H	1.9817461	2.6248605	-0.2541689
H	-0.3689385	2.7752863	-2.8676756
H	1.1480232	2.8739387	-1.9766195
H	1.8167090	2.6340809	3.2919792
H	0.0460535	2.8789112	3.4614526
H	-2.2148962	4.9577926	-0.5712414
H	-1.6233564	5.1671236	-2.2437831
H	1.9530159	-1.6579946	4.1540709
H	0.3601674	-1.5890092	4.9876861
H	0.4419100	-1.6674091	3.1973807
H	2.7255411	0.5812385	5.1942270
H	1.5052638	1.8954611	5.2230837
H	1.1995729	0.3916683	6.1221930
H	-4.6002964	1.8247166	-2.6710122
H	-5.5055900	3.0627582	-3.5987536
H	-5.7958412	2.8649248	-1.8413917
C	-4.3514384	5.2036038	-2.3685568

H	-5.1894786	5.3383259	-3.0661824
H	-4.6680404	5.5433199	-1.3669794
H	-3.5290311	5.8458149	-2.7095197
N	-3.6816272	3.9650327	1.5145067
O	-3.2571571	5.1258321	1.4445022
O	-3.2140641	3.0958503	0.6884691
O	-4.5416250	3.6202166	2.3228320
N	3.8838114	0.1060653	2.9435571
O	4.1496019	-0.6714437	3.8773190
O	3.4775988	-0.3500000	1.8423033
O	3.9878938	1.3422154	3.1004309
N	-1.0166272	-4.2538697	1.1924840
O	-0.2250683	-4.6846141	0.3326300
O	-0.6059039	-3.4453762	2.0711687
O	-2.2159311	-4.5818972	1.1724261

Starting coordinates for optimization

[Eu-(PIPDA)₂NO₃](NO₃)₂

C	0.34178810	0.05785770	11.38668160
H	1.41337930	0.30289920	11.29100050
H	-0.09159700	-0.01416290	10.36951620
C	0.04079980	-4.34846280	14.57412730
H	-0.75874490	-5.06464770	14.31651630
C	-0.30705180	1.19557520	12.17386500
O	-0.66659280	1.01453940	13.34809840
N	-0.45520880	2.38850960	11.55295060
C	-1.10689900	3.49753300	12.23559270
C	-0.02125810	2.65245790	10.18612640
C	-0.14973670	-3.83506250	15.99460370
O	-0.02386500	-2.60578990	16.23046520
N	-0.36926830	-4.71671990	16.96509540
C	-0.42667800	-4.24479420	18.35284380
C	-0.61669810	-6.12884040	16.66405280
H	-1.98384920	3.84008390	11.65972030
H	-1.43420320	3.16771910	13.22654580
H	0.34434450	3.68855410	10.12249620
H	0.80627210	1.99752580	9.89001290
H	-1.41548240	-6.22610480	15.91230950
H	-1.08355540	-3.36585270	18.42101100
H	0.57526130	-3.97830810	18.72503290
C	-1.94537290	1.12994610	16.31248390
C	3.25782400	-0.41521400	16.88052220
H	3.93036100	0.37333620	16.50882510
H	3.55874180	-0.68108060	17.90854970

