SUPPORTING INFORMATION

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Sterically Induced Conformational Relaxation and Structure of *meso*-Diaryloctaalkyl Porphyrins in the Excited Triplet State: Experimental and DFT Studies.

Alexander Kyrychenko[a,b], Joakim Andréasson[a], Jerker Mårtensson[c] and Bo Albinsson*[a]

[a]Department of Physical Chemistry and [c]Department of Organic Chemistry, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

[b]Permanent address: Research Institute for Chemistry, Kharkov State University, 4, Svobody, Sq., 310077 Kharkov, Ukraine

Correspondence to: Bo Albinsson, Department of Physical Chemistry, Chalmers University of Technology, SE-412 96 Göteborg, Sweden.
Phone: 46-31-772 30 44
Fax: 46-31-772 38 58
e-mail: balb@phc.chalmers.se

Cartesian coordinates

A listing of S_0 and T_1 optimized geometries (Cartesian coordinates).

H_2OMP
RB3LYP/6-31Gd (D_{2h})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.114761	0.000000	0.000000
2	1	0	1.099577	0.000000	0.000000
3	6	0	2.893735	1.127267	0.000000
4	6	0	2.893735	-1.127267	0.000000
5	6	0	4.269758	0.690559	0.000000
6	6	0	4.269758	-0.690559	0.000000
7	6	0	2.417790	2.436441	0.000000
8	6	0	2.417790	-2.436441	0.000000
9	6	0	1.082897	2.858555	0.000000
10	6	0	1.082897	-2.858555	0.000000
11	1	0	3.176685	3.212471	0.000000
12	1	0	3.176685	-3.212471	0.000000

13	6	0	5.444654	1.623958	0.000000
14	6	0	5.444654	-1.623958	0.000000
15	7	0	0.000000	2.032802	0.000000
16	7	0	0.000000	-2.032802	0.000000
17	6	0	0.682146	4.272350	0.000000
18	6	0	0.682146	-4.272350	0.000000
19	1	0	6.391404	1.077207	0.000000
20	1	0	6.391404	-1.077207	0.000000
21	1	0	5.441170	2.275963	0.882619
22	1	0	5.441170	2.275963	-0.882619
23	1	0	5.441170	-2.275963	-0.882619
24	1	0	5.441170	-2.275963	0.882619
25	6	0	-1.082897	2.858555	0.000000
26	6	0	-1.082897	-2.858555	0.000000
27	6	0	-0.682146	4.272350	0.000000
28	6	0	-0.682146	-4.272350	0.000000
29	6	0	1.626168	5.436217	0.000000
30	6	0	1.626168	-5.436217	0.000000
31	6	0	-2.417790	2.436441	0.000000
32	6	0	-2.417790	-2.436441	0.000000
33	6	0	-1.626168	5.436217	0.000000
34	6	0	-1.626168	-5.436217	0.000000
35	1	0	1.089228	6.389579	0.000000
36	1	0	1.089228	-6.389579	0.000000
37	1	0	2.279849	5.429250	-0.882234
38	1	0	2.279849	5.429250	0.882234
39	1	0	2.279849	-5.429250	0.882234
40	1	0	2.279849	-5.429250	-0.882234
41	6	0	-2.893735	1.127267	0.000000
42	6	0	-2.893735	-1.127267	0.000000
43	1	0	-3.176685	3.212471	0.000000
44	1	0	-3.176685	-3.212471	0.000000
45	1	0	-1.089228	6.389579	0.000000
46	1	0	-1.089228	-6.389579	0.000000
47	1	0	-2.279849	5.429250	0.882234
48	1	0	-2.279849	5.429250	-0.882234
49	1	0	-2.279849	-5.429250	-0.882234
50	1	0	-2.279849	-5.429250	0.882234
51	7	0	-2.114761	0.000000	0.000000
52	6	0	-4.269758	0.690559	0.000000
53	6	0	-4.269758	-0.690559	0.000000
54	1	0	-1.099577	0.000000	0.000000
55	6	0	-5.444654	1.623958	0.000000
56	6	0	-5.444654	-1.623958	0.000000
57	1	0	-6.391404	1.077207	0.000000
58	1	0	-6.391404	-1.077207	0.000000
59	1	0	-5.441170	2.275963	-0.882619
60	1	0	-5.441170	2.275963	0.882619
61	1	0	-5.441170	-2.275963	0.882619

