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Supplementary Material for:

TDDFT AND STRUCTURAL INVESTIGATION OF NATURAL PHOTOSENSITIVE PHENANTHROPERYLENE QUINONE DERIVATIVES

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Table S1. TD-DFT transitions in various methods and basis sets for **1**.[a]

Method / Basis Set	Wavelength[b] (λ/nm)	Probability[b] (*f*)	Excitations
MPW1PW91/TZVP	390	0.32	HOMO → LUMO
	388	0.09	HOMO -1 → LUMO
BLYP/TZVP	479	0.10	HOMO -3 → LUMO
	470	0.23	HOMO → LUMO
mPW1PW91/cc-pVTZ	389	0.30	HOMO → LUMO
	387	0.13	HOMO -1 → LUMO
PBE1PBE/TZVP	390	0.32	HOMO → LUMO
	388	0.13	HOMO -1 → LUMO
ωB97/TZVP	321	0.39	HOMO → LUMO
	313	0.13	HOMO -1 → LUMO
TPSSh/TZVP	424	0.12	HOMO -1 → LUMO
	421	0.28	HOMO → LUMO
B3LYP/TZVP	405	0.30	HOMO → LUMO
	405	0.13	HOMO -1 → LUMO
M06-L/TZVP (DMSO)	437 (459)	0.11 (0.18)	HOMO -3 → LUMO
	433 (456)	0.27 (0.43)	HOMO → LUMO

M06L/TZVP+	437	0.12	HOMO -3 → LUMO
	433	0.28	HOMO → LUMO
M06L/TZV2P+	439	0.11	HOMO -3 → LUMO
	436	0.26	HOMO → LUMO
M06L/TZV2P+f	438	0.11	HOMO -3 → LUMO
	435	0.23	HOMO → LUMO
M06L/cc-pVTZ	437	0.11	HOMO -3 → LUMO
	433	0.26	HOMO → LUMO

Method / Basis Set	Wavelength[b] (λ/nm)	Probability[b] (*f*)	Excitations
M06-L/TZVP+	437	0.12	HOMO -3 → LUMO
	433	0.28	HOMO → LUMO
M06-L/TZV2P+	439	0.11	HOMO -3 → LUMO
	436	0.26	HOMO → LUMO
M06-L/TZV2P+f	438	0.11	HOMO -3 → LUMO
	435	0.23	HOMO → LUMO
M06-L/cc-pVTZ	437	0.11	HOMO -3 → LUMO
	433	0.26	HOMO → LUMO
MPW1PW91/TZVP	390	0.32	HOMO → LUMO
	388	0.09	HOMO -1 → LUMO
B3LYP/TZVP	405	0.30	HOMO → LUMO
	405	0.13	HOMO -1 → LUMO
PBE0/TZVP	390	0.32	HOMO → LUMO
	388	0.13	HOMO -1 → LUMO
ωB97/TZVP	321	0.39	HOMO → LUMO
	313	0.13	HOMO -1 → LUMO
BLYP/TZVP	479	0.10	HOMO -3 → LUMO
	470	0.23	HOMO → LUMO
TPSSh/TZVP	424	0.12	HOMO -1 → LUMO
	421	0.28	HOMO → LUMO
LC-ωPBE/TZVP	316	0.40	HOMO → LUMO

	311	0.12	HOMO -1 → LUMO
CAM-B3LYP/cc-pVTZ	351	0.37	HOMO → LUMO
	345	0.14	HOMO -1 → LUMO

[a]Experimental λ_{max} = 423 and 410 nm in DMSO.[1] [b]Values in parentheses are for the IEF-PCM solvation model.

Table S2. Comparison of experimental UV-Vis bands to TD-DFT transitions (M06L/TZVP) for conformations of **6B** and **6C**.

	Wavelength (λ/nm)	Probability (*f*)	Excitations
6B Propeller	595	0.15	HOMO → LUMO
	519	0.19	HOMO -1 → LUMO
	349	0.03	HOMO → LUMO +2
6B Saddle	584	0.17	HOMO → LUMO
	512	0.19	HOMO -1 → LUMO
	349	0.05	HOMO → LUMO +2
6C Propeller	575	0.13	HOMO -1 → LUMO
	540	0.07	HOMO -2 → LUMO
	513	0.05	HOMO -3 → LUMO
	357	0.03	HOMO → LUMO +2
6C Saddle	595	0.14	HOMO → LUMO
	525	0.04	HOMO -2 → LUMO HOMO -1 → LUMO HOMO -3 → LUMO
	492	0.13	HOMO -2 → LUMO HOMO -1 → LUMO
	348	0.05	HOMO → LUMO +3

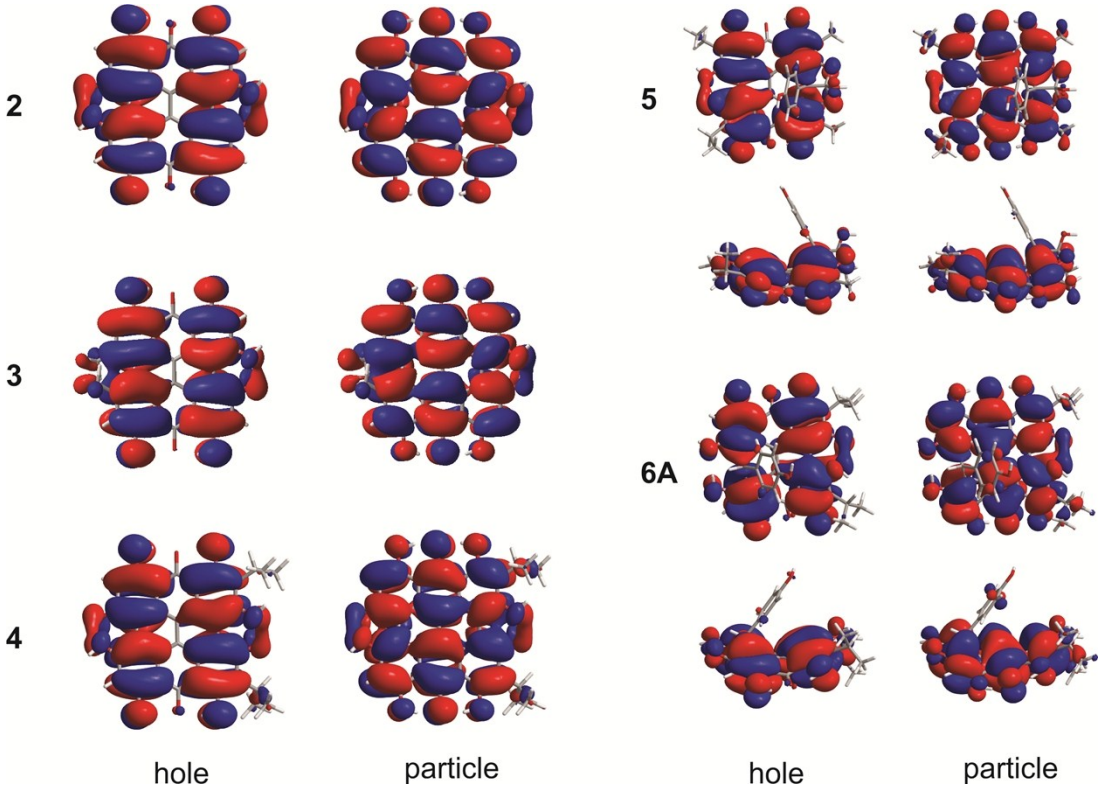

Figure S1. Natural transition orbitals for the first excited state of **2-5** and **6A**.

