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SUPPLEMENTARY INFORMATION

Tailoring the selectivity of phenanthroline derivatives for the partitioning of trivalent Am/Eu ions - A relativistic DFT study

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Contents :

Supplementary Information Table 1: Selected Bond Parameters of the metal complexes and the crystal structures.

	Bond Parameter	Am-1	Eu-1	Am-2	Eu-2	Am-3	Eu-3	905130
A	Bond Length							
1	C_1-C_2	1.446	1.453	1.446	1.453	1.444	1.451	1.444
2	C_1-N_1	1.359	1.356	1.360	1.357	1.360	1.357	1.351
3	C_2-N_2	1.359	1.355	1.359	1.355	1.360	1.357	1.353
4	N_2-C_8	1.346	1.341	1.345	1.341	1.346	1.340	1.329
5	N_1-C_7	1.346	1.340	1.347	1.340	1.345	1.340	1.336
B	Bond Angle							
1	C_1-N_1-C_7	118.43	118.73	118.66	118.95	118.57	118.89	118.14
2	C_2-N_2-C_8	118.41	118.78	118.40	118.73	118.60	118.92	118.56
C	Dihedral Angle							
1	C_5-C_1-N_1-C_7	0.60	0.10	2.42	1.43	1.84	1.30	1.21
2	C_3-C_2-N_2-C_8	1.88	1.20	1.24	0.68	2.08	1.51	-0.06
	Bond Parameter	Am-4	Eu-4	Am-5	Eu-5	Am-6	Eu-6	1891927
A	Bond Length							
1	C_1-C_2	1.446	1.453	1.446	1.453	1.444	1.451	1.431
2	C_1-N_1	1.359	1.355	1.358	1.355	1.359	1.357	1.355
3	C_2-N_2	1.358	1.356	1.360	1.357	1.360	1.356	1.352
4	N_2-C_8	1.347	1.341	1.346	1.340	1.345	1.341	1.334
5	N_1-C_7	1.347	1.341	1.347	1.341	1.346	1.341	1.332
B	Bond Angle							
1	C_1-N_1-C_7	118.45	118.80	118.44	118.75	118.63	118.92	118.33
2	C_2-N_2-C_8	118.44	118.77	118.64	118.98	118.65	118.92	119.02
C	Dihedral Angle							
1	C_5-C_1-N_1-C_7	1.43	1.11	2.15	1.08	2.18	1.56	1.09
2	C_3-C_2-N_2-C_8	1.07	0.46	1.49	1.47	1.78	1.15	-0.98

Supplementary Information Table 2: M-O Bond Parameters of the $M(NO_3)_3$ molecule and the complexes

	$M\text{-}O_1$	$M\text{-}O_3$	$M\text{-}O_7$	$M\text{-}O_9$	$M\text{-}O_{10}$	$M\text{-}O_{12}$
$Am(NO_3)_3$	2.471	2.473	2.472	2.472	2.476	2.475
$Eu(NO_3)_3$	2.479	2.481	2.480	2.479	2.486	2.484
Am-1	2.569	2.594	2.724	2.635	2.544	2.552
Eu-1	2.558	2.560	2.643	2.687	2.558	2.560
Am-2	2.601	2.564	2.562	2.554	2.632	2.727
Eu-2	2.669	2.663	2.563	2.569	2.673	2.661
Am-3	2.556	2.571	2.716	2.638	2.572	2.599
Eu-3	2.681	2.655	2.651	2.681	2.571	2.566
Am-4	2.729	2.638	2.585	2.561	2.550	2.562
Eu-4	2.696	2.641	2.555	2.566	2.632	2.698
Am-5	2.692	2.626	2.602	2.571	2.572	2.563
Eu-5	2.563	2.566	2.699	2.638	2.634	2.699
Am-6	2.707	2.635	2.563	2.572	2.599	2.567
Eu-6	2.700	2.638	2.564	2.567	2.634	2.699

Supplementary Information Table 3: HOMO-LUMO gap of ligands and SOMO-LUMO gap of metal complexes. (in eV)

	SOMO	LUMO	GAP
Am-1	-3.997	-3.921	0.076
Eu-1	-4.149	-3.986	0.163
Am-2	-3.932	-3.861	0.070
Eu-2	-4.068	-3.913	0.155
Am-3	-3.885	-3.806	0.078
Eu-3	-4.019	-3.850	0.168
Am-4	-4.005	-3.923	0.081
Eu-4	-4.136	-3.989	0.146
Am-5	-3.923	-3.855	0.068
Eu-5	-4.070	-3.907	0.163
Am-6	-3.874	-3.801	0.073
Eu-6	-3.989	-3.847	0.141
	HOMO	LUMO	GAP
1	-5.017	-3.061	1.956
2	-4.925	-3.069	1.855
3	-4.887	-3.045	1.842
4	-5.096	-3.045	2.051
5	-5.061	-3.017	2.043
6	-5.042	-2.976	2.065

Supplementary Information Table 4: Net charges obtained from Mulliken Population Analysis carried out at ZORA/ BP86 level using ADF software

Complexes	N_1	N_2	N_3	N_4	M
Am-1	-0.429	-0.293	-0.296	-0.430	1.571
Eu-1	-0.418	-0.296	-0.296	-0.417	1.573
Am-2	-0.429	-0.293	-0.297	-0.432	1.553
Eu-2	-0.417	-0.297	-0.296	-0.420	1.560
Am-3	-0.430	-0.296	-0.298	-0.431	1.547
Eu-3	-0.421	-0.298	-0.297	-0.420	1.555
Am-4	-0.430	-0.295	-0.294	-0.428	1.591
Eu-4	-0.414	-0.293	-0.293	-0.417	1.576
Am-5	-0.430	-0.296	-0.294	-0.428	1.575
Eu-5	-0.418	-0.292	-0.294	-0.416	1.565
Am-6	-0.429	-0.296	-0.296	-0.430	1.569
Eu-6	-0.418	-0.295	-0.294	-0.417	1.558

Supplementary Information Table 5: Net charges obtained from Natural Population Analysis carried out at ZORA/ BP86 level using ADF software

Complexes	N_1	N_2	N_3	N_4	M
Am-1	-0.4198	-0.2297	-0.2266	-0.4214	1.0156
Eu-1	-0.4001	-0.2229	-0.2225	-0.4009	1.0424
Am-2	-0.4203	-0.2301	-0.2285	-0.4224	1.0162
Eu-2	-0.4006	-0.2237	-0.2232	-0.4014	1.0427
Am-3	-0.4222	-0.2296	-0.2299	-0.4217	1.0164
Eu-3	-0.4025	-0.2249	-0.2246	-0.4031	1.0514
Am-4	-0.4192	-0.2382	-0.2367	-0.4211	1.0127
Eu-4	-0.4005	-0.2319	-0.2308	-0.3990	1.0416
Am-5	-0.4199	-0.2377	-0.2319	-0.4216	1.0117
Eu-5	-0.4008	-0.2325	-0.2319	-0.4009	1.0417
Am-6	-0.4210	-0.2398	-0.2385	-0.4214	1.0118
Eu-6	-0.4015	-0.2342	-0.2338	-0.4015	1.0518

Supplementary Information Table 6: M and O Mulliken Charges of the $M(NO_3)_3$ molecule and the complexes

	M^{3+}	O_1	O_3	O_7	O_9	O_{10}	O_{12}
$Am(NO_3)_3$	1.557	-0.541	-0.540	-0.541	-0.541	-0.541	-0.542
$Eu(NO_3)_3$	1.634	-0.553	-0.553	-0.554	-0.554	-0.554	-0.555
Am-1	1.571	-0.543	-0.545	-0.536	-0.535	-0.514	-0.525
Eu-1	1.574	-0.542	-0.548	-0.554	-0.555	-0.550	-0.541
Am-2	1.554	-0.533	-0.535	-0.543	-0.544	-0.527	-0.517
Eu-2	1.561	-0.546	-0.546	-0.554	-0.553	-0.549	-0.542
Am-3	1.548	-0.520	-0.525	-0.533	-0.535	-0.545	-0.542
Eu-3	1.555	-0.545	-0.547	-0.550	-0.543	-0.552	-0.554
Am-4	1.591	-0.517	-0.524	-0.531	-0.530	-0.545	-0.543
Eu-4	1.577	-0.543	-0.548	-0.550	-0.553	-0.549	-0.542
Am-5	1.576	-0.524	-0.528	-0.529	-0.528	-0.543	-0.540
Eu-5	1.565	-0.544	-0.548	-0.550	-0.552	-0.548	-0.542
Am-6	1.570	-0.522	-0.526	-0.529	-0.529	-0.545	-0.542
Eu-6	1.559	-0.550	-0.552	-0.544	-0.547	-0.548	-0.542

Supplementary Information Table 7: QTAIM analysis of electron density ρ(e/bohr^3) at Metal – Oxygen Bond Critical Points of the $M(NO_3)_3$ molecule and the complexes

	$M\text{-}O_1$	$M\text{-}O_3$	$M\text{-}O_7$	$M\text{-}O_9$	$M\text{-}O_{10}$	$M\text{-}O_{12}$
$Eu(NO_3)_3$	0.044	0.043	0.044	0.044	0.043	0.043
$Am(NO_3)_3$	0.054	0.054	0.054	0.054	0.054	0.054
Am-1	0.029	0.037	0.043	0.040	0.046	0.045
Eu-1	0.027	0.029	0.029	0.025	0.036	0.036
Am-2	0.029	0.037	0.027	0.040	0.044	0.044
Eu-2	0.027	0.028	0.027	0.028	0.035	0.036
Am-3	0.040	0.043	0.036	0.030	0.044	0.043
Eu-3	0.027	0.029	0.029	0.027	0.035	0.035
Am-4	0.036	0.029	0.041	0.044	0.045	0.044
Eu-4	0.030	0.026	0.026	0.030	0.035	0.036
Am-5	0.037	0.031	0.040	0.043	0.043	0.043
Eu-5	0.026	0.030	0.030	0.026	0.036	0.035
Am-6	0.031	0.037	0.043	0.040	0.043	0.044
Eu-6	0.030	0.026	0.026	0.030	0.035	0.036

Optimized Coordinates of 1 Ligand

1	H	7.3302	34.6144	11.3410
2	N	8.0508	29.3821	11.3835
3	N	8.2211	30.6849	11.5874
4	C	7.4436	31.3520	12.4597
5	C	6.4431	30.6660	13.1856
6	N	6.2805	29.3538	12.9910
7	C	7.0772	28.7634	12.0810
8	N	7.4095	26.7642	10.7470
9	C	6.8622	27.3020	11.8350
10	C	6.0894	26.5545	12.7569
11	H	5.6970	27.0409	13.6483
12	C	5.8547	25.2222	12.4951
13	H	5.2747	24.6168	13.1915
14	C	6.3785	24.6257	11.3238
15	C	6.1517	23.2337	10.9939
16	H	6.0322	33.3981	11.2375
17	C	6.7966	22.6980	9.9047
18	H	6.6289	21.6501	9.6447
19	C	7.6410	23.4760	9.0590
20	C	8.2861	22.9191	7.9302
21	H	8.1591	21.8571	7.7086
22	C	9.0604	23.7223	7.1235
23	H	9.5788	23.3341	6.2488
24	C	9.1764	25.1000	7.4455
25	C	9.9961	25.9822	6.5549
26	N	10.7448	25.3767	5.6148
27	C	11.4753	26.1592	4.8151
28	C	11.3982	27.5621	4.9660
29	N	10.6357	28.0937	5.9396
30	N	9.9299	27.3148	6.7533
31	N	8.5856	25.6535	8.5042
32	C	7.8375	24.8701	9.3072
33	C	7.1954	25.4577	10.4871
34	C	12.1644	28.5584	4.0992
35	C	12.7004	27.8395	2.8406
36	H	11.8711	27.7055	2.1270
37	H	13.4296	28.4966	2.3419
38	C	13.3365	26.4842	3.1523
39	H	14.1748	26.6234	3.8539
40	H	13.7713	26.0465	2.2401
41	C	12.3396	25.4704	3.7600
42	C	5.5435	31.3411	14.2203
43	C	5.6122	32.8766	14.0541
44	H	4.9903	33.1691	13.1927
45	H	5.1514	33.3464	14.9371
46	C	7.0362	33.3965	13.8573
47	H	7.6562	33.1220	14.7263
48	H	7.0375	34.4969	13.8162
49	C	7.7048	32.8524	12.5751
50	C	13.3257	29.1358	4.9448
51	H	12.9298	29.6097	5.8527
52	H	13.8727	29.8924	4.3627