62	1	0	-5.441170	-2.275963	-0.882619

Dipole moment (Debye):
X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Zero-point correction=	0.518837 (Hartree/Particle)
Thermal correction to Energy=	0.550552
Thermal correction to Enthalpy=	0.551496
Thermal correction to Gibbs Free Energy=	0.457614
Sum of electronic and zero-point Energies=	-1303.583954
Sum of electronic and thermal Energies=	-1303.552239
Sum of electronic and thermal Enthalpies=	-1303.551294
Sum of electronic and thermal Free Energies=	-1303.645176

H_2OMP
UB3LYP/6-31Gd (C_{2v})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.044480	0.000000	-0.000154
2	6	0	-2.877455	1.089927	-0.000235
3	6	0	-2.877455	-1.089927	-0.000235
4	6	0	-4.291957	0.680215	-0.000362
5	6	0	-2.458231	2.412509	-0.000168
6	6	0	-4.291957	-0.680215	-0.000362
7	6	0	-2.458231	-2.412509	-0.000168
8	6	0	-1.125802	2.925129	-0.000033
9	6	0	-5.454027	1.626131	-0.000422
10	6	0	-5.454027	-1.626131	-0.000422
11	6	0	-1.125802	-2.925129	-0.000033
12	1	0	-3.239400	3.165935	-0.000119
13	1	0	-3.239400	-3.165935	-0.000119
14	7	0	0.000000	2.140886	-0.000440
15	7	0	0.000000	-2.140886	-0.000440
16	6	0	-0.706718	4.272959	0.000457
17	6	0	-0.706718	-4.272959	0.000457
18	1	0	-6.408743	1.092012	-0.000670
19	1	0	-5.443259	2.279960	-0.882622
20	1	0	-5.443557	2.279680	0.881987
21	1	0	-6.408743	-1.092012	-0.000670
22	1	0	-5.443557	-2.279680	0.881987
23	1	0	-5.443259	-2.279960	-0.882622

24	1	0	0.000000	1.126621	-0.000191
25	1	0	0.000000	-1.126621	-0.000191
26	6	0	1.125802	2.925129	-0.000033
27	6	0	0.706718	4.272959	0.000457
28	6	0	-1.575398	5.494867	0.000874
29	6	0	1.125802	-2.925129	-0.000033
30	6	0	0.706718	-4.272959	0.000457
31	6	0	-1.575398	-5.494867	0.000874
32	6	0	2.458231	2.412509	-0.000168
33	6	0	1.575398	5.494867	0.000874
34	6	0	2.458231	-2.412509	-0.000168
35	6	0	1.575398	-5.494867	0.000874
36	1	0	-1.385945	6.124125	-0.879269
37	1	0	-1.388452	6.121885	0.883162
38	1	0	-2.640711	5.246607	-0.000959
39	1	0	-1.385945	-6.124125	-0.879269
40	1	0	-2.640711	-5.246607	-0.000959
41	1	0	-1.388452	-6.121885	0.883162
42	6	0	2.877455	1.089927	-0.000235
43	6	0	2.877455	-1.089927	-0.000235
44	1	0	3.239400	3.165935	-0.000119
45	1	0	1.385945	6.124125	-0.879269
46	1	0	2.640711	5.246607	-0.000959
47	1	0	1.388452	6.121885	0.883162
48	1	0	3.239400	-3.165935	-0.000119
49	1	0	1.385945	-6.124125	-0.879269
50	1	0	1.388452	-6.121885	0.883162
51	1	0	2.640711	-5.246607	-0.000959
52	7	0	2.044480	0.000000	-0.000154
53	6	0	4.291957	0.680215	-0.000362
54	6	0	4.291957	-0.680215	-0.000362
55	6	0	5.454027	1.626131	-0.000422
56	6	0	5.454027	-1.626131	-0.000422
57	1	0	6.408743	1.092012	-0.000670
58	1	0	5.443557	2.279680	0.881987
59	1	0	5.443259	2.279960	-0.882622
60	1	0	6.408743	-1.092012	-0.000670
61	1	0	5.443259	-2.279960	-0.882622
62	1	0	5.443557	-2.279680	0.881987

