

Supporting Information

Unique selectivity reversal between Am³⁺ and Eu³⁺ ions by incorporation of alkyl branching in diglycolamide derivatives: DFT validation of experimental results

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Extraction studies

Table S1: Extraction data of nitric acid and water in the organic phase comprising of 0.01 M nBuDGA or sBuDGA in toluene; Aq. Phase 3M HNO₃

[HNO ₃]	nBuDGA		sBuDGA	
	[HNO ₃] _{org} (M)	[H ₂ O] _{org} (M)	[HNO ₃] _{org} (M)	[H ₂ O] _{org} (M)
0.01	0.02	0.039	7.6 x10 ⁻³	0.044
0.5	0.016	0.044	6.7 x 10 ⁻³	0.056
1.0	0.011	0.056	4.9 x 10 ⁻³	0.044
2.0	0.011	0.067	0.015	0.044
3.0	0.018	0.089	0.012	0.044
4.0	0.022	0.100	0.015	0.044
6.0	0.032	0.106	0.02	0.061

FTIR studies

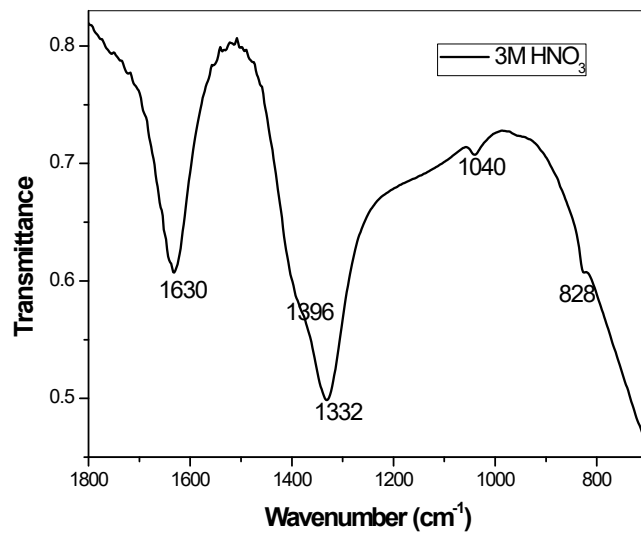


Figure S1: FTIR spectra of 3M HNO₃

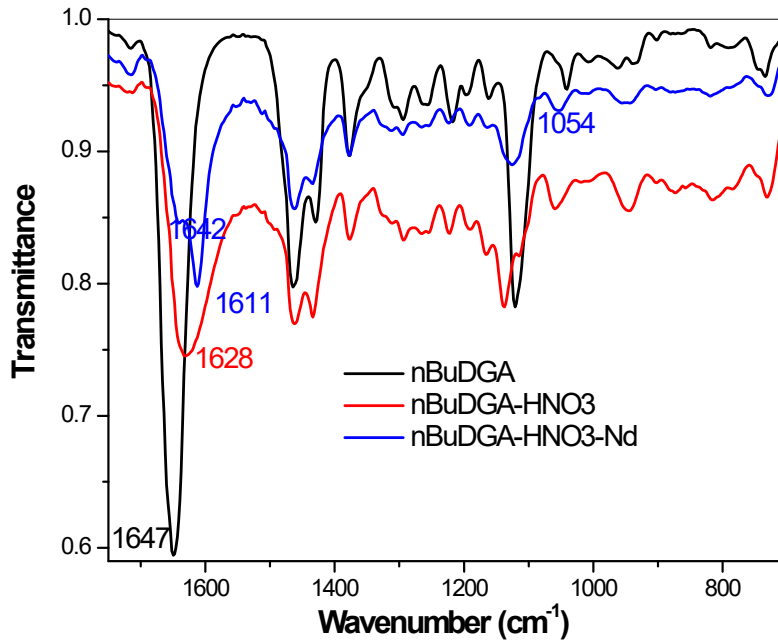


Figure S2: FTIR spectra of 0.01M nBuDGA in toluene before and after equilibration with 3M HNO₃ and 3M HNO₃+0.02M Nd³⁺

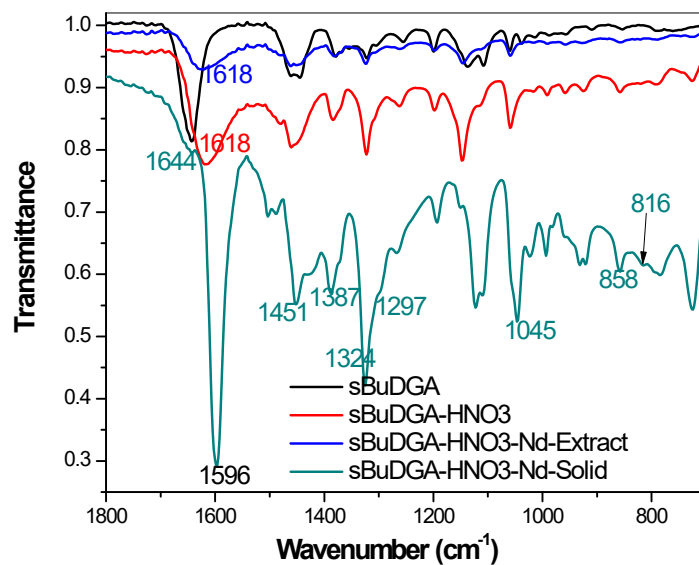


Figure S3: FTIR spectra of 0.01M sBuDGA in toluene before and after equilibration with 3M HNO₃ and 3M HNO₃+0.02M Nd³⁺ and solid precipitate of the Nd³⁺-sBuDGA complex

Computational Studies

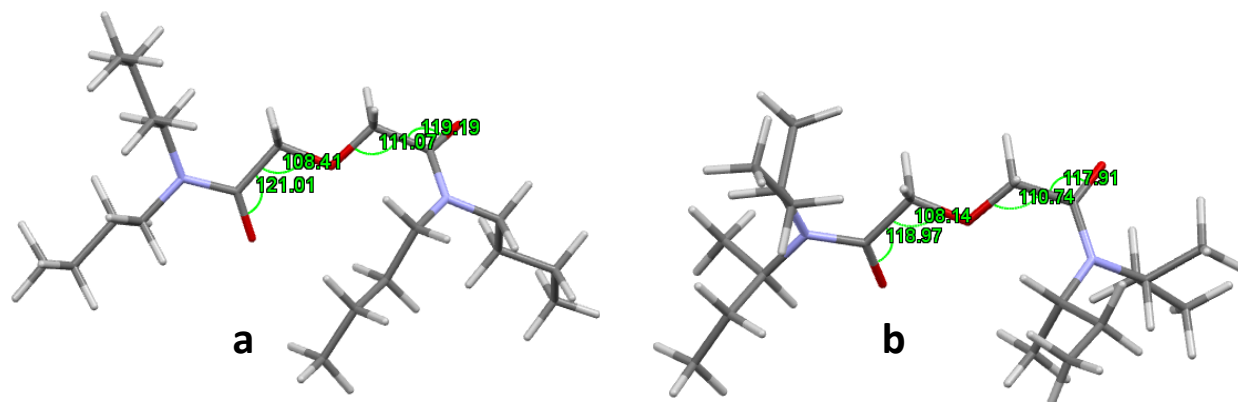


Figure S4: Energy optimized structures of (a) nBuDGA and (b) sBuDGA at the BP86/SV(P) level of theory showing the bond angles in the DGA part