All Cartesian coordinates are optimized at the DFT(M06-L)/TZVP level. Structures generated by other functionals and basis sets are not significantly different.

Cartesian Coordinates for **1** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001155	1.470006	3.663997
2	6	0	-0.000720	0.724220	2.476837
3	6	0	0.000694	1.419467	1.242797
4	6	0	-0.000053	2.833128	1.254040
5	6	0	0.000669	3.530347	2.449945
6	6	0	0.001385	2.848350	3.655997
7	6	0	-0.001649	0.696574	-0.000007
8	6	0	-0.000669	3.606611	-0.000001

9	6	0	-0.000328	2.833136	-1.254066
10	6	0	0.000433	1.419501	-1.242816
11	6	0	-0.000868	0.724229	-2.476865
12	6	0	0.000328	1.470079	-3.663976
13	6	0	0.000293	2.848448	-3.655967
14	6	0	-0.000053	3.530408	-2.449948
15	1	0	0.001637	0.959119	4.617117
16	1	0	0.000533	4.612130	2.403064
17	1	0	0.002403	3.392743	4.591890
18	1	0	0.000383	0.959233	-4.617074
19	1	0	0.000741	3.392825	-4.591878
20	1	0	-0.000197	4.612187	-2.402989
21	6	0	0.000868	-0.724229	-2.476865
22	6	0	-0.000433	-1.419501	-1.242816
23	6	0	-0.000328	-1.470079	-3.663976
24	6	0	0.001649	-0.696574	-0.000007
25	6	0	0.000328	-2.833136	-1.254066
26	6	0	-0.000293	-2.848448	-3.655967
27	1	0	-0.000383	-0.959233	-4.617074
28	6	0	-0.000694	-1.419467	1.242797
29	6	0	0.000669	-3.606611	-0.000001
30	6	0	0.000053	-3.530408	-2.449948
31	1	0	-0.000741	-3.392825	-4.591878
32	6	0	0.000720	-0.724220	2.476837
33	6	0	0.000053	-2.833128	1.254040
34	1	0	0.000197	-4.612187	-2.402989
35	6	0	-0.001155	-1.470006	3.663997
36	6	0	-0.000669	-3.530347	2.449945
37	6	0	-0.001385	-2.848350	3.655997
38	1	0	-0.001637	-0.959119	4.617117
39	1	0	-0.000533	-4.612130	2.403064
40	1	0	-0.002403	-3.392743	4.591890
41	8	0	-0.002066	4.830826	0.000009
42	8	0	0.002066	-4.830826	0.000009

Cartesian Coordinates for **2** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.730079	2.449388	0.163055
2	6	0	0.681021	2.481909	-0.137837
3	6	0	1.404045	1.262178	-0.091744
4	6	0	0.701484	0.013007	0.004933

5	6	0	-0.701510	-0.013902	0.016381
6	6	0	-1.431834	1.215914	0.108239
7	6	0	1.431015	-1.215889	0.112007
8	6	0	0.730835	-2.450670	0.158942
9	6	0	-0.682056	-2.483210	-0.132666
10	6	0	-1.403002	-1.261840	-0.098569
11	6	0	-2.820300	-1.253021	-0.206005
12	6	0	-3.562959	-0.047900	-0.005448
13	6	0	-2.846417	1.178174	0.219976
14	6	0	-1.408627	-3.634466	-0.590954
15	6	0	-2.776433	-3.604461	-0.751598
16	6	0	-3.503928	-2.451524	-0.510456
17	6	0	-3.565323	2.357914	0.491265
18	6	0	-2.860710	3.530419	0.741686
19	6	0	-1.497180	3.561081	0.597590
20	6	0	2.819314	1.250175	-0.222289
21	6	0	3.562813	0.048689	-0.002906
22	6	0	2.846873	-1.180138	0.208459
23	6	0	3.565560	-2.357831	0.489295
24	6	0	2.861548	-3.530940	0.738989
25	6	0	1.497816	-3.561254	0.597398
26	6	0	1.408151	3.634818	-0.590290
27	6	0	2.775809	3.604488	-0.752368
28	6	0	3.503689	2.451603	-0.512347
29	8	0	-4.836102	-0.053411	-0.014945
30	8	0	4.835947	0.056245	-0.004520
31	8	0	-4.888851	2.402602	0.573743
32	8	0	-4.826461	-2.520033	-0.612902
33	8	0	4.888942	-2.401691	0.574128
34	8	0	4.826399	2.520879	-0.612471
35	8	0	0.835538	4.778093	-1.007818
36	8	0	-0.827623	4.706549	0.947637
37	1	0	0.046664	4.963749	-0.476643
38	1	0	-1.465803	5.346024	1.283824
39	1	0	5.203347	-1.479534	0.368978
40	1	0	5.167464	1.613725	-0.404041
41	1	0	-5.167419	-1.612166	-0.407125
42	1	0	-5.203427	1.481352	0.365076
43	1	0	3.405682	-4.411582	1.059282
44	1	0	3.282170	4.501710	-1.077812
45	1	0	-3.404766	4.412165	1.059103
46	1	0	-3.282474	-4.500268	-1.081357
47	1	0	-0.045703	-4.962188	-0.479372
48	1	0	1.466490	-5.345932	1.284039
49	8	0	-0.836281	-4.777758	-1.008360
50	8	0	0.828500	-4.706889	0.946710

Cartesian Coordinates for **2** in gas phase (PBE0).

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.463963	-0.687130	0.171574
2	6	0	-2.471726	0.731266	-0.105830
3	6	0	-1.238146	1.423151	-0.088452
4	6	0	-0.000386	0.698899	0.021616
5	6	0	0.000386	-0.698899	0.021616
6	6	0	-1.245550	-1.406631	0.101045
7	6	0	1.245550	1.406631	0.101045
8	6	0	2.463963	0.687130	0.171574
9	6	0	2.471726	-0.731266	-0.105830
10	6	0	1.238146	-1.423151	-0.088452
11	6	0	1.202249	-2.838356	-0.199559
12	6	0	-0.020425	-3.556037	-0.038748
13	6	0	-1.232290	-2.821086	0.193428
14	6	0	3.618450	-1.486903	-0.535679
15	6	0	3.561355	-2.853342	-0.695121
16	6	0	2.383747	-3.553419	-0.489172
17	6	0	-2.420054	-3.531851	0.434752
18	6	0	-3.583909	-2.814192	0.694383
19	6	0	-3.588589	-1.447193	0.591874
20	6	0	-1.202249	2.838356	-0.199559
21	6	0	0.020425	3.556037	-0.038748
22	6	0	1.232290	2.821086	0.193428
23	6	0	2.420054	3.531851	0.434752
24	6	0	3.583909	2.814192	0.694383
25	6	0	3.588589	1.447193	0.591874
26	6	0	-3.618450	1.486903	-0.535679
27	6	0	-3.561355	2.853342	-0.695121
28	6	0	-2.383747	3.553419	-0.489172
29	8	0	-0.042815	-4.826732	-0.074095
30	8	0	0.042815	4.826732	-0.074095
31	8	0	-2.471726	-4.850969	0.478122
32	8	0	2.406707	-4.871148	-0.596232
33	8	0	2.471726	4.850969	0.478122
34	8	0	-2.406707	4.871148	-0.596232
35	8	0	-4.783327	0.939556	-0.906068
36	8	0	-4.720975	-0.774511	0.957431
37	1	0	-4.984028	0.171408	-0.344236
38	1	0	-5.373028	-1.397581	1.294457
39	1	0	1.544171	5.165069	0.268550

