Supporting Information for

Theoretical Prediction of Am(III)/Eu(III) Selectivity to Aid the Design of Actinide-Lanthanide Separation Agents

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Electronic Supplementary Information (ESI) Available: Complete reference 39, additional computational details, calculated bond distances to Am^{3+} and Eu^{3+}, gas-phase interaction energies with La^{3+}, structures of the selected optimized complexes, optimized geometries and absolute energies (in Hartrees) for all metal-ion complexes obtained at the B3LYP level.

Complete Reference 39. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, *Gaussian 09, Revision C.01*, Gaussian, Inc., Wallingford CT, 2009.

Additional Computational Details. For metal ion-ligand complexes with fused aromatic rings (ligands **9** and **10**), the SP diffuse basis function on carbon caused a singularity in the Pulay matrix using NWChem 6.3[1] software, leading to a problem of self-consistent field (SCF) convergence. We were able to get the converged wavefunctions for complexes with **9** and **10** by increasing an exponent of the most diffuse SP function of carbon from 0.0438 to 0.0738. Control calculations for complex with **1b** show that this procedure leads to only 0.09 kcal/mol decrease in Am/Eu selectivity when compared to results obtained with the standard 6-311++G** basis set. Geometries were optimized at each basis set and density functions, with the exception of M06 and M06-L, for which the addition of diffuse functions can cause numerical instabilities and fluctuations in gradient and energy during geometry optimization even when employing a very fine integration grid (NWChem "xfine" grid). The problem is likely to arise from a specific functional form used in these meta-GGA functionals that can cause large errors in individual

contributions to the exchange energy, a topic thoroughly discussed by Wheeler and Houk.[2] Therefore, only single-point energy calculations on B3LYP optimized geometries were run with the M06 and M06-L density functionals.

1. M. Valiev, E. J. Bylaska, N. Govind, K. Kowalski, T.P. Straatsma, H.J.J. van Dam, D. Wang, J. Nieplocha, E. Apra, T.L. Windus, W.A. de Jong, *Comput. Phys. Commun.* 2010, **181**, 1477-1489.

2. S. E. Wheeler, K. N. Houk, *J. Chem. Theory Comput.* 2010, **6**, 395-404.

Table S1. Gas-phase interaction energies (ΔE_1) for global minima of La^{3+} with ligand **1b** and **6**–**9** (kcal/mol)

ligand	ΔE_1
1b	-301.2
6	-300.5
7	-283.2
8	-281.6
9	-337.1

Obtained as E(1:1 La^{3+}-ligand complex) – E(ligand) – E(La^{3+}).

Table S2. Calculated distances (Å) from the central metal ion to neighboring ligand donor atoms in neutral Am(III) and Eu(III) complexes

complex	M−N/S		M−O		M−ONO_2	
	Am	Eu	Am	Eu	Am	Eu
$M(H_2O)_4(NO_3)_3$			2.572	2.512	2.498	2.466
M(**1b**)$_2(NO_3)_3$	2.721	2.730	2.531	2.494	2.554	2.514
M(**2**)$_3$	2.851	2.870				
M(**6**)$_2(NO_3)_3$	2.696	2.704	2.557	2.526	2.556	2.512
M(**7**)$_2(NO_3)_3$	2.722	2.732	2.547	2.511	2.542	2.506
M(**8**)$_2(NO_3)_3$	2.725	2.733	2.541	2.507	2.546	2.505
M(**9**)$_2(NO_3)_3$	2.676	2.672	2.508	2.474	2.576	2.534
M(**10**)$(NO_3)_3$	2.722	2.681	2.552	2.533	2.548	2.521

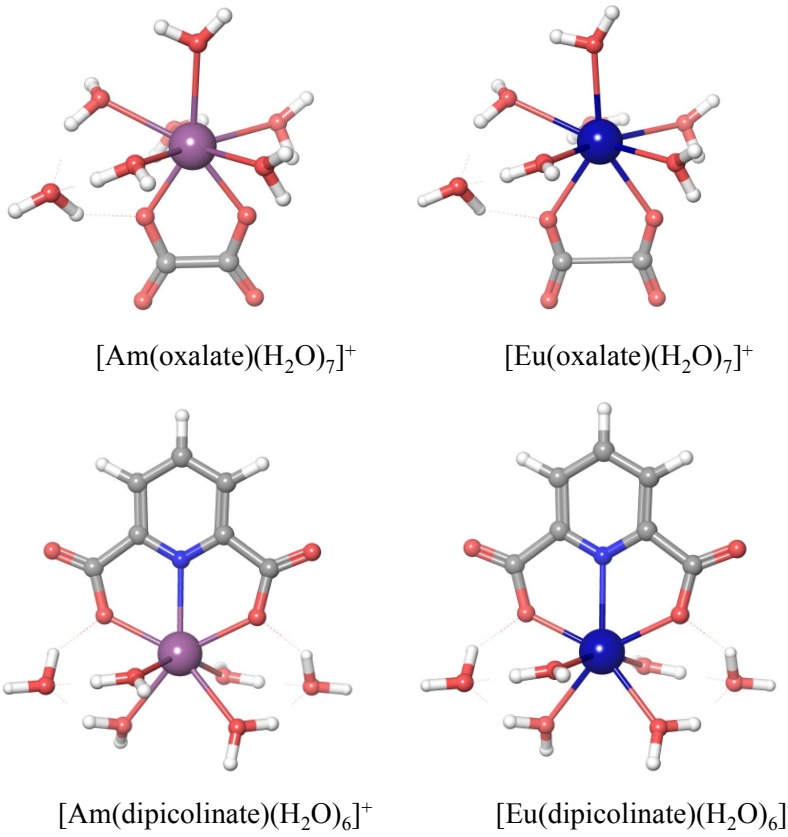

Figure S1. Initial set of optimized structures for aqueous 1:1 metal ion-ligand complexes

[Am(H2O)8]3+ B3LYP/6-311++G** Total energy: -1206.41802931

Am	-0.00000208	0.00000121	0.00553715
O	1.65052694	1.31809537	-1.38563387
H	1.43260086	1.89866999	-2.13223772
H	2.61524200	1.37004780	-1.29088640
O	0.40669460	2.06926792	1.37541664
H	1.09059871	2.74603133	1.24773320
H	-0.11054667	2.36317469	2.14239916
O	2.06989765	-0.40722191	1.37438167
H	2.36372793	0.10907190	2.14203305
H	2.74684270	-1.09076055	1.24570507
O	-1.31756435	1.65060845	-1.38598846
H	-1.89826476	1.43266851	-2.13249027
H	-1.36902386	2.61538863	-1.29162592
O	1.31774608	-1.64990476	-1.38664666
H	1.36912796	-2.61474389	-1.29284716
H	1.89858847	-1.43156072	-2.13291997
O	-2.07002775	0.40652702	1.37440356
H	-2.74697546	1.09012192	1.24603998
H	-2.36394561	-0.11022965	2.14170975
O	-0.40689094	-2.06995734	1.37432437
H	-1.09074466	-2.74668064	1.24615924
H	0.11026995	-2.36428975	2.14119789
O	-1.65036626	-1.31741124	-1.38647727
H	-2.61510020	-1.36934172	-1.29190926
H	-1.43236670	-1.89761907	-2.13334474

[Eu(H2O)8]3+ B3LYP/6-311++G** Total energy: -1321.35382096

Eu	0.00010192	0.00007144	0.00512192
O	1.66202087	1.25181203	-1.34555952
H	1.46198428	1.83234314	-2.09714707
H	2.62516217	1.29381733	-1.23293195
O	0.34605349	2.05055518	1.33444605
H	1.01726368	2.74009592	1.20785931
H	-0.18369377	2.33644171	2.09589050
O	2.05086067	-0.34626577	1.33403941
H	2.33681453	0.18342476	2.09550407
H	2.74040428	-1.01747059	1.20735457
O	-1.25144700	1.66229684	-1.34561193
H	-1.83167334	1.46199760	-2.09737288
H	-1.29404832	2.62540249	-1.23285463
O	1.25110805	-1.66154925	-1.34671488
H	1.29343635	-2.62464348	-1.23379716
H	1.83170347	-1.46154322	-2.09825974
O	-2.05082910	0.34561918	1.33359935
H	-2.74048181	1.01665603	1.20664122
H	-2.33692948	-0.18415671	2.09495474

O	-0.34588960	-2.05124619	1.33325222
H	-1.01702938	-2.74079785	1.20625206
H	0.18386041	-2.33751719	2.09456270
O	-1.66186560	-1.25072413	-1.34677756
H	-2.62493112	-1.29363821	-1.23378937
H	-1.46156937	-1.83099011	-2.09850588

[Am(H2O)9]3+ B3LYP/6-311++G** Total energy: -1282.91069370

Am	0.00292451	0.00679026	0.00272253
O	0.01737708	-0.09727988	2.53841693
H	0.78147213	-0.12326009	3.13410157
H	-0.76726664	-0.16012010	3.10395712
O	2.44495187	-0.26435372	0.76257111
H	3.07528820	0.45693053	0.91098119
H	2.91997412	-1.07809257	0.98991764
O	0.22805591	-2.46111018	0.59137802
H	0.45136819	-3.16896789	-0.03173623
H	0.17147233	-2.88434640	1.46132738
O	-2.25893062	-0.84397999	0.95808831
H	-3.06215159	-0.31683543	1.08377838
H	-2.49272794	-1.74490393	1.22774184
O	0.92011968	2.24359410	0.90336612
H	0.96268134	2.52912323	1.82872475
H	1.29369181	2.97382083	0.38680605
O	0.55466370	1.50114378	-1.97299138
H	1.24288422	1.33070799	-2.63386432
H	0.11419488	2.31959872	-2.24770988
O	-1.53841451	-0.73920328	-1.88235963
H	-1.54105103	-0.45837916	-2.80986626
H	-2.29563415	-1.33628069	-1.78583731
O	-1.80218081	1.83453453	-0.12694012
H	-1.79231595	2.67517185	0.35558989
H	-2.60269966	1.85563426	-0.67303491
O	1.40878752	-1.23343410	-1.79571196
H	2.36539061	-1.38548557	-1.77038323
H	1.09649674	-1.66670711	-2.60428845

[Eu(H2O)9]3+ B3LYP/6-311++G** Total energy: -1397.84647692

Eu	0.00388102	0.00510651	0.00117219
O	-0.01102388	-0.02312879	2.50140224
H	0.75234259	-0.04036345	3.09816702
H	-0.79545018	-0.09588820	3.06572079
O	2.39472466	-0.26528993	0.72737190
H	3.03965054	0.44599052	0.85946296
H	2.85148631	-1.08658520	0.96392486
O	0.26931360	-2.39661271	0.65258568
H	0.50420888	-3.12200604	0.05439526

