"Active Sites in Graphene and the Mechanism of CO_2 Formation in Carbon Oxidation"

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Complete Reference 17:

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery Jr, J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. 2004.

Figure S1a.

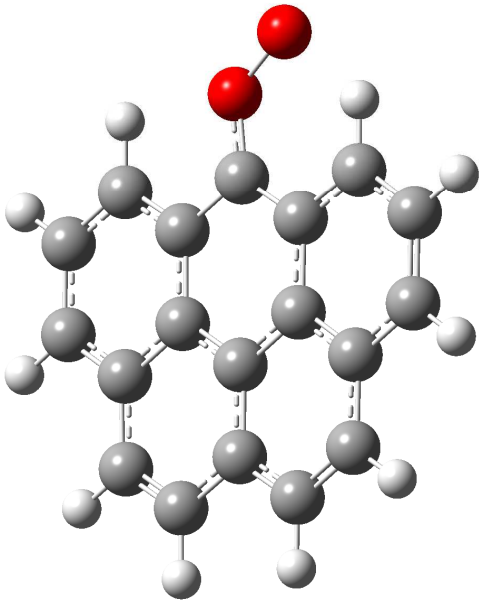

Figure S1b.

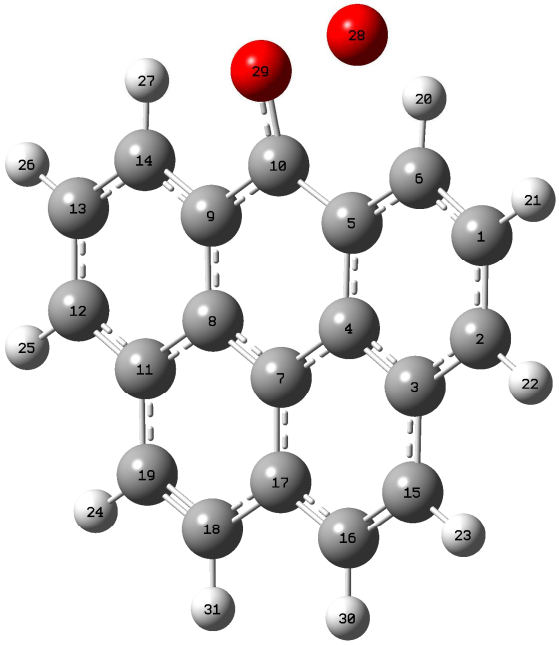

Figure S1. Adsorption of O_2 on a carbene site in graphene: (a) intermediate aryl-peroxy ground state, E = -880.4164 hartrees; (b) transition state, E = -880.3859 hartrees. The SCF energy of the triplet unbound state ($C_{19}H_{10}$+O_2) is -880.3286 hartrees.

Figure S2a.