53	H	14.0382	28.3579	5.2534
54	C	11.2385	29.7167	3.6748
55	H	10.3845	29.3467	3.0894
56	H	11.7994	30.4275	3.0500
57	H	10.8476	30.2462	4.5514
58	C	11.3982	24.9028	2.6704
59	H	10.6693	24.2153	3.1195
60	H	11.9854	24.3504	1.9221
61	H	10.8408	25.6961	2.1533
62	C	13.1201	24.3048	4.4015
63	H	13.7768	24.6646	5.2066
64	H	13.7469	23.8168	3.6411
65	H	12.4376	23.5595	4.8269
66	C	6.0374	30.9173	15.6250
67	H	6.0091	29.8240	15.7242
68	H	5.3867	31.3550	16.3961
69	H	7.0676	31.2475	15.8164
70	C	4.0860	30.8725	14.0412
71	H	3.7079	31.1307	13.0415
72	H	3.4457	31.3657	14.7868
73	H	4.0021	29.7865	14.1665
74	C	9.2210	33.1292	12.6310
75	H	9.6813	32.6292	13.4955
76	H	9.3947	34.2110	12.7287
77	H	9.7202	32.7685	11.7244
78	C	7.1199	33.5347	11.3143
79	H	7.5774	33.1115	10.4100
80	H	5.4880	22.6277	11.5929

Optimized Coordinates of 2 Ligand

1	H	5.1826	19.8790	14.1342
2	N	7.7560	29.4430	11.1086
3	N	7.9698	30.7293	11.3631
4	C	7.3304	31.3482	12.3735
5	C	6.3753	30.6445	13.1403
6	N	6.1813	29.3435	12.9047
7	C	6.8924	28.7838	11.9086
8	N	7.3458	26.7539	10.6533
9	C	6.6943	27.3184	11.6686
10	C	5.8409	26.5887	12.5320
11	H	5.3479	27.1006	13.3566
12	C	5.6650	25.2411	12.3065
13	H	5.0263	24.6515	12.9635
14	C	6.3236	24.6094	11.2235
15	C	6.1821	23.1935	10.9595
16	H	6.7719	21.2128	12.7609
17	C	6.9206	22.6014	9.9488
18	H	1.6867	20.3655	13.9516
19	C	7.7777	23.4102	9.1093
20	C	8.4823	22.8631	8.0094
21	H	8.4014	21.7978	7.7966
22	C	9.2506	23.6774	7.2070
23	H	9.8003	23.2863	6.3530
24	C	9.3112	25.0620	7.4993
25	C	10.1254	25.9546	6.6136
26	N	10.8115	25.3647	5.6174
27	C	11.5173	26.1569	4.8055
28	C	11.4756	27.5552	5.0011
29	N	10.8024	28.0679	6.0484
30	N	10.1263	27.2777	6.8760
31	N	8.6574	25.6125	8.5209
32	C	7.9068	24.8209	9.3143
33	C	7.1775	25.4354	10.4248
34	C	12.1959	28.5656	4.1119
35	C	12.6678	27.8689	2.8154
36	H	11.8063	27.7557	2.1371
37	H	13.3792	28.5307	2.2977
38	C	13.3046	26.5024	3.0706
39	H	14.1710	26.6189	3.7418
40	H	13.6991	26.0815	2.1325
41	C	12.3226	25.4843	3.6948
42	C	5.5523	31.2875	14.2558
43	C	5.6754	32.8265	14.1762
44	H	5.0243	33.1940	13.3664
45	H	5.2794	33.2599	15.1079
46	C	7.1087	33.3004	13.9348
47	H	7.7604	32.9401	14.7476
48	H	7.1582	34.3998	13.9683

49	C	7.6811	32.8195	12.5821
50	C	13.3989	29.1328	4.9040
51	H	13.0502	29.5876	5.8404
52	H	13.9110	29.9020	4.3072
53	H	14.1295	28.3520	5.1585
54	C	11.2449	29.7273	3.7563
55	H	10.3621	29.3633	3.2109
56	H	11.7687	30.4512	3.1148
57	H	10.8995	30.2398	4.6618
58	C	11.3267	24.9568	2.6341
59	H	10.6102	24.2657	3.0974
60	H	11.8730	24.4183	1.8458
61	H	10.7563	25.7696	2.1638
62	C	13.1147	24.2932	4.2713
63	H	13.8107	24.6238	5.0558
64	H	13.7016	23.8173	3.4723
65	H	12.4413	23.5453	4.7067
66	C	6.0899	30.7604	15.6082
67	H	6.0337	29.6642	15.6380
68	H	5.4850	31.1646	16.4330
69	H	7.1366	31.0494	15.7756
70	C	4.0711	30.8840	14.1153
71	H	3.6607	31.2146	13.1503
72	H	3.4821	31.3548	14.9159
73	H	3.9503	29.7961	14.1829
74	C	9.2134	32.9996	12.5777
75	H	9.6825	32.4146	13.3821
76	H	9.4619	34.0595	12.7355
77	H	9.6425	32.6718	11.6236
78	C	7.0810	33.6320	11.4093
79	H	7.4700	33.2551	10.4541
80	H	7.3571	34.6923	11.5086
81	H	5.9845	33.5635	11.3785
82	C	5.2398	22.3924	11.7979
83	C	3.8550	22.6151	11.7245
84	C	2.9591	21.8650	12.4879
85	C	3.4405	20.8759	13.3537
86	C	4.8182	20.6478	13.4522
87	C	5.7007	21.3995	12.6792
88	H	3.4684	23.3811	11.0500
89	H	1.8844	22.0480	12.4070
90	O	2.6083	20.1002	14.1311
91	H	6.8567	21.5355	9.7870

Optimized Coordinates of 3 Ligand

1	H	7.3371	16.5533	9.0748
2	N	7.6939	29.3962	11.0727
3	N	7.9498	30.6794	11.2898
4	C	7.3407	31.3208	12.2984
5	C	6.3818	30.6391	13.0930
6	N	6.1576	29.3386	12.8816
7	C	6.8332	28.7529	11.8839
8	N	7.2732	26.7323	10.6165
9	C	6.6248	27.3002	11.6438
10	C	5.7858	26.5653	12.5058
11	H	5.2983	27.0812	13.3307
12	C	5.6140	25.2164	12.2844
13	H	4.9795	24.6260	12.9439
14	C	6.2755	24.5821	11.2060
15	C	6.1465	23.1627	10.9532
16	H	6.7824	21.2162	12.7677
17	C	6.8889	22.5705	9.9450
18	H	8.8156	20.6736	10.3260
19	C	7.7426	23.3813	9.1042
20	C	8.4496	22.8365	8.0061
21	H	8.3658	21.7722	7.7919
22	C	9.2229	23.6504	7.2082
23	H	9.7726	23.2655	6.3520
24	C	9.2992	25.0270	7.5025
25	C	10.1146	25.9166	6.6340
26	N	10.7930	25.3638	5.6189
27	C	11.5025	26.1825	4.8369
28	C	11.4686	27.5815	5.0785
29	N	10.7952	28.0611	6.1348
30	N	10.1230	27.2312	6.9236
31	N	8.6401	25.5794	8.5311
32	C	7.8646	24.7873	9.3145
33	C	7.1228	25.4007	10.4009
34	C	12.1932	28.6163	4.2264
35	C	12.6612	27.9594	2.9078
36	H	11.8008	27.8761	2.2242
37	H	13.3774	28.6347	2.4163
38	C	13.2906	26.5824	3.1174
39	H	14.1569	26.6703	3.7925
40	H	13.6822	26.1898	2.1663
41	C	12.3019	25.5488	3.7036
42	C	5.5925	31.3131	14.2098
43	C	5.7418	32.8483	14.1049
44	H	5.0845	33.2158	13.3006
45	H	5.3682	33.2994	15.0368
46	C	7.1793	33.2920	13.8358
47	H	7.8380	32.9335	14.6434
48	H	7.2484	34.3901	13.8502

49	C	7.7228	32.7846	12.4808
50	C	13.3998	29.1445	5.0418
51	H	13.0570	29.5820	5.9881
52	H	13.9201	29.9224	4.4645
53	H	14.1206	28.3491	5.2771
54	C	11.2480	29.7949	3.9106
55	H	10.3591	29.4544	3.3606
56	H	11.7776	30.5276	3.2850
57	H	10.9133	30.2938	4.8270
58	C	11.2976	25.0715	2.6256
59	H	10.5799	24.3628	3.0595
60	H	11.8422	24.5660	1.8151
61	H	10.7294	25.9052	2.1915
62	C	13.0847	24.3292	4.2332
63	H	13.7789	24.6202	5.0342
64	H	13.6724	23.8894	3.4149
65	H	12.4072	23.5630	4.6286
66	C	6.1484	30.7949	15.5596
67	H	6.0696	29.7011	15.6110
68	H	5.5663	31.2267	16.3864
69	H	7.2031	31.0652	15.7030
70	C	4.1019	30.9324	14.1011
71	H	3.6818	31.2454	13.1348
72	H	3.5369	31.4364	14.8982
73	H	3.9598	29.8497	14.2024
74	C	9.2589	32.9343	12.4503
75	H	9.7311	32.3446	13.2490
76	H	9.5238	33.9905	12.6020
77	H	9.6729	32.6035	11.4911
78	C	7.1162	33.5892	11.3041
79	H	7.4868	33.2008	10.3468
80	H	7.4110	34.6448	11.3913
81	H	6.0187	33.5373	11.2888
82	C	5.2209	22.3601	11.8062
83	C	3.8325	22.5609	11.7406
84	C	2.9563	21.8047	12.5200
85	C	3.4618	20.8346	13.3940
86	C	4.8446	20.6298	13.4833
87	C	5.7076	21.3845	12.6934
88	H	3.4261	23.3094	11.0581
89	H	1.8780	21.9670	12.4446
90	O	2.6526	20.0541	14.1866
91	H	5.2267	19.8762	14.1723
92	H	1.7235	20.2993	14.0151
93	C	6.7994	21.1050	9.6710
94	C	5.6265	20.5367	9.1451
95	C	5.5429	19.1743	8.8716
96	C	6.6411	18.3442	9.1293
97	C	7.8188	18.8900	9.6547
98	C	7.8928	20.2590	9.9159

