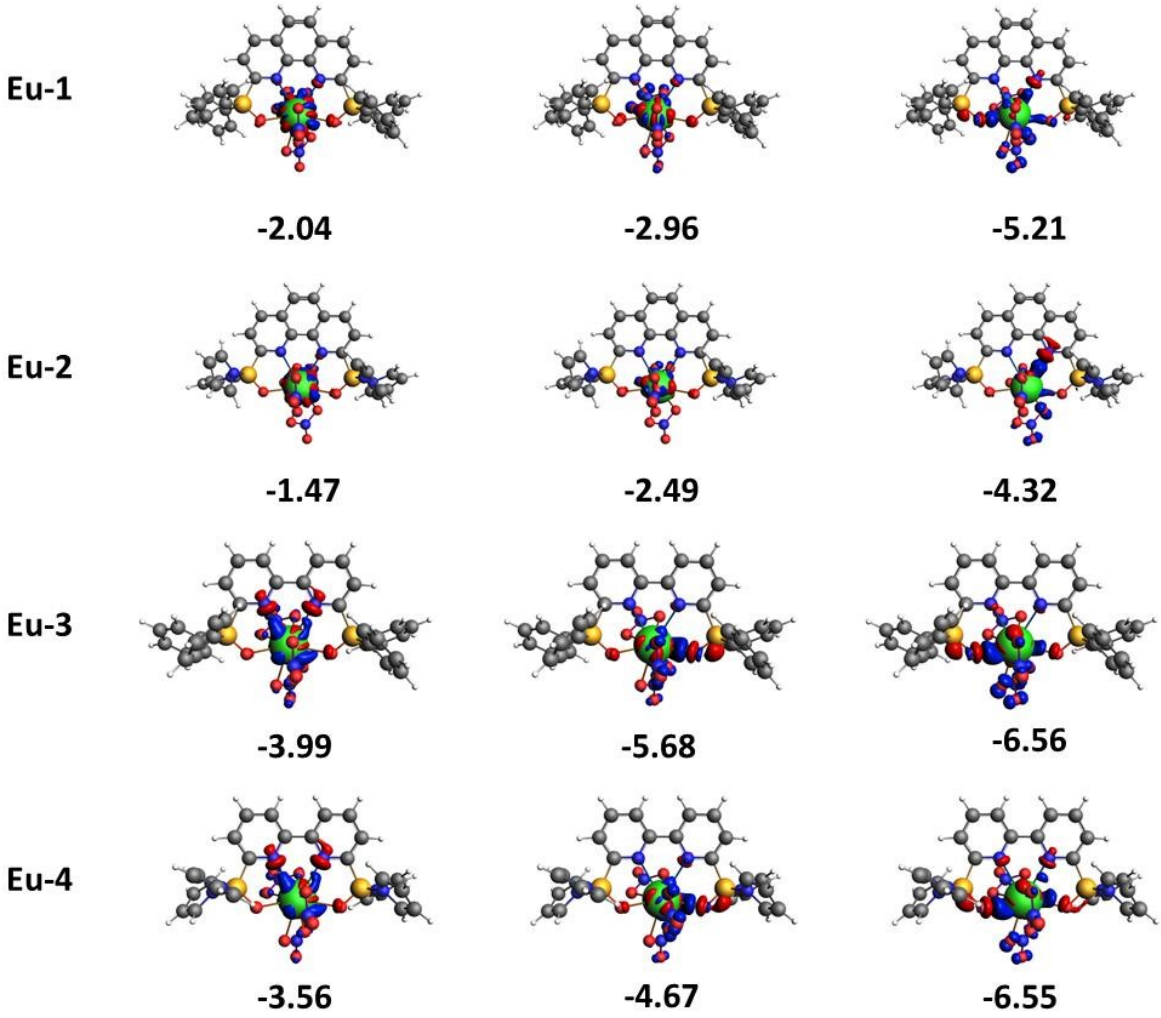

Figure 1 Natural orbitals for the chemical valence (NOCVs) for the four $[EuL(NO_3)_3]$ complexes. The corresponding orbital energy (kcal mol^{-1}) contribution for each NOCV pair is also presented.

Table 1. Computed bond parameters of ML_2NO_3 complexes where M= Am/Eu; L= 1-4

Complexes	$M-O_1$	$M-N_1$	$M-N_2$	$M-O_2$	$P_1C_1C_2P_2$	$M-O_3$	$M-N_3$	$M-N_4$	$M-O_4$	$P_3C_3C_4P_4$
Am-1	2.455	2.786	2.818	2.457	7.134	2.544	2.972	2.976	2.463	5.111
Eu-1	2.472	2.811	2.791	2.444	6.158	2.467	3.013	3.003	2.522	3.597
Am-2	2.548	2.759	2.738	2.482	1.514	2.504	2.841	2.805	2.601	13.330
Eu-2	2.520	2.696	2.757	2.570	2.628	2.546	2.899	2.847	2.600	14.687
Am-3	2.416	2.848	2.805	2.455	25.467	2.437	3.011	3.014	2.526	13.957
Eu-3	2.443	2.842	2.815	2.477	25.466	2.442	3.059	3.051	2.502	11.059
Am-4	2.472	2.758	2.746	2.569	14.270	2.581	2.787	2.820	2.512	7.159
Eu-4	2.568	2.774	2.755	2.507	9.402	2.576	2.860	2.911	2.530	14.217

Table 2. Mulliken charges on the oxygen, nitrogen, and metal ions in the ML_2NO_3 complexes where M=Am/Eu.

Complexes	O1	N1	N2	O2	O3	N3	N4	O4	M
Am-1	-0.842	-0.368	-0.383	-0.825	-0.826	-0.386	-0.383	-0.823	+1.500
Eu-1	-0.858	-0.386	-0.420	-0.844	-0.851	-0.399	-0.393	-0.846	+1.663
Am-2	-0.814	-0.388	-0.397	-0.803	-0.792	-0.412	-0.397	-0.796	+1.424
Eu-2	-0.826	-0.403	-0.417	-0.820	-0.809	-0.426	-0.407	-0.814	+1.557
Am-3	-0.843	-0.368	-0.373	-0.828	-0.830	-0.389	-0.373	-0.827	+1.514
Eu-3	-0.858	-0.388	-0.382	-0.845	-0.854	-0.397	-0.382	-0.852	+1.685
Am-4	-0.811	-0.391	-0.408	-0.799	-0.796	-0.416	-0.408	-0.797	+1.393
Eu-4	-0.825	-0.405	-0.422	-0.821	-0.811	-0.426	-0.408	-0.815	+1.561

Table 3. QTAIM analysis of electron density ρ(e/bohr^3) at Metal–Nitrogen and Metal-Oxygen Bond Critical Points of the ML_2NO_3 complexes.