Dipole moment (Debye):

X= 0.0000 Y= 0.0000 Z= 0.0016 Tot= 0.0016

Zero-point correction=	0.514479 (Hartree/Particle)
Thermal correction to Energy=	0.546896
Thermal correction to Enthalpy=	0.547840
Thermal correction to Gibbs Free Energy=	0.449030
Sum of electronic and zero-point Energies=	-1303.529949

Sum of electronic and thermal Energies=	-1303.497532
Sum of electronic and thermal Enthalpies=	-1303.496588
Sum of electronic and thermal Free Energies=	-1303.595398

H_2DPOMP
RB3LYP/6-31Gd (C_{2h})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.374170	1.634587	0.000000
2	6	0	-2.689835	1.263046	0.000000
3	6	0	-1.244411	3.005287	0.000000
4	6	0	-3.466564	2.477177	0.000000
5	6	0	-2.595901	3.549462	0.000000
6	6	0	-3.233866	-0.019213	0.000000
7	6	0	0.010792	3.652884	0.000000
8	6	0	-2.653143	-1.291803	0.000000
9	6	0	1.250274	2.960800	0.000000
10	6	0	0.009713	5.153077	0.000000
11	6	0	-4.967718	2.495574	0.000000
12	6	0	-3.015622	4.992452	0.000000
13	7	0	-1.331117	-1.595384	0.000000
14	7	0	1.331117	1.595384	0.000000
15	6	0	-3.473859	-2.503460	0.000000
16	6	0	2.608805	3.560264	0.000000
17	6	0	0.004727	5.869313	1.205361
18	6	0	0.004727	5.869313	-1.205361
19	6	0	-1.250274	-2.960800	0.000000
20	6	0	2.653143	1.291803	0.000000
21	6	0	-2.608805	-3.560264	0.000000
22	6	0	3.473859	2.503460	0.000000
23	6	0	-4.974417	-2.513093	0.000000
24	6	0	3.016475	5.006539	0.000000
25	6	0	-0.004727	7.265438	1.207002
26	6	0	-0.004727	7.265438	-1.207002
27	6	0	-0.010792	-3.652884	0.000000
28	6	0	3.233866	0.019213	0.000000
29	6	0	-3.016475	-5.006539	0.000000
30	6	0	4.974417	2.513093	0.000000
31	6	0	-0.009713	7.967433	0.000000
32	6	0	1.244411	-3.005287	0.000000
33	6	0	2.689835	-1.263046	0.000000
34	6	0	-0.009713	-5.153077	0.000000

35	7	0	1.374170	-1.634587	0.000000
36	6	0	2.595901	-3.549462	0.000000
37	6	0	3.466564	-2.477177	0.000000
38	6	0	-0.004727	-5.869313	-1.205361
39	6	0	-0.004727	-5.869313	1.205361
40	6	0	3.015622	-4.992452	0.000000
41	6	0	4.967718	-2.495574	0.000000
42	6	0	0.004727	-7.265438	1.207002
43	6	0	0.004727	-7.265438	-1.207002
44	6	0	0.009713	-7.967433	0.000000
45	1	0	-0.543114	1.040376	0.000000
46	1	0	-4.318696	-0.022254	0.000000
47	1	0	-5.362771	3.513686	0.000000
48	1	0	-5.376105	1.987262	0.882543
49	1	0	-5.376105	1.987262	-0.882543
50	1	0	-4.105655	5.071870	0.000000
51	1	0	-2.645159	5.531108	-0.877082
52	1	0	-2.645159	5.531108	0.877082
53	1	0	0.008945	5.323506	2.145427
54	1	0	0.008945	5.323506	-2.145427
55	1	0	-5.376750	-3.529301	0.000000
56	1	0	-5.382404	-2.002614	-0.882288
57	1	0	-5.382404	-2.002614	0.882288
58	1	0	4.106854	5.093797	0.000000
59	1	0	2.643983	5.545149	0.876813
60	1	0	2.643983	5.545149	-0.876813
61	1	0	-0.008145	7.804400	2.150999
62	1	0	-0.008145	7.804400	-2.150999
63	1	0	4.318696	0.022254	0.000000
64	1	0	-4.106854	-5.093797	0.000000
65	1	0	-2.643983	-5.545149	0.876813
66	1	0	-2.643983	-5.545149	-0.876813
67	1	0	5.376750	3.529301	0.000000
68	1	0	5.382404	2.002614	-0.882288
69	1	0	5.382404	2.002614	0.882288
70	1	0	-0.017227	9.054158	0.000000
71	1	0	0.543114	-1.040376	0.000000
72	1	0	-0.008945	-5.323506	-2.145427
73	1	0	-0.008945	-5.323506	2.145427
74	1	0	4.105655	-5.071870	0.000000
75	1	0	2.645159	-5.531108	-0.877082
76	1	0	2.645159	-5.531108	0.877082
77	1	0	5.362771	-3.513686	0.000000
78	1	0	5.376105	-1.987262	0.882543
79	1	0	5.376105	-1.987262	-0.882543
80	1	0	0.008145	-7.804400	2.150999
81	1	0	0.008145	-7.804400	-2.150999
82	1	0	0.017227	-9.054158	0.000000