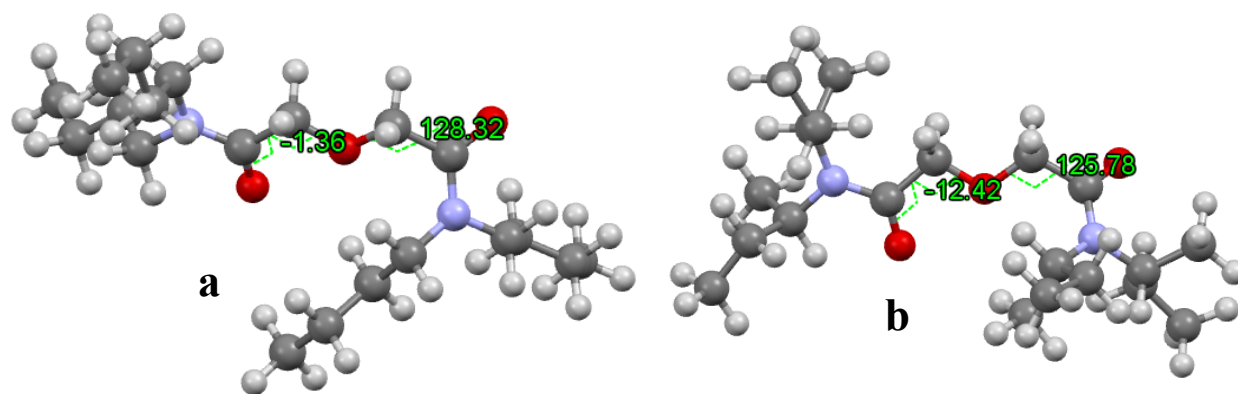


Figure S5: Energy optimized structures of (a) nBuDGA and (b) sBuDGA at the BP86/SV(P) level of theory showing the torsional angles in the coordination sites of the DGA part

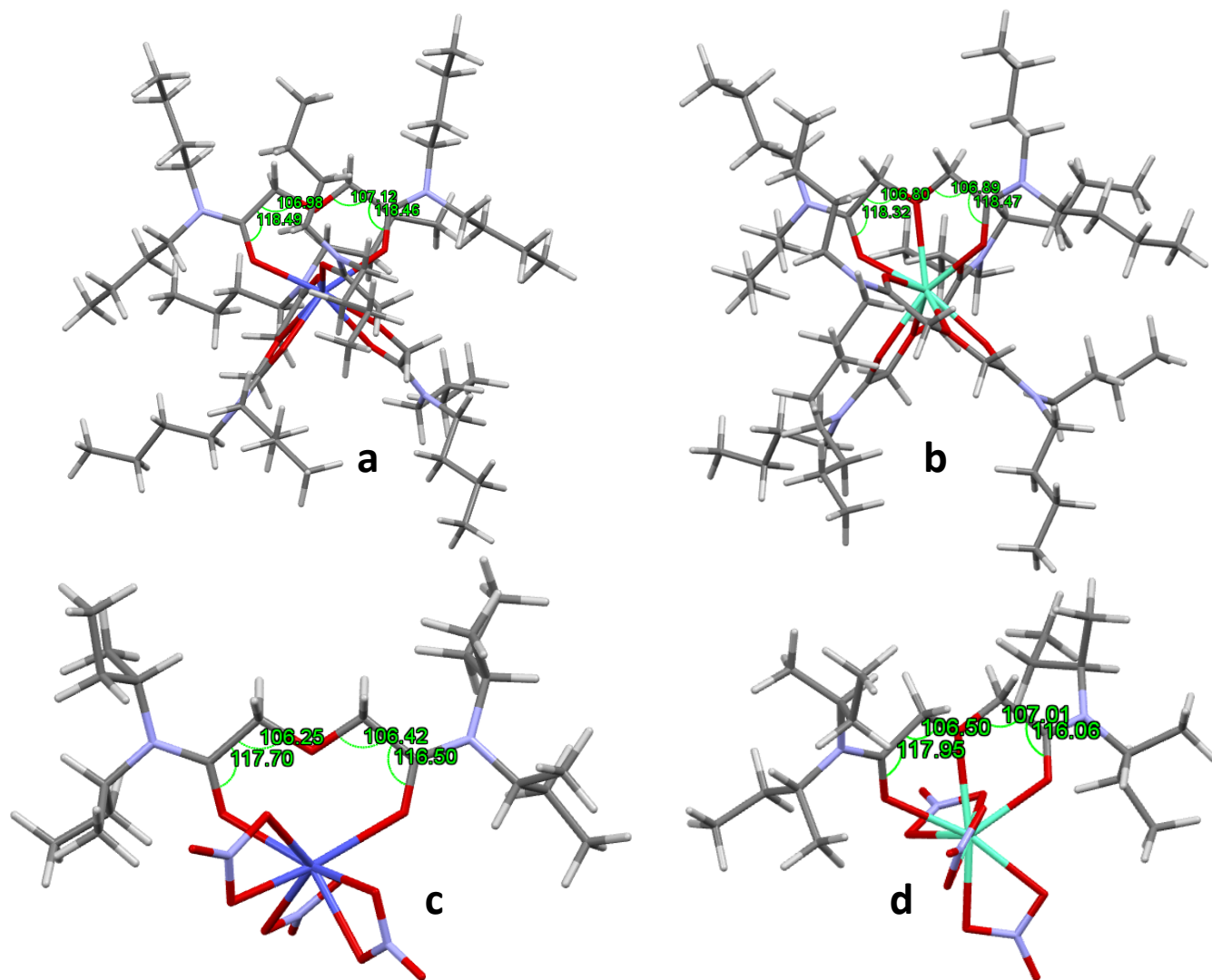


Figure S6: Energy optimized structures of Am^{3+} and Eu^{3+} complexes of nBuDGA and sBuDGA at the BP86/SV(P) level of theory showing the bond angles in the DGA part (a: $\text{Am}(\text{nBuDGA})_3^{3+}$; b: $\text{Eu}(\text{nBuDGA})_3^{3+}$; c: $\text{Am}(\text{sBuDGA})(\text{NO}_3)_3$; d: $\text{Eu}(\text{sBuDGA})(\text{NO}_3)_3$)