Complexes	M-O_1	M-N_1	M-N_2	M-O_2	M-O_3	M-N_3	M-N_4	M-O_4
Am-1	0.051	0.015	0.030	0.054	0.049	0.020	0.020	0.042
Eu-1	0.041	0.024	0.025	0.043	0.036	0.016	0.015	0.040
Am-2	0.042	0.033	0.034	0.048	0.045	0.027	0.029	0.036
Eu-2	0.032	0.026	0.026	0.036	0.030	0.022	0.020	0.033
Am-3	0.051	0.027	0.029	0.056	0.052	0.018	0.018	0.043
Eu-3	0.038	0.022	0.024	0.043	0.038	0.014	0.014	0.043
Am-4	0.040	0.034	0.032	0.048	0.044	0.028	0.030	0.044
Eu-4	0.032	0.026	0.027	0.037	0.031	0.031	0.019	0.034

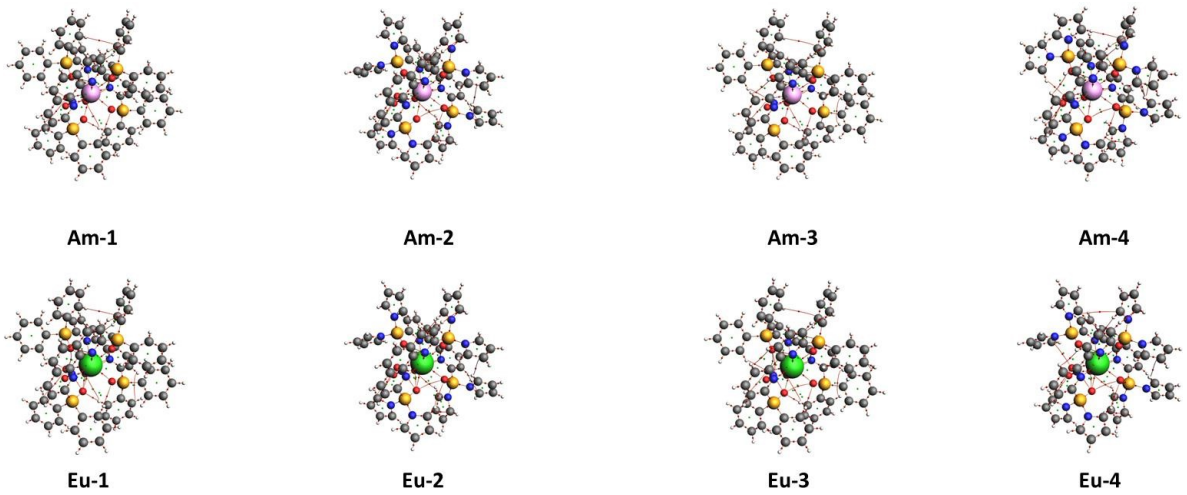

Figure 2: AIM molecular graphs of ML_2NO_3 complexes where red colour circles indicate BCPs while RCPs are represented by green colour circles.

Ligand 1

1	H	5.8855	20.9837	7.9361
2	C	7.8815	21.7806	7.8501
3	H	8.3048	20.9675	7.2720
4	C	8.6917	22.8647	8.2511
5	C	6.4463	25.0795	10.0662
6	N	8.2464	23.8976	8.9548
7	C	6.9457	23.9305	9.3115
8	N	7.2934	26.0855	10.3683
9	C	6.8274	27.1388	11.0341
10	C	5.4866	27.2597	11.4591
11	H	5.1517	28.1380	11.9977
12	C	4.6096	26.2322	11.1606
13	H	3.5685	26.2860	11.4646
14	C	5.0702	25.1071	10.4431
15	C	4.1987	24.0196	10.0837
16	H	3.1570	24.0703	10.3865
17	C	4.6639	22.9548	9.3733
18	H	4.0007	22.1396	9.0988
19	C	6.0424	22.8829	8.9663
20	C	6.5488	21.7962	8.2176
21	P	8.0720	28.4866	11.2306
22	P	10.4730	22.8751	7.7945
23	O	10.8320	21.6823	6.9481
24	O	8.5793	28.9701	9.8980
25	C	11.4225	22.9001	9.3537
26	C	11.1799	23.8193	10.3897

27	C	11.9641	23.7884	11.5455
28	C	12.9924	22.8471	11.6776
29	C	13.2352	21.9304	10.6500
30	C	12.4524	21.9552	9.4911
31	H	10.3764	24.5432	10.3032
32	H	11.7715	24.4992	12.3426
33	H	13.5996	22.8284	12.5777
34	H	14.0296	21.1965	10.7482
35	H	12.6352	21.2435	8.6930
36	C	10.8100	24.4485	6.9297
37	C	11.5655	24.3733	5.7475
38	C	11.8966	25.5381	5.0475
39	C	11.4739	26.7835	5.5229
40	C	10.7163	26.8626	6.6978
41	C	10.3833	25.7030	7.4034
42	H	11.8894	23.4055	5.3786
43	H	12.4809	25.4710	4.1346
44	H	11.7315	27.6883	4.9801
45	H	10.3821	27.8280	7.0664
46	H	9.7808	25.7740	8.3029
47	C	9.3967	27.8308	12.2909
48	C	9.1595	26.8875	13.3035
49	C	10.2062	26.4714	14.1322
50	C	11.4935	26.9891	13.9497
51	C	11.7375	27.9187	12.9323
52	C	10.6931	28.3399	12.1050
53	H	8.1677	26.4700	13.4479

54	H	10.0174	25.7420	14.9136
55	H	12.3056	26.6639	14.5933
56	H	12.7376	28.3138	12.7822
57	H	10.8825	29.0577	11.3129
58	C	7.2593	29.8320	12.1573
59	C	7.0739	29.7974	13.5498
60	C	6.4403	30.8600	14.2000
61	C	5.9919	31.9649	13.4669
62	C	6.1791	32.0079	12.0813
63	C	6.8107	30.9457	11.4276
64	H	7.4261	28.9524	14.1330
65	H	6.3024	30.8275	15.2764
66	H	5.5032	32.7908	13.9755
67	H	5.8382	32.8661	11.5102
68	H	6.9644	30.9811	10.3539