H	0.20805670	-2.78752138	1.53716002
O	-2.21460503	-0.90855724	0.89194381
H	-3.02993321	-0.41129695	1.05497851
H	-2.41202286	-1.82468601	1.13759946
O	0.91290023	2.20319187	0.88016675
H	0.94178010	2.49789560	1.80279013
H	1.30023870	2.92244080	0.35904695
O	0.59028050	1.50697864	-1.91652004
H	1.27466049	1.34584019	-2.58348916
H	0.14421013	2.32542864	-2.18161059
O	-1.51371168	-0.64968370	-1.87796375
H	-1.50029371	-0.33809854	-2.79542695
H	-2.28710225	-1.22859310	-1.80239126
O	-1.76986149	1.78044688	-0.09332512
H	-1.77017770	2.61319028	0.40250627
H	-2.57344415	1.79270028	-0.63479724
O	1.32512485	-1.26859329	-1.76922500
H	2.28217047	-1.41861481	-1.78572646
H	0.97605421	-1.70131865	-2.56271198

[Am(H2O)20]3+ B3LYP/6-311++G** Total energy: -2124.35328505

Am	0.17324049	0.10600762	-0.22191472
O	0.15414759	-2.86292038	3.32813710
H	0.54839760	-3.17764718	4.15251068
H	0.35178904	-3.53763217	2.64717538
O	0.57109512	-0.30292609	2.20544344
H	0.57764542	-1.17297561	2.65389807
H	0.58875431	0.39172942	2.89551843
O	-0.50534379	-0.89893791	-2.42323078
H	-1.01893666	-1.70087118	-2.63361113
H	-0.04007914	-0.63582905	-3.24538178
O	1.68318566	1.92800873	0.53258960
H	1.44115593	2.65995309	1.14547313
H	2.59077311	2.08445361	0.21140268
O	-2.44220007	-1.88551038	3.03132093
H	-3.20105579	-2.41861476	3.30291223
H	-1.63819979	-2.35343630	3.34109354
O	-1.50682002	-1.63798604	0.37024326
H	-1.97621122	-1.62351177	1.23069556
H	-1.63958575	-2.54299850	0.01647869
O	4.20236064	1.90120651	-0.76768962
H	4.54267981	2.66073873	-1.26071954
H	4.97394138	1.52370776	-0.32231300
O	-1.36890269	3.97705338	0.24481951
H	-0.72150853	4.21180841	0.93895397
H	-1.96674208	4.72753851	0.13572610
O	0.68894155	-4.37991914	0.98108554

H	1.22353492	-5.18440469	1.02364293
H	-0.09666872	-4.58835147	0.43563202
O	-1.84116277	-3.38548790	-3.22214152
H	-2.75237930	-3.30007211	-3.53769367
H	-1.38480926	-3.88427778	-3.91471779
O	-2.48446925	0.85539119	3.55018356
H	-3.29903278	1.22097105	3.91996412
H	-2.57643137	-0.12105182	3.56254275
O	-0.55956836	2.06537997	-1.60022322
H	-0.79458842	2.90352617	-1.15135334
H	-0.60587615	2.21860878	-2.56232447
O	1.09490583	0.23501572	-4.35693260
H	1.49850509	-0.13756852	-5.15179864
H	0.66138391	1.07254501	-4.61862696
O	-1.56962797	1.35766467	0.99221970
H	-1.97205739	1.19180557	1.87406895
H	-1.79682738	2.27569877	0.73680628
O	-0.46134900	2.57531658	-4.45756127
H	-0.05853922	3.41887981	-4.70809870
H	-1.28137423	2.52950785	-4.96971503
O	0.65807994	3.83005400	2.22306491
H	1.13209144	4.59936796	2.56577500
H	0.41940135	3.27717672	2.99790624
O	1.51206693	-2.00059219	-0.12055137
H	2.29683139	-2.06587829	-0.67779121
H	1.34422579	-2.87946474	0.28900653
O	2.18616493	0.20144519	-1.78135098
H	2.02922853	0.23249530	-2.74723001
H	2.97891012	0.74249933	-1.59391115
O	0.09315538	1.77566978	4.05863063
H	0.45489241	1.83648247	4.95276713
H	-0.85450816	1.54498346	4.14948432
O	-1.69183904	-4.27596276	-0.53835150
H	-2.40859236	-4.87234961	-0.28325993
H	-1.73868927	-4.19720896	-1.51232170

[Eu(H2O)20]3+ B3LYP/6-311++G** Total energy: -2239.29054901

Eu	0.19448273	0.11769604	-0.24867350
O	0.18113587	-2.85363245	3.28166520
H	0.57510915	-3.16342400	4.10803319
H	0.39590414	-3.52250789	2.60018957
O	0.56866261	-0.30611173	2.13546334
H	0.58654140	-1.17447830	2.58645716
H	0.60747458	0.38963514	2.82259176
O	-0.49006088	-0.87792923	-2.39876540
H	-1.02643029	-1.66502914	-2.60644601
H	-0.02495977	-0.62894204	-3.22557673

O	1.66904834	1.90327810	0.53431898
H	1.42680693	2.64039685	1.14097366
H	2.57821165	2.06136502	0.21895374
O	-2.41371645	-1.87011198	2.98158172
H	-3.17332553	-2.40554850	3.24618560
H	-1.61056539	-2.33820373	3.29302176
O	-1.46062932	-1.58483725	0.33629667
H	-1.92929676	-1.57158878	1.19698492
H	-1.59341418	-2.49092486	-0.01478931
O	4.18907350	1.92782462	-0.76471013
H	4.52064368	2.70564175	-1.23461503
H	4.96592284	1.54125116	-0.33668135
O	-1.31115963	3.98492667	0.18919408
H	-0.67860618	4.22389155	0.89550056
H	-1.90901961	4.73298285	0.06482593
O	0.74287910	-4.33451219	0.92115320
H	1.28681162	-5.13325741	0.95245084
H	-0.04546689	-4.54697968	0.38143055
O	-1.84980793	-3.33916027	-3.23661405
H	-2.76313244	-3.25806799	-3.54714666
H	-1.39271899	-3.82861712	-3.93528980
O	-2.45890011	0.87208513	3.47467773
H	-3.27540158	1.24632025	3.83126731
H	-2.55819804	-0.10351591	3.49290888
O	-0.49314537	2.04226438	-1.62779420
H	-0.71923948	2.88526993	-1.18390555
H	-0.55342102	2.19144458	-2.58950572
O	1.10152363	0.20928598	-4.36621514
H	1.51078292	-0.18066665	-5.14974241
H	0.66673067	1.03961993	-4.64846903
O	-1.49485171	1.37418571	0.93497936
H	-1.90822608	1.20394153	1.81100680
H	-1.72761959	2.28993776	0.67591329
O	-0.44024083	2.54577814	-4.49148907
H	-0.03394446	3.38393188	-4.75439490
H	-1.26838645	2.50335476	-4.99064938
O	0.67432227	3.83692875	2.20205519
H	1.15786999	4.60104751	2.54299212
H	0.43592203	3.28432149	2.97724743
O	1.52619994	-1.93815379	-0.17370826
H	2.30922252	-1.98167552	-0.73525414
H	1.37584268	-2.82370065	0.22794422
O	2.16712382	0.24955840	-1.79113460
H	2.01917908	0.26406039	-2.75881698
H	2.95734893	0.79424352	-1.60446216
O	0.11854476	1.76914723	4.01475272
H	0.47803936	1.81825137	4.91047939

H	-0.83076835	1.54447185	4.10098703
O	-1.65892576	-4.22700105	-0.56106378
H	-2.36980880	-4.82254604	-0.28817088
H	-1.72654417	-4.15390352	-1.53434785

Am(H2O)3(NO3)3 B3LYP/6-311++G** Total energy: -1666.320018

Am	-0.09351025	0.07696738	-0.05729135
O	-0.39448704	-2.12313272	-1.34104138
O	-2.31732989	0.71167141	-1.21697205
O	1.47858248	-0.17565743	-1.98377618
O	0.21499632	1.58184570	-2.03917474
O	1.59900013	1.18905351	-3.68597243
O	-1.95539213	-1.40245034	0.82851371
O	-3.00315958	-1.03929522	2.71133775
O	1.40376639	-1.57149886	1.05323453
O	3.27276511	-1.03312777	2.05059124
N	1.12512716	0.88074529	-2.62542340
N	-2.16943611	-0.73240364	1.90208164
N	2.28254912	-0.71978348	1.44878596
O	-0.12053562	2.44525890	0.92114771
O	-1.41704374	0.30706757	2.03873840
O	2.01027560	0.50587207	1.14663919
H	0.43348659	-2.38648009	-1.76487538
H	-0.65222254	-2.85246226	-0.76130929
H	-3.03373640	0.08503748	-1.37119333
H	-2.17697727	1.20471063	-2.03625047
H	0.75689483	2.79493378	1.12554684
H	-0.58479966	2.39978327	1.76930807

Eu(H2O)3(NO3)3 B3LYP/6-311++G** Total energy: -1781.260776

Eu	-0.06129844	0.00643927	-0.11331638
O	-0.41109354	-2.16170708	-1.32538857
O	-2.11877169	0.64895419	-1.41438583
O	1.33024076	-0.23101970	-2.13229145
O	0.52644511	1.74752658	-1.80766076
O	1.83981663	1.37986721	-3.51572135
O	-2.01569098	-1.31067916	0.71633668
O	-2.86915768	-1.08040399	2.71537706
O	1.38141068	-1.57688478	1.04517910
O	3.27268003	-1.03511975	1.99621675
N	1.26398873	0.98714365	-2.53587503
N	-2.07036413	-0.75896252	1.87604535
N	2.29095261	-0.72857727	1.37610274
O	-0.29655311	2.36015704	0.72361401
O	-1.20265024	0.17060240	2.06223351
O	2.05966938	0.47606588	0.98628786
H	0.30323567	-2.45283844	-1.90522569

H	-0.71896881	-2.92200747	-0.81765599
H	-2.96559834	0.19043616	-1.38756423
H	-2.17908337	1.38693717	-2.03077365
H	0.34385374	3.01687481	0.42503982
H	-0.42504517	2.47110256	1.67355465

Am(**1b**)2(NO3)3 B3LYP/6-311++G** Total energy: -2504.692918

Am	-0.03579777	-0.01574830	0.18487665
O	1.72642636	-0.15349105	1.99260280
O	0.14087478	1.24836227	2.44120518
O	1.84279572	1.07220032	3.79570951
N	1.25350265	0.73767746	2.78775613
O	1.57699135	-0.45553467	-1.75804039
O	-0.14746400	0.76828295	-2.21975624
O	1.31833506	0.33248233	-3.77743138
N	0.93335160	0.21843324	-2.63059813
O	-1.23289861	-1.60473678	1.87065975
O	-2.43469048	-0.09641697	0.89500028
O	-3.38576753	-1.54499021	2.22385560
N	-2.38638553	-1.10477026	1.69320000
C	1.44268920	5.58688796	0.32377052
C	0.21343133	5.88727587	-0.52798366
C	-0.81074410	4.79187459	-0.38985519
C	-0.36558964	3.48955058	-0.16056827
C	1.09503273	3.18152038	-0.03271698
N	1.94346272	4.22812596	0.07946060
C	3.36253022	3.97712269	0.32618423
O	1.48610804	2.00795887	-0.04175135
N	-1.18542181	2.43193520	-0.05855030
C	-2.49927481	2.63854374	-0.16632700
C	-3.03951677	3.90466062	-0.39682703
C	-2.18599186	4.99165340	-0.51555184
H	2.24752840	6.28299649	0.08155154
H	1.21162437	5.70739023	1.39044823
H	-0.20813958	6.85150927	-0.23294834
H	0.51018667	5.97313962	-1.58060912
H	3.59625123	4.09292718	1.39001457
H	3.96005285	4.68549808	-0.25134012
H	3.60005731	2.96126204	0.02226136
H	-3.13216705	1.76802198	-0.04944528
H	-4.11302992	4.02280873	-0.47692519
H	-2.57813042	5.98684830	-0.69776160
C	-1.35667576	-5.42337277	-1.39823785
C	0.13625440	-5.72666879	-1.47800816
C	0.92231395	-4.76060635	-0.63133494
C	0.43370950	-3.46344786	-0.47487237
C	-0.85247715	-3.03753459	-1.11105834