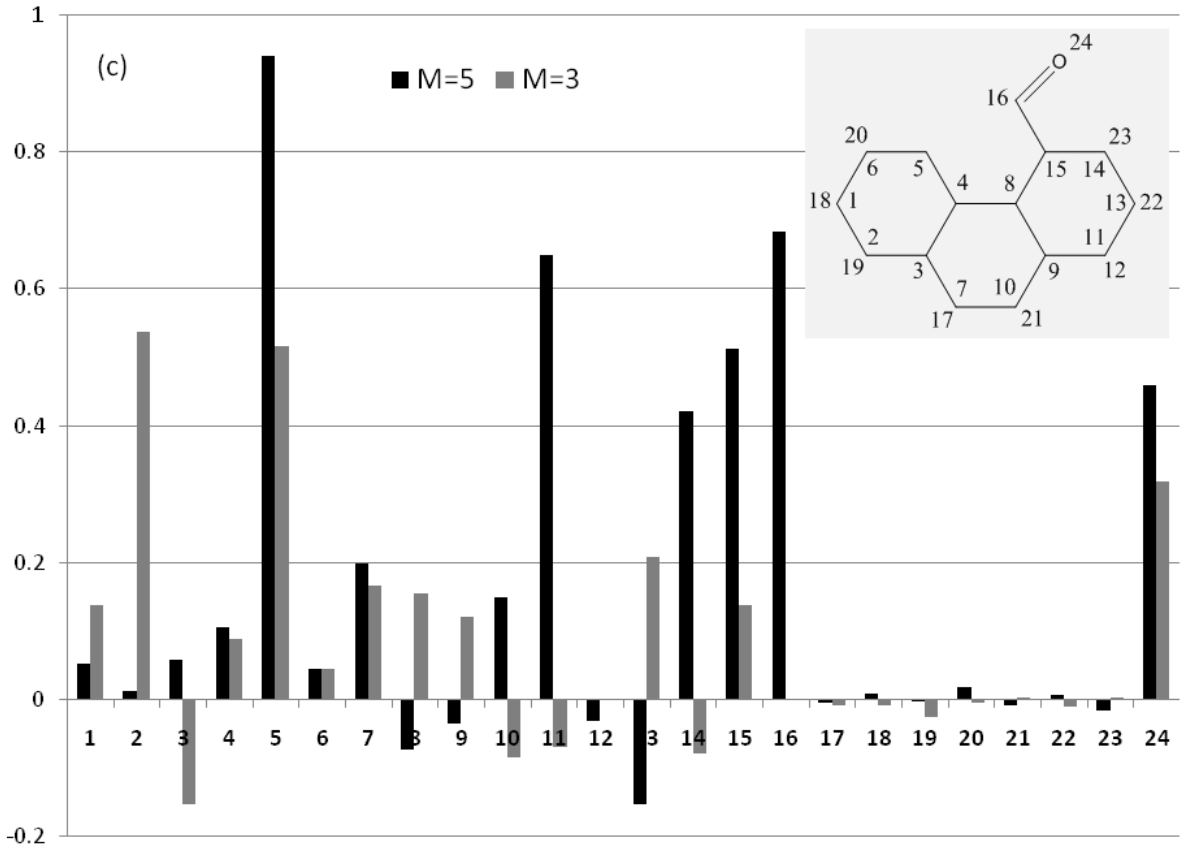
(c)
M=5
M=3
1
0.8
0.6
0.4
0.2
0
-0.2
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24
O
24
16
20
23
6
5
4
8
15
14
18
1
13
22
2
11
19
3
7
10
9
12
17
21

Figure S2b.

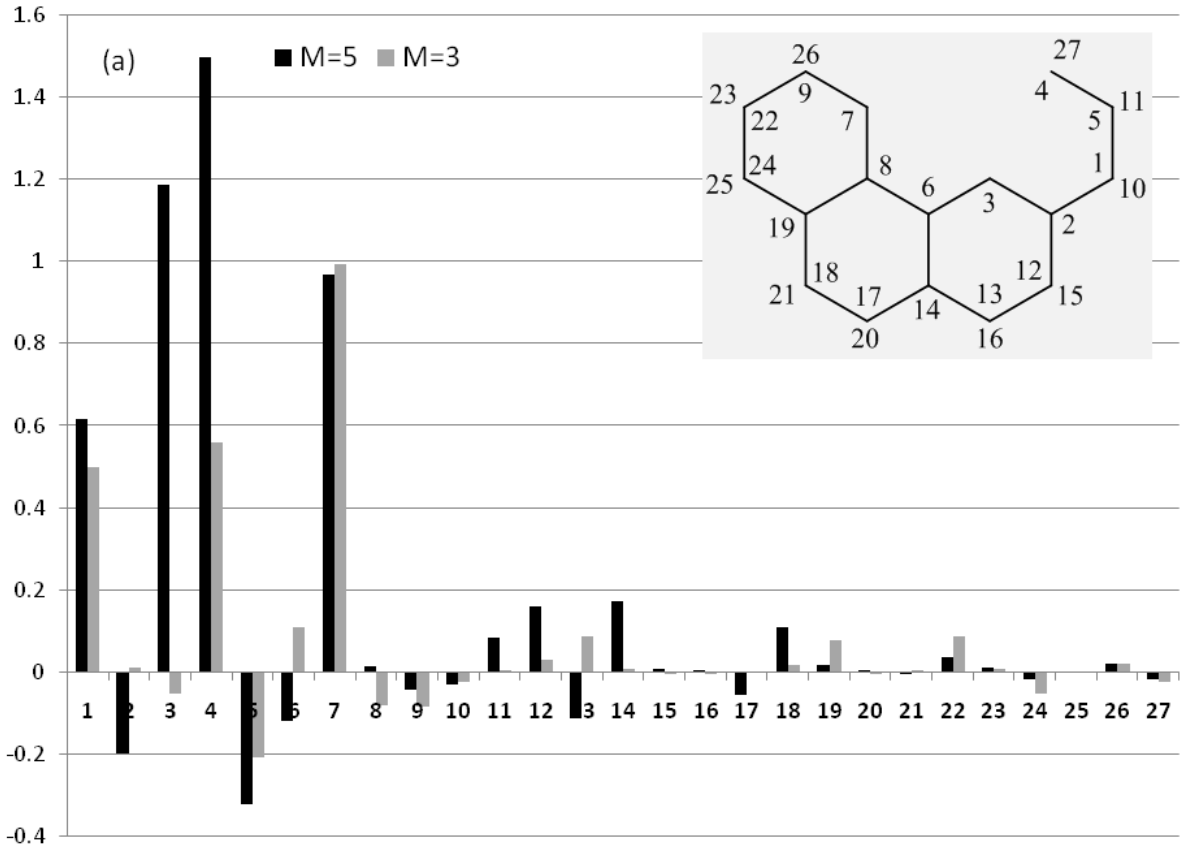
(a)
M=5
M=3
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27
26
27
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Figure S2c.