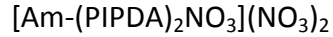
C	-2.64823130	-0.07533390	15.66805270
O	-1.94737190	-0.88266670	15.03483960
N	-3.97781080	-0.22548350	15.76107070
C	-4.59909200	-1.41816070	15.16172200
C	-4.88449800	0.74436070	16.35855720
C	3.45834010	-1.60145740	15.95167290
O	2.59833820	-1.87504140	15.07176780
N	4.60355320	-2.28234200	16.01463780
C	5.58434690	-2.06552500	17.08332610
C	4.81350100	-3.36076190	15.05428060
H	-3.98611670	-2.31863510	15.32069120
H	-4.38284070	1.69139790	16.58777630
H	4.16617560	-4.22360070	15.28520300
H	4.58840010	-3.01649950	14.03456890
H	6.27256770	-2.92000070	17.10151750
H	5.08319300	-2.00905550	18.06184560
H	0.99656680	-4.89819400	14.55774270
N	3.26784850	0.72764100	13.37486600
O	3.50868040	0.37797350	12.21498600
O	2.03447380	0.71307490	13.77315670
O	4.13576740	1.10889000	14.15316690
N	-3.38296340	-4.81726190	14.36474660
O	-4.34790510	-4.38611160	13.71936270
O	-2.98820680	-4.20981310	15.40216220
O	-2.75778150	-5.83862250	13.98486950
N	2.84350410	-2.65031230	19.52617860
O	2.07717050	-3.02867050	20.41875710
O	3.68978010	-1.74380040	19.75122980
O	2.76937080	-3.14741600	18.36681040
C	-0.38371580	0.06987370	17.85430990
C	1.07981060	-0.40223140	18.00457330
N	1.87019260	0.08369520	16.85050980
C	1.80119300	1.55445730	16.81203410
C	0.33263080	1.99203520	16.57467660
N	-0.54610520	0.80885100	16.58374450
H	-0.68657660	0.71738710	18.70216510
H	1.52256080	-0.03630500	18.94863200
H	2.18437190	1.98148650	17.75952380
H	0.01262190	2.72165140	17.34573290
C	1.16923610	-3.42992250	12.60327100
C	1.26714570	-2.17019850	11.70536190
N	0.22732950	-1.20479710	12.10422890
C	-1.10254890	-1.82897160	11.96869040
C	-1.19542670	-3.05997680	12.89944640
N	0.09838490	-3.24696750	13.59674430
H	0.97959680	-4.33232560	11.98958660
H	2.24401490	-1.67891150	11.81730480
H	-1.86657550	-1.09020600	12.24521960

H	-1.96803990	-2.90540250	13.65949420
H	2.11396440	-3.57819980	13.14307210
H	-1.46342540	-3.97160720	12.33534190
H	-1.27711060	-2.11361100	10.91081320
H	1.14943040	-2.44291460	10.63707730
H	2.43719290	1.90666730	15.99069780
H	0.23444590	2.47594190	15.59151140
H	1.13056540	-1.49584140	18.01426940
H	-1.05613590	-0.79890380	17.83746590
H	-1.98286890	1.94965430	15.57649810
H	-2.45755550	1.48048590	17.22662090
H	-0.93773480	-6.62839280	17.58582780
H	-5.70292970	0.96330790	15.65351570
H	-5.58038850	-1.56932610	15.63212360
Eu	0.49356080	-0.85319520	14.75149690
C	6.28538456	-3.80948863	15.11594986
H	6.92243242	-2.95160748	15.06018292
C	6.40734031	-0.78852674	16.83122040
H	6.42417650	-0.57626929	15.78261975
C	6.58545560	-4.74943776	13.93355695
H	7.56869201	-5.15716343	14.04267126
H	6.52686552	-4.19992613	13.01731235
C	5.55472710	-5.89345223	13.91282865
H	5.14893412	-6.02574265	14.89401737
H	4.76676500	-5.65127940	13.23064974
C	6.24211386	-7.19561477	13.46174976
H	6.72258370	-7.03718740	12.51890858
H	6.97128661	-7.48462195	14.18954229
C	5.18851936	-8.30983949	13.32018036
H	4.66217062	-8.42258429	14.24492120
H	4.49726454	-8.05074498	12.54562449
H	5.67408033	-9.23035804	13.07163228
C	6.54032388	-4.55297344	16.44027471
H	7.12744510	-3.93625619	17.08823189
H	5.60512424	-4.77526324	16.91026289
C	7.29623568	-5.86413855	16.15559353
H	6.59257263	-6.64725427	15.96457500
H	7.92614806	-5.73423171	15.30047096
H	7.89519761	-6.12193364	17.00393680
C	-5.51093116	0.19305929	17.65287102
H	-5.40088797	-0.87098711	17.67727884
C	-7.00711869	0.55547028	17.69387254
H	-7.12307498	1.60896827	17.54691629
H	-7.52316103	0.02830326	16.91882723
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H	-7.05238893	0.65797084	19.83921088
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C	8.01782770	-1.90602287	18.59425907
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C	7.41941992	-3.34168342	15.96215940
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C	8.87492514	-3.47241006	16.44797327
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[Am-(DADA)₂NO₃](NO₃)₂

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