N	-1.63011983	-4.00178548	-1.65005304
C	-2.94611083	-3.65173184	-2.18170926
O	-1.16531651	-1.83884488	-1.13924454
N	1.06823871	-2.50821062	0.22041131
C	2.22373780	-2.81790091	0.80995437
C	2.79258839	-4.08936341	0.71264133
C	2.13848433	-5.06881493	-0.02028631
H	-1.89885823	-6.00049930	-2.14917877
H	-1.75509369	-5.70407170	-0.41440502
H	0.31574889	-6.75672074	-1.15976722
H	0.47039235	-5.64828082	-2.51997972
H	-3.73173021	-3.89265122	-1.45747341
H	-3.12422067	-4.21118597	-3.10240478
H	-2.97166126	-2.58525085	-2.38823990
H	2.69552965	-2.02911902	1.38232116
H	3.73272933	-4.29495670	1.20933081
H	2.56041348	-6.06390988	-0.11587670

Eu(**1b**)2(NO3)3 B3LYP/6-311++G** Total energy: -2619.630694

Eu	-0.07085534	-0.02012470	0.24582137
O	1.69498599	-0.13227326	2.00444303
O	0.05068515	1.19112385	2.45030907
O	1.74478651	1.07598319	3.82179219
N	1.18210723	0.72625071	2.80564850
O	1.40074852	-0.49562687	-1.75473822
O	-0.27681097	0.81539868	-2.13316706
O	1.08795283	0.30870276	-3.75998628
N	0.75049041	0.21330309	-2.59517327
O	-1.29498887	-1.54481732	1.83237626
O	-2.50556993	-0.09561335	0.78912512
O	-3.46211862	-1.56280064	2.09203751
N	-2.46094356	-1.08835476	1.59795347
C	1.58462110	5.52108419	0.16520793
C	0.31925619	5.83982156	-0.62399107
C	-0.73855299	4.79493257	-0.38332690
C	-0.33519515	3.48379028	-0.12873311
C	1.11529578	3.11971507	-0.05901513
N	2.01200594	4.13110044	-0.04286216
C	3.43102786	3.82888888	0.13517808
O	1.45771669	1.93102137	-0.02437170
N	-1.18788512	2.46344008	0.04824190
C	-2.49552458	2.72080992	-0.00078301
C	-2.99711012	4.00153586	-0.24166995
C	-2.10947356	5.04808244	-0.44257559
H	2.40245427	6.16805752	-0.15646703
H	1.42511129	5.69840314	1.23715586
H	-0.04501165	6.83156843	-0.34446459

H	0.55444847	5.87185579	-1.69499407
H	3.73179395	3.98271554	1.17718952
H	4.02264593	4.48275360	-0.50878065
H	3.60761088	2.79063729	-0.13247476
H	-3.15438377	1.87809442	0.16583215
H	-4.06792416	4.16085811	-0.27017279
H	-2.47096471	6.05198868	-0.63953577
C	-1.18604142	-5.40955486	-1.53175730
C	0.31778170	-5.66042573	-1.56545551
C	1.03925010	-4.70976244	-0.64655011
C	0.50528122	-3.43547955	-0.45231730
C	-0.77505314	-3.02402070	-1.11032051
N	-1.49799952	-3.98707075	-1.72452178
C	-2.80655711	-3.65434446	-2.28454862
O	-1.13526984	-1.84041177	-1.08564716
N	1.08815520	-2.49085867	0.30102633
C	2.23189657	-2.79399585	0.91628920
C	2.84034771	-4.04447451	0.79015015
C	2.24178289	-5.00989953	-0.00557899
H	-1.67887842	-5.96539973	-2.33116384
H	-1.61260775	-5.75210498	-0.57956995
H	0.52104700	-6.69755969	-1.28720160
H	0.68898354	-5.52146778	-2.58833864
H	-3.60770849	-3.94910614	-1.59812046
H	-2.93670501	-4.17868196	-3.23342478
H	-2.85916027	-2.58115258	-2.44666007
H	2.66394502	-2.01497293	1.53149798
H	3.76849968	-4.24363563	1.31140396
H	2.69617820	-5.98756219	-0.12804382

Am(**2**)3 B3LYP/6-311+G** Total energy: -7422.35804026

Am	-0.00021015	-0.00084634	-0.17343653
S	-1.74443795	1.72840225	1.26716269
S	-0.15854115	2.46660895	-1.59871790
P	-1.41950038	3.17928220	-0.14372221
C	-0.65599078	4.63523959	0.73501412
C	-1.20393493	5.33425317	1.83376475
C	0.63171001	4.98211520	0.31337899
C	-0.45660447	6.33216552	2.46216730
C	1.36664010	5.97930648	0.94630968
H	1.05956148	4.45830880	-0.53089371
C	0.82316340	6.65753101	2.02832318
H	-0.89127120	6.86441034	3.29834540
H	2.36014792	6.22162446	0.58745448
H	1.38266189	7.43595881	2.53322274
C	-3.01533789	3.63627914	-0.99858834
C	-3.27472816	4.78228066	-1.78353699

C	-4.01244249	2.66101076	-0.90921154
C	-4.50687084	4.91654565	-2.42689851
C	-5.23190628	2.79947221	-1.56470961
H	-3.82923890	1.78193848	-0.30517141
C	-5.48380895	3.93216006	-2.32569145
H	-4.69707354	5.80137254	-3.01865995
H	-5.97969283	2.02036316	-1.47324042
H	-6.42965501	4.05679332	-2.83920960
S	-0.62181423	-2.36866241	1.28108965
S	-2.06255797	-1.37863930	-1.58556492
P	-2.04445645	-2.82005319	-0.12377513
C	-3.68472039	-2.88365533	0.75969089
C	-4.01263678	-3.70267186	1.86323872
C	-4.63079190	-1.94466748	0.33596916
C	-5.24899732	-3.55230787	2.49415249
C	-5.86032155	-1.80470175	0.97140783
H	-4.39379754	-1.31618472	-0.51201189
C	-6.17250337	-2.60947742	2.05814606
H	-5.48994048	-4.19100263	3.33404966
H	-6.56846184	-1.06779517	0.61076893
H	-7.12515189	-2.51244121	2.56505505
C	-1.64372815	-4.43443713	-0.97207632
C	-2.50810336	-5.23637504	-1.75087698
C	-0.30010298	-4.80908127	-0.88452541
C	-2.00929012	-6.37328973	-2.39019379
C	0.18868914	-5.93719090	-1.53597741
H	0.37082401	-4.20762732	-0.28510512
C	-0.66782547	-6.72582412	-2.29093285
H	-2.68166538	-6.98365317	-2.97725975
H	1.23771514	-6.19414626	-1.44608298
H	-0.30365169	-7.60945067	-2.80126763
S	2.36606965	0.65383845	1.26916609
S	2.21936758	-1.10650517	-1.58618071
P	3.46359491	-0.36099474	-0.13321732
C	4.34189169	-1.74412427	0.75585850
C	5.21884185	-1.61161540	1.85561675
C	4.00033820	-3.03559410	0.34144352
C	5.70890154	-2.75348161	2.49218197
C	4.49597341	-4.16633053	0.98245845
H	3.33472475	-3.14995418	-0.50359984
C	5.35263040	-4.02740747	2.06548748
H	6.38531876	-2.63747660	3.32908969
H	4.21061962	-5.15031998	0.62905952
H	5.74658738	-4.89771414	2.57664208
C	4.65832830	0.78795882	-0.99282263
C	5.78236449	0.43537813	-1.77315894
C	4.31117999	2.13941730	-0.91278774

C	6.51541900	1.43167545	-2.42134007
C	5.04154731	3.12257343	-1.57302625
H	3.45682360	2.42355931	-0.31234631
C	6.15027808	2.77029249	-2.32943428
H	7.37823133	1.15079616	-3.00950567
H	4.73981107	4.16008427	-1.48882872
H	6.73171772	3.52420741	-2.84654129
C	-3.11080516	-4.74802190	2.48539388
C	-3.99117331	-4.98154646	-1.90380049
C	-2.56205292	5.07978134	2.45334248
C	-2.31125386	5.93782994	-1.93923737
C	6.30249698	-0.97744729	-1.91871811
C	5.67528836	-0.30400440	2.46792653
F	-2.46638113	-4.27091275	3.57345915
F	-3.82455066	-5.82099259	2.90690284
F	-2.17402480	-5.22456560	1.64184439
F	-4.68435894	-5.35974155	-0.79928858
F	-4.28024366	-3.68194503	-2.12348620
F	-4.52265718	-5.67166704	-2.93664316
F	5.32064269	-1.87880522	-2.12923579
F	6.98023871	-1.38161899	-0.81382111
F	7.16239793	-1.09951488	-2.95369227
F	6.96281820	-0.38295404	2.88553857
F	5.61668290	0.74017162	1.61792189
F	4.94360770	0.02240876	3.55645244
F	-3.13477590	6.23676011	2.86776122
F	-2.47464633	4.28826328	3.54543100
F	-3.44120490	4.50337118	1.61008858
F	-1.04088431	5.53643647	-2.15334285
F	-2.29479435	6.73248435	-0.83844713
F	-2.63963014	6.73845405	-2.97686579

Eu(**2**)3 B3LYP/6-311+G** Total energy: -7537.29381624

Eu	-0.01505551	0.00462594	-0.18209022
S	-1.80684834	1.74677310	1.22085753
S	-0.15353430	2.50205897	-1.59545590
P	-1.43531272	3.21108294	-0.16034643
C	-0.67706716	4.64407417	0.75707141
C	-1.24376524	5.33563663	1.85091297
C	0.62800660	4.97415725	0.37808165
C	-0.49797557	6.31089526	2.51536498
C	1.36157632	5.94850644	1.04678520
H	1.07120779	4.45483466	-0.46091905
C	0.79912821	6.61992624	2.12314509
H	-0.94717231	6.83776081	3.34716397
H	2.36961681	6.17690943	0.72111629
H	1.35744313	7.38038603	2.65585069