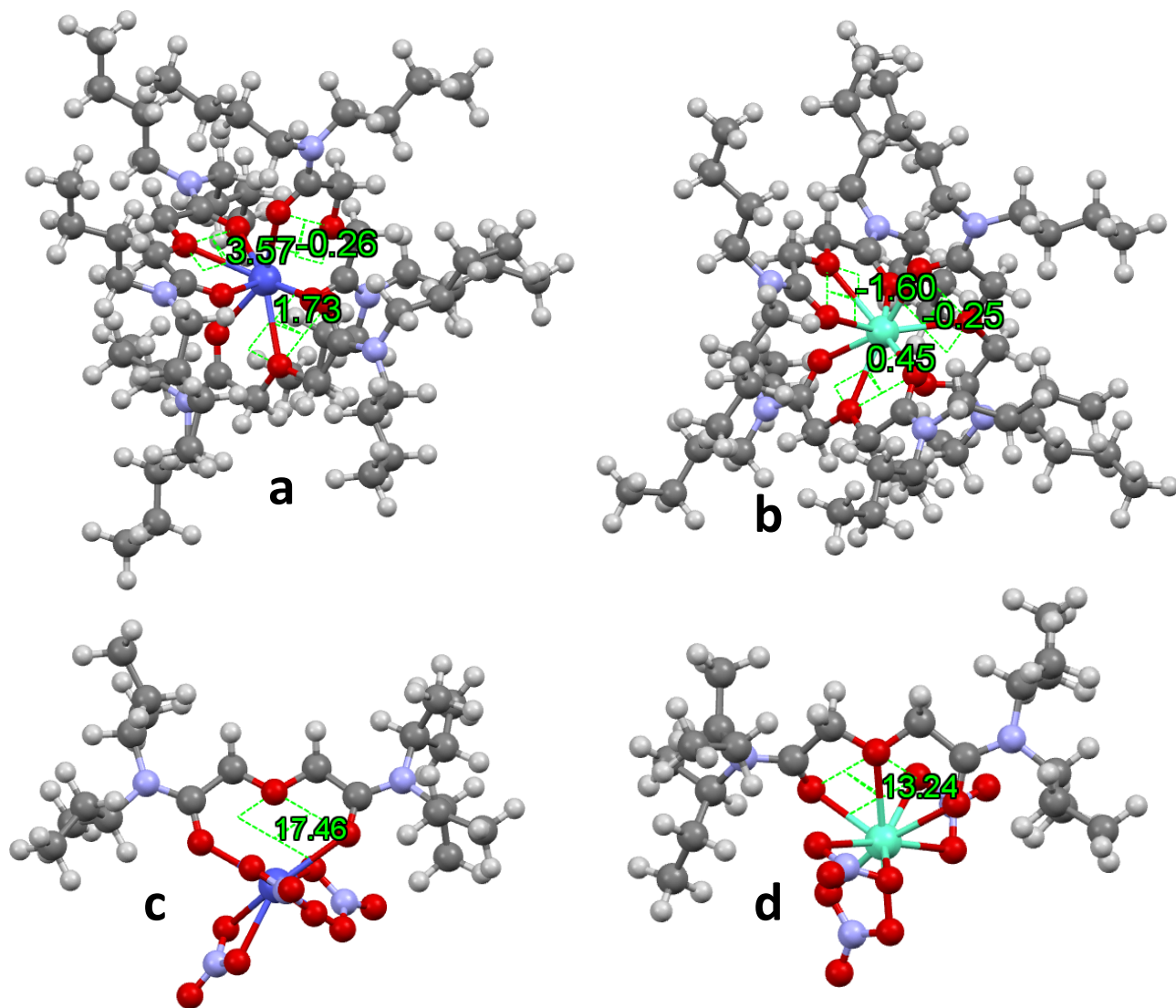


Figure S7: Energy optimized structures of Am^{3+} and Eu^{3+} complexes of nBuDGA and sBuDGA at the BP86/SV(P) level of theory showing the deviation from the coplanarity of the metal ion and the three coordinating 'O' atoms of the DGA units (a: $\text{Am}(\text{nBuDGA})_3^{3+}$; b: $\text{Eu}(\text{nBuDGA})_3^{3+}$; c: $\text{Am}(\text{sBuDGA})(\text{NO}_3)_3$; d: $\text{Eu}(\text{sBuDGA})(\text{NO}_3)_3$)

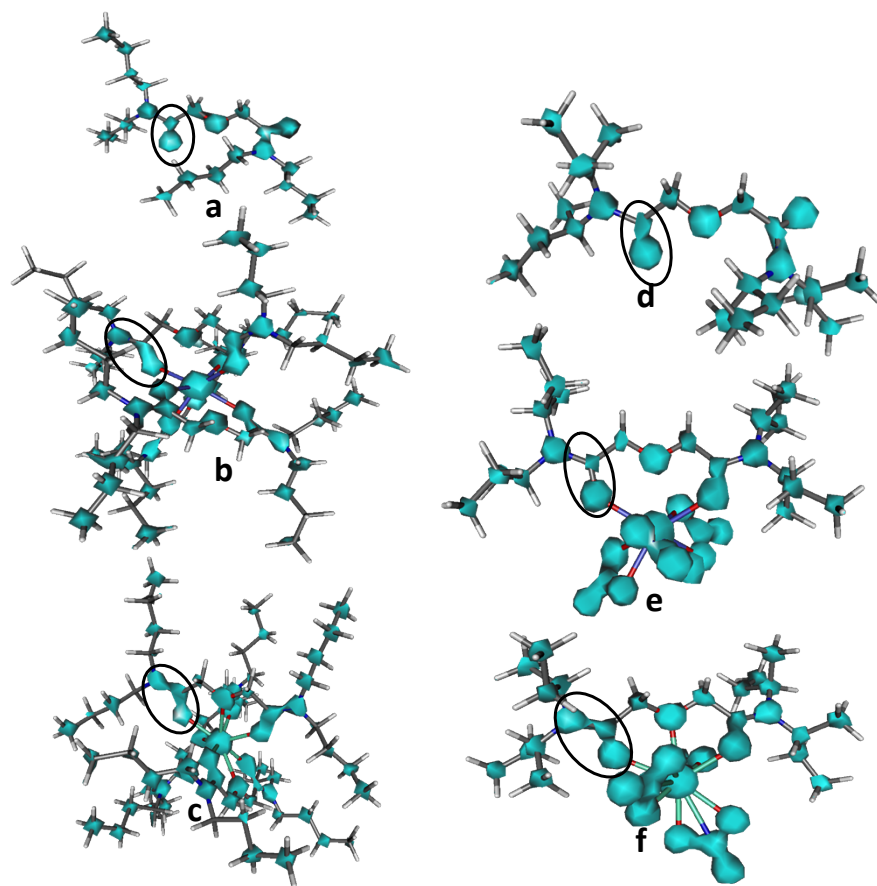


Figure S8: Electron density distribution in the free nBuDGA, sBuDGA and their complexes with Am^{3+} and Eu^{3+} (a: nBuDGA; b: $\text{Am}(\text{nBuDGA})_3^{3+}$; c: $\text{Eu}(\text{nBuDGA})_3^{3+}$; d: sBuDGA; e: $\text{Am}(\text{sBuDGA})(\text{NO}_3)_3$; f: $\text{Eu}(\text{sBuDGA})(\text{NO}_3)_3$) (encircled parts show the charge polarization in the coordination site of the ligand).