Dipole moment (Debye):
X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Zero-point correction=	0.681978 (Hartree/Particle)
Thermal correction to Energy=	0.722211
Thermal correction to Enthalpy=	0.723155
Thermal correction to Gibbs Free Energy=	0.609698
Sum of electronic and zero-point Energies=	-1765.494696
Sum of electronic and thermal Energies=	-1765.454463
Sum of electronic and thermal Enthalpies=	-1765.453519
Sum of electronic and thermal Free Energies=	-1765.566976

H_2DPOMP
UB3LYP/6-31Gd (C_2)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.265864	0.062224	-0.095689
2	6	0	-2.672851	1.308000	-0.194915
3	6	0	-2.732418	-1.249629	0.080300
4	7	0	-1.339241	1.597723	-0.056217
5	7	0	-1.415997	-1.614438	-0.020218
6	6	0	-3.449801	2.527982	-0.430596
7	6	0	-3.473867	-2.420469	0.344724
8	6	0	-1.236277	2.961169	-0.147842
9	6	0	-1.273142	-2.972838	0.151897
10	6	0	-2.567604	3.566053	-0.421072
11	6	0	-2.567604	-3.500728	0.410731
12	6	0	-4.932864	2.553701	-0.650621
13	6	0	-4.958015	-2.519466	0.546182
14	6	0	-0.007544	3.636524	0.014397
15	6	0	0.007544	-3.636524	0.014397
16	6	0	-2.914951	5.000342	-0.704378
17	6	0	-2.999192	-4.904265	0.736529
18	6	0	1.273142	2.972838	0.151897
19	6	0	1.236277	-2.961169	-0.147842
20	6	0	0.017236	5.130047	0.042047
21	6	0	-0.017236	-5.130047	0.042047
22	7	0	1.415997	1.614438	-0.020218
23	7	0	1.339241	-1.597723	-0.056217
24	6	0	2.567604	3.500728	0.410731
25	6	0	2.567604	-3.566053	-0.421072
26	6	0	-0.416488	5.831299	1.177257
27	6	0	0.493917	5.859829	-1.057442