C	-3.00353392	3.69348392	-1.04750017
C	-3.24080287	4.85556823	-1.81541968
C	-4.00065709	2.71486534	-1.01072290
C	-4.45534950	5.00487445	-2.48818527
C	-5.20216097	2.86857655	-1.69465676
H	-3.83286008	1.82136002	-0.42354670
C	-5.43456265	4.01905858	-2.43473227
H	-4.62923284	5.90230412	-3.06559115
H	-5.95067317	2.08661405	-1.64270093
H	-6.36665614	4.15583376	-2.96973171
S	-0.60623306	-2.40933268	1.24646656
S	-2.11694386	-1.38237080	-1.56488779
P	-2.05630138	-2.84667786	-0.13101459
C	-3.67205173	-2.93962823	0.79076288
C	-3.96749272	-3.78432715	1.88380320
C	-4.63164622	-1.99438517	0.41447073
C	-5.18733620	-3.65394290	2.55012246
C	-5.84426046	-1.87385675	1.08506718
H	-4.41898042	-1.34497371	-0.42404710
C	-6.12508062	-2.70496304	2.16035423
H	-5.40348697	-4.31244845	3.38131910
H	-6.56304450	-1.13030600	0.76123511
H	-7.06429102	-2.62328062	2.69421482
C	-1.66376594	-4.43781107	-1.02201956
C	-2.53996873	-5.23797991	-1.78914300
C	-0.31067839	-4.78633752	-0.99277819
C	-2.04363267	-6.35265356	-2.46835627
C	0.17512371	-5.89185305	-1.68338401
H	0.37048747	-4.18307364	-0.40682654
C	-0.69344392	-6.68213559	-2.42253485
H	-2.72484668	-6.96280323	-3.04508806
H	1.23163615	-6.12881274	-1.63787163
H	-0.33160732	-7.54865323	-2.96286457
S	2.38465031	0.70729167	1.22253119
S	2.22441857	-1.14324793	-1.56899451
P	3.47327636	-0.35874757	-0.14399471
C	4.34503924	-1.71308010	0.79171421
C	5.22513971	-1.54631155	1.88401811
C	3.98932463	-3.01622848	0.42968027
C	5.70652514	-2.66700762	2.56319881
C	4.47559668	-4.12579593	1.11306743
H	3.31969653	-3.15692762	-0.40806952
C	5.33679731	-3.95304353	2.18744176
H	6.38588808	-2.52478819	3.39355694
H	4.17790877	-5.11971684	0.80019616
H	5.72351624	-4.80651780	2.73133485
C	4.66929932	0.75205058	-1.04702959

C	5.79624588	0.37080799	-1.80934930
C	4.31326949	2.10341401	-1.03048477
C	6.52769788	1.34170018	-2.49673133
C	5.04186851	3.06054641	-1.72914767
H	3.45403486	2.40888133	-0.44767385
C	6.15642308	2.68135104	-2.46352887
H	7.39341528	1.03960266	-3.06965454
H	4.73329502	4.09878728	-1.69319182
H	6.73691763	3.41509459	-3.00976987
C	-3.04456546	-4.83876994	2.45722926
C	-4.03050753	-5.00131813	-1.89097498
C	-2.62358072	5.09603379	2.42631800
C	-2.26975808	6.00989559	-1.92504115
C	6.31710606	-1.04657226	-1.89767223
C	5.69503838	-0.21992193	2.44293015
F	-2.37769357	-4.38469193	3.54218415
F	-3.74057251	-5.92790841	2.86741780
F	-2.12463478	-5.28568242	1.57934018
F	-4.68424263	-5.40226402	-0.77078354
F	-4.34181954	-3.70214200	-2.08411975
F	-4.58684534	-5.68365829	-2.91603219
F	5.33503547	-1.95415269	-2.08189260
F	6.98635784	-1.41070651	-0.77410991
F	7.18397886	-1.20897293	-2.92140506
F	6.98566309	-0.29125630	2.85307387
F	5.63562170	0.79169670	1.55432383
F	4.97407953	0.15203243	3.52450601
F	-3.19186256	6.25723505	2.83569180
F	-2.58183875	4.29178375	3.51212428
F	-3.48487132	4.54179069	1.55021960
F	-0.99690549	5.60596012	-2.12209772
F	-2.27153608	6.78085500	-0.80767786
F	-2.57174956	6.83476173	-2.95179912

[Am(oxalate)(H2O)7]+ B3LYP/6-311++G** Total energy: -1508.032637

Am	-0.23350165	-0.44709886	-0.02503392
O	-0.01087183	-0.11118994	-2.57283482
O	3.45468774	-0.18311619	0.43660971
O	1.31698446	-0.96516754	1.90255478
O	-2.58236994	-0.19101187	-1.16099557
O	-0.82173657	-3.01231317	-0.05539358
O	-1.67983850	-0.32318620	2.10206875
O	1.76451843	-1.88113799	-0.88345426
H	-0.81266099	-0.01877446	-3.10375399
H	0.59167157	0.59204749	-2.85002493
H	4.38428629	0.05467359	0.52756185
H	2.95371740	0.61186820	0.13612969

H	1.14594713	-0.78493910	2.83353402
H	2.24995153	-0.72473347	1.71307573
H	-3.43252517	-0.62458973	-1.29519437
H	-2.74791550	0.71246450	-0.83467977
H	-1.56526499	-3.60096521	0.11908372
H	-0.03290898	-3.56709225	-0.12494189
H	-1.99676624	0.59456309	2.06883367
H	-2.12820545	-0.78257087	2.82041353
H	1.89783682	-2.01664652	-1.82949558
H	2.60177287	-1.50338961	-0.53369354
O	1.27082660	1.21740356	-0.22051319
O	-1.23469057	1.56618802	0.28657274
C	0.96335552	2.51085929	-0.05258382
C	-0.57394252	2.72459360	0.19268856
O	1.75399207	3.41062285	-0.07820738
O	-1.06332706	3.81392694	0.28034808

[Eu(oxalate)(H2O)7]+ B3LYP/6-311++G** Total energy: -1622.984020

Eu	-0.29367660	-0.58284006	-0.00606893
O	-0.32173461	-0.21771072	-2.61502375
O	3.55071745	-0.36741567	0.52096681
O	1.30848467	-1.03004992	1.99951757
O	-2.73758177	-0.16821332	-1.23259622
O	-0.61038678	-3.17687941	-0.07716921
O	-1.92352463	-0.34239075	2.06075133
O	1.81354338	-1.97255371	-0.93109050
H	-1.24890436	-0.09838983	-2.86312375
H	0.20920447	0.26818502	-3.25512926
H	4.49665670	-0.21944979	0.63306605
H	3.14961170	0.47431485	0.23201898
H	1.19172516	-1.07548253	2.95325981
H	2.25247143	-0.85981696	1.82481937
H	-3.59535783	-0.60242415	-1.30140345
H	-2.90462869	0.73077797	-0.91104441
H	-1.19834010	-3.92652560	0.06052968
H	0.27391991	-3.52891145	-0.24956640
H	-2.21030086	0.57863736	2.12027022
H	-2.33235083	-0.81362729	2.79434506
H	1.99133508	-2.08329578	-1.87182496
H	2.63922581	-1.63448811	-0.53120548
O	1.43629377	1.32569615	-0.15147675
O	-1.32010654	1.76278244	0.23185831
C	1.28764812	2.54848560	-0.07432902
C	-0.81154430	2.88466212	0.19001241
O	1.84687878	3.58821430	-0.07261858
O	-1.01225498	4.04446454	0.24916225

[Am(oxalate)(H2O)9]+ B3LYP/6-311++G** Total energy: -1660.999337

Am	0.00053897	-0.46058028	-0.06500160
O	0.98119315	0.47182868	-2.41675145
O	2.55176092	-0.95688058	-0.09856052
O	0.78465908	-0.74762546	2.45207723
O	-2.10553750	-1.35626050	-1.24380652
O	0.04513378	-2.91276166	0.97885914
O	-1.99480441	-0.42701653	1.57301729
O	0.50796050	-2.17324253	-2.08624916
H	0.44704772	1.18779708	-2.78709111
H	1.86793317	0.83789506	-2.29691144
H	3.02357763	-1.78270660	-0.24793454
H	3.05312547	-0.44721076	0.57762248
H	0.18476051	-0.30879140	3.06886415
H	1.66190564	-0.32001450	2.57558308
H	-2.13704043	-1.78813568	-2.10378314
H	-2.91760246	-0.81890604	-1.12933757
H	-0.43201890	-3.74839625	0.93337346
H	0.41085285	-2.82345275	1.87076860
H	-2.76629039	0.02148662	1.15873585
H	-2.34946246	-1.18769172	2.04668363
H	0.89061215	-1.64691727	-2.80276513
H	0.80720964	-3.08213093	-2.19719652
O	1.09706814	1.46693097	0.55551518
O	-1.21307294	1.41765266	-0.55774810
C	0.61363734	2.68802849	0.35691717
C	-0.81767747	2.65753689	-0.27367267
O	1.18734026	3.71039470	0.62365985
O	-1.46990702	3.64803518	-0.46683798
H	-2.98655052	1.25589900	-0.54136489
O	-3.70811550	0.62992458	-0.29192653
H	-4.55083750	1.09326297	-0.35016450
H	2.52284965	1.30980264	1.53861611
O	3.10109232	0.65020923	2.00073232
H	3.81461450	1.11660722	2.44990960

[Eu(oxalate)(H2O)9]+ B3LYP/6-311++G** Total energy: -1775.941980

Eu	0.01627761	-0.54858954	-0.07955913
O	0.99910365	0.37324549	-2.39026848
O	2.53747515	-0.99252768	-0.11228018
O	0.79994554	-0.82988212	2.43070445
O	-2.07831923	-1.41790629	-1.22836515
O	-0.03579372	-2.92297735	0.98655855
O	-1.94537727	-0.48210754	1.57520561
O	0.56774386	-2.25373520	-2.04065753
H	0.46576424	1.08032684	-2.77743764
H	1.88218694	0.74402523	-2.26084197

H	3.01938786	-1.79666205	-0.32955365
H	3.05204458	-0.50906617	0.57154523
H	0.18520548	-0.37463514	3.02030235
H	1.67408208	-0.40540857	2.57078091
H	-2.13174106	-1.85137040	-2.08567876
H	-2.88652400	-0.87841601	-1.10197566
H	-0.39535640	-3.81088850	0.89353248
H	0.36816418	-2.84166482	1.86280949
H	-2.71217092	-0.01046029	1.18543658
H	-2.30594822	-1.27899339	1.98009094
H	0.92467387	-1.73456959	-2.77481766
H	0.73208677	-3.18456805	-2.22261056
O	1.09390588	1.42201691	0.57609812
O	-1.18984347	1.36028120	-0.59218277
C	0.59103966	2.61791565	0.38346616
C	-0.82480174	2.59013358	-0.29507300
O	1.13432730	3.65240347	0.68835174
O	-1.46627829	3.58971108	-0.49265577
H	-3.00433018	1.20861069	-0.55992002
O	-3.70197346	0.57112737	-0.28799770
H	-4.55739412	1.01011801	-0.35157847
H	2.53801417	1.25300817	1.56039444
O	3.11901574	0.58528447	2.00271224
H	3.83532420	1.04209815	2.45674734