40	1	0	-1.477818	5.182524	-0.418022
41	1	0	1.477818	-5.182524	-0.418022
42	1	0	-1.544171	-5.165069	0.268550
43	1	0	4.474701	3.358219	0.991567
44	1	0	-4.454734	3.380762	-1.002247
45	1	0	-4.474701	-3.358219	0.991567
46	1	0	4.454734	-3.380762	-1.002247
47	1	0	4.984028	-0.171408	-0.344236
48	1	0	5.373028	1.397581	1.294457
49	8	0	4.783327	-0.939556	-0.906068
50	8	0	4.720975	0.774511	0.957431

Cartesian Coordinates for the excited state of **2** (td-dft(PBE0))

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.470381	-0.692805	0.185912
2	6	0	-2.480483	0.715394	-0.118364
3	6	0	-1.230750	1.418345	-0.091891
4	6	0	-0.000850	0.707745	0.028822
5	6	0	0.000850	-0.707745	0.028822
6	6	0	-1.230750	-1.410290	0.112023
7	6	0	1.230750	1.410290	0.112023
8	6	0	2.470381	0.692805	0.185912
9	6	0	2.480483	-0.715394	-0.118364
10	6	0	1.230750	-1.418345	-0.091891
11	6	0	1.206513	-2.828378	-0.179107
12	6	0	-0.012400	-3.552267	-0.031729
13	6	0	-1.218693	-2.821606	0.184973
14	6	0	3.622989	-1.467579	-0.553662
15	6	0	3.571997	-2.841216	-0.708251
16	6	0	2.402348	-3.541637	-0.484097
17	6	0	-2.419613	-3.540313	0.434340
18	6	0	-3.584061	-2.833651	0.694121
19	6	0	-3.588701	-1.456906	0.598197
20	6	0	-1.206513	2.828378	-0.179107
21	6	0	0.012400	3.552267	-0.031729
22	6	0	1.218693	2.821606	0.184973
23	6	0	2.419613	3.540313	0.434340
24	6	0	3.584061	2.833651	0.694121
25	6	0	3.588701	1.456906	0.598197
26	6	0	-3.622989	1.467579	-0.553662
27	6	0	-3.571997	2.841216	-0.708251
28	6	0	-2.402348	3.541637	-0.484097

29	8	0	-0.025151	-4.835324	-0.062034
30	8	0	0.025151	4.835324	-0.062034
31	8	0	-2.439267	-4.854330	0.469395
32	8	0	2.409036	-4.855287	-0.578926
33	8	0	2.439267	4.854330	0.469395
34	8	0	-2.409036	4.855287	-0.578926
35	8	0	-4.786662	0.919243	-0.922567
36	8	0	-4.731432	-0.792952	0.947580
37	1	0	-4.983450	0.145728	-0.365704
38	1	0	-5.382203	-1.421577	1.276784
39	1	0	1.492534	5.147533	0.260179
40	1	0	-1.468474	5.155684	-0.390420
41	1	0	1.468474	-5.155684	-0.390420
42	1	0	-1.492534	-5.147533	0.260179
43	1	0	4.476795	3.380819	0.977926
44	1	0	-4.466841	3.366529	-1.014062
45	1	0	-4.476795	-3.380819	0.977926
46	1	0	4.466841	-3.366529	-1.014062
47	1	0	4.983450	-0.145728	-0.365704
48	1	0	5.382203	1.421577	1.276784
49	8	0	4.786662	-0.919243	-0.922567
50	8	0	4.731432	0.792952	0.947580

Cartesian Coordinates for **3** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.720452	-2.470418	-0.154503
2	6	0	0.695951	-2.494716	0.138417
3	6	0	1.413204	-1.269377	0.095057
4	6	0	0.703056	-0.027474	0.002516
5	6	0	-0.699213	-0.012047	-0.012562
6	6	0	-1.426734	-1.238652	-0.105886
7	6	0	1.421147	1.207694	-0.110077
8	6	0	0.716588	2.433999	-0.183687
9	6	0	-0.677586	2.445819	0.177854
10	6	0	-1.400020	1.231435	0.104102
11	6	0	-2.813552	1.238874	0.204959
12	6	0	-3.561817	0.034024	-0.015013
13	6	0	-2.843628	-1.195309	-0.220268
14	6	0	-1.352118	3.583125	0.710787
15	6	0	-2.725056	3.567325	0.835422
16	6	0	-3.479979	2.443533	0.506010

17	6	0	-3.561442	-2.377080	-0.489132
18	6	0	-2.856211	-3.551876	-0.724141
19	6	0	-1.491253	-3.583315	-0.580278
20	6	0	2.829002	-1.239256	0.224402
21	6	0	3.563184	-0.025230	0.016535
22	6	0	2.833150	1.193831	-0.208863
23	6	0	3.517885	2.386511	-0.508194
24	6	0	2.780204	3.522945	-0.838414
25	6	0	1.408462	3.562172	-0.713330
26	6	0	1.437890	-3.642401	0.580224
27	6	0	2.806191	-3.597683	0.737589
28	6	0	3.523655	-2.434923	0.509187
29	8	0	-4.832858	0.053727	-0.030750
30	8	0	4.834508	-0.015981	0.035905
31	8	0	-4.884777	-2.419883	-0.580540
32	8	0	-4.805075	2.537324	0.575681
33	8	0	4.844049	2.461053	-0.576001
34	8	0	4.846755	-2.490861	0.613116
35	8	0	0.881287	-4.795791	0.992778
36	8	0	-0.827210	-4.732437	-0.925320
37	1	0	0.086388	-4.982886	0.471351
38	1	0	-1.468561	-5.373879	-1.251874
39	1	0	5.180700	1.556041	-0.349877
40	1	0	5.177854	-1.576548	0.417411
41	1	0	-5.157631	1.638996	0.353203
42	1	0	-5.200792	-1.496274	-0.390486
43	1	0	3.315932	4.374015	-1.241620
44	1	0	3.322080	-4.491915	1.056264
45	1	0	-3.399665	-4.435869	-1.036128
46	1	0	-3.246352	4.426699	1.239676
47	6	0	-0.631109	4.756000	1.306027
48	1	0	0.443025	4.604424	1.369284
49	1	0	-0.811987	5.679829	0.755697
50	1	0	-1.002054	4.921146	2.318109
51	6	0	0.706643	4.749446	-1.304034
52	1	0	-0.369464	4.614036	-1.372366
53	1	0	0.897926	5.667661	-0.747889
54	1	0	1.082915	4.915460	-2.313943