99	H	4.7668	21.1756	8.9406
100	H	4.6333	18.7375	8.4586
101	O	6.5040	17.0058	8.8432
102	H	8.6776	18.2462	9.8613

Optimized Coordinates of 4 Ligand

1	H	12.5239	-2.5579	1.4124
2	H	11.3175	-1.2441	1.3520
3	H	15.1227	-1.5874	6.2823
4	H	14.0741	-0.4057	7.1118
5	C	12.6213	-2.6974	6.5743
6	H	12.4008	-2.2679	7.5612
7	H	13.4231	-3.4408	6.6915
8	H	11.7209	-3.2178	6.2187
9	C	13.6427	-0.2435	2.4366
10	H	14.2280	0.3141	3.1807
11	N	8.0003	5.2929	5.5862
12	N	9.0002	2.8505	6.3787
13	N	9.0965	6.5912	3.3780
14	N	9.4880	7.0174	2.1641
15	N	6.9828	7.7444	3.1818
16	N	10.0284	1.1055	4.5023
17	N	10.7296	0.4350	3.5727
18	N	11.2639	0.0587	6.2941
19	H	13.1293	0.4855	1.7947
20	H	14.3417	-0.8241	1.8165
21	C	11.8370	-1.9471	2.0167
22	C	7.4758	6.4442	5.1747
23	C	6.5850	7.2128	5.9615
24	H	6.1871	8.1482	5.5703
25	C	6.2631	6.7617	7.2240
26	H	5.6139	7.3515	7.8708
27	C	6.7912	5.5365	7.6961
28	C	6.5096	5.0250	9.0223
29	H	6.9360	3.4874	10.4394
30	C	7.1384	3.8755	9.4387
31	H	11.0842	-2.6133	2.4612
32	C	8.0099	3.1313	8.5876
33	C	8.6316	1.9323	9.0084
34	H	8.4774	1.5766	10.0293
35	C	9.4161	1.2244	8.1232
36	H	9.9190	0.3020	8.4098
37	C	9.5509	1.7124	6.7979
38	C	7.6699	4.8302	6.8101
39	C	8.2572	3.5632	7.2488
40	C	7.8751	6.9446	3.8232
41	C	7.3854	8.1439	1.9831
42	C	6.6037	9.0072	1.0115
43	C	7.6862	9.3186	-0.0792
44	H	8.0623	10.3406	0.0750
45	H	7.2572	9.2809	-1.0905
46	C	8.8798	8.3112	0.0754
47	C	8.6348	7.7660	1.4679
48	C	6.0713	10.2833	1.6845

49	H	5.3695	10.0324	2.4917
50	H	5.5446	10.9092	0.9496
51	H	6.8900	10.8772	2.1149
52	C	5.4204	8.1888	0.4463
53	H	5.7612	7.2720	-0.0535
54	H	4.8638	8.7915	-0.2861
55	H	4.7343	7.9003	1.2548
56	C	10.2464	9.0099	-0.0289
57	H	10.3837	9.4312	-1.0356
58	H	11.0587	8.2967	0.1644
59	H	10.3316	9.8278	0.7005
60	C	8.8125	7.1582	-0.9505
61	H	7.8451	6.6383	-0.9183
62	H	9.5999	6.4201	-0.7453
63	H	8.9572	7.5497	-1.9680
64	C	10.3362	0.9217	5.8014
65	C	11.9456	-0.5894	5.3597
66	C	13.0547	-1.5978	5.5895
67	C	13.2838	-2.1554	4.1414
68	H	14.3532	-2.2941	3.9298
69	H	12.8076	-3.1439	4.0612
70	C	12.6159	-1.1866	3.1031
71	C	11.6943	-0.3798	3.9949
72	C	14.3008	-0.8704	6.1423
73	H	14.6474	-0.0818	5.4605
74	H	5.8172	5.5383	9.6730

Optimized Coordinates of 5 Ligand

1	H	12.6000	-2.4811	1.3492
2	H	11.3777	-1.1817	1.2967
3	C	5.5679	5.7248	9.9411
4	C	4.1962	5.8082	9.6530
5	C	3.3305	6.5475	10.4612
6	C	3.8312	7.2302	11.5762
7	C	5.1963	7.1631	11.8782
8	C	6.0477	6.4163	11.0664
9	H	3.7966	5.2822	8.7842
10	H	2.2646	6.5944	10.2226
11	N	7.9873	5.2346	5.6249
12	N	8.9661	2.7916	6.3940
13	N	9.0942	6.5658	3.4410
14	N	9.4941	7.0064	2.2351
15	N	6.9672	7.6914	3.2276
16	N	10.0108	1.0842	4.4781
17	N	10.7349	0.4435	3.5445
18	N	11.2290	0.0082	6.2644
19	O	3.0312	7.9845	12.4075
20	H	5.5755	7.7016	12.7471
21	H	2.1160	7.9429	12.0723
22	C	7.4537	6.3827	5.2160
23	C	6.5410	7.1314	5.9969
24	H	6.1273	8.0594	5.6043
25	C	6.2181	6.6720	7.2558
26	H	5.5487	7.2450	7.8965
27	C	6.7667	5.4550	7.7293
28	C	6.4896	4.9482	9.0570
29	H	7.1105	6.3725	11.3069
30	C	7.0980	3.7849	9.4968
31	H	11.1462	-2.5755	2.3754
32	C	7.9599	3.0357	8.6066
33	C	8.5459	1.8022	8.9826
34	H	8.3674	1.4050	9.9812
35	C	9.3251	1.1053	8.0834
36	H	9.7927	0.1578	8.3474
37	C	9.4979	1.6350	6.7821
38	C	7.6494	4.7623	6.8429
39	C	8.2229	3.4904	7.2764
40	C	7.8630	6.9000	3.8746
41	C	7.3785	8.1054	2.0370
42	C	6.5963	8.9650	1.0625
43	C	7.6867	9.2987	-0.0137
44	H	8.0459	10.3252	0.1503
45	H	7.2700	9.2602	-1.0301
46	C	8.8930	8.3076	0.1490
47	C	8.6392	7.7489	1.5345
48	C	6.0392	10.2289	1.7390

49	H	5.3325	9.9623	2.5368
50	H	5.5118	10.8529	1.0029
51	H	6.8450	10.8307	2.1826
52	C	5.4308	8.1348	0.4784
53	H	5.7896	7.2264	-0.0242
54	H	4.8738	8.7349	-0.2558
55	H	4.7402	7.8308	1.2774
56	C	10.2504	9.0267	0.0669
57	H	10.3949	9.4563	-0.9353
58	H	11.0704	8.3241	0.2667
59	H	10.3140	9.8410	0.8025
60	C	8.8549	7.1609	-0.8855
61	H	7.8948	6.6270	-0.8683
62	H	9.6503	6.4328	-0.6754
63	H	9.0062	7.5612	-1.8986
64	C	10.3000	0.8724	5.7772
65	C	11.9347	-0.6081	5.3264
66	C	13.0550	-1.6049	5.5515
67	C	13.3171	-2.1244	4.0948
68	H	14.3921	-2.2398	3.8981
69	H	12.8598	-3.1186	3.9834
70	C	12.6496	-1.1426	3.0680
71	C	11.7034	-0.3687	3.9632
72	C	14.2795	-0.8696	6.1413
73	H	14.6227	-0.0593	5.4837
74	H	15.1115	-1.5757	6.2776
75	H	14.0294	-0.4318	7.1174
76	C	12.6240	-2.7330	6.5040
77	H	12.3818	-2.3296	7.4968
78	H	13.4357	-3.4664	6.6170
79	H	11.7375	-3.2592	6.1228
80	C	13.6718	-0.1714	2.4358
81	H	14.2393	0.3781	3.1994
82	H	13.1566	0.5642	1.8030
83	H	14.3869	-0.7287	1.8130
84	C	11.8965	-1.8911	1.9551
85	H	6.9295	3.4358	10.5048

Optimized Coordinates of 6 Ligand

1	H	8.5084	2.9341	13.8888
2	H	5.4442	1.4791	14.8762
3	C	5.4822	5.6569	9.8813
4	C	4.1089	5.6577	9.5889
5	C	3.2041	6.3764	10.3720
6	C	3.6670	7.1231	11.4623
7	C	5.0336	7.1373	11.7671
8	C	5.9246	6.4083	10.9835
9	H	3.7382	5.0815	8.7394
10	H	2.1377	6.3573	10.1325
11	N	7.8433	5.1138	5.5418
12	N	9.1125	2.8793	6.4403
13	N	8.4561	5.9378	3.0315
14	N	8.8051	6.2846	1.7832
15	N	6.9773	7.8118	3.2636
16	N	10.6214	1.5392	4.6365
17	N	11.4002	0.9695	3.7048
18	N	11.2881	-0.0302	6.3234
19	O	2.8304	7.8639	12.2660
20	H	5.3823	7.7253	12.6163
21	H	1.9176	7.7646	11.9355
22	C	7.2529	6.2390	5.0984
23	C	6.3736	6.9950	5.8984
24	H	5.9407	7.9047	5.4872
25	C	6.0906	6.5671	7.1782
26	H	5.4170	7.1390	7.8143
27	C	6.6874	5.3853	7.6803
28	C	6.4444	4.9054	9.0214
29	H	6.9877	6.4289	11.2257
30	C	7.1186	3.7881	9.4921
31	H	8.8770	3.7906	11.5820
32	C	8.0326	3.0761	8.6270
33	C	8.6931	1.8900	9.0313
34	H	8.5245	1.4973	10.0326
35	C	9.5300	1.2314	8.1544
36	H	10.0446	0.3132	8.4307
37	C	9.7201	1.7527	6.8596
38	C	7.5889	4.7010	6.8126
39	C	8.2713	3.5223	7.2938
40	C	7.5742	6.6873	3.7255
41	C	7.3242	8.1468	2.0303
42	C	6.8077	9.3313	1.2418
43	C	7.7638	9.3278	-0.0006
44	H	8.5265	10.1079	0.1362
45	H	7.2189	9.5652	-0.9245
46	C	8.4784	7.9338	-0.1010
47	C	8.2443	7.3797	1.2864
48	C	6.9061	10.6362	2.0512

49	H	6.2744	10.5867	2.9483
50	H	6.5709	11.4851	1.4385
51	H	7.9398	10.8302	2.3694
52	C	5.3342	9.0728	0.8497
53	H	5.2233	8.1518	0.2618
54	H	4.9597	9.9116	0.2462
55	H	4.7074	8.9824	1.7476
56	C	9.9791	8.0697	-0.4142
57	H	10.1163	8.5218	-1.4070
58	H	10.4674	7.0865	-0.4099
59	H	10.4849	8.7044	0.3263
60	C	7.8146	7.0055	-1.1442
61	H	6.7382	6.8845	-0.9606
62	H	8.2773	6.0100	-1.1182
63	H	7.9465	7.4256	-2.1515
64	C	10.5920	1.0495	5.8947
65	C	12.0407	-0.5987	5.3936
66	C	12.9357	-1.8061	5.5761
67	C	13.3535	-2.1198	4.0974
68	H	14.4106	-2.4119	4.0343
69	H	12.7589	-2.9700	3.7332
70	C	13.0533	-0.8699	3.1972
71	C	12.1034	-0.0911	4.0790
72	C	14.1427	-1.4139	6.4588
73	H	14.7162	-0.5853	6.0224
74	H	14.8164	-2.2757	6.5694
75	H	13.8041	-1.1052	7.4576
76	C	12.1765	-2.9750	6.2284
77	H	11.8419	-2.7061	7.2396
78	H	12.8321	-3.8543	6.3034
79	H	11.2935	-3.2557	5.6377
80	C	14.3171	-0.0201	2.9288
81	H	14.8178	0.2766	3.8603
82	H	14.0529	0.8936	2.3801
83	H	15.0312	-0.5972	2.3238
84	C	12.4009	-1.2582	1.8586
85	H	13.0996	-1.8626	1.2622
86	H	12.1358	-0.3629	1.2813
87	H	11.4852	-1.8454	2.0162
88	C	6.8969	3.2777	10.8771
89	C	5.6715	2.7029	11.2465
90	C	5.4654	2.2137	12.5364
91	C	6.4890	2.2989	13.4880
92	C	7.7195	2.8690	13.1390
93	C	7.9156	3.3454	11.8445
94	H	4.8679	2.6307	10.5131
95	H	4.5055	1.7641	12.8032
96	O	6.3458	1.8389	14.7769