Table S2: Cartesian coordinates of the optimized structures of nBuDGA, sBuDGA and their Am³⁺ and Eu³⁺ complexes

nBuDGA

C	-3.8346370	-2.8084149	-3.3900037
C	-3.1563725	-3.9170095	-2.5624190
H	-3.8986115	-4.7179387	-2.2944512
H	-2.4028917	-4.3751421	-3.2462887
O	-2.5456062	-3.3842443	-1.4022189
C	-1.7869452	-4.3256372	-0.6948124
H	-2.4163440	-5.2007197	-0.3797951
H	-0.9668594	-4.7412126	-1.3401388
C	-1.1778982	-3.6304912	0.5436441
N	-0.4078870	-4.4220260	1.3746194
N	-4.7259025	-1.9707912	-2.7600108
O	-1.3712847	-2.4353459	0.7582325
O	-3.5777415	-2.7130364	-4.5940333
C	0.2159192	-3.7849991	2.5401649
H	0.1440959	-4.4834748	3.4053082
H	-0.3887600	-2.8856040	2.7784499
C	-0.2010902	-5.8595879	1.1949712
H	-0.2526527	-6.1125911	0.1146910
H	0.8440447	-6.0934270	1.5018173
C	1.6806533	-3.3769671	2.3054719
H	2.2851627	-4.2760518	2.0344877
H	1.7202092	-2.6928547	1.4272027
C	2.3094306	-2.6887257	3.5277216
H	2.2110017	-3.3534823	4.4190124
H	1.7247700	-1.7697100	3.7683772
C	3.7852814	-2.3209062	3.3263740
H	4.2019758	-1.8070103	4.2206144
H	4.4066374	-3.2262093	3.1393798
H	3.9178674	-1.6402113	2.4552357
C	-1.1776691	-6.7485813	1.9892122
H	-2.2218956	-6.5204062	1.6714418
H	-1.1196923	-6.4807523	3.0700035
C	-0.8960563	-8.2496153	1.8160843
H	0.1581096	-8.4625113	2.1137266
H	-0.9640299	-8.5146371	0.7342089
C	-1.8454437	-9.1447916	2.6232209
H	-2.9064066	-8.9835462	2.3261389
H	-1.6140653	-10.2220750	2.4712449
H	-1.7694353	-8.9349226	3.7141688
C	-5.3158349	-0.9070778	-3.5857002
H	-6.2621505	-0.5906192	-3.0936980
H	-5.5727459	-1.3498445	-4.5730257
C	-4.4000974	0.3088915	-3.8104353

H	-3.4580789	-0.0480634	-4.2825310
H	-4.1203625	0.7547019	-2.8282125
C	-5.0509742	1.3792401	-4.7012641
H	-5.3160358	0.9250687	-5.6852154
H	-6.0171222	1.7056803	-4.2466373
C	-4.1562537	2.6048417	-4.9287790
H	-3.1942711	2.3173447	-5.4102247
H	-4.6507108	3.3556322	-5.5847092
H	-3.9082146	3.1091880	-3.9672086
C	-5.1611350	-2.0939554	-1.3650845
H	-6.2737224	-1.9993165	-1.3520268
H	-4.9296374	-3.1183532	-1.0106800
C	-4.5362355	-1.0802767	-0.3925685
H	-3.4319630	-1.2044453	-0.4245305
H	-4.7717122	-0.0431924	-0.7284637
C	-5.0298390	-1.2722565	1.0496066
H	-4.8213836	-2.3218338	1.3655550
H	-6.1396938	-1.1519494	1.0909669
C	-4.3643445	-0.3100289	2.0421447
H	-4.7416626	-0.4656609	3.0776878
H	-3.2624849	-0.4615617	2.0511427
H	-4.5595730	0.7525140	1.7697921

sBuDGA

C	-3.6584196	-2.3801160	-3.1143610
C	-2.9956084	-3.6002142	-2.4376155
H	-3.7663284	-4.3269697	-2.0604588
H	-2.4333855	-4.1046513	-3.2582232
O	-2.1261195	-3.1866364	-1.3982668
C	-1.2427084	-4.1916732	-0.9743439
H	-1.7995258	-5.0842110	-0.5916217
H	-0.6151890	-4.5465036	-1.8320815
C	-0.3131497	-3.5916643	0.1017023
N	0.5120888	-4.4509311	0.8166296
N	-4.3279950	-1.4696011	-2.3306327
O	-0.2928432	-2.3712595	0.2584862
O	-3.5516028	-2.2700157	-4.3410491
C	1.4999414	-3.7972957	1.7167625
H	1.2821929	-2.7168196	1.5925256
C	0.5087817	-5.9351946	0.7822726
H	1.3845599	-6.2083754	1.4085650
C	1.2602151	-4.1445023	3.2041798
H	0.1776376	-3.9938949	3.4157889
H	1.4730950	-5.2236886	3.3933687
C	2.0817826	-3.2914300	4.1826179
H	1.9054533	-2.2049027	4.0147855

H	3.1749209	-3.4748864	4.0887245
C	-0.7183497	-6.5562275	1.4987376
H	-1.6457660	-6.3534489	0.9166825
H	-0.8448921	-6.0312550	2.4707995
C	-0.5972745	-8.0666669	1.7469368
H	0.3372413	-8.3147394	2.3009200
H	-0.5927357	-8.6506821	0.8007193
C	-4.8245227	-0.2156669	-2.9636924
H	-5.2710856	0.3665680	-2.1289380
C	-3.6566351	0.6373399	-3.5180970
H	-3.1888791	0.0941513	-4.3659547
H	-2.8839562	0.7072338	-2.7191974
C	-4.0656611	2.0514582	-3.9511855
H	-4.7453662	2.0434550	-4.8319986
H	-4.5829053	2.6023844	-3.1313798
C	-4.5520241	-1.6426376	-0.8740016
H	-4.1458176	-2.6385556	-0.6153149
C	-6.0647926	-1.6767782	-0.5407326
H	-6.5251561	-0.6778141	-0.7225349
H	-6.5524589	-2.3784548	-1.2553408
C	-6.3790375	-2.1224375	0.8949964
H	-6.0110187	-1.3961181	1.6522972
H	-5.9159516	-3.1094613	1.1245297
H	-3.1699399	2.6464975	-4.2366057
H	-7.4765838	-2.2258541	1.0433254
H	1.8003387	-3.5186239	5.2344209
H	-1.4516908	-8.4341029	2.3566632
C	2.9412279	-4.0487200	1.2417805
H	3.2487907	-5.1143656	1.3490400
H	3.0563893	-3.7594036	0.1745738
H	3.6589834	-3.4382013	1.8310964
C	0.7934205	-6.5513341	-0.6035206
H	-0.1043924	-6.5896494	-1.2560636
H	1.5873141	-5.9809227	-1.1314723
H	1.1535861	-7.5966111	-0.4879357
C	-3.7445001	-0.6256525	-0.0488541
H	-3.8885674	-0.8042286	1.0391748
H	-2.6616896	-0.7449473	-0.2640943
H	-4.0506043	0.4238337	-0.2594775
C	-5.9450870	-0.4826598	-3.9859553
H	-6.3911367	0.4749642	-4.3335923
H	-5.5473299	-1.0360403	-4.8604044
H	-6.7597586	-1.0844616	-3.5266984