Cartesian Coordinates for **4** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.733045	-0.407507	-0.086612
2	6	0	1.497553	1.006415	0.091808
3	6	0	0.181756	1.514678	-0.035375
4	6	0	-0.932339	0.618003	-0.060377
5	6	0	-0.708207	-0.759589	0.073919
6	6	0	0.626417	-1.281538	0.026524
7	6	0	-2.264941	1.126745	-0.217186
8	6	0	-3.372168	0.240458	-0.179364
9	6	0	-3.141978	-1.120461	0.245014
10	6	0	-1.820996	-1.643641	0.243151
11	6	0	-1.578464	-3.022830	0.476442
12	6	0	-0.258475	-3.571169	0.312440
13	6	0	0.828897	-2.685011	0.028907
14	6	0	-4.132274	-1.997470	0.755649
15	6	0	-3.907024	-3.325388	1.016579
16	6	0	-2.644993	-3.875544	0.820468
17	6	0	2.118524	-3.206172	-0.214520
18	6	0	3.183787	-2.366652	-0.558108
19	6	0	2.978402	-0.991918	-0.498600
20	6	0	-0.040384	2.913692	-0.070039
21	6	0	-1.352606	3.428517	-0.356058
22	6	0	-2.444678	2.512390	-0.478071
23	6	0	-3.730035	2.994129	-0.814350
24	6	0	-4.773927	2.096922	-0.960467
25	6	0	-4.615692	0.757630	-0.676224
26	6	0	2.483012	1.953082	0.478024
27	6	0	2.303089	3.324362	0.477394
28	6	0	1.031013	3.804548	0.128351
29	8	0	-0.073022	-4.827304	0.423269
30	8	0	-1.535842	4.682054	-0.498287
31	8	0	2.352473	-4.517118	-0.177053
32	8	0	-2.502626	-5.180060	1.020634
33	8	0	-3.981789	4.279112	-1.040821
34	8	0	0.869709	5.124116	0.054909
35	8	0	3.672500	1.434006	0.927234
36	8	0	3.994480	-0.244718	-0.980077
37	1	0	4.225370	2.152565	1.257166
38	1	0	4.071678	0.570190	-0.460181
39	1	0	-3.127143	4.758165	-0.891495
40	1	0	-0.089245	5.268364	-0.184373
41	1	0	-1.544550	-5.377315	0.839165
42	1	0	1.490960	-4.947675	0.070647
43	1	0	-5.733243	2.444222	-1.315612
44	1	0	-4.703113	-3.959896	1.388241
45	8	0	-5.363552	-1.471879	1.057614
46	1	0	-5.904653	-2.164052	1.454564

47	8	0	-5.672895	0.000622	-1.021119
48	1	0	-5.742940	-0.761653	-0.426191
49	6	0	4.521403	-2.934211	-0.981576
50	6	0	4.412423	-3.796172	-2.237582
51	6	0	5.211728	-3.683995	0.157069
52	1	0	5.146131	-2.077259	-1.230113
53	1	0	3.960571	-3.241370	-3.060543
54	1	0	5.404035	-4.117211	-2.560115
55	1	0	3.812775	-4.687608	-2.059779
56	1	0	5.321458	-3.051811	1.039224
57	1	0	4.655919	-4.574039	0.446322
58	1	0	6.210427	-3.996384	-0.152272
59	6	0	3.391747	4.315578	0.836454
60	6	0	4.613549	4.237394	-0.079727
61	6	0	3.778998	4.278451	2.316263
62	1	0	2.943419	5.294009	0.666370
63	1	0	4.322935	4.278713	-1.128613
64	1	0	5.284549	5.073994	0.115898
65	1	0	5.206907	3.328477	0.052453
66	1	0	2.901907	4.363052	2.956606
67	1	0	4.303788	3.366316	2.619037
68	1	0	4.449584	5.105213	2.551855

Cartesian Coordinates for **5** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.600483	1.177007	-0.139677
2	6	0	1.785752	-0.252403	-0.136421
3	6	0	0.730722	-1.056435	-0.624563
4	6	0	-0.618366	-0.592220	-0.519512
5	6	0	-0.845351	0.775439	-0.278664
6	6	0	0.281715	1.670955	-0.331728
7	6	0	-1.653699	-1.606411	-0.720793
8	6	0	-2.876701	-1.564344	-0.056238
9	6	0	-3.226143	0.704813	0.495513
10	6	0	-2.167064	1.380333	-0.116431
11	6	0	-2.374420	2.711193	-0.562081
12	6	0	-1.249813	3.547370	-0.881804
13	6	0	0.070250	3.045647	-0.621200
14	6	0	-4.506554	1.268902	0.457086
15	6	0	-4.747356	2.517904	-0.068341
16	6	0	-3.678006	3.264082	-0.553143

17	6	0	1.173341	3.923266	-0.711829
18	6	0	2.475388	3.481814	-0.457780
19	6	0	2.674140	2.129693	-0.212508
20	6	0	1.012880	-2.344700	-1.137429
21	6	0	-0.016774	-3.090356	-1.818399
22	6	0	-1.376780	-2.718335	-1.562628
23	6	0	-2.425137	-3.611696	-1.900963
24	6	0	-3.701142	-3.419647	-1.390784
25	6	0	-3.920208	-2.416285	-0.465346
26	6	0	2.934278	-0.985240	0.278948
27	6	0	3.241766	-2.261787	-0.160111
28	6	0	2.299110	-2.886173	-1.000967
29	8	0	-1.435637	4.734942	-1.298754
30	8	0	0.276460	-4.109524	-2.517251
31	8	0	1.016794	5.204648	-1.040692
32	8	0	-3.938751	4.494558	-0.988575
33	8	0	-2.225578	-4.660727	-2.700390
34	8	0	2.631337	-4.048080	-1.564775
35	8	0	3.727652	-0.367645	1.217108
36	8	0	3.969134	1.768363	-0.175916
37	1	0	4.446270	-0.971013	1.451594
38	1	0	4.080808	0.971097	0.370638
39	1	0	-1.255641	-4.690202	-2.886565
40	1	0	1.833805	-4.335078	-2.088458
41	1	0	-3.063661	4.882788	-1.249963
42	1	0	0.048764	5.329897	-1.229219
43	1	0	-4.503850	-4.084600	-1.675617
44	1	0	-5.741241	2.948382	-0.086342
45	8	0	-5.522499	0.503644	0.971103
46	1	0	-6.351148	0.988582	0.892119
47	8	0	-5.165193	-2.319767	0.051682
48	1	0	-5.281939	-1.458828	0.483695
49	6	0	-3.029335	-0.640416	1.114245
50	1	0	-3.939252	-0.902810	1.657776
51	6	0	-1.892614	-0.747028	2.123803
52	6	0	-1.290959	-1.979024	2.376441
53	6	0	-1.420715	0.360754	2.816306
54	6	0	-0.230515	-2.100467	3.255152
55	1	0	-1.641733	-2.860279	1.849962
56	6	0	-0.355288	0.257143	3.697033
57	1	0	-1.867331	1.333127	2.642289
58	6	0	0.254891	-0.973046	3.907831
59	1	0	0.239127	-3.058815	3.434961
60	1	0	0.014137	1.138897	4.211048
61	8	0	1.323641	-1.133631	4.739594
62	1	0	1.548767	-0.275822	5.114347