Ligand 2

1	H	5.7597	21.2025	7.7826
2	C	7.7930	21.8999	7.7443
3	H	8.1911	21.0608	7.1865
4	C	8.6363	22.9494	8.1626
5	C	6.4619	25.2652	9.9336
6	N	8.2288	24.0102	8.8483
7	C	6.9249	24.1030	9.1753
8	N	7.3479	26.2192	10.2828
9	C	6.9102	27.2688	10.9734
10	C	5.5684	27.4555	11.3643
11	H	5.2646	28.3318	11.9242
12	C	4.6515	26.4821	11.0093
13	H	3.6066	26.5785	11.2865
14	C	5.0793	25.3528	10.2795
15	C	4.1669	24.3112	9.8872
16	H	3.1223	24.4074	10.1670
17	C	4.5998	23.2303	9.1821
18	H	3.9078	22.4467	8.8888
19	C	5.9828	23.0968	8.8076
20	C	6.4533	21.9842	8.0762
21	P	8.1998	28.5136	11.3024
22	P	10.4093	22.8456	7.7768
23	O	10.8243	21.6137	7.0626
24	O	8.8682	29.0694	10.1002
25	H	13.5561	22.0671	11.4141
26	H	10.2750	25.7552	14.7827

27	H	6.0910	31.1686	14.8454
28	H	12.6061	25.8141	4.6162
29	N	7.4740	29.7574	12.2149
30	C	6.9201	30.9117	11.6469
31	C	6.2943	31.6200	12.6424
32	C	6.4541	30.8852	13.8667
33	C	7.1721	29.7504	13.5816
34	H	7.0399	31.1170	10.5940
35	N	9.2801	27.7705	12.3792
36	C	10.5736	28.2526	12.6247
37	C	11.1288	27.4958	13.6246
38	C	10.1551	26.5167	14.0243
39	C	9.0353	26.7033	13.2552
40	H	10.9703	29.0779	12.0530
41	N	10.8035	24.2389	6.8757
42	C	10.4149	25.5671	7.0939
43	C	11.0969	26.3618	6.2058
44	C	11.9429	25.5104	5.4153
45	C	11.7520	24.2207	5.8437
46	H	9.6822	25.8073	7.8492
47	N	11.2388	22.9857	9.2640
48	C	11.0860	23.9566	10.2613
49	C	12.0046	23.7013	11.2497
50	C	12.7569	22.5406	10.8591
51	C	12.2751	22.1218	9.6440
52	H	10.3214	24.7143	10.1803
53	H	12.5592	21.2961	9.0104

54	H	12.1866	23.2890	5.5161
55	H	12.1218	24.2766	12.1584
56	H	5.7882	32.5676	12.5152
57	H	7.5084	28.9479	14.2210
58	H	12.1270	27.6181	14.0233
59	H	8.0965	26.1718	13.2370
60	H	10.9982	27.4359	6.1220

Ligand 3

1	H	5.8406	21.2404	7.3882
2	C	7.8797	21.9367	7.5516
3	H	8.3072	21.2071	6.8735
4	C	8.6880	22.8985	8.1655
5	C	6.4427	24.9573	10.1891
6	N	8.2235	23.8246	9.0100
7	C	6.9107	23.8604	9.2803
8	N	7.2288	26.0412	10.2786
9	C	6.8434	27.0617	11.0572
10	C	5.6521	27.0574	11.7903
11	H	5.3663	27.9048	12.4021
12	C	4.8388	25.9226	11.7119
13	H	3.9122	25.8702	12.2737
14	C	5.2355	24.8596	10.9061
15	H	6.4943	30.7127	10.1077
16	H	5.3164	32.5796	11.2354
17	H	5.3771	32.7726	13.7163
18	H	6.6302	31.0958	15.0603
19	C	6.0193	22.9333	8.7102
20	C	6.5131	21.9609	7.8426
21	P	8.0304	28.4774	11.0387
22	P	10.4923	22.9514	7.8172
23	O	10.9013	21.8737	6.8478
24	O	8.4087	28.8913	9.6424
25	C	11.3349	22.7619	9.4247
26	C	11.1311	23.6382	10.5052

27	C	11.8051	23.4278	11.7105
28	C	12.6860	22.3479	11.8473
29	C	12.8922	21.4749	10.7749
30	C	12.2185	21.6798	9.5659
31	H	10.4396	24.4688	10.4143
32	H	11.6423	24.1068	12.5417
33	H	13.2074	22.1883	12.7867
34	H	13.5742	20.6358	10.8764
35	H	12.3738	21.0031	8.7321
36	C	10.8622	24.6203	7.1762
37	C	11.7238	24.6919	6.0685
38	C	12.0647	25.9322	5.5201
39	C	11.5479	27.1081	6.0741
40	C	10.6867	27.0416	7.1757
41	C	10.3413	25.8051	7.7287
42	H	12.1172	23.7780	5.6354
43	H	12.7289	25.9772	4.6619
44	H	11.8113	28.0712	5.6465
45	H	10.2750	27.9481	7.6099
46	H	9.6530	25.7677	8.5669
47	C	9.4561	27.9312	12.0295
48	C	9.3276	27.0230	13.0930
49	C	10.4471	26.6663	13.8506
50	C	11.7004	27.2085	13.5462
51	C	11.8359	28.1050	12.4801
52	C	10.7182	28.4671	11.7233
53	H	8.3628	26.5863	13.3324

54	H	10.3402	25.9642	14.6720
55	H	12.5699	26.9283	14.1335
56	H	12.8093	28.5201	12.2369
57	H	10.8237	29.1568	10.8917
58	C	7.2190	29.8365	11.9454
59	C	7.2585	29.9558	13.3444
60	C	6.5945	31.0103	13.9786
61	C	5.8912	31.9538	13.2216
62	C	5.8556	31.8457	11.8268
63	C	6.5169	30.7920	11.1899
64	H	7.8073	29.2361	13.9434
65	H	4.9574	22.9829	8.9204
66	H	4.6262	23.9655	10.8464