Am(nBuDGA)₃³⁺

C	-5.0909299	-4.2683953	4.3971062
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C	-3.8566979	-3.3864562	4.1365377
C	-2.9335498	-3.9821010	3.0602556
N	-1.6997611	-3.2030094	2.8189133
C	-1.5606439	-2.3218253	1.8165874
C	-2.7349164	-2.1104477	0.8523640
O	-2.3674267	-1.0556832	-0.0233137
C	-3.3211089	-0.7909208	-1.0388614
C	-2.7703968	0.3622240	-1.8856643
N	-3.5562268	0.8884920	-2.8377193
C	-4.9512762	0.4521322	-3.0715482
C	-6.0045059	1.2864926	-2.3222626
C	-7.4428336	0.8544121	-2.6633062
C	-0.5736474	-3.4375551	3.7473036
C	0.3095924	-4.6293331	3.3422420
C	1.4336190	-4.8961732	4.3577815
O	-0.4972505	-1.6675814	1.6237061
Am	0.0428993	0.0408993	-0.0162005
O	0.0994373	-1.8366459	-1.6041729
C	1.0242498	-2.6596078	-1.8544697
N	0.9213632	-3.6220998	-2.7850739
C	1.9800736	-4.6234641	-3.0447346
C	1.7954142	-5.9444949	-2.2781837
C	2.8621071	-6.9908317	-2.6494317
O	-1.2959392	1.3525805	1.5555883
C	-1.3355785	2.5983274	1.7573726
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C	-2.1235882	4.6147024	2.9843467
C	-1.1701450	5.1020611	4.0884043
C	-1.3351603	6.6051863	4.3774712
O	0.2619630	2.6706492	-0.0038151
C	1.0127558	3.3798160	-0.9798001
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N	2.6350864	2.7644618	-2.7436207
C	2.9531415	4.1925380	-2.9681451
C	4.1900739	4.6904060	-2.2006527
C	4.5390619	6.1505731	-2.5420426
O	1.5164572	1.1149737	-1.6136437
O	-1.5954396	0.7695519	-1.6577084
O	2.1492984	-1.5287755	-0.0881953
C	3.2728508	-1.3444395	0.7629675
C	2.9155361	-0.2205839	1.7435794
N	3.7808700	0.0821074	2.7220955
C	5.0628650	-0.6284506	2.9269778
C	5.0041943	-1.7455105	3.9826258
C	6.3785113	-2.4015194	4.2102420
C	-0.5173013	3.5131099	0.8367270
C	2.3322170	-2.5493770	-1.0606746
O	1.8185628	0.3881487	1.5821047

C	-3.0518787	1.9803646	-3.6975336
C	-2.5583469	1.5004299	-5.0720438
C	-2.1261664	2.6691626	-5.9754135
C	3.4708641	1.1776445	3.6665152
C	4.1176711	2.5167911	3.2760748
C	3.8600301	3.6178630	4.3194730
C	-0.3098298	-3.7389425	-3.5950611
C	-0.1983663	-3.0786109	-4.9788816
C	-1.4577498	-3.3046200	-5.8344347
C	-2.8830249	2.2989869	3.6187236
C	-4.3349617	2.1377411	3.1392972
C	-5.1858034	1.3071495	4.1155439
C	3.3569828	1.7854811	-3.5845418
C	2.7011476	1.5505361	-4.9546637
C	3.5260256	0.5960244	-5.8362956
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H	-5.8363293	1.2041191	-1.2217197
H	-3.3661700	0.9260355	-5.5823021
H	5.2171865	2.3817442	3.1514166
H	4.2608293	-2.5173390	3.6714900
H	1.8231856	-5.7484815	-1.1798637
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H	-2.9293792	-3.0462686	0.2718591
H	-3.6684500	-1.8519532	1.4065318
H	-2.6124145	-5.0030635	3.3611811
H	-3.4806518	-4.1128278	2.1033356
H	-3.2851279	-3.2606126	5.0848603
C	-6.0048023	-3.7142191	5.4970550
H	-4.7534057	-5.2936671	4.6760935
H	-5.6689744	-4.3845990	3.4500838
H	-1.0114220	-3.6059510	4.7547081
H	0.0233969	-2.5043229	3.7920892
H	0.7453066	-4.4303777	2.3350132
H	0.9844779	-5.0912502	5.3590548
H	2.0485718	-3.9722465	4.4765500
C	2.3351408	-6.0738106	3.9657116
H	-4.3047759	-0.5211479	-0.5875685
H	-3.4740012	-1.6965678	-1.6764652
H	-5.0494668	-0.6249936	-2.8203727
H	-5.1254305	0.5181572	-4.1666056
H	-5.8701167	2.3633403	-2.5758589
H	-7.5986263	0.9455589	-3.7633197
C	-8.5072976	1.6750979	-1.9243458

H	-7.5708003	-0.2281193	-2.4257030
H	-2.2354628	2.4871713	-3.1459653
H	-3.8823639	2.7093269	-3.8197739
H	-1.7089088	0.7931149	-4.9271926
C	-1.6509744	2.2160161	-7.3616032
H	-1.3158339	3.2458913	-5.4689401
H	-2.9785242	3.3787035	-6.0909631
H	4.1724992	-1.0626390	0.1621413
H	3.5079812	-2.2904219	1.3059539
H	5.8069650	0.1392517	3.2295653
H	5.4246760	-1.0254135	1.9555290
H	4.6299651	-1.3255106	4.9444081
C	6.3517730	-3.4973472	5.2828683
H	7.1133203	-1.6151577	4.5003121
H	6.7504951	-2.8258454	3.2478117
H	3.8286684	0.8539489	4.6671872
H	2.3676715	1.2731503	3.7177017
H	3.7250104	2.8329630	2.2813386
H	4.2486885	3.2825677	5.3087581
H	2.7596298	3.7482896	4.4542592
C	4.5020862	4.9607499	3.9492438
H	2.5796646	-3.5167191	-0.5627711
H	3.1799686	-2.2886028	-1.7400570
H	2.9737734	-4.1776185	-2.8282826
H	1.9736505	-4.8172403	-4.1385161
H	0.7823509	-6.3566296	-2.4934227
H	2.8304758	-7.1680770	-3.7495239
C	2.6790585	-8.3222894	-1.9103709
H	3.8763777	-6.5780246	-2.4361125
H	-1.1361141	-3.2840998	-3.0126996
H	-0.5284011	-4.8234090	-3.7017220
H	-0.0155415	-1.9868491	-4.8478259
C	-1.3661041	-2.6600583	-7.2230352
H	-2.3483873	-2.9071103	-5.2916021
H	-1.6337667	-4.3998306	-5.9453949
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H	-1.9384975	5.1615322	2.0358842
H	-1.3584613	4.5222047	5.0213219
C	-0.4026724	7.1118199	5.4845245
H	-2.3941642	6.8060937	4.6617983
H	-1.1566360	7.1843409	3.4408722
H	-2.8582730	2.7590040	4.6296156
H	-2.3800226	1.3130921	3.6850501
H	-4.3313063	1.6578074	2.1327487
H	-5.1801670	1.7981297	5.1160364
H	-4.7064084	0.3097700	4.2646902