Optimized Coordinates of Am-1

1	Am	8.7802	28.2486	8.9229
2	N	7.5890	29.4044	10.9737
3	N	7.8372	30.6887	11.1987
4	C	7.2806	31.3013	12.2537
5	C	6.4255	30.5741	13.1260
6	N	6.1761	29.2850	12.8785
7	C	6.7651	28.7410	11.8050
8	N	7.1809	26.7552	10.4847
9	C	6.5166	27.3040	11.5124
10	C	5.6156	26.5716	12.3162
11	H	5.1039	27.0832	13.1289
12	C	5.4153	25.2351	12.0465
13	H	4.7222	24.6425	12.6463
14	C	6.1217	24.6190	10.9897
15	C	5.9788	23.2288	10.6815
16	H	5.2904	22.6307	11.2812
17	C	6.6925	22.6588	9.6664
18	H	6.5861	21.5965	9.4402
19	C	7.5947	23.4384	8.8751
20	C	8.3517	22.8792	7.8218
21	H	8.2598	21.8142	7.6013
22	C	9.1927	23.6823	7.0824
23	H	9.7917	23.2953	6.2608
24	C	9.2746	25.0573	7.3942
25	C	10.1382	25.9467	6.5727
26	N	10.8849	25.3959	5.6069
27	C	11.6263	26.2201	4.8600
28	C	11.5448	27.6210	5.0780
29	N	10.8048	28.0986	6.0905
30	N	10.1095	27.2635	6.8526
31	N	8.5843	25.6150	8.3995
32	C	7.7552	24.8326	9.1340
33	C	7.0063	25.4362	10.2242
34	C	12.2838	28.6606	4.2454
35	C	12.8257	27.9945	2.9607
36	H	11.9965	27.8693	2.2455
37	H	13.5390	28.6831	2.4837
38	C	13.4898	26.6431	3.2248
39	H	14.3242	26.7736	3.9321
40	H	13.9330	26.2453	2.2991
41	C	12.5115	25.5885	3.7915
42	C	5.8104	31.1800	14.3817
43	C	5.8698	32.7222	14.3049
44	H	5.0753	33.0753	13.6276
45	H	5.6285	33.1303	15.2982
46	C	7.2240	33.2494	13.8305
47	H	8.0152	32.9264	14.5262
48	H	7.2307	34.3496	13.8511
49	C	7.5936	32.7849	12.4038

50	C	13.4380	29.2315	5.1060
51	H	13.0422	29.6752	6.0284
52	H	13.9657	30.0125	4.5396
53	H	14.1669	28.4589	5.3882
54	C	11.3269	29.8114	3.8668
55	H	10.4720	29.4418	3.2828
56	H	11.8681	30.5460	3.2535
57	H	10.9404	30.3175	4.7586
58	C	11.5895	25.0372	2.6761
59	H	10.8726	24.3179	3.0934
60	H	12.1976	24.5248	1.9170
61	H	11.0195	25.8343	2.1795
62	C	13.3121	24.4193	4.4041
63	H	13.9503	24.7653	5.2293
64	H	13.9592	23.9772	3.6334
65	H	12.6442	23.6400	4.7902
66	C	6.6307	30.6549	15.5884
67	H	6.5974	29.5579	15.6247
68	H	6.2042	31.0494	16.5221
69	H	7.6849	30.9585	15.5357
70	C	4.3452	30.7272	14.5374
71	H	3.7387	31.0431	13.6769
72	H	3.9182	31.1822	15.4425
73	H	4.2731	29.6371	14.6274
74	C	9.0920	33.0507	12.1492
75	H	9.7200	32.4874	12.8539
76	H	9.2972	34.1218	12.2881
77	H	9.3831	32.7680	11.1315
78	C	6.7617	33.5448	11.3399
79	H	7.0135	33.1873	10.3330
80	H	6.9887	34.6193	11.3954
81	H	5.6804	33.4128	11.4857
82	O	9.4556	28.0071	10.8310
83	N	10.5182	27.4187	10.4045
84	O	11.3915	27.0200	11.1881
85	O	10.8394	27.1707	9.4794
86	O	7.2033	27.8494	6.8396
87	N	6.1550	28.4527	7.2821
88	O	6.2155	28.9160	8.4768
89	O	5.1370	28.5751	6.5875
90	O	8.7870	30.5583	7.8183
91	O	10.5713	30.0730	9.0004
92	N	9.9393	30.9248	8.2662
93	O	10.4145	32.0355	8.0058

Optimized Coordinates of Eu-1

1	Eu	8.3070	28.1040	8.6970
2	N	7.3600	29.3660	10.6380
3	N	7.7780	30.6100	10.8890
4	C	7.4550	31.1890	12.0390
5	C	6.6210	30.5170	12.9740
6	N	6.1930	29.2860	12.7010
7	C	6.5960	28.7480	11.5430
8	N	6.8890	26.7620	10.2540
9	C	6.2440	27.3370	11.2730
10	C	5.3590	26.6310	12.0920
11	H	4.8810	27.0720	12.7560
12	C	5.2020	25.2790	11.9050
13	H	4.6040	24.8000	12.4340
14	C	5.9450	24.6210	10.9120
15	C	5.9440	23.2050	10.7230
16	H	5.4010	22.6730	11.2590
17	C	6.7230	22.6250	9.7760
18	H	6.7300	21.6990	9.6950
19	C	7.5360	23.4130	8.8970
20	C	8.3560	22.8700	7.8960
21	H	8.4010	21.9470	7.7780
22	C	9.0890	23.7000	7.0950
23	H	9.6290	23.3500	6.4250
24	C	9.0220	25.0910	7.2960
25	C	9.8410	26.0270	6.4910
26	N	10.7760	25.5070	5.6880
27	C	11.5500	26.3820	5.0420
28	C	11.2610	27.7600	5.1230
29	N	10.3290	28.2100	5.9640
30	N	9.6300	27.3310	6.6890
31	N	8.2650	25.6330	8.2450
32	C	7.5330	24.8140	9.0350
33	C	6.7530	25.4290	10.0830
34	C	11.9930	28.8250	4.3200
35	C	12.9450	28.1440	3.3310
36	H	12.4390	27.8880	2.5440
37	H	13.6120	28.7900	3.0520
38	C	13.6330	26.9640	3.8410
39	H	14.1700	27.2270	4.6050
40	H	14.2390	26.6400	3.1550
41	C	12.7230	25.8100	4.2650
42	C	6.2050	31.1150	14.3090
43	C	6.4490	32.6140	14.2790
44	H	5.7550	33.0350	13.7470
45	H	6.3790	32.9610	15.1820
46	C	7.7980	32.9910	13.7130
47	H	8.4890	32.5710	14.2480
48	H	7.9090	33.9510	13.7870

49	C	7.9960	32.5860	12.2470
50	C	12.7440	29.7570	5.2780
51	H	12.1290	30.1180	5.9200
52	H	13.1450	30.4730	4.7790
53	H	13.4290	29.2610	5.7330
54	C	10.9610	29.6350	3.5310
55	H	10.4180	29.0390	3.0070
56	H	11.4130	30.2510	2.9490
57	H	10.4030	30.1220	4.1410
58	C	12.2210	24.9850	3.1060
59	H	11.6690	24.2750	3.4360
60	H	12.9680	24.6160	2.6300
61	H	11.7080	25.5410	2.5160
62	C	13.5170	24.8860	5.1990
63	H	13.8000	25.3800	5.9720
64	H	14.2870	24.5490	4.7360
65	H	12.9600	24.1520	5.4720
66	C	7.0120	30.4040	15.3930
67	H	6.7940	29.4710	15.3930
68	H	6.8020	30.7820	16.2500
69	H	7.9500	30.5120	15.2160
70	C	4.7140	30.8480	14.5580
71	H	4.1960	31.2530	13.8590
72	H	4.4590	31.2240	15.4040
73	H	4.5550	29.9020	14.5660
74	C	9.4750	32.6230	11.8950
75	H	9.9490	31.9880	12.4390
76	H	9.8200	33.5030	12.0590
77	H	9.5900	32.4010	10.9690
78	C	7.2090	33.5240	11.3230
79	H	7.3160	33.2420	10.4120
80	H	7.5380	34.4180	11.4200
81	H	6.2780	33.4960	11.5570
82	O	9.3293	27.7407	10.8052
83	N	10.3853	27.2357	10.3332
84	O	11.3133	26.8907	11.0472
85	O	10.7464	26.9633	9.2241
86	O	6.8910	27.7850	6.7470
87	N	5.8220	28.3090	7.1950
88	O	5.8650	28.6960	8.4030
89	O	4.8180	28.4140	6.5010
90	O	8.1920	30.2650	7.7030
91	O	9.9920	29.7800	8.7780
92	N	9.3300	30.6470	8.1110
93	O	9.7590	31.7550	7.8980

Optimized Coordinates of Am-2

1	Am	8.8438	28.2202	8.9998
2	N	7.6586	29.3984	11.0414
3	N	7.9485	30.6684	11.2907
4	C	7.3508	31.3023	12.3108
5	C	6.3667	30.6293	13.0822
6	N	6.1036	29.3424	12.8347
7	C	6.7706	28.7617	11.8282
8	N	7.2086	26.7553	10.5436
9	C	6.5276	27.3213	11.5519
10	C	5.6219	26.5985	12.3599
11	H	5.0915	27.1248	13.1509
12	C	5.4466	25.2524	12.1269
13	H	4.7593	24.6642	12.7378
14	C	6.1754	24.6186	11.0944
15	C	6.0876	23.2162	10.8532
16	H	5.4471	22.6211	11.5070
17	C	6.8205	22.5899	9.8725
18	H	8.8618	20.7623	9.8982
19	C	7.6681	23.3951	9.0166
20	C	8.3585	22.8565	7.9069
21	O	10.5904	31.9713	8.1118
22	C	9.1445	23.6688	7.1185
23	H	9.6838	23.2877	6.2540
24	C	9.2480	25.0385	7.4360
25	C	10.0891	25.9262	6.5893
26	N	10.7735	25.3765	5.5772
27	C	11.5019	26.1957	4.8127
28	C	11.4779	27.5925	5.0675
29	N	10.8035	28.0671	6.1258
30	N	10.1147	27.2361	6.8985
31	N	8.5874	25.5905	8.4633
32	C	7.7988	24.8022	9.2371
33	C	7.0496	25.4289	10.3135
34	C	12.2152	28.6296	4.2296
35	C	12.6942	27.9792	2.9117
36	H	11.8410	27.9048	2.2183
37	H	13.4192	28.6541	2.4326
38	C	13.3140	26.5976	3.1196
39	H	14.1718	26.6765	3.8065
40	H	13.7161	26.2096	2.1710
41	C	12.3122	25.5653	3.6857
42	C	5.5953	31.2963	14.2157
43	C	5.7864	32.8289	14.1498
44	H	5.1407	33.2349	13.3546
45	H	5.4236	33.2663	15.0924
46	C	7.2363	33.2398	13.8947
47	H	7.8823	32.8438	14.6949
48	H	7.3354	34.3348	13.9360