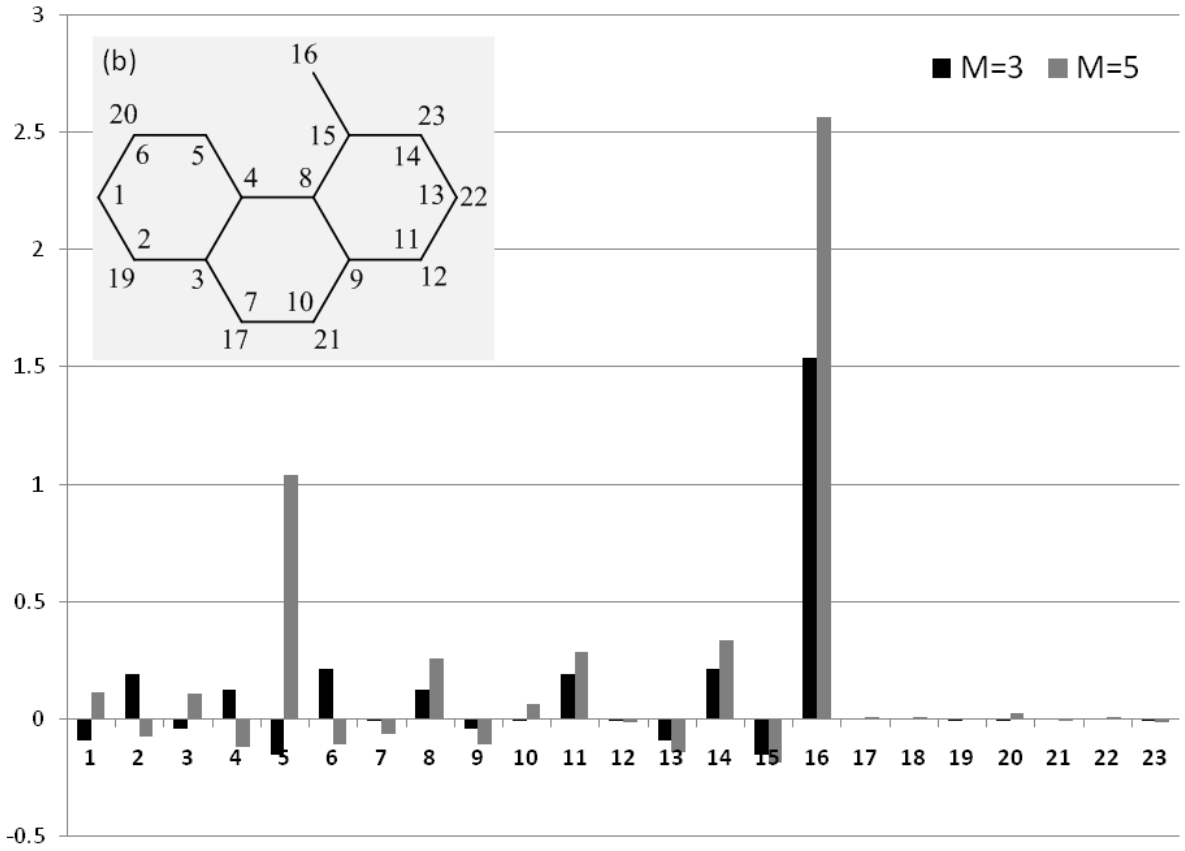

Figure S2. Distribution of Mulliken spin densities for the graphene clusters shown in Figures 9e, 9b and 9d: (a) $C_{15}H_8O$; (b) $C_{17}H_{10}$; (c) $C_{15}H_8$.