C	-6.6347248	1.1217264	3.6472601
H	1.7264774	4.0821882	-0.4878511
H	0.3303822	3.9841495	-1.6269670
H	2.0639099	4.8122194	-2.7271119
H	3.1117988	4.3134767	-4.0612879
H	5.0600345	4.0357440	-2.4389935
H	4.7078111	6.2362477	-3.6406245
C	5.7740396	6.6642446	-1.7912712
H	3.6631908	6.8035221	-2.3159512
H	3.4170206	0.8362051	-3.0155106
H	4.3922465	2.1693528	-3.7120632
H	1.6758943	1.1403613	-4.8020451
C	2.8928187	0.3448046	-7.2103170
H	3.6620873	-0.3742646	-5.3015106
H	4.5503490	1.0150524	-5.9714229
H	-6.8822329	-4.3768824	5.6537165
H	-5.4695355	-3.6349990	6.4693627
H	-6.3914617	-2.7031064	5.2379313
H	3.1342795	-6.2343971	4.7206847
H	1.7569950	-7.0213926	3.8897362
H	2.8300881	-5.9027657	2.9823048
H	-9.5290120	1.3388303	-2.2010216
H	-8.4092723	1.5738428	-0.8199712
H	-8.4335111	2.7567609	-2.1744701
H	-1.3455268	3.0847783	-7.9832402
H	-0.7778432	1.5286758	-7.2913298
H	-2.4571746	1.6825660	-7.9121861
H	-7.2166575	0.5170712	4.3754669
H	-7.1551621	2.0991339	3.5395853
H	-6.6851045	0.6032948	2.6626474
H	-0.5565639	8.1968241	5.6656409
H	-0.5879559	6.5838133	6.4462335
H	0.6679772	6.9660370	5.2172834
H	5.9964426	7.7163354	-2.0692551
H	5.6260336	6.6338043	-0.6883911
H	6.6762485	6.0586607	-2.0302655
H	3.5175950	-0.3440849	-7.8181743
H	1.8807606	-0.1103441	-7.1180866
H	2.7863937	1.2903193	-7.7866780
H	-2.2889254	-2.8469544	-7.8127302
H	-1.2272835	-1.5575989	-7.1539718
H	-0.5123019	-3.0715947	-7.8056508
H	3.4640282	-9.0504836	-2.2058298
H	2.7428236	-8.1907355	-0.8069572
H	1.6930893	-8.7838833	-2.1414338
H	7.3599262	-3.9435653	5.4178919
H	6.0313966	-3.0936297	6.2688672
H	5.6549248	-4.3212640	5.0098307

H	4.2983876	5.7293321	4.7252909
H	5.6069746	4.8705356	3.8553463
H	4.1129365	5.3485581	2.9805454

Eu(nBuDGA)₃³⁺

C	-5.0572116	-4.2771682	4.4080142
C	-3.8213888	-3.4163744	4.0904854
C	-2.9581602	-4.0265001	2.9732851
N	-1.7140075	-3.2779867	2.6928455
C	-1.5929674	-2.3770905	1.7045696
C	-2.8002070	-2.1069312	0.7966976
O	-2.4315090	-1.0478796	-0.0711941
C	-3.4242568	-0.7175764	-1.0267678
C	-2.8678622	0.4398961	-1.8657829
N	-3.6585853	0.9914127	-2.8048555
C	-5.0580290	0.5764131	-3.0389764
C	-6.0981199	1.4351914	-2.2960959
C	-7.5422503	1.0144719	-2.6270154
C	-0.5527054	-3.5660797	3.5601939
C	0.2716266	-4.7761888	3.0908428
C	1.4420196	-5.0919447	4.0369403
O	-0.5231355	-1.7484413	1.4801035
Eu	-0.0056322	0.0306269	-0.0727091
O	0.1396579	-1.8162803	-1.6482463
C	1.0552105	-2.6594573	-1.8466085
N	0.9578654	-3.6489756	-2.7527056
C	2.0073210	-4.6697732	-2.9612381
C	1.7891328	-5.9630619	-2.1548419
C	2.8518909	-7.0318956	-2.4685588
O	-1.2606793	1.3259386	1.5480363
C	-1.3188518	2.5692734	1.7439311
N	-2.0219336	3.1184389	2.7478838
C	-2.1048203	4.5745836	2.9926451
C	-1.1170526	5.0940724	4.0509969
C	-1.3046592	6.5945899	4.3390352
O	0.2054091	2.6572153	-0.0715949
C	0.9698707	3.3628599	-1.0344009
C	1.7382903	2.3138148	-1.8478541
N	2.6424993	2.7286378	-2.7481210
C	2.9764601	4.1523314	-2.9732993
C	4.1904694	4.6435925	-2.1659389
C	4.5593120	6.1024155	-2.4909223
O	1.4843379	1.0939956	-1.6424149
O	-1.6890998	0.8270442	-1.6479054
O	2.1454743	-1.5033703	-0.0827554
C	3.2521732	-1.2947319	0.7798606

C	2.8811926	-0.1281367	1.7064660
N	3.7336374	0.2058205	2.6931078
C	4.9982962	-0.5122512	2.9569261
C	4.8959596	-1.5993005	4.0419531
C	6.2576247	-2.2563888	4.3330937
C	-0.5588332	3.4940803	0.7823663
C	2.3432604	-2.5468522	-1.0216783
O	1.7975776	0.4783709	1.5006815
C	-3.1344615	2.0763194	-3.6592151
C	-2.6062833	1.5823940	-5.0169940
C	-2.1386061	2.7394866	-5.9169434
C	3.4106856	1.3356933	3.5891775
C	4.0949638	2.6509356	3.1778172
C	3.8117287	3.7919376	4.1705723
C	-0.2510156	-3.7578859	-3.5947340
C	-0.0871957	-3.1172788	-4.9838010
C	-1.3297269	-3.3177207	-5.8692303
C	-2.7653269	2.2404996	3.6761053
C	-4.2177533	1.9879556	3.2407373
C	-4.9947785	1.1396026	4.2619779
C	3.3716336	1.7352059	-3.5646011
C	2.7287467	1.4810973	-4.9375332
C	3.5424861	0.4901809	-5.7881377
H	-4.1388546	-2.3873666	3.7972803
H	-0.3875588	-5.6717196	3.0105613
H	-5.9252612	1.3646330	-1.1957259
H	-3.4047005	1.0094842	-5.5434798
H	5.1962643	2.4956946	3.1033345
H	4.1580444	-2.3751139	3.7270385
H	1.7967578	-5.7301475	-1.0632858
H	0.8007350	-3.5556004	-5.4959247
H	-4.7408205	2.9617760	3.0952152
H	-0.0710194	4.8984815	3.7134003
H	3.9803152	4.5405834	-1.0743850
H	2.6317092	2.4449345	-5.4891060
H	-3.0541342	-3.0238213	0.2085160
H	-3.6982067	-1.8295608	1.3988296
H	-2.6541269	-5.0589836	3.2513829
H	-3.5453615	-4.1313699	2.0370041
H	-3.2044076	-3.2996219	5.0111516
C	-5.9213132	-3.6956939	5.5335810
H	-4.7235383	-5.3034868	4.6877438
H	-5.6722579	-4.3972484	3.4851154
H	-0.9455268	-3.7399050	4.5851059
H	0.0756187	-2.6529493	3.5906831
H	0.6560663	-4.5749470	2.0634149
H	1.0468249	-5.2649352	5.0647074
H	2.1041247	-4.1961828	4.1147316