[Am(dipicolinate)(H2O)6]+ B3LYP/6-311++G** Total energy: -1678.758122

Am	-0.51753586	0.40257090	0.34169376
O	-0.95636724	-0.94690907	2.39279908
O	0.71079847	0.68928175	3.83383432
O	-0.80767929	2.21011790	2.15149097
O	-3.07549657	0.89059566	-2.35876715
O	-1.03975241	2.33560222	-1.20652698
O	-3.07953809	0.50344860	0.33798617
H	-1.62749123	-1.56390867	2.70270633
H	-0.42855283	-0.63365887	3.16112736
H	1.16447138	0.71713394	4.68413468
H	1.38993105	0.67890479	3.12020744
H	-0.84496636	3.17219744	2.11015514
H	-0.32229658	1.96507850	2.96811011
H	-2.51267754	0.08289857	-2.40927203
H	-3.65439022	0.90721337	-3.12928229
H	-0.54620590	3.04481388	-1.63333025
H	-1.78203156	2.08203484	-1.80141265
H	-3.69714749	0.89772344	0.96371741
H	-3.46120365	0.59302437	-0.56012356
C	2.54928395	-0.88321911	-0.30582902
C	3.58379289	-1.59266160	-0.90612439

C	3.30313004	-2.31330890	-2.06782943
C	2.01009675	-2.30873740	-2.59186447
C	1.03234825	-1.57561212	-1.92748715
C	-0.40495843	-1.45879475	-2.39003595
C	2.69341119	-0.08672918	0.97449431
N	1.31095090	-0.88297814	-0.81539757
O	1.56787549	0.52014549	1.32310546
O	3.72697264	-0.05495353	1.60019898
O	-1.14654798	-0.74901208	-1.55457339
O	-0.78971635	-1.94521670	-3.42743464
H	4.56924658	-1.57023446	-0.45879326
H	4.08738760	-2.87613885	-2.56020487
H	1.74393755	-2.85107064	-3.49015998

[Eu(dipicolinate)(H2O)6]+ B3LYP/6-311++G** Total energy: -1793.699026

Eu	-0.63031399	0.47352075	0.39966502
O	-0.94519877	-0.92367632	2.39840023
O	0.64384595	0.77094885	3.86285402
O	-0.97923396	2.19203430	2.21100920
O	-3.08151249	1.01939364	-2.32868776
O	-0.93328333	2.32231603	-1.20640836
O	-3.12343146	0.73129873	0.37602375
H	-1.44980269	-1.70073464	2.66096595
H	-0.43996637	-0.59214014	3.17289282
H	1.10354100	0.81730914	4.70879939
H	1.31585276	0.80080718	3.14416167
H	-1.27033011	3.10884544	2.24353949
H	-0.46997934	1.99774729	3.02586342
H	-2.59000461	0.16679582	-2.34355344
H	-3.64937441	1.05337303	-3.10680407
H	-0.45861750	3.10247026	-1.51206535
H	-1.67524312	2.13971981	-1.82532469
H	-3.79441409	0.93131956	1.03618659
H	-3.51557085	0.83164338	-0.51552326
C	2.43124114	-0.77985611	-0.26064344
C	3.46735697	-1.48760800	-0.86079733
C	3.17823476	-2.23862198	-2.00100095
C	1.87687664	-2.26613980	-2.50437396
C	0.89949519	-1.53471231	-1.83777396
C	-0.54852534	-1.44215807	-2.26880770
C	2.57570956	0.05871842	0.99111981
N	1.18598510	-0.81450191	-0.74771643
O	1.45327293	0.67506652	1.32101982
O	3.60822900	0.11298776	1.61969222
O	-1.28282519	-0.73335268	-1.42846397
O	-0.95358415	-1.94263624	-3.29331500
H	4.46125592	-1.44094857	-0.43434058

H 3.96299921 -2.79970293 -2.49466124
H 1.60903059 -2.83226237 -3.38734871

[Am(dipicolinate)(H2O)8]+ B3LYP/6-311++G** Total energy: -1831.723315
Am -0.06661727 -0.11873810 -0.66332505
C -0.14609280 1.52850975 2.30755194
C -0.02915292 1.81219826 3.66509333
H -0.28995145 2.80010734 4.02262178
C 0.42405114 0.80381759 4.51592056
H 0.52624982 0.99333681 5.57812125
C 0.74671889 -0.44905538 3.99396349
H 1.10474036 -1.26149832 4.61331016
C 0.59986756 -0.65234050 2.62500398
C 0.91513194 -1.96448631 1.93058798
C -0.61509265 2.53655932 1.27447895
N 0.16166666 0.32099964 1.81480440
O -0.62199850 2.04786860 0.05353963
O -0.93853684 3.66142385 1.58959213
O 0.68463659 -1.92321226 0.63638045
O 1.33405122 -2.92127315 2.54564968
O 2.50442737 0.53506602 -0.43167999
H 2.97959125 -0.22423974 -0.79908349
H 3.00222685 0.84272137 0.33500413
O 1.68584493 -1.43215085 -2.17908326
O 0.82035709 1.42800389 -2.55252615
H 1.69777606 1.76317242 -2.32889606
H 0.25398659 2.21071598 -2.71097795
O -2.09125033 0.65942777 -2.20687520
H -2.32516305 0.20251200 -3.02348275
O -2.53390208 -0.58219552 0.21572621
H -2.87607837 -0.60114859 1.11726666
H -3.09225341 0.02425627 -0.29190344
O -1.21258590 -2.19406293 -1.72946315
H -2.02745257 -2.40782098 -1.25748837
H -0.65440467 -2.99822121 -1.70327941
H -1.09267271 3.14693882 -1.26752826
O -1.25130920 3.22519471 -2.23988094
H -1.55178705 4.11969283 -2.43333265
H 0.95744275 -3.41837423 -0.29015614
O 0.94209874 -3.83132417 -1.18802346
H 1.23294308 -4.74653027 -1.11280978
H -2.05264821 1.62247941 -2.40491038
H 1.64768183 -2.40412423 -2.03220393
H 1.75252887 -1.28130698 -3.12904181

[Eu(dipicolinate)(H2O)8]+ B3LYP/6-311++G** Total energy: -1946.664275
Eu -0.06821150 -0.13155241 -0.76469939

C	-0.11968064	1.52137190	2.18551939
C	0.00187123	1.80723634	3.54234281
H	-0.24314704	2.80003307	3.89776335
C	0.43447458	0.79196885	4.39597887
H	0.53909743	0.98201653	5.45783657
C	0.72721136	-0.47035204	3.87856963
H	1.06020633	-1.29063461	4.50168501
C	0.57792893	-0.67341875	2.50971867
C	0.84288613	-1.99757616	1.81569816
C	-0.59268149	2.52299905	1.14745359
N	0.17003657	0.30925300	1.69702840
O	-0.63514065	2.01831624	-0.06407041
O	-0.89069599	3.65855134	1.45194635
O	0.57254781	-1.96045111	0.53116493
O	1.25918357	-2.96004991	2.42503593
O	2.42676290	0.53679036	-0.47733765
H	2.95389187	-0.19082254	-0.83653562
H	2.89002794	0.88084300	0.29489850
O	1.66544694	-1.40350800	-2.22904245
O	0.79105927	1.36838941	-2.63901572
H	1.66369599	1.71985375	-2.42226037
H	0.21598854	2.14347153	-2.80759814
O	-2.05436519	0.58731429	-2.27974830
H	-2.27896607	0.09382356	-3.07710482
O	-2.45536973	-0.62339137	0.14258544
H	-2.75627309	-0.70819938	1.05455509
H	-3.06171584	-0.02099221	-0.31037911
O	-1.19968886	-2.13368771	-1.89799591
H	-2.01337157	-2.34787757	-1.42426113
H	-0.65291415	-2.94525095	-1.88146784
H	-1.12064898	3.10349283	-1.39028277
O	-1.27197846	3.16894407	-2.36465677
H	-1.56893743	4.06092671	-2.57411256
H	0.88061589	-3.43603489	-0.41352215
O	0.90773455	-3.82357077	-1.32241672
H	1.19291649	-4.74149185	-1.26066363
H	-2.05140384	1.54366513	-2.50541755
H	1.63273066	-2.37832654	-2.09859926
H	1.74242280	-1.23532627	-3.17550398

[Am(ADPTZ)(H2O)6]3+ B3LYP/6-311++G** Total energy: -1883.780723

Am	0.22929294	-0.95038027	-0.32012878
O	0.48904329	-1.15661854	2.26224370
O	1.76462930	-2.95428191	0.42925287
O	-1.12540753	-2.90916385	0.78382586
O	-0.25113456	0.16167047	-2.59859706
O	-0.26811482	-2.74172158	-2.19823400

O	2.16378851	-1.17539166	-2.14102781
H	0.98397260	-0.55696388	2.83693522
H	-0.17305656	-1.58654135	2.82108451
H	2.34433800	-3.56007388	-0.05291201
H	2.00177675	-3.03913477	1.36362751
H	-2.07641862	-3.00365842	0.93160609
H	-0.73148480	-3.76825936	0.98954903
H	0.45121246	0.39237756	-3.22238234
H	-1.02564487	0.68348321	-2.84891668
H	-0.54728654	-2.46484838	-3.08228854
H	-0.42132459	-3.69582901	-2.15663195
H	3.00718580	-0.70730947	-2.21041267
H	2.19997635	-1.89119756	-2.79026776
N	-2.27177169	-0.33980777	-0.42339607
N	-0.34466936	1.33371139	0.46216352
N	-1.98954851	2.97918609	0.92615166
N	0.32620881	3.45359363	1.28633735
N	2.24535575	0.53480701	0.42983114
C	-3.20492262	-1.18025903	-0.91255952
C	-4.56196748	-0.87675526	-0.94392741
C	-4.98293464	0.35472181	-0.44850758
C	-4.02864458	1.24117149	0.04482744
C	-2.68756512	0.86502787	0.03923842
C	-1.62856970	1.79038814	0.51498392
C	-0.98545223	3.80862423	1.31691349
C	0.58910447	2.24113829	0.86761863
C	2.00842230	1.80423189	0.84384869
C	3.02735749	2.66220476	1.25198051
C	4.34276261	2.20455468	1.24338046
C	4.59352912	0.89648988	0.83859796
C	3.52122230	0.10273436	0.44394602
N	-1.30023322	5.01805801	1.74476140
H	-2.84783338	-2.12697482	-1.30208778
H	-5.26659205	-1.59172425	-1.35079822
H	-6.03267608	0.62460967	-0.45324543
H	-4.30226429	2.21484952	0.42838366
H	2.77779932	3.66551358	1.56958865
H	5.15263526	2.85439838	1.55408263
H	5.59828411	0.49205366	0.82822125
H	3.68770312	-0.92331079	0.13652897
H	-0.57761391	5.66151043	2.03914964
H	-2.26671554	5.31417855	1.77872956

[Eu(ADPTZ)(H2O)6]3+ B3LYP/6-311++G** Total energy: -1998.717262

Eu	0.27226863	-1.08919535	-0.36880738
O	0.45519819	-1.24201471	2.18306685
O	1.80517671	-3.03819324	0.36469484