Ligand 4

1	H	5.7269	21.4475	7.1499
2	C	7.7880	22.0265	7.4376
3	H	8.2146	21.2638	6.7968
4	C	8.6031	22.9507	8.0960
5	C	6.3608	25.1297	9.9886
6	N	8.1468	23.9132	8.9035
7	C	6.8242	24.0205	9.0930
8	N	7.2104	26.1485	10.1788
9	C	6.8341	27.1573	10.9766
10	C	5.5983	27.2229	11.6246
11	H	5.3353	28.0623	12.2575
12	C	4.7136	26.1579	11.4290
13	H	3.7448	26.1520	11.9162
14	C	5.0963	25.1015	10.6090
15	H	7.8943	29.0706	14.0601
16	H	12.3438	27.9015	13.3613
17	H	8.3441	26.2040	13.0810
18	H	10.9324	27.6104	6.6207
19	C	5.9205	23.1405	8.4682
20	C	6.4093	22.1338	7.6398
21	P	8.0839	28.4740	11.0876
22	P	10.4024	22.8804	7.8585
23	O	10.8884	21.7222	7.0697
24	O	8.5584	29.0067	9.7872
25	H	13.1536	21.7004	11.7035
26	H	10.7000	25.9736	14.3882

27	H	6.5126	31.2779	14.8003
28	H	12.8525	26.1957	5.2831
29	N	7.4285	29.7219	12.0498
30	C	6.7196	30.8103	11.5261
31	C	6.2626	31.5683	12.5754
32	C	6.6921	30.9338	13.7907
33	C	7.3985	29.8078	13.4467
34	H	6.6268	30.9427	10.4589
35	N	9.3298	27.8282	12.0416
36	C	10.6107	28.3921	12.1241
37	C	11.3168	27.7085	13.0808
38	C	10.4532	26.6945	13.6207
39	C	9.2466	26.7860	12.9755
40	H	10.8923	29.2150	11.4842
41	N	10.8388	24.3607	7.1312
42	C	10.3342	25.6466	7.3706
43	C	11.0876	26.5400	6.6500
44	C	12.0981	25.7973	5.9485
45	C	11.9312	24.4713	6.2600
46	H	9.4909	25.7939	8.0288
47	N	11.1237	22.8988	9.4063
48	C	10.9894	23.8583	10.4164
49	C	11.7936	23.4883	11.4661
50	C	12.4500	22.2625	11.1036
51	C	12.0274	21.9209	9.8433
52	H	10.3181	24.6950	10.2986
53	H	12.2799	21.0867	9.2075

54	H	12.4691	23.5921	5.9405
55	H	11.8980	24.0319	12.3954
56	H	5.6934	32.4841	12.4879
57	H	4.8525	23.2481	8.6125
58	H	4.4286	24.2604	10.4665

Am-1

1	H	6.6808	20.3829	9.3742
2	C	8.4851	21.3092	8.6658
3	H	8.8857	20.4065	8.2194
4	C	9.2048	22.5179	8.6109
5	C	7.0349	24.9152	10.2876
6	N	8.7624	23.6582	9.1465
7	C	7.5513	23.6644	9.7594
8	N	7.7702	26.0461	10.1365
9	C	7.2485	27.2129	10.5275
10	C	5.9883	27.3203	11.1453
11	H	5.5977	28.2855	11.4445
12	C	5.2508	26.1707	11.3511
13	H	4.2781	26.2152	11.8295
14	C	5.7534	24.9294	10.9038
15	C	5.0011	23.7112	11.0296
16	H	4.0333	23.7511	11.5184
17	C	5.4826	22.5399	10.5302
18	H	4.9077	21.6233	10.6111
19	C	6.7582	22.4893	9.8699
20	C	7.2617	21.2965	9.3058
21	P	8.2913	28.6853	10.0875
22	P	10.8689	22.6555	7.8080
23	O	11.3963	24.0522	8.1517
24	O	9.5601	28.1390	9.4286
25	C	10.6535	22.3832	6.0227
26	C	9.4260	22.6687	5.3994

27	C	9.3092	22.5676	4.0113
28	C	10.4139	22.1896	3.2410
29	C	11.6397	21.9111	3.8560
30	C	11.7632	22.0065	5.2431
31	H	8.5643	22.9695	5.9859
32	H	8.3588	22.7841	3.5344
33	H	10.3204	22.1127	2.1621
34	H	12.4971	21.6191	3.2581
35	H	12.7172	21.7896	5.7122
36	C	11.9542	21.3594	8.4775
37	C	12.8674	21.7175	9.4846
38	C	13.6904	20.7426	10.0532
39	C	13.6024	19.4138	9.6252
40	C	12.6957	19.0554	8.6208
41	C	11.8735	20.0245	8.0432
42	H	12.9382	22.7499	9.8105
43	H	14.3996	21.0208	10.8264
44	H	14.2438	18.6588	10.0695
45	H	12.6334	18.0262	8.2827
46	H	11.1867	19.7394	7.2524
47	C	8.6923	29.6824	11.5583
48	C	10.0469	29.8061	11.9091
49	C	10.4135	30.5909	13.0057
50	C	9.4333	31.2465	13.7563
51	C	8.0820	31.1233	13.4104
52	C	7.7089	30.3483	12.3111
53	H	10.8033	29.2954	11.3236

54	H	11.4617	30.6900	13.2698
55	H	9.7203	31.8568	14.6072
56	H	7.3217	31.6368	13.9899
57	H	6.6599	30.2843	12.0412
58	C	7.2958	29.7077	8.9549
59	C	6.4716	29.0884	7.9974
60	C	5.8042	29.8613	7.0459
61	C	5.9590	31.2524	7.0404
62	C	6.7811	31.8727	7.9867
63	C	7.4506	31.1052	8.9425
64	H	6.3504	28.0098	7.9871
65	H	5.1672	29.3795	6.3113
66	H	5.4392	31.8518	6.2993
67	H	6.9031	32.9512	7.9809
68	H	8.0891	31.5939	9.6702
69	Am	10.3357	25.8331	9.3837
70	O	10.9992	26.8328	7.0754
71	N	9.8888	26.6132	6.4876
72	O	8.9874	26.0221	7.1699
73	O	9.6955	26.9544	5.3165
74	O	12.3896	27.3710	9.6256
75	N	13.1753	26.5537	10.2159
76	O	12.7163	25.3884	10.4395
77	O	14.3172	26.8830	10.5503
78	O	10.3810	26.5273	11.9528
79	N	10.2923	25.3451	12.4148
80	O	10.1526	24.4038	11.5631