28	6	0	-0.493917	-5.859829	-1.057442
29	6	0	0.416488	-5.831299	1.177257
30	6	0	2.732418	1.249629	0.080300
31	6	0	2.672851	-1.308000	-0.194915
32	6	0	3.473867	2.420469	0.344724
33	6	0	3.449801	-2.527982	-0.430596
34	6	0	2.999192	4.904265	0.736529
35	6	0	2.914951	-5.000342	-0.704378
36	6	0	-0.374932	7.226113	1.212659
37	6	0	0.523144	7.254310	-1.028365
38	6	0	-0.523144	-7.254310	-1.028365
39	6	0	0.374932	-7.226113	1.212659
40	6	0	3.265864	-0.062224	-0.095689
41	6	0	4.958015	2.519466	0.546182
42	6	0	4.932864	-2.553701	-0.650621
43	6	0	0.091637	7.941795	0.108344
44	6	0	-0.091637	-7.941795	0.108344
45	1	0	-4.349364	0.074802	-0.152602
46	1	0	-0.606734	-1.008453	-0.134699
47	1	0	-5.301929	3.566212	-0.833237
48	1	0	-5.474462	2.165518	0.222553
49	1	0	-5.226129	1.935791	-1.509275
50	1	0	-5.417977	-3.220037	-0.162500
51	1	0	-5.458937	-1.555549	0.422122
52	1	0	-5.205798	-2.879170	1.553942
53	1	0	-3.931453	5.072625	-1.102761
54	1	0	-2.240080	5.446635	-1.440716
55	1	0	-2.864527	5.633079	0.187960
56	1	0	-3.959691	-4.882512	1.262075
57	1	0	-2.284733	-5.426348	1.376045
58	1	0	-3.135557	-5.524812	-0.158420
59	1	0	0.606734	1.008453	-0.134699
60	1	0	-0.781066	5.274331	2.036313
61	1	0	0.836629	5.325547	-1.939620
62	1	0	-0.836629	-5.325547	-1.939620
63	1	0	0.781066	-5.274331	2.036313
64	1	0	3.959691	4.882512	1.262075
65	1	0	2.284733	5.426348	1.376045
66	1	0	3.135557	5.524812	-0.158420
67	1	0	3.931453	-5.072625	-1.102761
68	1	0	2.240080	-5.446635	-1.440716
69	1	0	2.864527	-5.633079	0.187960
70	1	0	-0.708560	7.753264	2.102771
71	1	0	0.884985	7.804533	-1.893145
72	1	0	-0.884985	-7.804533	-1.893145
73	1	0	0.708560	-7.753264	2.102771
74	1	0	4.349364	-0.074802	-0.152602
75	1	0	5.417977	3.220037	-0.162500
76	1	0	5.458937	1.555549	0.422122

77	1	0	5.205798	2.879170	1.553942
78	1	0	5.301929	-3.566212	-0.833237
79	1	0	5.474462	-2.165518	0.222553
80	1	0	5.226129	-1.935791	-1.509275
81	1	0	0.119915	9.027842	0.133366
82	1	0	-0.119915	-9.027842	0.133366

Dipole moment (Debye):
X= 0.0000 Y= 0.0000 Z= -0.3216 Tot= 0.3216

Zero-point correction=	0.678032 (Hartree/Particle)
Thermal correction to Energy=	0.718817
Thermal correction to Enthalpy=	0.719761
Thermal correction to Gibbs Free Energy=	0.604468
Sum of electronic and zero-point Energies=	-1765.441453
Sum of electronic and thermal Energies=	-1765.400669
Sum of electronic and thermal Enthalpies=	-1765.399725
Sum of electronic and thermal Free Energies=	-1765.515017

ZnDPOMP
RB3LYP/6-31Gd (D_{2h})

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	30	0	0.000000	0.000000	0.000000
2	7	0	-1.489656	1.410842	0.000000
3	7	0	-1.489656	-1.410842	0.000000
4	7	0	1.489656	1.410842	0.000000
5	7	0	1.489656	-1.410842	0.000000
6	6	0	-2.862477	1.254851	0.000000
7	6	0	-1.250835	2.759113	0.000000
8	6	0	-2.862477	-1.254851	0.000000
9	6	0	1.250835	2.759113	0.000000
10	6	0	-1.250835	-2.759113	0.000000
11	6	0	2.862477	1.254851	0.000000
12	6	0	1.250835	-2.759113	0.000000
13	6	0	2.862477	-1.254851	0.000000
14	6	0	-3.513402	0.000000	0.000000
15	6	0	0.000000	3.364095	0.000000
16	6	0	0.000000	-3.364095	0.000000
17	6	0	3.513402	0.000000	0.000000
18	6	0	-3.504970	2.582766	0.000000