49	C	7.7709	32.7506	12.5296
50	C	13.4154	29.1491	5.0601
51	H	13.0650	29.5818	6.0057
52	H	13.9436	29.9287	4.4924
53	H	14.1314	28.3500	5.2973
54	C	11.2766	29.8131	3.9121
55	H	10.3925	29.4791	3.3506
56	H	11.8146	30.5487	3.2971
57	H	10.9340	30.3066	4.8286
58	C	11.3198	25.1005	2.5911
59	H	10.5935	24.3920	3.0105
60	H	11.8727	24.5987	1.7840
61	H	10.7610	25.9400	2.1560
62	C	13.0814	24.3381	4.2176
63	H	13.7672	24.6202	5.0290
64	H	13.6769	23.8999	3.4041
65	H	12.3947	23.5732	4.5996
66	C	6.1388	30.7296	15.5512
67	H	6.0368	29.6366	15.5727
68	H	5.5651	31.1509	16.3892
69	H	7.1989	30.9736	15.7024
70	C	4.0951	30.9577	14.1005
71	H	3.6823	31.3036	13.1424
72	H	3.5445	31.4580	14.9100
73	H	3.9246	29.8773	14.1776
74	C	9.3103	32.8621	12.5069
75	H	9.7647	32.2448	13.2949
76	H	9.6009	33.9080	12.6809
77	H	9.7196	32.5407	11.5426
78	C	7.1894	33.5983	11.3706
79	H	7.5550	33.2245	10.4056
80	H	7.5100	34.6437	11.4847
81	H	6.0910	33.5742	11.3495
82	O	9.5023	27.9022	10.9328
83	N	10.5582	27.3300	10.4740
84	O	11.4369	26.8909	11.2289
85	O	10.8914	27.1134	9.5426
86	O	7.2282	27.8266	6.9228
87	N	6.2192	28.4918	7.3638
88	O	6.3321	29.0051	8.5347
89	O	5.1874	28.6243	6.6915
90	O	8.9716	30.5012	7.8257
91	O	10.6361	30.0428	9.1801
92	N	10.0819	30.8729	8.3642
93	C	6.7333	21.1160	9.7104
94	C	5.4845	20.4834	9.5622
95	C	5.3811	19.0998	9.4501
96	C	6.5374	18.3099	9.4938
97	C	7.7897	18.9180	9.6514
98	C	7.8818	20.3053	9.7525

99	H	4.5798	21.0911	9.5133
100	H	4.4120	18.6168	9.3211
101	O	6.3808	16.9501	9.3779
102	H	8.6942	18.3068	9.7036
103	H	7.2596	16.5293	9.4307
104	H	8.2511	21.7984	7.6718

Optimized Coordinates of Eu-2

1	Eu	8.7878	28.2204	8.9796
2	N	7.5937	29.4155	11.0006
3	N	7.8900	30.6852	11.2438
4	C	7.3346	31.3120	12.2915
5	C	6.3727	30.6374	13.0891
6	N	6.1126	29.3474	12.8541
7	C	6.7492	28.7695	11.8268
8	N	7.1838	26.7563	10.5504
9	C	6.5278	27.3201	11.5758
10	C	5.6705	26.5896	12.4280
11	H	5.1607	27.1146	13.2332
12	C	5.5168	25.2371	12.2172
13	H	4.8681	24.6409	12.8617
14	C	6.2140	24.6082	11.1614
15	C	6.1320	23.2032	10.9198
16	H	5.5195	22.5940	11.5871
17	C	6.8186	22.6246	9.8904
18	H	8.8725	20.8339	9.6453
19	C	7.6353	23.4033	9.0079
20	C	8.3662	22.8258	7.9234
21	O	10.4758	31.9945	8.0794
22	C	9.1866	23.6644	7.1807
23	H	9.7570	23.2848	6.3355
24	C	9.2574	25.0373	7.4738
25	C	10.0948	25.9215	6.6181
26	N	10.7995	25.3661	5.6228
27	C	11.5172	26.1849	4.8481
28	C	11.4688	27.5854	5.0791
29	N	10.7733	28.0671	6.1199
30	N	10.0909	27.2374	6.9002
31	N	8.5694	25.6027	8.4769
32	C	7.7744	24.8085	9.2365
33	C	7.0422	25.4239	10.3354
34	C	12.2007	28.6199	4.2329
35	C	12.6950	27.9589	2.9263
36	H	11.8467	27.8663	2.2289
37	H	13.4150	28.6361	2.4429
38	C	13.3294	26.5871	3.1540
39	H	14.1846	26.6842	3.8419
40	H	13.7381	26.1916	2.2113
41	C	12.3379	25.5506	3.7305
42	C	5.6167	31.3081	14.2309
43	C	5.8178	32.8396	14.1641
44	H	5.1645	33.2517	13.3784
45	H	5.4713	33.2784	15.1121
46	C	7.2673	33.2389	13.8891
47	H	7.9219	32.8305	14.6759
48	H	7.3780	34.3326	13.9366

49	C	7.7748	32.7538	12.5121
50	C	13.3897	29.1605	5.0661
51	H	13.0281	29.5999	6.0045
52	H	13.9144	29.9391	4.4937
53	H	14.1119	28.3712	5.3173
54	C	11.2542	29.7909	3.8940
55	H	10.3758	29.4421	3.3325
56	H	11.7897	30.5224	3.2720
57	H	10.9029	30.2943	4.8017
58	C	11.3527	25.0627	2.6395
59	H	10.6316	24.3530	3.0657
60	H	11.9124	24.5557	1.8403
61	H	10.7876	25.8915	2.1919
62	C	13.1196	24.3381	4.2775
63	H	13.7989	24.6368	5.0884
64	H	13.7229	23.8987	3.4705
65	H	12.4400	23.5695	4.6645
66	C	6.1640	30.7381	15.5627
67	H	6.0574	29.6456	15.5843
68	H	5.5967	31.1617	16.4037
69	H	7.2259	30.9775	15.7083
70	C	4.1133	30.9791	14.1239
71	H	3.6970	31.3292	13.1688
72	H	3.5701	31.4814	14.9371
73	H	3.9368	29.8994	14.2004
74	C	9.3159	32.8429	12.4672
75	H	9.7737	32.2103	13.2410
76	H	9.6244	33.8826	12.6480
77	H	9.7050	32.5272	11.4926
78	C	7.1900	33.6183	11.3679
79	H	7.5346	33.2450	10.3952
80	H	7.5294	34.6575	11.4842
81	H	6.0910	33.6125	11.3636
82	O	9.9367	27.7354	11.3100
83	N	10.9986	27.1436	10.8854
84	O	11.8668	26.7365	11.6702
85	O	11.1086	26.9924	9.6169
86	O	7.2338	27.8457	6.8870
87	N	6.1740	28.4407	7.3137
88	O	6.2128	28.9065	8.5069
89	O	5.1662	28.5499	6.6014
90	O	8.8314	30.5384	7.8776
91	O	10.6049	30.0257	9.0645
92	N	9.9859	30.8878	8.3323
93	C	6.7437	21.1021	9.6715
94	C	5.4982	20.4692	9.5734
95	C	5.4301	19.0847	9.3743
96	C	6.6073	18.3330	9.2733
97	C	7.8528	18.9658	9.3713
98	C	7.9210	20.3504	9.5704

99	H	4.5987	21.0436	9.6507
100	H	4.4785	18.6012	9.2994
101	O	6.5392	16.9489	9.0743
102	H	8.7523	18.3915	9.2941
103	H	6.5236	16.5037	9.9246
104	H	8.2832	21.7745	7.6900

Optimized Coordinates of Am-3

1	Am	8.8604	28.2059	9.0316
2	N	7.6939	29.3962	11.0727
3	N	7.9498	30.6794	11.2898
4	C	7.3407	31.3208	12.2984
5	C	6.3818	30.6391	13.0930
6	N	6.1576	29.3386	12.8816
7	C	6.8332	28.7529	11.8839
8	N	7.2732	26.7323	10.6165
9	C	6.6248	27.3002	11.6438
10	C	5.7858	26.5653	12.5058
11	H	5.2983	27.0812	13.3307
12	C	5.6140	25.2164	12.2844
13	H	4.9795	24.6260	12.9439
14	C	6.2755	24.5821	11.2060
15	C	6.1465	23.1627	10.9532
16	H	6.7824	21.2162	12.7677
17	C	6.8889	22.5705	9.9450
18	H	8.8156	20.6736	10.3260
19	C	7.7426	23.3813	9.1042
20	C	8.4496	22.8365	8.0061
21	O	10.5412	31.9646	8.0385
22	C	9.2229	23.6504	7.2082
23	H	9.7726	23.2655	6.3520
24	C	9.2992	25.0270	7.5025
25	C	10.1146	25.9166	6.6340
26	N	10.7930	25.3638	5.6189
27	C	11.5025	26.1825	4.8369
28	C	11.4686	27.5815	5.0785
29	N	10.7952	28.0611	6.1348
30	N	10.1230	27.2312	6.9236
31	N	8.6401	25.5794	8.5311
32	C	7.8646	24.7873	9.3145
33	C	7.1228	25.4007	10.4009
34	C	12.1932	28.6163	4.2264
35	C	12.6612	27.9594	2.9078
36	H	11.8008	27.8761	2.2242
37	H	13.3774	28.6347	2.4163
38	C	13.2906	26.5824	3.1174
39	H	14.1569	26.6703	3.7925
40	H	13.6822	26.1898	2.1663
41	C	12.3019	25.5488	3.7036
42	C	5.5925	31.3131	14.2098
43	C	5.7418	32.8483	14.1049
44	H	5.0845	33.2158	13.3006
45	H	5.3682	33.2994	15.0368
46	C	7.1793	33.2920	13.8358
47	H	7.8380	32.9335	14.6434
48	H	7.2484	34.3901	13.8502

49	C	7.7228	32.7846	12.4808
50	C	13.3998	29.1445	5.0418
51	H	13.0570	29.5820	5.9881
52	H	13.9201	29.9224	4.4645
53	H	14.1206	28.3491	5.2771
54	C	11.2480	29.7949	3.9106
55	H	10.3591	29.4544	3.3606
56	H	11.7776	30.5276	3.2850
57	H	10.9133	30.2938	4.8270
58	C	11.2976	25.0715	2.6256
59	H	10.5799	24.3628	3.0595
60	H	11.8422	24.5660	1.8151
61	H	10.7294	25.9052	2.1915
62	C	13.0847	24.3292	4.2332
63	H	13.7789	24.6202	5.0342
64	H	13.6724	23.8894	3.4149
65	H	12.4072	23.5630	4.6286
66	C	6.1484	30.7949	15.5596
67	H	6.0696	29.7011	15.6110
68	H	5.5663	31.2267	16.3864
69	H	7.2031	31.0652	15.7030
70	C	4.1019	30.9324	14.1011
71	H	3.6818	31.2454	13.1348
72	H	3.5369	31.4364	14.8982
73	H	3.9598	29.8497	14.2024
74	C	9.2589	32.9343	12.4503
75	H	9.7311	32.3446	13.2490
76	H	9.5238	33.9905	12.6020
77	H	9.6729	32.6035	11.4911
78	C	7.1162	33.5892	11.3041
79	H	7.4868	33.2008	10.3468
80	H	7.4110	34.6448	11.3913
81	H	6.0187	33.5373	11.2888
82	O	10.0335	27.6644	11.3507
83	N	11.0966	27.1085	10.8872
84	O	11.9836	26.6815	11.6397
85	O	11.1903	27.0122	9.6104
86	O	7.2078	27.7731	7.0042
87	N	6.2046	28.4486	7.4435
88	O	6.3301	28.9817	8.6041
89	O	5.1668	28.5725	6.7785
90	O	8.9467	30.4606	7.7985
91	O	10.6194	30.0697	9.1634
92	N	10.0512	30.8654	8.3235
93	C	6.7994	21.1050	9.6710
94	C	5.6265	20.5367	9.1451
95	C	5.5429	19.1743	8.8716
96	C	6.6411	18.3442	9.1293
97	C	7.8188	18.8900	9.6547
98	C	7.8928	20.2590	9.9159