O	-1.05944560	-3.06087207	0.72019247
O	-0.19204994	0.07665673	-2.59731369
O	-0.28797868	-2.78896968	-2.23070634
O	2.18853774	-1.29704362	-2.16487847
H	0.92183022	-0.65527487	2.79297239
H	-0.18712972	-1.73383049	2.71231033
H	2.38268500	-3.63663176	-0.12855540
H	2.04424064	-3.13801269	1.29671954
H	-2.00718582	-3.16367823	0.88076432
H	-0.65710250	-3.91688145	0.92092072
H	0.52242930	0.28367270	-3.21482584
H	-0.94513319	0.62528925	-2.85390380
H	-0.55731585	-2.47841151	-3.10634101
H	-0.45391302	-3.74139875	-2.21749302
H	3.03368395	-0.82982320	-2.21112787
H	2.22730229	-1.98775015	-2.84030555
N	-2.24052200	-0.48705190	-0.44808520
N	-0.30632099	1.21774994	0.37600406
N	-1.95277443	2.85152382	0.86252495
N	0.36364303	3.32648101	1.22418599
N	2.28003644	0.39401114	0.39749094
C	-3.17760816	-1.33401069	-0.91172227
C	-4.53609327	-1.02997523	-0.93866724
C	-4.95266479	0.20974477	-0.46331699
C	-3.99281101	1.10386449	0.00568361
C	-2.65203637	0.72618622	-0.00519815
C	-1.59283158	1.65962891	0.45139852
C	-0.94659759	3.68069145	1.24170747
C	0.62856577	2.11279255	0.80136883
C	2.04508067	1.66863131	0.79552014
C	3.06183973	2.52872507	1.20504767
C	4.37631638	2.06732039	1.21512956
C	4.62581260	0.75517639	0.82586247
C	3.55358173	-0.03933064	0.42853184
N	-1.26049802	4.89921255	1.65248295
H	-2.82505133	-2.28748047	-1.28800204
H	-5.24344669	-1.75232633	-1.32748196
H	-6.00227238	0.48001975	-0.46389132
H	-4.26303800	2.08393553	0.37529642
H	2.81360694	3.53638083	1.50940958
H	5.18517187	2.71759362	1.52728305
H	5.62908889	0.34690784	0.82926535
H	3.72059177	-1.06884557	0.13340051
H	-0.53685742	5.54285611	1.94672659
H	-2.22772931	5.19548090	1.68666540

[Am(**6**)2(NO3)3] B3LYP/6-311++G** Total energy: -2536.691316

Am	-0.00412597	0.00315460	-0.01887571
O	1.56354275	-0.09812169	1.96040502
O	-0.01163257	1.36263963	2.21600833
O	1.62363026	1.26904998	3.66056911
N	1.07528202	0.85393654	2.65468806
O	1.56703977	-0.38570266	-1.95999024
O	-0.22558452	0.73018967	-2.42704849
O	1.23187287	0.31765372	-3.99996132
N	0.87312595	0.22459044	-2.84467443
O	-1.17186246	-1.66063052	1.63256047
O	-2.39922309	-0.10409621	0.76628525
O	-3.33256124	-1.68136207	1.95096308
N	-2.33789552	-1.16355433	1.47470054
C	1.24619345	5.36318785	1.29267286
C	0.13371333	5.89617279	0.38949971
C	-0.83738251	4.79984910	0.04934925
C	-0.35875341	3.48805881	-0.00442504
C	1.08701300	3.16484556	0.21804529
N	1.85455053	4.14531911	0.73685724
C	3.23793801	3.84647489	1.11175654
O	1.52521514	2.05235922	-0.09717430
N	-1.13292588	2.43633959	-0.28259665
N	-2.41040727	2.59321631	-0.56649205
C	-2.92047667	3.82659724	-0.55292396
C	-2.18152154	4.96626663	-0.23932056
H	2.03614123	6.10897696	1.39104435
H	0.86027568	5.15299791	2.29791403
H	-0.37735700	6.72669105	0.88239222
H	0.56839058	6.28710624	-0.53858321
H	3.30339620	3.62128545	2.18106919
H	3.86728773	4.70793168	0.88069363
H	3.57609211	2.98022413	0.54928177
H	-3.97472985	3.88394331	-0.79879642
H	-2.65173557	5.94324318	-0.22342945
C	-1.56344841	-5.42408649	-0.41586832
C	-0.11664102	-5.87553923	-0.61649324
C	0.83546184	-4.79107975	-0.19445877
C	0.41643066	-3.46314723	-0.31143955
C	-0.92070003	-3.10407239	-0.88342626
N	-1.80802384	-4.10971178	-1.02819757
C	-3.17667374	-3.80086576	-1.44620708
O	-1.15333146	-1.93743665	-1.22124158
N	1.17284193	-2.42189574	0.04418988
N	2.39730206	-2.59933691	0.49818094
C	2.86153328	-3.84563961	0.61197012
C	2.11855056	-4.98056487	0.29093107
H	-2.24458395	-6.13591211	-0.88413757

H	-1.81010916	-5.38120654	0.65228134
H	0.06658251	-6.79281862	-0.05176588
H	0.05369867	-6.10640102	-1.67516893
H	-3.83672203	-3.73833178	-0.57509256
H	-3.53306331	-4.58361492	-2.11849718
H	-3.18057855	-2.84289822	-1.95939444
H	3.87564969	-3.91908568	0.98795088
H	2.53856201	-5.97173144	0.42137985

[Eu(**6**)2(NO3)3] B3LYP/6-311++G** Total energy: -2651.627614

Eu	-0.07480216	-0.01828948	0.23719983
O	1.61793782	-0.09532550	2.08708300
O	-0.02347925	1.27868944	2.37734888
O	1.62105156	1.23972909	3.81368909
N	1.09466296	0.81560421	2.80276157
O	1.41551591	-0.50655647	-1.75778391
O	-0.25437648	0.81192071	-2.13721778
O	1.11065675	0.30185449	-3.76270793
N	0.77193298	0.20555587	-2.59894856
O	-1.18239617	-1.59279002	1.83831297
O	-2.48052566	-0.14793711	0.89455516
O	-3.33773398	-1.69469739	2.17334647
N	-2.37506336	-1.15938982	1.65939003
C	1.39519267	5.46340204	0.92261626
C	0.22199722	5.89827402	0.04539574
C	-0.80204461	4.80158921	-0.04754879
C	-0.36615269	3.47695916	0.04869903
C	1.08377080	3.13409871	0.20741008
N	1.91789918	4.15234951	0.51297813
C	3.32277671	3.86281422	0.80217953
O	1.46847591	1.97400588	0.03600886
N	-1.18836771	2.42714720	-0.03129678
N	-2.47830201	2.59635510	-0.23404510
C	-2.95340702	3.83939890	-0.34403070
C	-2.16030835	4.98080496	-0.25046288
H	2.21076289	6.18299614	0.83834067
H	1.09437041	5.42640840	1.97739395
H	-0.22347200	6.81130598	0.44774798
H	0.58352786	6.13062395	-0.96375124
H	3.49187528	3.82404999	1.88320667
H	3.94937665	4.64283108	0.36513293
H	3.57931906	2.89840120	0.37196216
H	-4.02271438	3.90271011	-0.51087166
H	-2.59867261	5.96887179	-0.33662616
C	-1.44364544	-5.47626556	-0.80878955
C	0.03454427	-5.82226892	-0.98309641
C	0.90092764	-4.77401988	-0.34225361

C	0.42229178	-3.46208413	-0.28566723
C	-0.90286880	-3.08089311	-0.87029318
N	-1.72664755	-4.09341067	-1.21878884
C	-3.08094202	-3.78758583	-1.68075395
O	-1.18800228	-1.89090765	-1.03456143
N	1.11266072	-2.45125069	0.24906110
N	2.31840887	-2.64622410	0.74043690
C	2.83419405	-3.87756565	0.70670750
C	2.16547035	-4.98179513	0.18311903
H	-2.05619254	-6.13382928	-1.42722303
H	-1.75250414	-5.62105583	0.23431936
H	0.23745841	-6.80727212	-0.55586072
H	0.27638887	-5.87565882	-2.05160375
H	-3.80225003	-3.91904438	-0.86764490
H	-3.34023816	-4.45394802	-2.50587419
H	-3.11374592	-2.75433029	-2.01582676
H	3.82984761	-3.96326587	1.12694506
H	2.62673583	-5.96314947	0.18886088

[Am(**7**)2(NO3)3] B3LYP/6-311++G** Total energy: -2536.766921

Am	-0.03257774	-0.01325003	0.14901166
O	1.72137158	-0.16809079	1.95338232
O	0.17263509	1.28068299	2.38004323
O	1.89975065	1.12175542	3.70597235
N	1.28390199	0.76058006	2.72525184
O	1.55812263	-0.46929172	-1.79383447
O	-0.15342643	0.77735995	-2.23936775
O	1.29960082	0.33454285	-3.80758112
N	0.91950343	0.21770107	-2.66152501
O	-1.26572030	-1.62150226	1.78450602
O	-2.42977155	-0.06878950	0.83305376
O	-3.42946335	-1.56320829	2.07204674
N	-2.41311107	-1.10801336	1.59224116
C	1.43896011	5.57811673	0.45717379
C	0.20250444	5.91275842	-0.37384646
C	-0.79943161	4.79428711	-0.29193646
C	-0.34529713	3.49154466	-0.12122144
C	1.12010737	3.18348279	-0.00984501
N	1.95277030	4.23337960	0.14993800
C	3.37712035	3.98943828	0.37906087
O	1.51117651	2.01376728	-0.08085946
N	-1.17444086	2.44168478	-0.06825056
C	-2.48135113	2.70007812	-0.17503110
N	-3.02129895	3.90979078	-0.34476705
C	-2.18278155	4.94126492	-0.40599820
H	2.23869009	6.28900700	0.24465206
H	1.21311194	5.64465288	1.52907120

H	-0.23208758	6.85158319	-0.02173058
H	0.49188656	6.06280328	-1.42095649
H	3.61571734	4.08344844	1.44347739
H	3.96339400	4.71605767	-0.18685438
H	3.62115152	2.98301442	0.04994124
H	-3.15228841	1.85345586	-0.10454894
H	-2.62719253	5.92413571	-0.54554510
C	-1.37526027	-5.45564241	-1.27419860
C	0.11666121	-5.77388668	-1.34243140
C	0.90231136	-4.76525179	-0.55056638
C	0.42020289	-3.46603084	-0.44519077
C	-0.86845407	-3.05542858	-1.09500321
N	-1.64640437	-4.04185859	-1.58507986
C	-2.96349429	-3.71466298	-2.13159545
O	-1.16432333	-1.85662038	-1.17416814
N	1.07672720	-2.50432501	0.21351335
C	2.23149370	-2.84943540	0.78999911
N	2.78379218	-4.06548772	0.75020460
C	2.12336275	-5.00726268	0.08143847
H	-1.92247913	-6.05910926	-1.99975413
H	-1.77478476	-5.69044225	-0.27949544
H	0.29169231	-6.78560602	-0.96823771
H	0.45061082	-5.75328896	-2.38682896
H	-3.74815906	-3.94555512	-1.40380331
H	-3.13267273	-4.29693873	-3.03950658
H	-2.99670216	-2.65358318	-2.36333660
H	2.75034553	-2.07585644	1.34179722
H	2.57869679	-5.99456597	0.05050420