63	6	0	3.618041	4.472246	-0.530109
64	6	0	4.468635	4.283636	-1.784597
65	6	0	4.471918	4.508031	0.734617
66	1	0	3.142074	5.449809	-0.616112
67	1	0	3.856630	4.334576	-2.685751
68	1	0	5.223136	5.069082	-1.852402
69	1	0	4.983916	3.323915	-1.778442
70	1	0	3.856213	4.628956	1.626939
71	1	0	5.064751	3.603370	0.852668
72	1	0	5.159126	5.354470	0.692843
73	6	0	4.517037	-2.979858	0.231265
74	6	0	4.245495	-4.277291	0.989244
75	6	0	5.447682	-3.197136	-0.961142
76	1	0	5.082856	-2.342706	0.927206
77	1	0	3.745710	-5.001848	0.350043
78	1	0	5.181572	-4.719905	1.331110
79	1	0	3.616037	-4.104286	1.862543
80	1	0	5.665922	-2.259061	-1.471970
81	1	0	6.392619	-3.627698	-0.627796
82	1	0	5.001174	-3.877811	-1.681993

Cartesian Coordinates for **6A** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.567552	-0.701862	-0.188456
2	6	0	-2.617949	0.737039	-0.250885
3	6	0	-1.414596	1.475008	-0.434438
4	6	0	-0.145901	0.802146	-0.386067
5	6	0	-0.132835	-0.603696	-0.555354
6	6	0	-1.371544	-1.322462	-0.624688
7	6	0	1.045451	1.645520	-0.381007
8	6	0	2.288189	1.218096	0.034952
9	6	0	2.303894	-1.091126	-0.273184
10	6	0	1.064441	-1.406885	-0.776864
11	6	0	1.013122	-2.602405	-1.547137
12	6	0	-0.252217	-3.256228	-1.722279
13	6	0	-1.396024	-2.672114	-1.072465
14	6	0	3.474189	-1.694716	-0.714733
15	6	0	3.490392	-2.769950	-1.574722
16	6	0	2.214513	-3.247702	-1.937033
17	6	0	-2.573993	-3.424629	-0.918314
18	6	0	-3.640287	-2.924240	-0.160075

19	6	0	-3.605820	-1.598392	0.241252
20	6	0	-1.463832	2.875148	-0.705341
21	6	0	-0.268494	3.625407	-1.014776
22	6	0	0.999732	2.987000	-0.855783
23	6	0	2.203989	3.720791	-1.045436
24	6	0	3.476259	3.175039	-0.795868
25	6	0	3.458133	1.914721	-0.241996
26	6	0	-3.828206	1.473319	-0.363295
27	6	0	-3.902099	2.831632	-0.591615
28	6	0	-2.705710	3.535541	-0.766531
29	8	0	-0.344589	-4.359456	-2.346709
30	8	0	-0.342506	4.844750	-1.376015
31	8	0	-2.690039	-4.663936	-1.394685
32	8	0	2.193675	-4.360314	-2.674729
33	8	0	2.189712	4.977085	-1.494235
34	8	0	-2.815839	4.839058	-1.017143
35	8	0	-4.995690	0.764147	-0.309580
36	8	0	-4.550146	-1.260049	1.145777
37	1	0	-5.729810	1.362716	-0.495615
38	1	0	-4.806422	-0.334985	1.017671
39	1	0	1.235148	5.231593	-1.581094
40	1	0	-1.891473	5.158520	-1.212647
41	1	0	1.239482	-4.613123	-2.770854
42	1	0	-1.853173	-4.845796	-1.896225
43	8	0	4.587679	-1.099922	-0.190299
44	8	0	4.575651	1.211754	0.104675
45	6	0	2.613660	-0.049579	0.724379
46	6	0	1.996231	-0.219358	2.093703
47	6	0	1.914743	0.871765	2.956153
48	6	0	1.519480	-1.447561	2.532351
49	6	0	1.370956	0.748865	4.219076
50	1	0	2.282717	1.838004	2.627684
51	6	0	0.966136	-1.584988	3.795367
52	1	0	1.568373	-2.309538	1.876699
53	6	0	0.890457	-0.486456	4.642850
54	1	0	1.306879	1.596374	4.888421
55	1	0	0.588040	-2.547544	4.123927
56	8	0	0.355068	-0.557290	5.892058
57	1	0	0.065647	-1.461631	6.051392
58	6	0	4.168142	-0.040352	0.689989
59	8	0	4.756982	-0.190953	1.902924
60	1	0	5.713240	-0.176451	1.772812
61	6	0	4.713930	3.952790	-1.073244
62	1	0	4.761519	4.253077	-2.120763
63	1	0	4.737322	4.875267	-0.490861
64	1	0	5.602610	3.372575	-0.838346

65	6	0	4.726608	-3.446815	-2.050798
66	1	0	4.733275	-4.499168	-1.763769
67	1	0	4.789257	-3.428502	-3.139905
68	1	0	5.616209	-2.969976	-1.646693
69	6	0	-4.767558	-3.826304	0.237372
70	6	0	-4.460075	-4.617073	1.503276
71	1	0	-4.967298	-4.517082	-0.583030
72	1	0	-5.664282	-3.225900	0.389571
73	1	0	-5.291642	-5.268108	1.773365
74	1	0	-3.578298	-5.243873	1.366298
75	1	0	-4.271800	-3.948259	2.343592
76	6	0	-5.211453	3.560092	-0.684445
77	6	0	-5.736630	4.012763	0.673266
78	1	0	-5.968332	2.951501	-1.197850
79	1	0	-5.074846	4.426406	-1.330309
80	1	0	-6.685256	4.540147	0.576638
81	1	0	-5.889702	3.170805	1.350888
82	1	0	-5.026295	4.687232	1.149723