81	O	10.3348	25.1142	13.6284

Am-2

1	H	6.7345	20.3480	9.5207
2	C	8.5036	21.2791	8.7330
3	H	8.8830	20.3812	8.2598
4	C	9.2150	22.4893	8.6584
5	C	7.1261	24.8777	10.4393
6	N	8.8025	23.6277	9.2254
7	C	7.6212	23.6280	9.8859
8	N	7.8454	26.0063	10.2464
9	C	7.3421	27.1684	10.6777
10	C	6.1400	27.2730	11.3973
11	H	5.7956	28.2327	11.7646
12	C	5.4123	26.1189	11.6296
13	H	4.4790	26.1562	12.1807
14	C	5.8792	24.8870	11.1261
15	C	5.1357	23.6654	11.2796
16	H	4.1955	23.6993	11.8196
17	C	5.5904	22.4992	10.7456
18	H	5.0198	21.5822	10.8479
19	C	6.8337	22.4511	10.0242
20	C	7.3104	21.2627	9.4316
21	P	8.3346	28.6141	10.1487
22	P	10.8155	22.6528	7.7851
23	O	11.4097	23.9961	8.1308
24	O	9.6853	28.1492	9.6690
25	N	10.4926	22.3563	6.1527
26	O	9.0111	26.0781	7.3349

27	O	12.4843	27.2649	9.7156
28	N	13.2697	26.3983	10.2358
29	O	12.7807	25.2352	10.4178
30	O	14.4289	26.6764	10.5414
31	O	9.7056	27.0204	5.4805
32	O	10.5079	26.4562	12.0258
33	N	10.3984	25.2709	12.4835
34	O	10.2272	24.3432	11.6193
35	O	10.4503	25.0282	13.6895
36	N	11.8891	21.4145	8.1972
37	O	11.0394	26.8403	7.2122
38	N	9.9132	26.6576	6.6383
39	N	7.5003	29.4239	8.9159
40	N	8.3793	29.7134	11.4356
41	Am	10.4154	25.7875	9.4816
42	C	9.2824	22.6665	5.4970
43	C	9.4992	22.5962	4.1497
44	C	10.8821	22.2560	3.9407
45	C	11.4742	22.1266	5.1659
46	H	8.3887	22.8950	6.0564
47	H	8.7511	22.7589	3.3864
48	H	11.3758	22.1147	2.9888
49	H	12.4893	21.8868	5.4429
50	C	11.8367	20.0634	7.8050
51	C	12.7699	19.3765	8.5328
52	C	13.4189	20.3102	9.4148
53	C	12.8648	21.5431	9.2045

54	H	11.1601	19.7346	7.0313
55	H	12.9823	18.3201	8.4395
56	H	14.2141	20.0926	10.1145
57	H	13.0710	22.5056	9.6471
58	C	6.1218	29.6799	8.8147
59	C	5.9200	30.4849	7.7259
60	C	7.2009	30.7515	7.1292
61	C	8.1521	30.1002	7.8667
62	H	5.4195	29.2527	9.5129
63	H	4.9588	30.8407	7.3811
64	H	7.3937	31.3510	6.2498
65	H	9.2239	30.0415	7.7587
66	C	8.0765	31.0878	11.3951
67	C	8.4267	31.6330	12.5995
68	C	8.9762	30.5844	13.4180
69	C	8.9454	29.4249	12.6921
70	H	7.6365	31.5324	10.5163
71	H	8.3035	32.6714	12.8758
72	H	9.3514	30.6823	14.4276
73	H	9.2861	28.4273	12.9282

Am-3

1	H	6.6561	20.3686	9.2715
2	C	8.4784	21.3137	8.6035
3	H	8.8789	20.4291	8.1223
4	C	9.1871	22.5143	8.6029
5	C	7.0178	24.8961	10.3821
6	N	8.7342	23.6416	9.1871
7	C	7.5296	23.6170	9.7978
8	N	7.7467	26.0132	10.1724
9	C	7.2522	27.2017	10.5767
10	C	6.0409	27.3297	11.2541
11	H	5.6680	28.3008	11.5566
12	C	5.3169	26.1708	11.5328
13	H	4.3803	26.2220	12.0761
14	C	5.8015	24.9483	11.0823
15	O	10.3235	26.5150	11.9983
16	N	10.2347	25.3351	12.4663
17	O	10.1079	24.3880	11.6189
18	O	10.2643	25.1123	13.6819
19	C	6.7634	22.4412	9.8417
20	C	7.2409	21.2807	9.2436
21	P	8.2826	28.6654	10.0839
22	P	10.8581	22.6647	7.8189
23	O	11.3933	24.0462	8.2092
24	O	9.5516	28.1058	9.4360
25	C	10.6683	22.4435	6.0233
26	C	9.4550	22.7564	5.3860

27	C	9.3631	22.6946	3.9939
28	C	10.4782	22.3272	3.2335
29	C	11.6901	22.0211	3.8625
30	C	11.7889	22.0782	5.2535
31	H	8.5856	23.0489	5.9653
32	H	8.4237	22.9331	3.5058
33	H	10.4035	22.2796	2.1514
34	H	12.5556	21.7370	3.2725
35	H	12.7323	21.8398	5.7335
36	C	11.9345	21.3468	8.4620
37	C	12.8445	21.6783	9.4809
38	C	13.6644	20.6884	10.0279
39	C	13.5762	19.3709	9.5667
40	C	12.6722	19.0389	8.5508
41	C	11.8538	20.0234	7.9942
42	H	12.9160	22.7023	9.8323
43	H	14.3716	20.9465	10.8098
44	H	14.2151	18.6041	9.9941
45	H	12.6096	18.0184	8.1871
46	H	11.1702	19.7590	7.1936
47	C	8.6876	29.7052	11.5236
48	C	10.0374	29.7992	11.9007
49	C	10.4051	30.6119	12.9765
50	C	9.4307	31.3254	13.6803
51	C	8.0842	31.2336	13.3072
52	C	7.7104	30.4307	12.2283
53	H	10.7902	29.2451	11.3512