[Eu(**7**)2(NO3)3] B3LYP/6-311++G** Total energy: -2651.705217

Eu	-0.07564256	-0.02148126	0.26212141
O	1.69788140	-0.15670650	2.00008403
O	0.07548194	1.19321480	2.44912268
O	1.77710373	1.06155089	3.80987057
N	1.20433690	0.71347762	2.80098797
O	1.38061464	-0.51688990	-1.73794047
O	-0.26847581	0.83309427	-2.10503899
O	1.08222962	0.30700244	-3.73749229
N	0.74511116	0.21165838	-2.57419562
O	-1.31500692	-1.54541279	1.81840739
O	-2.50662248	-0.07113105	0.78750163
O	-3.48354228	-1.54543677	2.06729339
N	-2.47762394	-1.07418668	1.58438949
C	1.57561367	5.53187988	0.18695801
C	0.30120204	5.84554750	-0.59327409
C	-0.73478086	4.78242469	-0.35326522
C	-0.32100881	3.47911338	-0.10288271

C	1.13461266	3.12049288	-0.03792879
N	2.01576174	4.14259811	-0.02074091
C	3.44145735	3.85864743	0.14192653
O	1.47638450	1.93336307	-0.01183025
N	-1.18147234	2.46960295	0.07193511
C	-2.48116472	2.77254601	0.01841086
N	-2.98612401	3.98989730	-0.20389303
C	-2.11621167	4.97829456	-0.39428416
H	2.38703230	6.18326162	-0.14091291
H	1.42390024	5.70781337	1.25972200
H	-0.07367510	6.82949036	-0.30064896
H	0.52773599	5.89159085	-1.66530228
H	3.75479747	4.04580871	1.17429242
H	4.01610681	4.49974872	-0.52949155
H	3.62389839	2.81495786	-0.09924410
H	-3.17645341	1.95813443	0.17716717
H	-2.53220730	5.96565641	-0.58171535
C	-1.19081509	-5.42353284	-1.51061278
C	0.31559502	-5.67166445	-1.53112735
C	1.01840384	-4.70212580	-0.62165122
C	0.47858548	-3.43432488	-0.43774078
C	-0.80306865	-3.02691408	-1.10344648
N	-1.51322076	-4.00114999	-1.71011571
C	-2.81825681	-3.68344469	-2.28946344
O	-1.15767062	-1.84344159	-1.08594807
N	1.06985624	-2.50055759	0.31632145
C	2.21111521	-2.84798921	0.91687332
N	2.80945506	-4.03896771	0.81756707
C	2.21753880	-4.94917543	0.04874392
H	-1.67488456	-5.98298489	-2.31241592
H	-1.62466231	-5.76424651	-0.56167473
H	0.52014312	-6.70355587	-1.23504171
H	0.69541096	-5.54698743	-2.55234162
H	-3.62369606	-4.00877147	-1.62281345
H	-2.92007672	-4.19186725	-3.25028250
H	-2.88968020	-2.60857552	-2.43191730
H	2.67956469	-2.09741527	1.54064466
H	2.71201753	-5.91440116	-0.03429132

[Am(**8**)2(NO3)3] B3LYP/6-311++G** Total energy: -2536.769124

Am	-0.04061241	-0.01548813	0.18254474
O	1.71853926	-0.18478857	1.97824418
O	0.16910292	1.25741929	2.42536134
O	1.88628798	1.06640539	3.75965506
N	1.27651582	0.72961964	2.76687501
O	1.54785829	-0.47536129	-1.75976014
O	-0.15955938	0.77818991	-2.20536772

O	1.29343914	0.33209112	-3.77238080
N	0.91187141	0.21523255	-2.62699529
O	-1.27470145	-1.61212541	1.82958570
O	-2.43517262	-0.06135275	0.87019133
O	-3.43418176	-1.52923057	2.14100531
N	-2.41885606	-1.09202617	1.64325626
C	1.44665522	5.59553063	0.29955246
C	0.17050369	5.90010511	-0.48071756
C	-0.82669367	4.78695890	-0.33053249
C	-0.35663590	3.48730347	-0.13057661
C	1.10573636	3.18390210	-0.04351258
N	1.94678614	4.23697948	0.03307244
C	3.37662767	3.99860441	0.22636838
O	1.49434865	2.00944720	-0.05589117
N	-1.18680332	2.44168064	-0.03158668
C	-2.49225096	2.69600345	-0.11109929
C	-2.95560632	4.00023199	-0.31024881
N	-2.13465602	5.04211950	-0.42713216
H	2.23440523	6.29453482	0.01538126
H	1.27627382	5.71230603	1.37759134
H	-0.27160599	6.83674919	-0.13673635
H	0.40148229	6.02125045	-1.54616384
H	3.65118742	4.13671659	1.27745615
H	3.94523178	4.69934256	-0.38812472
H	3.60854703	2.97860532	-0.06807458
H	-3.16726356	1.85647692	-0.00246162
H	-4.02024612	4.19900609	-0.37645104
C	-1.30728999	-5.44320136	-1.41386079
C	0.18879812	-5.74703367	-1.41513342
C	0.93690807	-4.75451028	-0.57156419
C	0.42908382	-3.46007301	-0.45023751
C	-0.84242475	-3.04696617	-1.11861922
N	-1.58513904	-4.02194760	-1.68199234
C	-2.88615867	-3.69045354	-2.26134533
O	-1.16450410	-1.85074338	-1.14778360
N	1.06514591	-2.51071619	0.24598863
C	2.20386850	-2.85852454	0.84234963
C	2.70564522	-4.15868742	0.71983704
N	2.08631258	-5.10295363	0.01409129
H	-1.80789207	-6.02468168	-2.18918906
H	-1.75610113	-5.72178869	-0.45178983
H	0.37159895	-6.75648850	-1.04271592
H	0.58078245	-5.70219067	-2.43862074
H	-3.69347298	-3.95441317	-1.57012420
H	-3.01738816	-4.24337939	-3.19354732
H	-2.92411068	-2.62249561	-2.45847235
H	2.70861738	-2.09848206	1.42556019

H	3.63469931	-4.43501193	1.20753497

[Eu(**8**)2(NO3)3] B3LYP/6-311++G** Total energy: -2651.707238

Eu	-0.07494404	-0.02078507	0.25483907
O	1.69790121	-0.16333320	1.99589947
O	0.07899727	1.19097963	2.44569120
O	1.77282115	1.04244077	3.81416416
N	1.20354766	0.70467748	2.79966713
O	1.39112104	-0.51325779	-1.73480515
O	-0.26865342	0.82320073	-2.10791560
O	1.08848529	0.30305121	-3.73661912
N	0.75105805	0.20804212	-2.57391933
O	-1.30973996	-1.53194834	1.83226024
O	-2.50214759	-0.06701269	0.78872132
O	-3.47625910	-1.51821132	2.09657743
N	-2.47110444	-1.06002238	1.59979340
C	1.55947413	5.53871347	0.14100311
C	0.25741006	5.85093662	-0.59217281
C	-0.76878876	4.78347029	-0.34015714
C	-0.33463351	3.47808645	-0.10145582
C	1.11790274	3.12704508	-0.05923214
N	1.99829563	4.15020256	-0.07464336
C	3.42665999	3.86889439	0.06091308
O	1.46481415	1.93983935	-0.02115330
N	-1.19179580	2.46571927	0.07320058
C	-2.48956095	2.76153866	0.03629592
C	-2.91870611	4.07310417	-0.19219145
N	-2.07056848	5.08069465	-0.38865107
H	2.35613382	6.19204478	-0.21736490
H	1.44709101	5.71806739	1.21818046
H	-0.13433782	6.81919688	-0.27580790
H	0.43989192	5.91084466	-1.67213197
H	3.75841070	4.04462517	1.08976366
H	3.98753544	4.51979747	-0.61259201
H	3.60836269	2.82872220	-0.19585668
H	-3.18577429	1.94772040	0.19571313
H	-3.97818366	4.30603085	-0.21851282
C	-1.15741688	-5.42269916	-1.54744715
C	0.34712015	-5.67881454	-1.51215655
C	1.03450239	-4.70909939	-0.59385506
C	0.48428385	-3.43667133	-0.42806890
C	-0.78119017	-3.03105577	-1.11243583
N	-1.47346249	-3.99909622	-1.74923135
C	-2.76512617	-3.67741760	-2.35408946
O	-1.14583836	-1.84869355	-1.08458433
N	1.07227198	-2.50157284	0.32681345
C	2.20185602	-2.84619317	0.94184300

C	2.74266345	-4.12623589	0.78126316
N	2.17365616	-5.05364365	0.01356628
H	-1.61183743	-5.97743046	-2.36946056
H	-1.62844927	-5.76812195	-0.61797739
H	0.55127167	-6.70048330	-1.18719858
H	0.77064434	-5.56644602	-2.51773880
H	-3.58590918	-3.99290259	-1.70120892
H	-2.85203739	-4.19192290	-3.31304442
H	-2.82722070	-2.60310958	-2.50543178
H	2.67074841	-2.09757473	1.56805648
H	3.66241285	-4.39974760	1.28791429

[Am(**9**)2(NO3)3] B3LYP/6-311++G** Total energy: -2878.570127

Am	0.02442059	0.00672176	-0.08383502
O	1.57593072	0.12448177	1.94136343
O	-0.15674119	1.40012620	2.14318998
O	1.46367478	1.53519332	3.60241825
N	0.97088598	1.03112273	2.60295440
O	1.62883520	-0.23857820	-2.03762800
O	-0.29800320	0.60449719	-2.53135353
O	1.19453431	0.32844245	-4.10103403
N	0.85563931	0.23526203	-2.93755483
O	-0.95189095	-1.70491577	1.66291288
O	-2.36193625	-0.34057320	0.75709978
O	-3.09355813	-1.98330686	1.99321569
N	-2.16539414	-1.35952839	1.49796675
C	2.29974176	5.06820124	1.59991576
C	1.44701663	6.06883605	0.82720853
C	0.13561322	5.44403354	0.41771768
C	0.11406967	4.07122170	0.18971305
C	1.34931635	3.24763703	0.26966550
N	2.42599044	3.80447976	0.86336861
C	3.62333489	2.99816679	1.10407550
O	1.38444029	2.10873476	-0.22609833
C	-2.23379549	5.67887569	-0.15690544
C	-1.02824555	6.22839361	0.23952047
H	3.30603122	5.46345851	1.74804621
H	1.86893456	4.87135275	2.58995311
H	1.27363717	6.95226708	1.44706569
H	1.99006837	6.40390121	-0.06582754
H	3.63595842	2.63839852	2.13790473
H	4.51004670	3.60705989	0.91554887
H	3.61338308	2.14156161	0.43580855
H	-0.96695504	7.29607894	0.41977616
C	-2.57955294	-5.14513391	-0.63926871
C	-1.40414044	-6.05704876	-0.97438962
C	-0.10476533	-5.43555691	-0.52359812