Cartesian Coordinates for **6B** propeller in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.435473	-0.559697	-0.099295
2	6	0	-2.493414	0.877599	-0.119606
3	6	0	-1.291448	1.613883	-0.286712
4	6	0	-0.029670	0.930108	-0.306549
5	6	0	-0.009513	-0.457764	-0.571474
6	6	0	-1.258386	-1.163240	-0.606887
7	6	0	1.149526	1.756279	-0.130994
8	6	0	2.329632	1.247317	0.360305
9	6	0	2.481941	-0.951675	-0.488847
10	6	0	1.186260	-1.227000	-0.945338
11	6	0	1.025558	-2.334556	-1.824061
12	6	0	-0.245796	-3.004788	-1.893511
13	6	0	-1.319642	-2.492536	-1.096197
14	6	0	3.572918	-1.477030	-1.194158
15	6	0	3.439229	-2.444415	-2.182106
16	6	0	2.156698	-2.932906	-2.428374
17	6	0	-2.470869	-3.267176	-0.869548
18	6	0	-3.484654	-2.794818	-0.027539
19	6	0	-3.448068	-1.466049	0.364584
20	6	0	-1.330097	3.028624	-0.464937

21	6	0	-0.122524	3.804682	-0.619884
22	6	0	1.129497	3.157653	-0.368183
23	6	0	2.312666	3.928374	-0.212767
24	6	0	3.520403	3.376136	0.254496
25	6	0	3.456959	2.034494	0.549989
26	6	0	-3.702999	1.621177	-0.187820
27	6	0	-3.769258	2.989576	-0.347117
28	6	0	-2.569765	3.692708	-0.509934
29	8	0	-0.391489	-4.070548	-2.571669
30	8	0	-0.174536	5.047950	-0.884461
31	8	0	-2.603720	-4.496332	-1.367187
32	8	0	2.041788	-3.968346	-3.263819
33	8	0	2.330706	5.238197	-0.465282
34	8	0	-2.676936	5.002975	-0.722797
35	8	0	-4.870934	0.910829	-0.158366
36	8	0	-4.364995	-1.129733	1.296752
37	1	0	-5.609889	1.525904	-0.242502
38	1	0	-4.614744	-0.202010	1.184864
39	1	0	1.407158	5.486773	-0.724066
40	1	0	-1.746491	5.338661	-0.845049
41	1	0	1.086008	-4.237614	-3.238314
42	1	0	-1.820196	-4.638635	-1.958039
43	8	0	4.483915	1.324358	1.116724
44	6	0	2.621469	-0.138700	0.779790
45	6	0	1.750041	-0.689288	1.905924
46	6	0	1.097060	0.159871	2.794182
47	6	0	1.627495	-2.061862	2.090008
48	6	0	0.315036	-0.339912	3.819377
49	1	0	1.184652	1.233991	2.673441
50	6	0	0.851009	-2.575934	3.113374
51	1	0	2.137606	-2.740963	1.416208
52	6	0	0.183929	-1.714598	3.978752
53	1	0	-0.203448	0.321243	4.501089
54	1	0	0.757155	-3.649429	3.240898
55	8	0	-0.605190	-2.159456	4.993940
56	1	0	-0.601568	-3.122109	4.986123
57	6	0	4.053681	0.011062	1.336409
58	6	0	4.727695	4.221700	0.452214
59	1	0	5.043846	4.675858	-0.488111
60	1	0	4.521650	5.047570	1.134518
61	1	0	5.553750	3.638313	0.850768
62	6	0	4.636454	-2.993927	-2.882200
63	1	0	4.343425	-3.755849	-3.598481
64	1	0	5.178864	-2.216653	-3.427624
65	1	0	5.342756	-3.462086	-2.188357
66	6	0	-4.561257	-3.715981	0.455311

67	6	0	-4.172387	-4.427817	1.746574
68	1	0	-4.767117	-4.453200	-0.321236
69	1	0	-5.474271	-3.142580	0.616694
70	1	0	-4.967356	-5.092938	2.084382
71	1	0	-3.273381	-5.029848	1.606593
72	1	0	-3.974762	-3.710030	2.543431
73	6	0	-5.073295	3.723377	-0.468193
74	6	0	-5.580646	3.807522	-1.903928
75	1	0	-4.933788	4.730042	-0.074566
76	1	0	-5.835999	3.272420	0.179624
77	1	0	-6.527959	4.343085	-1.958727
78	1	0	-4.861468	4.335012	-2.528976
79	1	0	-5.729324	2.818891	-2.341908
80	8	0	4.793673	-0.980405	-0.880260
81	1	0	5.478989	-1.517823	-1.294449
82	8	0	4.708961	-0.756843	1.959050

Cartesian Coordinates for **6B** saddle in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.402902	0.736400	-0.002327
2	6	0	2.365182	-0.704397	-0.000540
3	6	0	1.226808	-1.343753	-0.546199
4	6	0	-0.025873	-0.653940	-0.540719
5	6	0	-0.063178	0.743268	-0.361456
6	6	0	1.200225	1.438537	-0.312113
7	6	0	-1.184757	-1.514695	-0.688182
8	6	0	-2.370753	-1.234310	-0.059678
9	6	0	-2.561603	1.109361	-0.053367
10	6	0	-1.290524	1.550571	-0.455104
11	6	0	-1.197124	2.855113	-1.012094
12	6	0	0.079062	3.508229	-1.097723
13	6	0	1.246246	2.825113	-0.618782
14	6	0	-3.694589	1.791801	-0.517774
15	6	0	-3.630795	3.014020	-1.170024
16	6	0	-2.369566	3.577717	-1.349575
17	6	0	2.475642	3.517174	-0.576006
18	6	0	3.652486	2.868184	-0.207810
19	6	0	3.618708	1.502576	0.024964
20	6	0	1.309311	-2.683824	-1.012446
21	6	0	0.175328	-3.335813	-1.624340
22	6	0	-1.114498	-2.768016	-1.354719

23	6	0	-2.278875	-3.566522	-1.490059
24	6	0	-3.506173	-3.228310	-0.883962
25	6	0	-3.475535	-2.069299	-0.141768
26	6	0	3.363469	-1.602965	0.467031
27	6	0	3.484028	-2.910334	0.039163
28	6	0	2.495636	-3.410082	-0.822192
29	8	0	0.159306	4.702991	-1.532476
30	8	0	0.307303	-4.435935	-2.241691
31	8	0	2.580289	4.805913	-0.894878
32	8	0	-2.320916	4.801565	-1.877638
33	8	0	-2.248124	-4.729512	-2.145653
34	8	0	2.683898	-4.624792	-1.335795
35	8	0	4.217395	-1.144549	1.441813
36	8	0	4.843904	0.960458	0.151983
37	1	0	4.796699	-1.870245	1.708737
38	1	0	4.808404	0.148686	0.685951
39	1	0	-1.306277	-4.881005	-2.408384
40	1	0	1.856939	-4.838687	-1.844161
41	1	0	-1.359113	5.053900	-1.895632
42	1	0	1.680565	5.085713	-1.210027
43	8	0	-4.496696	-1.632730	0.662982
44	6	0	-2.659081	-0.104859	0.845416
45	6	0	-1.749510	0.006597	2.065957
46	6	0	-1.027718	-1.086548	2.535747
47	6	0	-1.649458	1.210806	2.753067
48	6	0	-0.194678	-0.977508	3.633806
49	1	0	-1.097202	-2.038255	2.020410
50	6	0	-0.824610	1.333032	3.857218
51	1	0	-2.216672	2.069114	2.411510
52	6	0	-0.083768	0.239995	4.295099
53	1	0	0.377789	-1.824507	3.988568
54	1	0	-0.749837	2.280566	4.380850
55	8	0	0.758925	0.303058	5.362147
56	1	0	0.731408	1.195484	5.722215
57	6	0	-4.071020	-0.483590	1.345538
58	6	0	-4.684970	-4.129889	-0.986515
59	1	0	-5.001814	-4.241345	-2.024728
60	1	0	-4.443292	-5.133270	-0.633072
61	1	0	-5.522405	-3.748336	-0.407991
62	6	0	-4.873003	3.711757	-1.613008
63	1	0	-4.631209	4.658644	-2.086576
64	1	0	-5.436774	3.115134	-2.336132
65	1	0	-5.543375	3.933328	-0.775957
66	6	0	4.948262	3.620341	-0.190300
67	6	0	5.651505	3.615563	-1.542437
68	1	0	5.601799	3.178320	0.561778