54	H	11.4500	30.6880	13.2606
55	H	9.7189	31.9573	14.5149
56	H	7.3288	31.7945	13.8480
57	H	6.6667	30.3926	11.9337
58	C	7.2849	29.6597	8.9289
59	C	6.4123	29.0274	8.0246
60	C	5.7469	29.7800	7.0552
61	C	5.9517	31.1624	6.9793
62	C	6.8231	31.7950	7.8718
63	C	7.4908	31.0482	8.8448
64	H	6.2495	27.9553	8.0707
65	H	5.0717	29.2891	6.3618
66	H	5.4326	31.7459	6.2250
67	H	6.9840	32.8667	7.8117
68	H	8.1673	31.5459	9.5308
69	Am	10.3175	25.8082	9.4331
70	O	11.0013	26.7966	7.1162
71	N	9.8977	26.5647	6.5216
72	O	8.9936	25.9750	7.2013
73	O	9.7126	26.8933	5.3452
74	O	12.3831	27.3329	9.6776
75	N	13.1562	26.5135	10.2817
76	O	12.6809	25.3581	10.5213
77	O	14.3021	26.8319	10.6134
78	H	5.2327	24.0500	11.2773
79	H	5.7985	22.4264	10.3281

Am-4

1	H	6.6174	20.4000	9.2770
2	C	8.4410	21.3257	8.5867
3	H	8.7980	20.4558	8.0486
4	C	9.1771	22.5086	8.6161
5	C	7.1462	24.8608	10.5735
6	N	8.7813	23.6196	9.2695
7	C	7.6008	23.5961	9.9199
8	N	7.8395	25.9797	10.2923
9	C	7.3877	27.1593	10.7664
10	C	6.2816	27.2800	11.6022
11	H	5.9694	28.2455	11.9827
12	C	5.5985	26.1110	11.9487
13	H	4.7451	26.1497	12.6157
14	C	6.0217	24.8991	11.4179
15	O	10.4798	26.4688	12.0531
16	N	10.3682	25.2893	12.5264
17	O	10.2065	24.3497	11.6739
18	O	10.4073	25.0644	13.7363
19	C	6.8022	22.4402	9.9367
20	C	7.2259	21.2964	9.2714
21	P	8.3393	28.5941	10.1479
22	P	10.8003	22.6666	7.7864
23	O	11.4081	23.9929	8.1714
24	O	9.6836	28.1338	9.6457
25	N	10.5231	22.3989	6.1413
26	O	12.7580	25.2143	10.4863

27	O	14.4140	26.6462	10.6127
28	H	5.4914	23.9923	11.6737
29	H	5.8507	22.4358	10.4499
30	Am	10.4090	25.7665	9.5182
31	N	7.4531	29.3407	8.9118
32	O	11.0422	26.8146	7.2451
33	N	8.4027	29.7403	11.3918
34	N	9.9243	26.6140	6.6616
35	O	9.0249	26.0208	7.3500
36	N	11.8462	21.4068	8.2078
37	O	9.7219	26.9722	5.5012
38	O	12.4834	27.2374	9.7568
39	N	13.2568	26.3722	10.2965
40	C	11.7762	20.0584	7.8100
41	C	12.6868	19.3526	8.5484
42	C	13.3396	20.2719	9.4427
43	C	12.8098	21.5149	9.2291
44	H	11.1063	19.7437	7.0248
45	H	12.8817	18.2930	8.4546
46	H	14.1209	20.0383	10.1528
47	H	13.0259	22.4720	9.6785
48	C	9.3553	22.7803	5.4470
49	C	9.6220	22.7298	4.1078
50	C	10.9942	22.3270	3.9440
51	C	11.5314	22.1442	5.1875
52	H	8.4527	23.0398	5.9776
53	H	8.9132	22.9448	3.3201

54	H	11.5176	22.1819	3.0086
55	H	12.5223	21.8505	5.4976
56	C	8.0729	31.1068	11.3112
57	C	8.4505	31.7019	12.4833
58	C	9.0437	30.6937	13.3218
59	C	9.0121	29.5079	12.6398
60	H	7.5975	31.5103	10.4310
61	H	8.3173	32.7475	12.7255
62	H	9.4474	30.8345	14.3151
63	H	9.3753	28.5251	12.9026
64	C	6.0655	29.5532	8.8441
65	C	5.8079	30.3126	7.7345
66	C	7.0622	30.5939	7.0899
67	C	8.0538	29.9973	7.8207
68	H	5.3984	29.1299	9.5787
69	H	4.8270	30.6277	7.4058
70	H	7.2105	31.1650	6.1834
71	H	9.1233	29.9645	7.6821

Eu-1

1	H	6.6763	20.3432	9.3848
2	C	8.4845	21.2597	8.6750
3	H	8.8812	20.3531	8.2330
4	C	9.2086	22.4657	8.6170
5	C	7.0453	24.8781	10.2845
6	N	8.7696	23.6092	9.1474
7	C	7.5593	23.6230	9.7598
8	N	7.7821	26.0082	10.1344
9	C	7.2627	27.1753	10.5260
10	C	6.0013	27.2866	11.1409
11	H	5.6123	28.2525	11.4397
12	C	5.2613	26.1385	11.3443
13	H	4.2875	26.1845	11.8203
14	C	5.7625	24.8960	10.8990
15	C	5.0060	23.6808	11.0268
16	H	4.0373	23.7252	11.5136
17	C	5.4849	22.5067	10.5319
18	H	4.9072	21.5919	10.6144
19	C	6.7613	22.4509	9.8741
20	C	7.2607	21.2544	9.3142
21	P	8.3100	28.6495	10.0993
22	P	10.8735	22.5924	7.8149
23	O	11.4239	23.9788	8.1648
24	O	9.5866	28.1093	9.4496
25	C	10.6542	22.3325	6.0277
26	C	9.4252	22.6154	5.4068