C	-0.02354487	-4.04633697	-0.50046160
C	-1.14460446	-3.19135353	-0.97242422
N	-2.34699479	-3.78275914	-1.13453051
C	-3.52112403	-2.97005869	-1.45492463
O	-0.95830205	-1.99157043	-1.23685098
C	2.21300465	-5.68460362	0.22830648
C	1.00677794	-6.23430286	-0.16580276
H	-3.49154515	-5.51446115	-1.11113396
H	-2.75267929	-5.11433985	0.44405799
H	-1.55086012	-7.02849064	-0.49531998
H	-1.37168170	-6.23387785	-2.05714751
H	-4.09906682	-2.76572331	-0.54793798
H	-4.14328127	-3.50620847	-2.17465711
H	-3.19258950	-2.02586148	-1.88037638
H	0.90443485	-7.31327463	-0.20513256
N	-2.73386302	2.16031844	-0.75965283
N	-3.22865658	3.40795482	-0.72571582
C	-2.25285891	4.29412006	-0.36254755
C	-1.11397440	3.49228393	-0.18885980
N	-1.48127467	2.19078294	-0.43722599
N	2.80666028	-2.14031179	0.50977070
N	1.57802431	-2.16419025	0.10511604
C	1.19089044	-3.47114425	-0.07516401
C	2.27968256	-4.28675570	0.27048930
N	3.25973414	-3.39941973	0.61904968
H	3.05546624	-6.31001151	0.49697518
H	-3.11542402	6.29351303	-0.29111375
C	4.61509882	-3.65115164	1.07560276
H	4.60047559	-4.24301326	1.99299546
H	5.18431752	-4.17560446	0.30537068
H	5.07279092	-2.68454217	1.27460441
C	-4.62775924	3.64766129	-1.03210951
H	-5.13047474	4.09719545	-0.17343593
H	-4.71971239	4.30341788	-1.90035223
H	-5.07916891	2.68278446	-1.25269857

[Eu(**9**)2(NO3)3] B3LYP/6-311++G** Total energy: -2993.505803

Eu	-0.01941431	-0.00577390	0.07150181
O	1.61876540	0.15680045	2.02419946
O	-0.16845634	1.35659516	2.18637955
O	1.42596432	1.58666091	3.66138403
N	0.97498117	1.04314726	2.66511983
O	1.57125124	-0.36577053	-1.89103456
O	-0.24696718	0.70966721	-2.33464313
O	1.19909474	0.33245532	-3.92592941
N	0.85678911	0.22832261	-2.76209695
O	-0.93080315	-1.63522610	1.76751905

O	-2.41430424	-0.39269043	0.81374619
O	-3.05125802	-2.01301654	2.12883264
N	-2.16651683	-1.36339783	1.59589149
C	2.41434055	5.19805001	1.20807030
C	1.55423196	6.10113466	0.33158547
C	0.21119086	5.46401835	0.07149323
C	0.14932025	4.07357818	0.02772761
C	1.36859042	3.23492746	0.17860092
N	2.47871053	3.83893151	0.65935283
C	3.65789708	3.03487006	0.98093846
O	1.36303302	2.03868085	-0.14558920
C	-2.17679358	5.68860735	-0.42088755
C	-0.94179770	6.25114012	-0.15495311
H	3.43513237	5.58071352	1.25962679
H	2.02048353	5.16236146	2.23238793
H	1.43156447	7.07163841	0.81908205
H	2.06547895	6.28168535	-0.62267807
H	3.69053327	2.81792401	2.05366011
H	4.55670376	3.58344203	0.69134176
H	3.60568193	2.09605166	0.43668204
H	-0.84846388	7.33097243	-0.11773995
C	-2.49921038	-5.18862437	-1.05545411
C	-1.27480652	-5.99868121	-1.46600482
C	-0.02221558	-5.40440642	-0.87004856
C	0.00695208	-4.02802970	-0.66050161
C	-1.13036308	-3.15567658	-1.05525420
N	-2.30576231	-3.76134797	-1.33640218
C	-3.50025418	-2.95118277	-1.57502812
O	-0.99097921	-1.92622470	-1.13950078
C	2.26633886	-5.68033103	-0.04395366
C	1.09978454	-6.20960011	-0.56571090
H	-3.37657693	-5.51781776	-1.61484740
H	-2.71484236	-5.32647554	0.01231917
H	-1.40009660	-7.03539037	-1.14337378
H	-1.19135611	-6.00923749	-2.56029816
H	-4.11356446	-2.90038422	-0.66946180
H	-4.08155998	-3.39719540	-2.38487777
H	-3.19690682	-1.94428521	-1.84761840
H	1.03820229	-7.27659239	-0.74971486
N	-2.77911401	2.13845823	-0.55525988
N	-3.24567348	3.39438953	-0.65364899
C	-2.23483212	4.29049897	-0.44672711
C	-1.10638183	3.48444846	-0.22492968
N	-1.51324016	2.17268048	-0.29518635
N	2.72316651	-2.18556896	0.70889922
N	1.51613262	-2.19163824	0.24646825
C	1.18237002	-3.47593724	-0.11267187

C	2.28195183	-4.29891040	0.18011214
N	3.21473369	-3.43601344	0.68288774
H	3.11729593	-6.31053318	0.18374581
H	-3.05089440	6.30481135	-0.59220269
C	4.55828232	-3.70192585	1.16494990
H	4.52886283	-4.41099316	1.99475717
H	5.17980668	-4.09951831	0.35990214
H	4.96881075	-2.75561757	1.51067873
C	-4.65175295	3.63165879	-0.92710456
H	-5.10394384	4.20253665	-0.11355241
H	-4.77062936	4.17148725	-1.86886014
H	-5.13396844	2.65914376	-0.99942047

[Am(**10**)(NO3)3] B3LYP/6-311++G** Total energy: -2579.730010

C	-2.83243710	2.61378421	2.50913420
N	-1.34699629	0.88199174	0.91529393
C	-0.72139952	1.78778793	1.68283250
C	-1.42475844	2.68804743	2.52002583
C	0.72122861	1.83941975	1.62631232
C	1.42450129	2.75552832	2.44620596
C	0.68010758	3.64410897	3.29372504
C	-0.68045049	3.61337186	3.32734582
N	1.34690748	0.99223738	0.79459072
C	2.83218431	2.73795788	2.37331752
O	-2.54051923	-0.65527377	-0.92137475
O	2.54059692	-0.97735956	-0.56806589
H	-3.40850655	3.28477603	3.13908429
H	1.22547223	4.34723144	3.91360476
H	-1.22588083	4.29497253	3.97075964
N	0.00013697	-2.97652169	-2.71556989
O	0.00016965	-3.86972126	-3.53045875
O	0.58796715	-3.08017222	-1.57980473
O	-0.58773062	-1.85502937	-2.92272885
N	-0.44019580	-2.29521416	1.85696817
O	-1.30809264	-2.26384952	0.91704595
O	-0.64245881	-2.87170809	2.90688592
O	0.64198496	-1.66112522	1.61960903
N	0.44021933	1.63914131	-2.45550588
O	-0.64199694	1.46073074	-1.80243617
O	0.64245096	2.63189694	-3.12567069
O	1.30818497	0.70610826	-2.33816840
Am	0.00003758	-0.80889307	-0.73795809
C	-2.66779231	0.84990066	0.90615747
C	-3.47254051	1.69985703	1.69261339
C	-4.96663794	1.56906607	1.55310480
C	-3.26091093	-0.12801372	-0.06938733
H	-5.47092773	1.85627018	2.47911815

C	2.66770555	0.98026938	0.76353299
C	3.47237287	1.84125364	1.53798435
C	4.96648362	1.69043721	1.42058053
C	3.26092072	-0.08065182	-0.12096469
H	5.47071545	2.63887486	1.62185498
C	5.21061429	-0.94199348	-1.28744580
H	6.16042925	-1.29004555	-0.87591808
H	4.54173676	-1.78566274	-1.43599537
H	5.39078807	-0.45639629	-2.25196458
N	4.58908844	-0.00518099	-0.35227118
C	-5.21050092	-1.36853402	-0.82044714
H	-5.39065933	-2.28456825	-0.24861857
N	-4.58907114	-0.35151069	0.02687307
C	-5.35455152	0.13721442	1.18249823
C	5.35448828	1.19036351	0.02867392
H	6.41153122	0.92061463	0.01228264
H	5.20343831	1.97842486	-0.72019219
H	-5.20351027	-0.53637782	2.03579614
H	-6.41157929	0.09615157	0.91532943
H	5.31377253	0.97221472	2.17339491
H	-5.31392545	2.25297194	0.76898318
H	3.40818985	3.42670297	2.98386715
H	-6.16031433	-0.99063718	-1.20475471
H	-4.54156794	-1.59364437	-1.64694321

[Eu(**10**)(NO3)3] B3LYP/6-311++G** Total energy: -2694.668052

C	-2.83309839	2.52114169	2.41247314
N	-1.34245062	0.77534270	0.83874112
C	-0.72070652	1.68840153	1.60029011
C	-1.42534852	2.59308892	2.43070933
C	0.72053342	1.74813094	1.53489394
C	1.42508728	2.65793531	2.35977880
C	0.68029130	3.54616429	3.20753783
C	-0.68064069	3.51865298	3.23762242
N	1.34236233	0.90622029	0.69542240
C	2.83284167	2.63326723	2.28986623
O	-2.52419436	-0.78333396	-0.98374148
O	2.52428170	-1.05124928	-0.68979970
H	-3.41184304	3.19682662	3.03491670
H	1.22537408	4.24760083	3.82960657
H	-1.22579087	4.20230569	3.87912695
N	0.00012046	-3.01520816	-2.75104880
O	0.00016348	-3.90814889	-3.56580314
O	0.51957513	-3.14489454	-1.58709665
O	-0.51938046	-1.86800525	-2.98657055
N	-0.38111237	-2.32309210	1.79701880
O	-1.26911283	-2.30838591	0.87876983

O	-0.55764143	-2.87801284	2.86351085
O	0.69463454	-1.69536032	1.51992107
N	0.38118785	1.57686139	-2.47772083
O	-0.69461520	1.35827035	-1.82739315
O	0.55769300	2.58810807	-3.12789666
O	1.26926898	0.66390345	-2.37893125
Eu	0.00004491	-0.87176667	-0.79528026
C	-2.66297478	0.74597105	0.82153389
C	-3.47002023	1.60432937	1.59650587
C	-4.96338040	1.48120383	1.44388750
C	-3.25103022	-0.24084192	-0.14812493
H	-5.47467464	1.77764872	2.36315626
C	2.66288821	0.88646808	0.66780860
C	3.46985088	1.73682031	1.45164243
C	4.96322463	1.57365588	1.34306955
C	3.25104341	-0.16942776	-0.22606228
H	5.47445707	2.51623146	1.55413582
C	5.20100447	-1.03896613	-1.38568743
H	6.14377701	-1.40205529	-0.97079394
H	4.52364822	-1.87347870	-1.54701756
H	5.39420409	-0.54677853	-2.34441102
N	4.58270763	-0.10499166	-0.44600295
C	-5.20089596	-1.47528082	-0.90796868
H	-5.39409068	-2.38493113	-0.33009516
N	-4.58269066	-0.45401694	-0.06390209
C	-5.35794435	0.05001269	1.07826903
C	5.35787414	1.07857331	-0.04862392
H	6.41186832	0.79660972	-0.05688132
H	5.22345645	1.87397811	-0.79301769
H	-5.22354501	-0.61843022	1.93848998
H	-6.41192121	0.01592822	0.79818641
H	5.29832139	0.84780894	2.09409135
H	-5.29846800	2.16260785	0.65231811
H	3.41152069	3.31499593	2.90574609
H	-6.14366142	-1.09540718	-1.30756806
H	-4.52348284	-1.71229788	-1.72416997