69	1	0	4.748500	4.649332	0.110260
70	1	0	6.587897	4.172203	-1.500144
71	1	0	5.881778	2.598608	-1.860079
72	1	0	5.026977	4.075024	-2.308657
73	6	0	4.640063	-3.777750	0.445251
74	6	0	5.894001	-3.515155	-0.381400
75	1	0	4.342408	-4.820654	0.340732
76	1	0	4.860164	-3.659094	1.515209
77	1	0	6.722004	-4.145990	-0.059567
78	1	0	5.704639	-3.721652	-1.433945
79	1	0	6.217737	-2.474706	-0.309991
80	8	0	-4.890152	1.185726	-0.321368
81	1	0	-5.604205	1.794537	-0.543172
82	8	0	-4.709727	-0.024495	2.232844

Cartesian Coordinates for **6C** saddle in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.373221	-0.613014	-0.345729
2	6	0	-2.418253	0.824852	-0.422686
3	6	0	-1.202654	1.539925	-0.575260
4	6	0	0.051780	0.855017	-0.449058
5	6	0	0.077654	-0.536950	-0.630262
6	6	0	-1.170519	-1.232986	-0.762246
7	6	0	1.238459	1.669068	-0.249518
8	6	0	2.369089	1.187751	0.409022
9	6	0	2.469028	-1.146522	-0.007989
10	6	0	1.290301	-1.358549	-0.745891
11	6	0	1.227883	-2.470637	-1.628843
12	6	0	-0.038356	-3.097627	-1.893673
13	6	0	-1.193582	-2.566021	-1.226381
14	6	0	3.642156	-1.835810	-0.410773
15	6	0	3.638006	-2.765728	-1.451684
16	6	0	2.417623	-3.130308	-2.009053
17	6	0	-2.360384	-3.331749	-1.085444
18	6	0	-3.428498	-2.844450	-0.321175
19	6	0	-3.412330	-1.511940	0.066646
20	6	0	-1.215480	2.929971	-0.868878
21	6	0	0.015158	3.647540	-1.080079
22	6	0	1.249256	3.004573	-0.734481
23	6	0	2.453414	3.747186	-0.738449
24	6	0	3.638918	3.182386	-0.268155

25	6	0	3.564475	1.920239	0.302023
26	6	0	-3.611751	1.577600	-0.578475
27	6	0	-3.653762	2.928613	-0.865466
28	6	0	-2.440262	3.606393	-1.018891
29	8	0	-0.128613	-4.153439	-2.593515
30	8	0	0.000998	4.853074	-1.490520
31	8	0	-2.458307	-4.565941	-1.583080
32	8	0	2.404998	-4.147470	-2.876833
33	8	0	2.508499	4.999631	-1.195647
34	8	0	-2.510214	4.903247	-1.320665
35	8	0	-4.790510	0.890558	-0.506769
36	8	0	-4.384398	-1.170387	0.941014
37	1	0	-5.515443	1.493234	-0.713667
38	1	0	-4.610427	-0.235711	0.829836
39	1	0	1.578813	5.242116	-1.446543
40	1	0	-1.571720	5.200302	-1.467561
41	1	0	1.452279	-4.367911	-3.031028
42	1	0	-1.631149	-4.712619	-2.109323
43	6	0	2.345095	-0.139089	1.131693
44	6	0	1.056242	-0.404731	1.962990
45	6	0	0.332277	0.635181	2.540844
46	6	0	0.618608	-1.707598	2.171517
47	6	0	-0.844714	0.393948	3.220407
48	1	0	0.679796	1.654905	2.427208
49	6	0	-0.559083	-1.965109	2.854248
50	1	0	1.180087	-2.536256	1.755698
51	6	0	-1.310410	-0.910837	3.360290
52	1	0	-1.423892	1.206906	3.638781
53	1	0	-0.903597	-2.986457	2.980767
54	8	0	-2.490581	-1.087474	4.009583
55	1	0	-2.727485	-2.020420	3.974848
56	6	0	4.935321	3.919968	-0.329323
57	1	0	4.797446	4.897643	-0.781046
58	1	0	5.364597	4.081589	0.664589
59	1	0	5.680597	3.387861	-0.928674
60	6	0	4.904567	-3.446039	-1.842315
61	1	0	4.714754	-4.224105	-2.575617
62	1	0	5.618085	-2.736372	-2.264714
63	1	0	5.395636	-3.885785	-0.973311
64	6	0	-4.543602	-3.755557	0.089006
65	6	0	-4.279218	-4.425146	1.432746
66	1	0	-4.669804	-4.519391	-0.678771
67	1	0	-5.471970	-3.186248	0.143886
68	1	0	-5.097157	-5.088838	1.713679
69	1	0	-3.365354	-5.020142	1.402302
70	1	0	-4.171970	-3.680043	2.222827

71	6	0	-4.946080	3.674708	-1.029429
72	6	0	-5.495165	4.214049	0.286239
73	1	0	-5.701483	3.051357	-1.526540
74	1	0	-4.777091	4.500996	-1.719265
75	1	0	-6.429462	4.754286	0.135117
76	1	0	-5.683691	3.415451	1.006080
77	1	0	-4.782704	4.900220	0.742283
78	8	0	4.856010	-1.645806	0.137542
79	1	0	4.751922	-1.404952	1.076854
80	8	0	4.683895	1.322405	0.783097
81	1	0	5.438651	1.910653	0.665349
82	6	0	3.338321	-0.192331	2.288400
83	8	0	4.055939	-1.122390	2.591513
84	8	0	3.228253	0.892524	3.070871
85	1	0	3.816155	0.738027	3.824434