27	C	9.3074	22.5188	4.0183
28	C	10.4123	22.1471	3.2456
29	C	11.6399	21.8707	3.8583
30	C	11.7643	21.9617	5.2455
31	H	8.5633	22.9119	5.9951
32	H	8.3558	22.7342	3.5431
33	H	10.3178	22.0732	2.1665
34	H	12.4975	21.5831	3.2586
35	H	12.7193	21.7453	5.7131
36	C	11.9431	21.2773	8.4736
37	C	12.8635	21.6147	9.4809
38	C	13.6735	20.6237	10.0405
39	C	13.5649	19.2996	9.6032
40	C	12.6509	18.9617	8.5982
41	C	11.8418	19.9470	8.0296
42	H	12.9501	22.6436	9.8139
43	H	14.3887	20.8859	10.8136
44	H	14.1959	18.5319	10.0406
45	H	12.5728	17.9360	8.2528
46	H	11.1497	19.6784	7.2378
47	C	8.6985	29.6417	11.5766
48	C	10.0497	29.7651	11.9393
49	C	10.4063	30.5475	13.0410
50	C	9.4194	31.2009	13.7846
51	C	8.0712	31.0780	13.4266
52	C	7.7081	30.3053	12.3224
53	H	10.8123	29.2576	11.3592

54	H	11.4521	30.6467	13.3144
55	H	9.6990	31.8095	14.6392
56	H	7.3055	31.5902	14.0003
57	H	6.6616	30.2422	12.0426
58	C	7.3264	29.6751	8.9601
59	C	6.5067	29.0589	7.9967
60	C	5.8486	29.8343	7.0408
61	C	6.0083	31.2248	7.0367
62	C	6.8262	31.8419	7.9886
63	C	7.4863	31.0719	8.9490
64	H	6.3805	27.9808	7.9859
65	H	5.2146	29.3548	6.3020
66	H	5.4957	31.8264	6.2924
67	H	6.9518	32.9200	7.9842
68	H	8.1211	31.5584	9.6815
69	Eu	10.3927	25.8110	9.3738
70	O	11.0545	26.8271	7.0355
71	N	9.9499	26.5847	6.4451
72	O	9.0526	25.9863	7.1259
73	O	9.7583	26.9130	5.2700
74	O	12.4931	27.3617	9.6140
75	N	13.2748	26.5332	10.1909
76	O	12.8102	25.3688	10.4119
77	O	14.4235	26.8491	10.5171
78	O	10.4341	26.4703	11.9431
79	N	10.3654	25.2869	12.4104
80	O	10.2392	24.3400	11.5638

81	O	10.4148	25.0648	13.6244

Eu-2

1	H	6.7145	20.3117	9.5066
2	C	8.4903	21.2318	8.7216
3	H	8.8646	20.3311	8.2500
4	C	9.2090	22.4383	8.6485
5	C	7.1322	24.8395	10.4277
6	N	8.8009	23.5786	9.2128
7	C	7.6206	23.5864	9.8734
8	N	7.8546	25.9663	10.2343
9	C	7.3576	27.1282	10.6729
10	C	6.1582	27.2364	11.3964
11	H	5.8198	28.1962	11.7690
12	C	5.4257	26.0849	11.6256
13	H	4.4938	26.1242	12.1788
14	C	5.8866	24.8527	11.1177
15	C	5.1363	23.6352	11.2700
16	H	4.1964	23.6740	11.8101
17	C	5.5840	22.4673	10.7340
18	H	5.0073	21.5537	10.8341
19	C	6.8262	22.4138	10.0116
20	C	7.2960	21.2230	9.4181
21	P	8.3515	28.5756	10.1504
22	P	10.8143	22.5886	7.7818
23	O	11.4257	23.9244	8.1287
24	O	9.7027	28.1157	9.6661
25	N	10.4957	22.2963	6.1483
26	O	9.0698	26.0479	7.2790

27	O	12.5773	27.2641	9.7049
28	N	13.3576	26.3834	10.2030
29	O	12.8657	25.2181	10.3707
30	O	14.5224	26.6467	10.5044
31	O	9.7594	27.0002	5.4296
32	O	10.5416	26.3980	12.0132
33	N	10.4529	25.2098	12.4728
34	O	10.2963	24.2777	11.6126
35	O	10.5127	24.9730	13.6791
36	N	11.8711	21.3378	8.1992
37	O	11.0916	26.8362	7.1626
38	N	9.9685	26.6392	6.5880
39	N	7.5188	29.3915	8.9212
40	N	8.3975	29.6671	11.4433
41	Eu	10.4664	25.7618	9.4604
42	C	9.2940	22.6258	5.4861
43	C	9.5181	22.5559	4.1400
44	C	10.8972	22.1959	3.9385
45	C	11.4800	22.0550	5.1668
46	H	8.4007	22.8661	6.0410
47	H	8.7772	22.7313	3.3726
48	H	11.3944	22.0493	2.9892
49	H	12.4897	21.7994	5.4496
50	C	11.7950	19.9853	7.8149
51	C	12.7125	19.2854	8.5501
52	C	13.3755	20.2120	9.4292
53	C	12.8457	21.4538	9.2091

54	H	11.1153	19.6649	7.0404
55	H	12.9048	18.2246	8.4644
56	H	14.1636	19.9838	10.1335
57	H	13.0688	22.4147	9.6467
58	C	6.1421	29.6598	8.8280
59	C	5.9427	30.4771	7.7479
60	C	7.2237	30.7407	7.1500
61	C	8.1724	30.0745	7.8771
62	H	5.4388	29.2306	9.5240
63	H	4.9830	30.8435	7.4100
64	H	7.4179	31.3478	6.2762
65	H	9.2434	30.0084	7.7650
66	C	8.0967	31.0422	11.4107
67	C	8.4447	31.5790	12.6195
68	C	8.9915	30.5247	13.4324
69	C	8.9607	29.3697	12.6991
70	H	7.6595	31.4931	10.5337
71	H	8.3224	32.6158	12.9020
72	H	9.3650	30.6158	14.4432
73	H	9.2994	28.3701	12.9298

Eu-3

1	H	6.6368	20.3668	9.2978
2	C	8.4685	21.2875	8.6232
3	H	8.8441	20.4024	8.1236
4	C	9.1984	22.4759	8.6305
5	C	7.1058	24.8642	10.4891
6	N	8.7746	23.5993	9.2410
7	C	7.5812	23.5869	9.8708
8	N	7.8263	25.9807	10.2483
9	C	7.3583	27.1676	10.6848
10	C	6.1875	27.2962	11.4301
11	H	5.8422	28.2659	11.7683
12	C	5.4751	26.1373	11.7391
13	H	4.5720	26.1875	12.3366
14	C	5.9300	24.9158	11.2555
15	O	10.4779	26.3927	12.0879
16	N	10.3858	25.2047	12.5401
17	O	10.2412	24.2727	11.6805
18	O	10.4281	24.9659	13.7512
19	C	6.7904	22.4268	9.9030
20	C	7.2385	21.2681	9.2787
21	P	8.3733	28.6316	10.1580
22	P	10.8546	22.6159	7.8159
23	O	11.4431	23.9639	8.2462
24	O	9.7086	28.0888	9.6423
25	C	10.6153	22.4670	6.0182
26	C	9.3864	22.7983	5.4222