99	H	4.7668	21.1756	8.9406
100	H	4.6333	18.7375	8.4586
101	O	6.5040	17.0058	8.8432
102	H	8.6776	18.2462	9.8613
103	H	7.3371	16.5533	9.0748
104	H	8.3658	21.7722	7.7919
105	C	5.2209	22.3601	11.8062
106	C	3.8325	22.5609	11.7406
107	C	2.9563	21.8047	12.5200
108	C	3.4618	20.8346	13.3940
109	C	4.8446	20.6298	13.4833
110	C	5.7076	21.3845	12.6934
111	H	3.4261	23.3094	11.0581
112	H	1.8780	21.9670	12.4446
113	O	2.6526	20.0541	14.1866
114	H	5.2267	19.8762	14.1723
115	H	1.7235	20.2993	14.0151

Optimized Coordinates of Eu-3

1	Eu	8.8611	28.2107	9.0280
2	N	7.6862	29.4015	11.0647
3	N	7.9470	30.6829	11.2883
4	C	7.3434	31.3209	12.3020
5	C	6.3858	30.6376	13.0971
6	N	6.1590	29.3385	12.8810
7	C	6.8278	28.7560	11.8765
8	N	7.2729	26.7334	10.6134
9	C	6.6178	27.3038	11.6350
10	C	5.7721	26.5710	12.4924
11	H	5.2792	27.0886	13.3128
12	C	5.6020	25.2216	12.2730
13	H	4.9632	24.6327	12.9296
14	C	6.2713	24.5844	11.2010
15	C	6.1447	23.1647	10.9517
16	H	6.7563	21.2098	12.7693
17	C	6.8961	22.5692	9.9517
18	H	8.8169	20.6722	10.3627
19	C	7.7547	23.3783	9.1142
20	C	8.4723	22.8302	8.0245
21	O	10.5325	31.9754	8.0501
22	C	9.2466	23.6429	7.2264
23	H	9.8037	23.2554	6.3762
24	C	9.3126	25.0219	7.5116
25	C	10.1238	25.9116	6.6392
26	N	10.8055	25.3587	5.6266
27	C	11.5056	26.1792	4.8377
28	C	11.4607	27.5790	5.0718
29	N	10.7894	28.0584	6.1297
30	N	10.1254	27.2273	6.9241
31	N	8.6455	25.5771	8.5334
32	C	7.8710	24.7858	9.3182
33	C	7.1232	25.4016	10.3990
34	C	12.1735	28.6154	4.2117
35	C	12.6444	27.9553	2.8958
36	H	11.7834	27.8609	2.2145
37	H	13.3537	28.6341	2.3991
38	C	13.2861	26.5850	3.1116
39	H	14.1531	26.6839	3.7843
40	H	13.6788	26.1905	2.1618
41	C	12.3076	25.5461	3.7060
42	C	5.6024	31.3082	14.2200
43	C	5.7540	32.8435	14.1206
44	H	5.0949	33.2153	13.3198
45	H	5.3840	33.2917	15.0554
46	C	7.1915	33.2858	13.8487
47	H	7.8520	32.9227	14.6528
48	H	7.2627	34.3837	13.8674

49	C	7.7298	32.7829	12.4899
50	C	13.3771	29.1599	5.0209
51	H	13.0329	29.5987	5.9661
52	H	13.8880	29.9399	4.4382
53	H	14.1065	28.3729	5.2580
54	C	11.2164	29.7833	3.8916
55	H	10.3295	29.4315	3.3456
56	H	11.7376	30.5176	3.2609
57	H	10.8791	30.2839	4.8062
58	C	11.3050	25.0543	2.6327
59	H	10.5940	24.3424	3.0722
60	H	11.8522	24.5483	1.8243
61	H	10.7294	25.8808	2.1947
62	C	13.1022	24.3363	4.2404
63	H	13.7950	24.6376	5.0388
64	H	13.6925	23.8976	3.4234
65	H	12.4322	23.5661	4.6407
66	C	6.1630	30.7834	15.5653
67	H	6.0816	29.6895	15.6127
68	H	5.5859	31.2135	16.3965
69	H	7.2192	31.0502	15.7050
70	C	4.1107	30.9305	14.1160
71	H	3.6869	31.2491	13.1531
72	H	3.5500	31.4314	14.9181
73	H	3.9673	29.8476	14.2125
74	C	9.2661	32.9291	12.4553
75	H	9.7395	32.3347	13.2498
76	H	9.5339	33.9840	12.6110
77	H	9.6764	32.6018	11.4934
78	C	7.1215	33.5940	11.3186
79	H	7.4879	33.2087	10.3585
80	H	7.4195	34.6485	11.4092
81	H	6.0238	33.5454	11.3067
82	O	10.0349	27.6902	11.3566
83	N	11.0970	27.1323	10.8937
84	O	11.9889	26.7150	11.6458
85	O	11.1846	27.0232	9.6172
86	O	7.2200	27.7643	6.9871
87	N	6.2089	28.4259	7.4285
88	O	6.3282	28.9580	8.5902
89	O	5.1696	28.5397	6.7638
90	O	8.9380	30.4714	7.8086
91	O	10.6205	30.0714	9.1590
92	N	10.0451	30.8740	8.3305
93	C	6.8096	21.1032	9.6797
94	C	5.6445	20.5343	9.1377
95	C	5.5647	19.1715	8.8643
96	C	6.6591	18.3416	9.1380
97	C	7.8292	18.8880	9.6794
98	C	7.8997	20.2573	9.9403

99	H	4.7874	21.1725	8.9203
100	H	4.6603	18.7357	8.4390
101	O	6.5265	17.0030	8.8505
102	H	8.6857	18.2452	9.8987
103	H	7.3567	16.5512	9.0935
104	H	8.3952	21.7642	7.8161
105	C	5.2094	22.3650	11.7972
106	C	3.8226	22.5746	11.7223
107	C	2.9360	21.8228	12.4940
108	C	3.4292	20.8479	13.3699
109	C	4.8097	20.6343	13.4684
110	C	5.6834	21.3850	12.6862
111	H	3.4258	23.3273	11.0388
112	H	1.8596	21.9932	12.4113
113	O	2.6096	20.0722	14.1565
114	H	5.1832	19.8774	14.1586
115	H	1.6832	20.3221	13.9780

Optimized Coordinates of Am-4

1	Am	9.4574	3.7660	3.8725
2	O	11.3491	4.0526	2.1631
3	O	9.5859	2.9588	1.4513
4	O	11.2923	3.2916	0.0944
5	O	6.9095	3.5081	3.0310
6	O	7.7976	1.7120	3.9129
7	O	5.7322	1.6493	3.1492
8	O	10.5631	5.7204	4.6909
9	O	11.6392	3.8768	5.1769
10	O	12.4667	5.8226	5.7960
11	N	7.8019	5.1690	5.4628
12	N	9.0785	2.9045	6.3851
13	N	8.3891	5.9984	2.9366
14	N	8.7291	6.3588	1.6896
15	N	6.9260	7.8789	3.2042
16	N	10.6511	1.5390	4.6280
17	N	11.4403	0.9378	3.7254
18	N	11.2880	0.0199	6.3699
19	N	10.7597	3.4301	1.2008
20	N	6.7821	2.2738	3.3547
21	N	11.5853	5.1569	5.2360
22	C	7.2016	6.2843	5.0220
23	C	6.2977	7.0271	5.8140
24	H	5.8431	7.9209	5.3916
25	C	6.0218	6.5967	7.0940
26	H	5.3243	7.1461	7.7289
27	C	6.6503	5.4352	7.5947
28	C	6.4131	4.9460	8.9186
29	H	5.7156	5.4905	9.5575
30	C	7.0440	3.8240	9.3748
31	H	6.8609	3.4549	10.3853
32	C	7.9602	3.1063	8.5418
33	C	8.6335	1.9460	8.9840
34	H	8.4594	1.5767	9.9961
35	C	9.4980	1.2904	8.1340
36	H	10.0350	0.3922	8.4315
37	C	9.6930	1.7987	6.8304
38	C	7.5496	4.7473	6.7262
39	C	8.2220	3.5534	7.2125
40	C	7.5194	6.7439	3.6431
41	C	7.2715	8.2338	1.9746
42	C	6.7651	9.4374	1.2084
43	C	7.7127	9.4419	-0.0405
44	H	8.4834	10.2133	0.1003
45	H	7.1634	9.6966	-0.9571
46	C	8.4134	8.0429	-0.1649
47	C	8.1790	7.4698	1.2142
48	C	6.8862	10.7283	2.0368

49	H	6.2599	10.6743	2.9375
50	H	6.5584	11.5902	1.4385
51	H	7.9246	10.9043	2.3500
52	C	5.2861	9.2033	0.8212
53	H	5.1600	8.2905	0.2237
54	H	4.9208	10.0536	0.2283
55	H	4.6621	9.1117	1.7208
56	C	9.9141	8.1674	-0.4818
57	H	10.0522	8.6286	-1.4702
58	H	10.3929	7.1794	-0.4899
59	H	10.4295	8.7894	0.2631
60	C	7.7363	7.1357	-1.2183
61	H	6.6602	7.0195	-1.0300
62	H	8.1924	6.1367	-1.2107
63	H	7.8653	7.5712	-2.2194
64	C	10.5981	1.0826	5.8928
65	C	12.0669	-0.5691	5.4740
66	C	12.9689	-1.7613	5.7113
67	C	13.4128	-2.1207	4.2503
68	H	14.4742	-2.4012	4.2134
69	H	12.8348	-2.9909	3.9072
70	C	13.1110	-0.9066	3.3030
71	C	12.1456	-0.1052	4.1456
72	C	14.1585	-1.3271	6.5982
73	H	14.7327	-0.5104	6.1406
74	H	14.8367	-2.1788	6.7506
75	H	13.8019	-0.9850	7.5797
76	C	12.2094	-2.9135	6.3917
77	H	11.8576	-2.6137	7.3883
78	H	12.8708	-3.7842	6.5058
79	H	11.3374	-3.2213	5.7981
80	C	14.3684	-0.0520	3.0182
81	H	14.8592	0.2774	3.9440
82	H	14.0987	0.8420	2.4404
83	H	15.0920	-0.6405	2.4362
84	C	12.4756	-1.3465	1.9722
85	H	13.1848	-1.9662	1.4049
86	H	12.2104	-0.4738	1.3614
87	H	11.5624	-1.9348	2.1404