19	6	0	-2.487499	3.501617	0.000000
20	6	0	-3.504970	-2.582766	0.000000
21	6	0	2.487499	3.501617	0.000000
22	6	0	-2.487499	-3.501617	0.000000
23	6	0	3.504970	2.582766	0.000000
24	6	0	2.487499	-3.501617	0.000000
25	6	0	3.504970	-2.582766	0.000000
26	6	0	-4.962260	2.956001	0.000000
27	6	0	-2.561068	5.000963	0.000000
28	6	0	-4.962260	-2.956001	0.000000
29	6	0	2.561068	5.000963	0.000000
30	6	0	-2.561068	-5.000963	0.000000
31	6	0	4.962260	2.956001	0.000000
32	6	0	2.561068	-5.000963	0.000000
33	6	0	4.962260	-2.956001	0.000000
34	6	0	-5.015132	0.000000	0.000000
35	6	0	5.015132	0.000000	0.000000
36	6	0	-5.731350	0.000000	1.204912
37	6	0	-7.127474	0.000000	1.207067
38	6	0	-7.829525	0.000000	0.000000
39	6	0	-7.127474	0.000000	-1.207067
40	6	0	-5.731350	0.000000	-1.204912
41	6	0	5.731350	0.000000	-1.204912
42	6	0	7.127474	0.000000	-1.207067
43	6	0	7.829525	0.000000	0.000000
44	6	0	7.127474	0.000000	1.207067
45	6	0	5.731350	0.000000	1.204912
46	1	0	0.000000	4.448406	0.000000
47	1	0	0.000000	-4.448406	0.000000
48	1	0	-5.068802	4.044060	0.000000
49	1	0	-5.493647	2.575386	0.876517
50	1	0	-5.493647	2.575386	-0.876517
51	1	0	-3.591603	5.363063	0.000000
52	1	0	-2.066579	5.427567	-0.882183
53	1	0	-2.066579	5.427567	0.882183
54	1	0	-5.068802	-4.044060	0.000000
55	1	0	-5.493647	-2.575386	-0.876517
56	1	0	-5.493647	-2.575386	0.876517
57	1	0	3.591603	5.363063	0.000000
58	1	0	2.066579	5.427567	0.882183
59	1	0	2.066579	5.427567	-0.882183
60	1	0	-3.591603	-5.363063	0.000000
61	1	0	-2.066579	-5.427567	0.882183
62	1	0	-2.066579	-5.427567	-0.882183
63	1	0	5.068802	4.044060	0.000000
64	1	0	5.493647	2.575386	-0.876517
65	1	0	5.493647	2.575386	0.876517
66	1	0	3.591603	-5.363063	0.000000
67	1	0	2.066579	-5.427567	-0.882183

68	1	0	2.066579	-5.427567	0.882183
69	1	0	5.068802	-4.044060	0.000000
70	1	0	5.493647	-2.575386	0.876517
71	1	0	5.493647	-2.575386	-0.876517
72	1	0	-5.185264	0.000000	2.144915
73	1	0	-7.666452	0.000000	2.151094
74	1	0	-8.916316	0.000000	0.000000
75	1	0	-7.666452	0.000000	-2.151094
76	1	0	-5.185264	0.000000	-2.144915
77	1	0	5.185264	0.000000	-2.144915
78	1	0	7.666452	0.000000	-2.151094
79	1	0	8.916316	0.000000	0.000000
80	1	0	7.666452	0.000000	2.151094
81	1	0	5.185264	0.000000	2.144915

Dipole moment (Debye):

X= 0.0000 Y= 0.0000 Z= 0.0000 Tot= 0.0000

Zero-point correction=	0.660109 (Hartree/Particle)
Thermal correction to Energy=	0.701256
Thermal correction to Enthalpy=	0.702200
Thermal correction to Gibbs Free Energy=	0.586705
Sum of electronic and zero-point Energies=	-3543.547980
Sum of electronic and thermal Energies=	-3543.506833
Sum of electronic and thermal Enthalpies=	-3543.505889
Sum of electronic and thermal Free Energies=	-3543.621384

ZnDPOMP

UB3LYP/6-31Gd (C_1)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.052350	3.374178	-0.276123
2	6	0	1.281434	2.730718	-0.419661
3	6	0	-1.190194	2.780754	-0.027635
4	1	0	0.064703	4.456891	-0.345331
5	7	0	1.495690	1.385990	-0.164697
6	7	0	-1.451867	1.451356	-0.106210
7	6	0	2.507310	3.367202	-0.788391
8	6	0	-2.381378	3.528265	0.345588
9	30	0	-0.000592	0.002716	-0.077030
10	6	0	2.837603	1.176962	-0.315662
11	6	0	-2.822116	1.299368	0.154418