Cartesian Coordinates for **6C** propeller in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.393836	-0.855719	0.064197
2	6	0	-2.676883	0.545636	-0.079588
3	6	0	-1.607961	1.439472	-0.341076
4	6	0	-0.248920	0.961779	-0.389260
5	6	0	-0.066317	-0.410718	-0.642885
6	6	0	-1.180887	-1.301808	-0.507031
7	6	0	0.786986	1.961063	-0.114328
8	6	0	1.998836	1.639344	0.517362
9	6	0	2.429081	-0.376848	-0.955246
10	6	0	1.171620	-0.966167	-1.178938
11	6	0	1.088230	-2.138351	-1.969862
12	6	0	-0.007523	-3.049373	-1.771366
13	6	0	-1.052977	-2.662728	-0.872605
14	6	0	3.450062	-0.704381	-1.876738
15	6	0	3.335921	-1.749057	-2.799546
16	6	0	2.194941	-2.534945	-2.758640
17	6	0	-2.010762	-3.593771	-0.437711
18	6	0	-3.020037	-3.208985	0.455182
19	6	0	-3.203742	-1.855959	0.693586
20	6	0	-1.883762	2.805060	-0.619013
21	6	0	-0.815177	3.760039	-0.711713
22	6	0	0.472964	3.341022	-0.240830
23	6	0	1.348622	4.328787	0.271514

24	6	0	2.353654	3.977843	1.173276
25	6	0	2.582356	2.622704	1.340421
26	6	0	-3.991657	1.077109	-0.172656
27	6	0	-4.283522	2.391066	-0.476058
28	6	0	-3.210886	3.256871	-0.718846
29	8	0	-0.019667	-4.194181	-2.323365
30	8	0	-1.033281	4.963547	-1.054277
31	8	0	-1.954260	-4.877394	-0.793941
32	8	0	2.164534	-3.640771	-3.508088
33	8	0	1.155376	5.632447	0.064189
34	8	0	-3.515261	4.512864	-1.042598
35	8	0	-5.022566	0.191781	-0.018972
36	8	0	-4.120977	-1.563373	1.642340
37	1	0	-5.856472	0.664296	-0.133293
38	1	0	-4.536767	-0.716204	1.430469
39	1	0	0.331288	5.711533	-0.477767
40	1	0	-2.646456	4.985643	-1.155986
41	1	0	1.321751	-4.106395	-3.277645
42	1	0	-1.226071	-4.940452	-1.464922
43	6	0	2.621830	0.261491	0.448980
44	6	0	2.029249	-0.689177	1.507023
45	6	0	1.164307	-0.230434	2.495419
46	6	0	2.319140	-2.052547	1.471627
47	6	0	0.595023	-1.094021	3.418937
48	1	0	0.886293	0.817816	2.527110
49	6	0	1.756686	-2.925144	2.381691
50	1	0	2.985038	-2.437908	0.708272
51	6	0	0.884705	-2.449469	3.359824
52	1	0	-0.091004	-0.731500	4.172709
53	1	0	1.987998	-3.984353	2.335230
54	8	0	0.294158	-3.264236	4.273484
55	1	0	0.553122	-4.173231	4.089494
56	6	0	3.078691	5.025514	1.943815
57	1	0	3.755770	5.585410	1.295198
58	1	0	2.384712	5.755354	2.360844
59	1	0	3.661554	4.586499	2.748439
60	6	0	4.463970	-2.055253	-3.723927
61	1	0	4.186369	-2.843522	-4.417696
62	1	0	4.756757	-1.169763	-4.288484
63	1	0	5.353379	-2.377139	-3.178525
64	6	0	-3.862064	-4.240846	1.137129
65	6	0	-3.236528	-4.713214	2.445369
66	1	0	-3.990747	-5.090039	0.465247
67	1	0	-4.849317	-3.823218	1.334836
68	1	0	-3.858880	-5.464606	2.931727
69	1	0	-2.255362	-5.157480	2.269950

70	1	0	-3.105727	-3.883267	3.140455
71	6	0	-5.689518	2.890363	-0.635530
72	6	0	-6.214996	2.750740	-2.060400
73	1	0	-5.714170	3.939650	-0.342101
74	1	0	-6.364359	2.387767	0.069379
75	1	0	-7.233486	3.128274	-2.146446
76	1	0	-5.589337	3.315067	-2.750494
77	1	0	-6.213730	1.711707	-2.394557
78	8	0	4.644483	-0.075823	-1.960065
79	1	0	4.630241	0.754668	-1.464855
80	8	0	3.423758	2.260144	2.356316
81	1	0	3.159247	1.389960	2.690721
82	6	0	4.143899	0.350566	0.745331
83	8	0	4.772304	-0.435318	1.393440
84	8	0	4.740916	1.438787	0.166859
85	1	0	5.665306	1.412320	0.458779

Cartesian Coordinates for **7** in gas phase.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.656695	1.466543	0.000001
2	6	0	-2.461547	0.718629	0.000000
3	6	0	-1.237188	1.422381	-0.000002
4	6	0	-1.239605	2.845840	-0.000002
5	6	0	-2.463508	3.545975	0.000000
6	6	0	-3.668529	2.831897	0.000002
7	6	0	0.000000	0.704574	-0.000003
8	6	0	0.000000	3.579395	-0.000004
9	6	0	1.239605	2.845840	-0.000002
10	6	0	1.237188	1.422381	-0.000002
11	6	0	2.461547	0.718629	0.000000
12	6	0	3.656695	1.466543	0.000001
13	6	0	3.668529	2.831897	0.000002
14	6	0	2.463508	3.545975	0.000000
15	1	0	-4.607982	0.952451	0.000003
16	1	0	-4.594907	3.390220	0.000003
17	1	0	4.607982	0.952451	0.000003
18	1	0	4.594907	3.390220	0.000003
19	6	0	2.461547	-0.718629	0.000000
20	6	0	1.237188	-1.422381	-0.000002
21	6	0	3.656695	-1.466543	0.000001
22	6	0	0.000000	-0.704574	-0.000003

23	6	0	1.239605	-2.845840	-0.000002
24	6	0	3.668529	-2.831897	0.000002
25	1	0	4.607982	-0.952451	0.000003
26	6	0	-1.237188	-1.422381	-0.000002
27	6	0	0.000000	-3.579395	-0.000004
28	6	0	2.463508	-3.545975	0.000000
29	1	0	4.594907	-3.390220	0.000003
30	6	0	-2.461547	-0.718629	0.000000
31	6	0	-1.239605	-2.845840	-0.000002
32	6	0	-3.656695	-1.466543	0.000001
33	6	0	-2.463508	-3.545975	0.000000
34	6	0	-3.668529	-2.831897	0.000002
35	1	0	-4.607982	-0.952451	0.000003
36	1	0	-4.594907	-3.390220	0.000003
37	8	0	0.000000	4.848922	0.000007
38	8	0	0.000000	-4.848922	0.000007
39	8	0	-2.539708	4.871895	0.000000
40	1	0	-1.605397	5.203985	-0.000004
41	8	0	2.539708	4.871895	0.000000
42	1	0	1.605397	5.203985	-0.000004
43	8	0	2.539708	-4.871895	0.000000
44	1	0	1.605397	-5.203985	-0.000004
45	8	0	-2.539708	-4.871895	0.000000
46	1	0	-1.605397	-5.203985	-0.000004