C	2.2631658	-6.3101982	3.5962297
H	-4.3741614	-0.4209450	-0.5208335
H	-3.6470102	-1.5974974	-1.6792133
H	-5.1761973	-0.4955132	-2.7754663
H	-5.2314015	0.6364251	-4.1347978
H	-5.9512944	2.5064283	-2.5658206
H	-7.6965115	1.0783788	-3.7291213
C	-8.5944281	1.8707632	-1.9109177
H	-7.6855668	-0.0592072	-2.3602278
H	-2.3294743	2.5848380	-3.0922378
H	-3.9610258	2.8040532	-3.8084994
H	-1.7666537	0.8708787	-4.8410674
C	-1.6165573	2.2670092	-7.2798214
H	-1.3439467	3.3184008	-5.3885939
H	-2.9829877	3.4509932	-6.0703607
H	4.1666335	-1.0425841	0.1875758
H	3.4719462	-2.2180742	1.3669356
H	5.7423194	0.2544388	3.2623557
H	5.3850242	-0.9405798	2.0087359
H	4.4919042	-1.1496204	4.9778013
C	6.1842933	-3.3352971	5.4207129
H	6.9836319	-1.4679500	4.6391176
H	6.6651639	-2.6972322	3.3927918
H	3.7274026	1.0419525	4.6130087
H	2.3086065	1.4523877	3.5969401
H	3.7472284	2.9361737	2.1574201
H	4.1394268	3.4807593	5.1895206
H	2.7094208	3.9532924	4.2418610
C	4.5076401	5.1053459	3.7917992
H	2.5657465	-3.5077238	-0.4991830
H	3.2107351	-2.3144548	-1.6873714
H	3.0025758	-4.2310010	-2.7380428
H	2.0191623	-4.8994781	-4.0479970
H	0.7755614	-6.3694216	-2.3781669
H	2.8320659	-7.2553569	-3.5603655
C	2.6485867	-8.3286314	-1.6747915
H	3.8666269	-6.6180395	-2.2598169
H	-1.0843446	-3.2787914	-3.0424722
H	-0.4837342	-4.8401769	-3.6940603
H	0.1221309	-2.0296221	-4.8592819
C	-1.1767775	-2.7020899	-7.2657198
H	-2.2201567	-2.8796419	-5.3586437
H	-1.5397774	-4.4083100	-5.9659032
H	-1.2769388	4.1094945	0.1857177
H	0.1058401	4.1932887	1.3424456
H	-3.1484257	4.7845433	3.3135162
H	-1.9750565	5.1183287	2.0334115
H	-1.2494287	4.5159274	4.9943973

C	-0.3341223	7.1296367	5.3991196
H	-2.3538581	6.7725007	4.6710503
H	-1.1833904	7.1716217	3.3922239
H	-2.7392016	2.7255906	4.6750476
H	-2.2096168	1.2839499	3.7515235
H	-4.2116703	1.4792436	2.2484902
H	-4.9938505	1.6597868	5.2476077
H	-4.4535104	0.1770573	4.4271089
C	-6.4408745	0.8547541	3.8375584
H	1.6707912	4.0729212	-0.5346295
H	0.3031388	3.9589730	-1.7058142
H	2.0844560	4.7798206	-2.7648952
H	3.1719431	4.2656838	-4.0613428
H	5.0637597	3.9836987	-2.3760928
H	4.7718473	6.1898592	-3.5816786
C	5.7659143	6.6074321	-1.6899170
H	3.6784199	6.7591417	-2.2978707
H	3.4188250	0.7947185	-2.9795323
H	4.4099708	2.1124382	-3.6862183
H	1.6941606	1.0939302	-4.7877007
C	2.9220174	0.2282896	-7.1660604
H	3.6459789	-0.4723606	-5.2324479
H	4.5789600	0.8804900	-5.9165261
H	-6.7985141	-4.3465621	5.7353347
H	-5.3478863	-3.6063616	6.4829788
H	-6.3078688	-2.6850175	5.2725337
H	3.1028987	-6.5024218	4.2978249
H	1.6393787	-7.2309952	3.5676136
H	2.6985376	-6.1680590	2.5805410
H	-9.6205197	1.5366285	-2.1743964
H	-8.4943375	1.8037080	-0.8042950
H	-8.5098761	2.9428869	-2.1960296
H	-1.2900938	3.1272793	-7.9026774
H	-0.7464371	1.5809703	-7.1700258
H	-2.4035239	1.7254249	-7.8499192
H	-6.9671481	0.2380802	4.5975516
H	-7.0217740	1.7957173	3.7160250
H	-6.4841236	0.3048776	2.8697468
H	-0.5043774	8.2119850	5.5816725
H	-0.4621171	6.6033909	6.3710728
H	0.7260806	7.0068852	5.0830764
H	6.0039992	7.6596902	-1.9541724
H	5.5738678	6.5730789	-0.5938929
H	6.6742848	5.9987247	-1.8952628
H	3.5340006	-0.4919978	-7.7500601
H	1.8952743	-0.1939799	-7.0795760
H	2.8525620	1.1640243	-7.7634785
H	-2.0910012	-2.8637218	-7.8759091

H	-0.9965587	-1.6047782	-7.2117964
H	-0.3251527	-3.1570135	-7.8183645
H	3.4292986	-9.0755841	-1.9326064
H	2.7051861	-8.1509409	-0.5774160
H	1.6603703	-8.7908079	-1.8945506
H	7.1853497	-3.7808498	5.6033437
H	5.8247548	-2.9162887	6.3865388
H	5.4976994	-4.1624922	5.1320268
H	4.2788445	5.9056469	4.5279395
H	5.6133999	4.9859396	3.7662634
H	4.1853706	5.4672864	2.7892746

Am(sBuDGA)(NO₃)₃

C	-2.6572745	-0.8235789	-1.8457364
C	-2.1515559	-2.2818303	-1.8042752
H	-2.9748333	-2.9874150	-1.5352114
H	-1.7341690	-2.5799670	-2.7960009
O	-1.1418096	-2.3236323	-0.8095029
C	-0.6035744	-3.6136562	-0.5797170
H	-1.4109934	-4.3203821	-0.2849739
H	-0.1166042	-4.0073431	-1.5064492
C	0.4653716	-3.4502677	0.5116297
N	0.9289911	-4.5178901	1.2119660
N	-3.6909227	-0.4961566	-2.6554849
O	0.9183494	-2.2971764	0.6806098
O	-2.0794930	0.0113226	-1.1211191
C	2.0672556	-4.2638073	2.1535421
H	2.2961917	-3.1895241	2.0129722
C	0.3902892	-5.9063378	1.1524361
H	1.0892319	-6.4752774	1.7991304
C	1.6345247	-4.4524365	3.6244605
H	0.6941673	-3.8767481	3.7781612
H	1.3934908	-5.5237428	3.8246519
C	2.6820898	-3.9708138	4.6394055
H	2.9593522	-2.9084134	4.4583535
H	3.6133091	-4.5776161	4.6077299
C	-1.0000883	-6.0395408	1.8230603
H	-1.7828263	-5.5447473	1.2041057
H	-0.9701261	-5.4791836	2.7821432
C	-1.4165542	-7.4922148	2.0937318
H	-0.6535171	-8.0272787	2.7035143
H	-1.5673168	-8.0716086	1.1563363
C	-4.1571748	0.9295632	-2.7157677
H	-5.0072691	0.9032779	-3.4308760
C	-4.7297162	1.4033204	-1.3585736
H	-3.9009229	1.5032133	-0.6263795