Optimized Coordinates of Eu-4

1	Eu	11.0796	3.3712	0.8328
2	O	12.9821	3.6983	-0.8573
3	O	11.2528	2.5615	-1.5848
4	O	12.9651	2.9312	-2.9245
5	O	8.5476	3.0513	-0.0348
6	O	9.4684	1.2788	0.8612
7	O	7.4132	1.1655	0.0759
8	O	12.2366	5.5539	1.7411
9	O	13.3507	3.7374	2.2434
10	O	14.1255	5.7037	2.8660
11	N	7.8019	5.1690	5.4628
12	N	9.0785	2.9045	6.3851
13	N	8.3891	5.9984	2.9366
14	N	8.7291	6.3588	1.6896
15	N	6.9260	7.8789	3.2042
16	N	10.6511	1.5390	4.6280
17	N	11.4403	0.9378	3.7254
18	N	11.2880	0.0199	6.3699
19	N	12.4178	3.0598	-1.8242
20	N	8.4459	1.8151	0.2909
21	N	13.2660	5.0160	2.2985
22	C	7.2016	6.2843	5.0220
23	C	6.2977	7.0271	5.8140
24	H	5.8431	7.9209	5.3916
25	C	6.0218	6.5967	7.0940
26	H	5.3243	7.1461	7.7289
27	C	6.6503	5.4352	7.5947
28	C	6.4131	4.9460	8.9186
29	H	5.7156	5.4905	9.5575
30	C	7.0440	3.8240	9.3748
31	H	6.8609	3.4549	10.3853
32	C	7.9602	3.1063	8.5418
33	C	8.6335	1.9460	8.9840
34	H	8.4594	1.5767	9.9961
35	C	9.4980	1.2904	8.1340
36	H	10.0350	0.3922	8.4315
37	C	9.6930	1.7987	6.8304
38	C	7.5496	4.7473	6.7262
39	C	8.2220	3.5534	7.2125
40	C	7.5194	6.7439	3.6431
41	C	7.2715	8.2338	1.9746
42	C	6.7651	9.4374	1.2084
43	C	7.7127	9.4419	-0.0405
44	H	8.4834	10.2133	0.1003
45	H	7.1634	9.6966	-0.9571
46	C	8.4134	8.0429	-0.1649
47	C	8.1790	7.4698	1.2142
48	C	6.8862	10.7283	2.0368

49	H	6.2599	10.6743	2.9375
50	H	6.5584	11.5902	1.4385
51	H	7.9246	10.9043	2.3500
52	C	5.2861	9.2033	0.8212
53	H	5.1600	8.2905	0.2237
54	H	4.9208	10.0536	0.2283
55	H	4.6621	9.1117	1.7208
56	C	9.9141	8.1674	-0.4818
57	H	10.0522	8.6286	-1.4702
58	H	10.3929	7.1794	-0.4899
59	H	10.4295	8.7894	0.2631
60	C	7.7363	7.1357	-1.2183
61	H	6.6602	7.0195	-1.0300
62	H	8.1924	6.1367	-1.2107
63	H	7.8653	7.5712	-2.2194
64	C	10.5981	1.0826	5.8928
65	C	12.0669	-0.5691	5.4740
66	C	12.9689	-1.7613	5.7113
67	C	13.4128	-2.1207	4.2503
68	H	14.4742	-2.4012	4.2134
69	H	12.8348	-2.9909	3.9072
70	C	13.1110	-0.9066	3.3030
71	C	12.1456	-0.1052	4.1456
72	C	14.1585	-1.3271	6.5982
73	H	14.7327	-0.5104	6.1406
74	H	14.8367	-2.1788	6.7506
75	H	13.8019	-0.9850	7.5797
76	C	12.2094	-2.9135	6.3917
77	H	11.8576	-2.6137	7.3883
78	H	12.8708	-3.7842	6.5058
79	H	11.3374	-3.2213	5.7981
80	C	14.3684	-0.0520	3.0182
81	H	14.8592	0.2774	3.9440
82	H	14.0987	0.8420	2.4404
83	H	15.0920	-0.6405	2.4362
84	C	12.4756	-1.3465	1.9722
85	H	13.1848	-1.9662	1.4049
86	H	12.2104	-0.4738	1.3614
87	H	11.5624	-1.9348	2.1404

Optimized Coordinates of Am-5

1	Am	9.5677	3.5827	3.9334
2	O	11.4793	3.8815	2.2473
3	O	9.7260	2.7952	1.4997
4	O	11.4589	3.1243	0.1768
5	O	7.0295	3.3249	3.0515
6	O	7.9086	1.5319	3.9483
7	O	5.8478	1.4687	3.1714
8	O	10.7787	5.7262	4.8696
9	O	11.8450	3.8758	5.3512
10	O	12.5780	5.9861	5.9425
11	N	7.8083	5.1240	5.4645
12	N	9.0827	2.8617	6.3808
13	N	8.4105	5.9898	2.9508
14	N	8.7628	6.3718	1.7134
15	N	6.9011	7.8338	3.2153
16	N	10.6598	1.5185	4.6053
17	N	11.4518	0.9306	3.6961
18	N	11.2710	-0.0406	6.3200
19	N	10.9056	3.2627	1.2735
20	N	6.8975	2.0927	3.3807
21	N	11.7930	5.1552	5.4216
22	C	7.1889	6.2290	5.0217
23	C	6.2613	6.9492	5.8077
24	H	5.7909	7.8339	5.3836
25	C	5.9869	6.5122	7.0847
26	H	5.2759	7.0463	7.7176
27	C	6.6393	5.3637	7.5879
28	C	6.4298	4.8929	8.9169
29	H	5.7514	5.4549	9.5617
30	C	7.0857	3.7952	9.4223
31	H	8.9383	3.4507	11.4163
32	C	7.9902	3.0648	8.5570
33	C	8.6271	1.8683	8.9581
34	H	8.4336	1.4653	9.9511
35	C	9.4723	1.2085	8.0917
36	H	9.9739	0.2835	8.3682
37	C	9.6867	1.7422	6.8045
38	C	7.5556	4.6956	6.7253
39	C	8.2385	3.5118	7.2213
40	C	7.5143	6.7080	3.6522
41	C	7.2597	8.2109	1.9965
42	C	6.7385	9.4118	1.2360
43	C	7.7071	9.4534	0.0038
44	H	8.4580	10.2394	0.1685
45	H	7.1682	9.7078	-0.9190
46	C	8.4404	8.0717	-0.1257
47	C	8.1973	7.4770	1.2428
48	C	6.8168	10.6947	2.0823

49	H	6.1746	10.6162	2.9700
50	H	6.4820	11.5570	1.4885
51	H	7.8449	10.8883	2.4178
52	C	5.2719	9.1506	0.8213
53	H	5.1759	8.2451	0.2075
54	H	4.8963	10.0019	0.2362
55	H	4.6359	9.0304	1.7092
56	C	9.9431	8.2331	-0.4178
57	H	10.0855	8.7106	-1.3979
58	H	10.4427	7.2557	-0.4321
59	H	10.4332	8.8557	0.3433
60	C	7.8002	7.1625	-1.2002
61	H	6.7232	7.0241	-1.0331
62	H	8.2748	6.1722	-1.1938
63	H	7.9390	7.6099	-2.1947
64	C	10.5920	1.0361	5.8592
65	C	12.0528	-0.6167	5.4181
66	C	12.9476	-1.8173	5.6394
67	C	13.4030	-2.1499	4.1756
68	H	14.4639	-2.4325	4.1424
69	H	12.8252	-3.0112	3.8108
70	C	13.1133	-0.9164	3.2494
71	C	12.1451	-0.1268	4.1000
72	C	14.1312	-1.4049	6.5449
73	H	14.7119	-0.5812	6.1087
74	H	14.8053	-2.2618	6.6859
75	H	13.7671	-1.0815	7.5299
76	C	12.1787	-2.9802	6.2906
77	H	11.8202	-2.6991	7.2902
78	H	12.8365	-3.8551	6.3927
79	H	11.3106	-3.2733	5.6841
80	C	14.3764	-0.0626	2.9900
81	H	14.8606	0.2492	3.9253
82	H	14.1156	0.8422	2.4250
83	H	15.1029	-0.6440	2.4043
84	C	12.4861	-1.3282	1.9056
85	H	13.1984	-1.9374	1.3308
86	H	12.2272	-0.4427	1.3108
87	H	11.5709	-1.9181	2.0557
88	C	6.8539	3.3854	10.8306
89	C	5.5478	3.1693	11.3018
90	C	5.3071	2.8295	12.6328
91	C	6.3786	2.7078	13.5263
92	C	7.6882	2.9278	13.0789
93	C	7.9167	3.2578	11.7464
94	H	4.7080	3.2491	10.6100
95	H	4.2846	2.6518	12.9748
96	O	6.2110	2.3736	14.8487
97	H	8.5126	2.8455	13.7873
98	H	5.2574	2.2555	15.0202

Optimized Coordinates of Eu-5

1	Eu	9.4755	3.7547	3.8770
2	O	11.3861	4.0538	2.1901
3	O	9.6326	2.9672	1.4435
4	O	11.3642	3.2974	0.1192
5	O	6.9368	3.4970	2.9969
6	O	7.8166	1.7036	3.8925
7	O	5.7557	1.6404	3.1161
8	O	10.6867	5.8986	4.8121
9	O	11.7536	4.0484	5.2935
10	O	12.5777	5.9865	5.9405
11	N	7.8077	5.1242	5.4643
12	N	9.0826	2.8620	6.3809
13	N	8.4095	5.9892	2.9503
14	N	8.7617	6.3709	1.7127
15	N	6.9010	7.8338	3.2149
16	N	10.6593	1.5183	4.6060
17	N	11.4507	0.9302	3.6966
18	N	11.2724	-0.0394	6.3213
19	N	10.8118	3.4352	1.2165
20	N	6.8053	2.2645	3.3255
21	N	11.7015	5.3278	5.3637
22	C	7.1890	6.2296	5.0218
23	C	6.2621	6.9504	5.8080
24	H	5.7918	7.8352	5.3839
25	C	5.9874	6.5132	7.0849
26	H	5.2765	7.0473	7.7178
27	C	6.6396	5.3645	7.5881
28	C	6.4300	4.8938	8.9170
29	H	5.7523	5.4563	9.5620
30	C	7.0857	3.7960	9.4223
31	H	8.9386	3.4397	11.4136
32	C	7.9908	3.0659	8.5573
33	C	8.6280	1.8699	8.9590
34	H	8.4339	1.4667	9.9518
35	C	9.4745	1.2107	8.0933
36	H	9.9768	0.2862	8.3701
37	C	9.6879	1.7435	6.8055
38	C	7.5555	4.6960	6.7252
39	C	8.2386	3.5124	7.2214
40	C	7.5140	6.7080	3.6520
41	C	7.2597	8.2108	1.9961
42	C	6.7390	9.4120	1.2358
43	C	7.7075	9.4533	0.0035
44	H	8.4588	10.2391	0.1683
45	H	7.1687	9.7080	-0.9192
46	C	8.4403	8.0714	-0.1260
47	C	8.1970	7.4766	1.2423
48	C	6.8176	10.6948	2.0822

49	H	6.1754	10.6163	2.9700
50	H	6.4829	11.5573	1.4886
51	H	7.8458	10.8882	2.4177
52	C	5.2723	9.1513	0.8210
53	H	5.1761	8.2457	0.2073
54	H	4.8970	10.0027	0.2358
55	H	4.6362	9.0315	1.7088
56	C	9.9432	8.2323	-0.4179
57	H	10.0858	8.7098	-1.3979
58	H	10.4424	7.2547	-0.4322
59	H	10.4334	8.8547	0.3433
60	C	7.8000	7.1626	-1.2007
61	H	6.7230	7.0244	-1.0337
62	H	8.2744	6.1722	-1.1946
63	H	7.9389	7.6103	-2.1951
64	C	10.5929	1.0369	5.8604
65	C	12.0535	-0.6159	5.4191
66	C	12.9489	-1.8161	5.6405
67	C	13.4032	-2.1495	4.1766
68	H	14.4641	-2.4320	4.1428
69	H	12.8252	-3.0111	3.8126
70	C	13.1127	-0.9166	3.2500
71	C	12.1447	-0.1269	4.1006
72	C	14.1330	-1.4030	6.5449
73	H	14.7132	-0.5795	6.1079
74	H	14.8073	-2.2597	6.6861
75	H	13.7695	-1.0791	7.5300
76	C	12.1806	-2.9788	6.2930
77	H	11.8228	-2.6973	7.2927
78	H	12.8387	-3.8535	6.3950
79	H	11.3121	-3.2724	5.6872
80	C	14.3755	-0.0625	2.9896
81	H	14.8599	0.2497	3.9247
82	H	14.1141	0.8420	2.4244
83	H	15.1018	-0.6439	2.4039
84	C	12.4851	-1.3291	1.9065
85	H	13.1973	-1.9384	1.3318
86	H	12.2259	-0.4439	1.3114
87	H	11.5701	-1.9191	2.0572
88	C	6.8533	3.3858	10.8301
89	C	5.5467	3.1755	11.3024
90	C	5.3058	2.8333	12.6327
91	C	6.3779	2.7020	13.5241
92	C	7.6880	2.9170	13.0758
93	C	7.9164	3.2510	11.7445
94	H	4.7064	3.2601	10.6116
95	H	4.2827	2.6607	12.9756
96	O	6.2101	2.3675	14.8463
97	H	8.5129	2.8284	13.7830
98	H	5.2562	2.2529	15.0183