12	6	0	3.492354	2.389092	-0.756792
13	6	0	-3.389214	2.621865	0.509017
14	6	0	2.638736	4.814428	-1.161826
15	6	0	-2.408121	5.015425	0.533471
16	7	0	1.450326	-1.447769	-0.097895
17	7	0	-1.496520	-1.381961	-0.170593
18	6	0	3.488210	-0.094091	0.028659
19	6	0	-3.489726	0.097859	0.018524
20	6	0	4.919463	2.607795	-1.181182
21	6	0	-4.760253	2.955132	1.025081
22	1	0	3.685496	5.116265	-1.254415
23	1	0	2.181803	5.466732	-0.406571
24	1	0	2.146655	5.039502	-2.117830
25	1	0	-3.395158	5.372257	0.839943
26	1	0	-2.148062	5.538903	-0.395872
27	1	0	-1.686384	5.338815	1.294492
28	6	0	2.819588	-1.295506	0.164127
29	6	0	1.187976	-2.776680	-0.023260
30	6	0	-1.281816	-2.726006	-0.428239
31	6	0	-2.837196	-1.172900	-0.328042
32	6	0	4.964824	-0.038525	0.253273
33	6	0	-4.964046	0.034830	0.256316
34	1	0	5.006033	3.553548	-1.724804
35	1	0	5.274175	1.819085	-1.850749
36	1	0	5.621830	2.647468	-0.340787
37	1	0	-4.748025	3.933998	1.514286
38	1	0	-5.110632	2.223403	1.756050
39	1	0	-5.515990	2.992225	0.232473
40	6	0	-0.052718	-3.370421	-0.279443
41	6	0	3.383771	-2.618386	0.521487
42	6	0	2.378116	-3.524663	0.354431
43	6	0	-2.505313	-3.362014	-0.803479
44	6	0	-3.490471	-2.382105	-0.773998
45	6	0	5.482906	0.577479	1.404170
46	6	0	5.865399	-0.573124	-0.680182
47	6	0	-5.877488	0.561229	-0.669773
48	6	0	-5.465588	-0.585362	1.412274
49	6	0	4.752604	-2.949095	1.046734
50	6	0	2.402913	-5.011094	0.544078
51	6	0	-2.636549	-4.808796	-1.177913
52	6	0	-4.915658	-2.595975	-1.205675
53	6	0	6.860962	0.639045	1.622514
54	6	0	7.241888	-0.502562	-0.469751
55	6	0	-7.251897	0.479287	-0.444827
56	6	0	-6.839799	-0.658324	1.645239
57	1	0	-0.064866	-4.453665	-0.352410
58	1	0	4.796953	1.004131	2.130855
59	1	0	5.474410	-1.040307	-1.580543
60	1	0	-5.499959	1.029027	-1.574845

61	1	0	-4.769476	-1.005525	2.132784
62	6	0	7.745381	0.101129	0.684821
63	6	0	-7.738487	-0.127609	0.715449
64	1	0	4.739329	-3.927183	1.538710
65	1	0	5.095994	-2.214284	1.779792
66	1	0	5.513818	-2.986927	0.261259
67	1	0	3.381555	-5.364189	0.878755
68	1	0	2.171616	-5.535897	-0.392109
69	1	0	1.658971	-5.335833	1.282845
70	1	0	-3.681658	-5.103902	-1.298634
71	1	0	-2.204619	-5.462589	-0.408216
72	1	0	-2.118089	-5.040144	-2.118372
73	1	0	-5.004333	-3.541221	-1.750204
74	1	0	-5.262534	-1.805733	-1.876023
75	1	0	-5.623793	-2.633238	-0.368856
76	1	0	7.242929	1.110039	2.524318
77	1	0	7.923066	-0.919271	-1.208198
78	1	0	-7.944323	0.886563	-1.177558
79	1	0	-7.210187	-1.130978	2.550959
80	1	0	8.816748	0.153570	0.851784
81	1	0	-8.808182	-0.189141	0.892782

Dipole moment (Debye):

X= 0.1271 Y= -0.6473 Z= -0.2477 Tot= 0.7047