27	C	9.2568	22.7726	4.0316
28	C	10.3501	22.4242	3.2320
29	C	11.5783	22.1011	3.8200
30	C	11.7143	22.1215	5.2087
31	H	8.5327	23.0750	6.0317
32	H	8.3047	23.0237	3.5754
33	H	10.2457	22.4035	2.1515
34	H	12.4271	21.8308	3.1999
35	H	12.6692	21.8674	5.6570
36	C	11.9081	21.2399	8.3702
37	C	12.8688	21.4970	9.3630
38	C	13.6773	20.4584	9.8319
39	C	13.5264	19.1660	9.3187
40	C	12.5706	18.9076	8.3293
41	C	11.7644	19.9413	7.8502
42	H	12.9888	22.5017	9.7541
43	H	14.4242	20.6596	10.5929
44	H	14.1565	18.3608	9.6842
45	H	12.4592	17.9066	7.9254
46	H	11.0418	19.7348	7.0674
47	C	8.6091	29.7637	11.5627
48	C	9.8609	29.7850	12.1999
49	C	10.0741	30.6415	13.2829
50	C	9.0421	31.4696	13.7355
51	C	7.7938	31.4502	13.1024
52	C	7.5760	30.6041	12.0139
53	H	10.6600	29.1439	11.8450

54	H	11.0441	30.6625	13.7693
55	H	9.2114	32.1350	14.5766
56	H	6.9953	32.0990	13.4478
57	H	6.6128	30.6168	11.5139
58	C	7.4265	29.5130	8.8757
59	C	6.4651	28.8495	8.0939
60	C	5.8352	29.5225	7.0441
61	C	6.1645	30.8531	6.7665
62	C	7.1266	31.5159	7.5369
63	C	7.7573	30.8506	8.5893
64	H	6.2027	27.8163	8.2960
65	H	5.0902	29.0082	6.4456
66	H	5.6721	31.3740	5.9508
67	H	7.3839	32.5481	7.3212
68	H	8.5007	31.3720	9.1835
69	Eu	10.4433	25.7707	9.5068
70	O	11.1462	26.8292	7.1967
71	N	10.0428	26.6197	6.5925
72	O	9.1257	26.0313	7.2560
73	O	9.8696	26.9687	5.4207
74	O	12.5853	27.2640	9.7737
75	N	13.3398	26.4082	10.3462
76	O	12.8398	25.2570	10.5595
77	O	14.4973	26.6867	10.6765
78	H	5.3737	24.0164	11.4803
79	H	5.8296	22.4240	10.3983

Eu-4

1	H	6.6118	20.3638	9.2506
2	C	8.4458	21.2841	8.5802
3	H	8.8068	20.4134	8.0462
4	C	9.1824	22.4666	8.6171
5	C	7.1384	24.8216	10.5591
6	N	8.7842	23.5779	9.2670
7	C	7.5987	23.5573	9.9063
8	N	7.8384	25.9423	10.3014
9	C	7.3787	27.1175	10.7793
10	C	6.2491	27.2326	11.5847
11	H	5.9249	28.1951	11.9622
12	C	5.5582	26.0620	11.9067
13	H	4.6875	26.0961	12.5511
14	C	5.9967	24.8540	11.3808
15	O	10.4849	26.4144	12.0478
16	N	10.4281	25.2266	12.5148
17	O	10.3076	24.2841	11.6606
18	O	10.4798	25.0016	13.7240
19	C	6.7958	22.4034	9.9119
20	C	7.2233	21.2583	9.2517
21	P	8.3293	28.5639	10.1846
22	P	10.8102	22.6216	7.7949
23	O	11.4306	23.9403	8.1889
24	O	9.6670	28.1116	9.6556
25	N	10.5369	22.3683	6.1474
26	O	12.8523	25.2711	10.4393

27	O	14.4809	26.7327	10.5600
28	H	5.4607	23.9458	11.6188
29	H	5.8386	22.4000	10.4142
30	Eu	10.4498	25.7647	9.5009
31	N	7.4617	29.3509	8.9588
32	O	11.0489	26.8155	7.1831
33	N	8.3564	29.6824	11.4521
34	N	9.9405	26.5566	6.6043
35	O	9.0583	25.9526	7.3051
36	N	11.8488	21.3539	8.2102
37	O	9.7295	26.8743	5.4334
38	O	12.5322	27.2973	9.7301
39	N	13.3245	26.4414	10.2530
40	C	11.7700	20.0085	7.8038
41	C	12.6775	19.2923	8.5359
42	C	13.3373	20.2018	9.4351
43	C	12.8151	21.4493	9.2300
44	H	11.0966	19.7027	7.0180
45	H	12.8654	18.2321	8.4351
46	H	14.1185	19.9590	10.1424
47	H	13.0388	22.4021	9.6844
48	C	9.3647	22.7358	5.4530
49	C	9.6304	22.6833	4.1138
50	C	11.0068	22.2951	3.9499
51	C	11.5466	22.1199	5.1933
52	H	8.4604	22.9890	5.9837
53	H	8.9187	22.8890	3.3264

54	H	11.5307	22.1534	3.0143
55	H	12.5405	21.8364	5.5034
56	C	8.3418	31.0858	11.3117
57	C	8.7071	31.6347	12.5088
58	C	8.9821	30.5589	13.4253
59	C	8.7758	29.3806	12.7641
60	H	8.0606	31.5448	10.3771
61	H	8.7649	32.6940	12.7195
62	H	9.2925	30.6523	14.4570
63	H	8.8935	28.3570	13.0862
64	C	6.1218	29.7718	8.9804
65	C	5.8486	30.3756	7.7821
66	C	7.0458	30.3386	6.9858
67	C	8.0170	29.7096	7.7166
68	H	5.4927	29.5987	9.8400
69	H	4.8951	30.7989	7.4977
70	H	7.1720	30.7324	5.9867
71	H	9.0489	29.4877	7.4950