Optimized Coordinates of Am-6

1	Am	9.5762	3.5894	3.9540
2	O	11.4737	3.8705	2.2483
3	O	9.7061	2.7945	1.5196
4	O	11.4292	3.1082	0.1802
5	O	7.0273	3.3468	3.0958
6	O	7.9018	1.5508	3.9913
7	O	5.8323	1.5005	3.2366
8	O	10.8122	5.7268	4.8724
9	O	11.8709	3.8703	5.3473
10	O	12.6230	5.9759	5.9290
11	N	7.8425	5.1425	5.5069
12	N	9.1113	2.8771	6.4043
13	N	8.4279	5.9991	2.9765
14	N	8.7621	6.3734	1.7314
15	N	6.9389	7.8562	3.2594
16	N	10.6634	1.5196	4.6163
17	N	11.4384	0.9216	3.6991
18	N	11.2865	-0.0364	6.3297
19	N	10.8867	3.2532	1.2818
20	N	6.8897	2.1170	3.4316
21	N	11.8275	5.1499	5.4163
22	C	7.2460	6.2609	5.0691
23	C	6.3653	7.0116	5.8744
24	H	5.9258	7.9204	5.4686
25	C	6.0914	6.5769	7.1525
26	H	5.4190	7.1432	7.7950
27	C	6.6926	5.3953	7.6461
28	C	6.4498	4.9147	8.9893
29	H	6.9929	6.4419	11.1907
30	C	7.1255	3.8007	9.4576
31	H	8.8838	3.8173	11.5490
32	C	8.0377	3.0897	8.5878
33	C	8.6969	1.9062	8.9966
34	H	8.5272	1.5195	10.0002
35	C	9.5356	1.2444	8.1263
36	H	10.0532	0.3299	8.4083
37	C	9.7232	1.7615	6.8280
38	C	7.5924	4.7171	6.7711
39	C	8.2756	3.5294	7.2513
40	C	7.5507	6.7275	3.6905
41	C	7.2745	8.2223	2.0311
42	C	6.7443	9.4207	1.2733
43	C	7.6906	9.4510	0.0236
44	H	8.4478	10.2346	0.1705
45	H	7.1363	9.7027	-0.8907
46	C	8.4154	8.0652	-0.1110
47	C	8.1935	7.4785	1.2645
48	C	6.8417	10.7081	2.1107

49	H	6.2156	10.6363	3.0104
50	H	6.4987	11.5682	1.5184
51	H	7.8764	10.9002	2.4264
52	C	5.2695	9.1618	0.8871
53	H	5.1592	8.2525	0.2813
54	H	4.8859	10.0106	0.3034
55	H	4.6497	9.0496	1.7874
56	C	9.9135	8.2182	-0.4294
57	H	10.0417	8.6906	-1.4138
58	H	10.4083	7.2385	-0.4473
59	H	10.4190	8.8420	0.3206
60	C	7.7527	7.1532	-1.1692
61	H	6.6782	7.0206	-0.9824
62	H	8.2229	6.1608	-1.1655
63	H	7.8760	7.5946	-2.1685
64	C	10.6095	1.0441	5.8738
65	C	12.0493	-0.6238	5.4191
66	C	12.9352	-1.8327	5.6322
67	C	13.3665	-2.1754	4.1635
68	H	14.4239	-2.4690	4.1165
69	H	12.7748	-3.0320	3.8099
70	C	13.0764	-0.9424	3.2369
71	C	12.1273	-0.1406	4.0977
72	C	14.1357	-1.4297	6.5193
73	H	14.7186	-0.6137	6.0717
74	H	14.8029	-2.2930	6.6541
75	H	13.7891	-1.0988	7.5082
76	C	12.1636	-2.9854	6.2983
77	H	11.8221	-2.6973	7.3019
78	H	12.8137	-3.8668	6.3941
79	H	11.2841	-3.2714	5.7051
80	C	14.3443	-0.1021	2.9573
81	H	14.8439	0.2085	3.8850
82	H	14.0847	0.8030	2.3924
83	H	15.0575	-0.6926	2.3644
84	C	12.4269	-1.3526	1.9032
85	H	13.1251	-1.9707	1.3206
86	H	12.1682	-0.4666	1.3091
87	H	11.5081	-1.9330	2.0682
88	C	6.9076	3.2894	10.8433
89	C	5.6862	2.7056	11.2112
90	C	5.4820	2.2169	12.5016
91	C	6.5038	2.3112	13.4543
92	C	7.7305	2.8904	13.1062
93	C	7.9251	3.3662	11.8113
94	H	4.8844	2.6258	10.4766
95	H	4.5253	1.7606	12.7680
96	O	6.3627	1.8526	14.7434
97	H	8.5172	2.9622	13.8575
98	H	5.4643	1.4851	14.8429

99	C	5.4872	5.6645	9.8494
100	C	4.1135	5.6610	9.5586
101	C	3.2078	6.3768	10.3431
102	C	3.6703	7.1260	11.4320
103	C	5.0375	7.1443	11.7348
104	C	5.9295	6.4173	10.9505
105	H	3.7432	5.0840	8.7095
106	H	2.1411	6.3543	10.1057
107	O	2.8336	7.8641	12.2371
108	H	5.3850	7.7341	12.5830
109	H	1.9200	7.7621	11.9095

Optimized Coordinates of Eu-6

1	Eu	9.4764	3.7552	3.8772
2	O	11.3879	4.0540	2.1912
3	O	9.6347	2.9678	1.4435
4	O	11.3676	3.2969	0.1206
5	O	6.9382	3.4975	2.9953
6	O	7.8173	1.7044	3.8921
7	O	5.7565	1.6413	3.1152
8	O	10.6874	5.8987	4.8134
9	O	11.7537	4.0483	5.2950
10	O	12.5780	5.9861	5.9425
11	N	7.8083	5.1240	5.4645
12	N	9.0827	2.8617	6.3808
13	N	8.4105	5.9898	2.9508
14	N	8.7628	6.3718	1.7134
15	N	6.9011	7.8338	3.2153
16	N	10.6598	1.5185	4.6053
17	N	11.4518	0.9306	3.6961
18	N	11.2710	-0.0406	6.3200
19	N	10.8143	3.4353	1.2174
20	N	6.8062	2.2653	3.3245
21	N	11.7017	5.3277	5.3655
22	C	7.1889	6.2290	5.0217
23	C	6.2613	6.9492	5.8077
24	H	5.7909	7.8339	5.3836
25	C	5.9869	6.5122	7.0847
26	H	5.2759	7.0463	7.7176
27	C	6.6393	5.3637	7.5879
28	C	6.4298	4.8929	8.9169
29	H	7.2063	6.4707	10.9851
30	C	7.0857	3.7952	9.4223
31	H	8.8074	3.7878	11.5337
32	C	7.9902	3.0648	8.5570
33	C	8.6271	1.8683	8.9581
34	H	8.4336	1.4653	9.9511
35	C	9.4723	1.2085	8.0917
36	H	9.9739	0.2835	8.3682
37	C	9.6867	1.7422	6.8045
38	C	7.5556	4.6956	6.7253
39	C	8.2385	3.5118	7.2213
40	C	7.5143	6.7080	3.6522
41	C	7.2597	8.2109	1.9965
42	C	6.7385	9.4118	1.2360
43	C	7.7071	9.4534	0.0038
44	H	8.4580	10.2394	0.1685
45	H	7.1682	9.7078	-0.9190
46	C	8.4404	8.0717	-0.1257
47	C	8.1973	7.4770	1.2428
48	C	6.8168	10.6947	2.0823

49	H	6.1746	10.6162	2.9700
50	H	6.4820	11.5570	1.4885
51	H	7.8449	10.8883	2.4178
52	C	5.2719	9.1506	0.8213
53	H	5.1759	8.2451	0.2075
54	H	4.8963	10.0019	0.2362
55	H	4.6359	9.0304	1.7092
56	C	9.9431	8.2331	-0.4178
57	H	10.0855	8.7106	-1.3979
58	H	10.4427	7.2557	-0.4321
59	H	10.4332	8.8557	0.3433
60	C	7.8002	7.1625	-1.2002
61	H	6.7232	7.0241	-1.0331
62	H	8.2748	6.1722	-1.1938
63	H	7.9390	7.6099	-2.1947
64	C	10.5920	1.0361	5.8592
65	C	12.0528	-0.6167	5.4181
66	C	12.9476	-1.8173	5.6394
67	C	13.4030	-2.1499	4.1756
68	H	14.4639	-2.4325	4.1424
69	H	12.8252	-3.0112	3.8108
70	C	13.1133	-0.9164	3.2494
71	C	12.1451	-0.1268	4.1000
72	C	14.1312	-1.4049	6.5449
73	H	14.7119	-0.5812	6.1087
74	H	14.8053	-2.2618	6.6859
75	H	13.7671	-1.0815	7.5299
76	C	12.1787	-2.9802	6.2906
77	H	11.8202	-2.6991	7.2902
78	H	12.8365	-3.8551	6.3927
79	H	11.3106	-3.2733	5.6841
80	C	14.3764	-0.0626	2.9900
81	H	14.8606	0.2492	3.9253
82	H	14.1156	0.8422	2.4250
83	H	15.1029	-0.6440	2.4043
84	C	12.4861	-1.3282	1.9056
85	H	13.1984	-1.9374	1.3308
86	H	12.2272	-0.4427	1.3108
87	H	11.5709	-1.9181	2.0557
88	C	6.8263	3.3158	10.8096
89	C	5.5689	2.7954	11.1530
90	C	5.3158	2.3670	12.4586
91	C	6.3245	2.4438	13.4387
92	C	7.5810	2.9536	13.0894
93	C	7.8316	3.3905	11.7851
94	H	4.7847	2.7261	10.4094
95	H	4.3363	1.9763	12.7038
96	O	6.1149	2.0289	14.7366
97	H	8.3660	3.0130	13.8325
98	H	5.1833	1.6988	14.8189

99	C	5.5568	5.6704	9.8398
100	C	4.1610	5.6068	9.7208
101	C	3.3468	6.2831	10.6337
102	C	3.9218	7.0227	11.6864
103	C	5.3157	7.0883	11.7959
104	C	6.1295	6.4210	10.8776
105	H	3.7081	5.0257	8.9275
106	H	2.2713	6.2232	10.5252
107	O	3.1530	7.6823	12.6218
108	H	5.7710	7.6528	12.5997
109	H	2.1959	7.5323	12.4092