H	-5.4076796	0.6072734	-0.9730330
C	-5.5059755	2.7233964	-1.4546400
H	-4.8486100	3.5744487	-1.7359367
H	-6.3309850	2.6675809	-2.2026866
C	-4.3577860	-1.4860535	-3.5387080
H	-3.8753452	-2.4645587	-3.3383647
C	-4.0949804	-1.1718255	-5.0321106
H	-4.5732628	-0.2030544	-5.3028873
H	-2.9991036	-1.0228460	-5.1594969
C	-4.5774799	-2.2657107	-5.9948217
H	-5.6846830	-2.3685026	-5.9991337
H	-4.1455128	-3.2596261	-5.7359273
H	-5.9617013	2.9759287	-0.4726488
H	-4.2655063	-2.0303629	-7.0353700
H	2.2787704	-4.0388176	5.6730247
H	-2.3735606	-7.5234030	2.6582392
C	3.3113967	-5.0676275	1.7454934
H	3.1921358	-6.1638671	1.9020394
H	3.5666702	-4.8864450	0.6792273
H	4.1833344	-4.7424451	2.3516568
C	0.4918018	-6.5546252	-0.2415492
H	-0.3035977	-6.2190535	-0.9411616
H	1.4795257	-6.3440443	-0.7052805
H	0.3953116	-7.6575936	-0.1509045
C	-5.8466872	-1.6459575	-3.1806634
H	-6.2946122	-2.4860210	-3.7530852
H	-5.9708865	-1.8667766	-2.0983887
H	-6.4346931	-0.7317396	-3.4159296
C	-3.0848721	1.8617348	-3.3048867
H	-3.5319591	2.8547454	-3.5251699
H	-2.2381310	2.0115667	-2.6044773
H	-2.6809799	1.4592447	-4.2578650
Am	0.2890339	-0.1240321	-0.2776749
N	3.1131001	0.3882042	0.1088472
O	2.6817717	-0.4651435	-0.7626322
O	2.1854622	1.0276127	0.7451353
O	4.2954506	0.5703168	0.3170120
N	-1.1235645	1.0323550	1.9839667
N	0.3720869	0.6628920	-3.0934256
O	0.3440126	-0.5758082	-2.7006003
O	0.3509885	0.9595129	-4.2744329
O	0.4050528	1.5354907	-2.1526718
O	-0.6505031	-0.1829390	1.9742475
O	-0.8472431	1.7303422	0.9427284
O	-1.7874857	1.4539115	2.9111291

Eu(sBuDGA)(NO₃)₃

C	-2.7780542	-0.8717226	-1.8388788
C	-2.3758804	-2.3624180	-1.8330140
H	-3.2795220	-3.0139506	-1.7448742
H	-1.8323268	-2.6205883	-2.7729862
O	-1.5240142	-2.5447593	-0.7162112
C	-1.0110010	-3.8599415	-0.5525422
H	-1.7240459	-4.4737392	0.0353364
H	-0.8605910	-4.3459235	-1.5478032
C	0.3784334	-3.7239685	0.0959271
N	0.8922923	-4.7066545	0.8733393
N	-3.6655144	-0.4272394	-2.7578964
O	1.0202072	-2.6888821	-0.1913963
O	-2.2672312	-0.1234079	-0.9771189
C	2.2841152	-4.4909502	1.3818108
H	2.6508064	-3.6260208	0.7950460
C	0.1328896	-5.8658804	1.4226451
H	0.8635710	-6.3397591	2.1092156
C	2.2712339	-4.0610213	2.8673135
H	1.4615129	-3.3091049	2.9936195
H	2.0116225	-4.9313832	3.5172598
C	3.5978123	-3.4418713	3.3317935
H	3.8495820	-2.5464236	2.7209590
H	4.4497572	-4.1551405	3.2690481
C	-1.0818409	-5.4676356	2.3101933
H	-2.0153243	-5.4536296	1.7013243
H	-0.9389230	-4.4295917	2.6820583
C	-1.2873461	-6.4232867	3.4939370
H	-0.4119717	-6.4081774	4.1812355
H	-1.4399901	-7.4755534	3.1628880
C	-4.1069064	1.0061887	-2.7355276
H	-4.8066519	1.0847399	-3.5945977
C	-4.9269450	1.3070162	-1.4584026
H	-4.2606770	1.2314091	-0.5726775
H	-5.6970840	0.5092992	-1.3490261
C	-5.6180264	2.6769101	-1.4801621
H	-4.8864428	3.5142062	-1.4704269
H	-6.2645732	2.8009137	-2.3795845
C	-4.1386722	-1.2835763	-3.8766477
H	-3.7461391	-2.3021069	-3.6828308
C	-3.5119855	-0.8203349	-5.2158896
H	-3.8980866	0.1910998	-5.4782928
H	-2.4169958	-0.7002289	-5.0533541
C	-3.7562180	-1.7818906	-6.3870386
H	-4.8298320	-1.8427030	-6.6708433
H	-3.4084236	-2.8133970	-6.1491908
H	-6.2652576	2.7982963	-0.5844240
H	-3.1968455	-1.4440990	-7.2861628
H	3.5213218	-3.1123133	4.3907700

H	-2.1803040	-6.1281486	4.0865578
C	3.1871709	-5.6942557	1.0750442
H	2.9140309	-6.6030999	1.6580710
H	3.1635787	-5.9487705	-0.0069277
H	4.2382306	-5.4455369	1.3349413
C	-0.2015087	-6.9233636	0.3552588
H	-0.9403628	-6.5572644	-0.3908980
H	0.7111373	-7.2454238	-0.1906915
H	-0.6435391	-7.8210421	0.8401966
C	-5.6721605	-1.4048845	-3.9019058
H	-5.9820501	-2.1639786	-4.6513348
H	-6.0608242	-1.7271397	-2.9116709
H	-6.1678602	-0.4477037	-4.1748437
C	-2.9562283	1.9927331	-2.9952457
H	-3.3728431	2.9994359	-3.2132806
H	-2.2755828	2.0773981	-2.1248259
H	-2.3480044	1.6844764	-3.8714310
Eu	-0.0311946	-0.4899460	0.0046976
N	2.1502855	0.9829869	1.2181386
O	2.2945004	-0.2156246	0.7593831
O	0.9669897	1.4720282	1.1186507
O	3.0734340	1.6016555	1.7141353
N	-1.3891952	-1.1140211	2.5433554
N	0.2442680	0.3683752	-2.7911849
O	0.1999034	-0.8804716	-2.4817908
O	0.1993613	0.7511259	-3.9522351
O	0.3241550	1.1846392	-1.8027604
O	-0.4716366	-1.8820753	2.0444248
O	-1.5990327	-0.0274700	1.9062441
O	-2.0061445	-1.4256499	3.5480638