Figure S3.

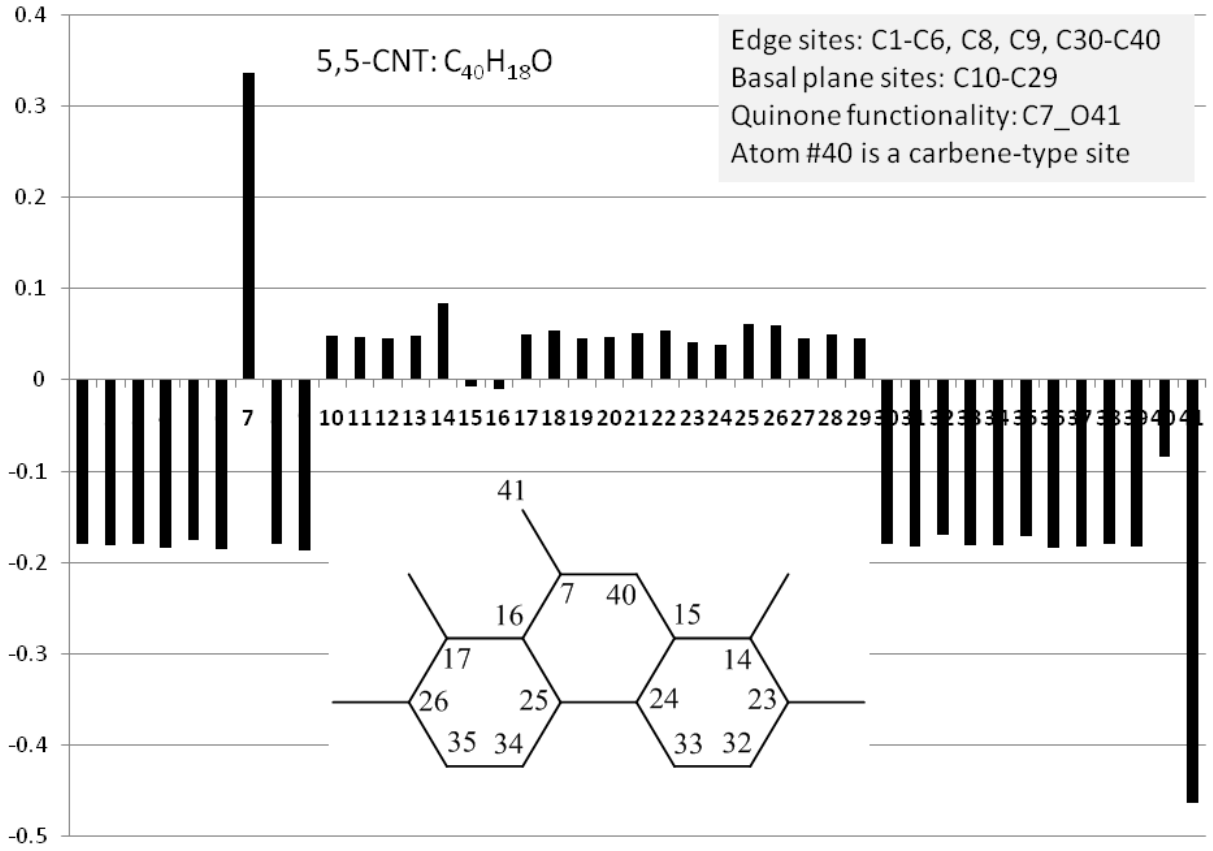

Figure S3. Mulliken population analysis of 5,5-CNT $C_{40}H_{18}O$ (M=1).

Figure 1a

$C_{22}H_{12}$, M=3 (E = -845.61199 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.995950	-3.012185	-0.000231
2	6	0	-1.652498	-3.378598	-0.000218
3	6	0	-0.628751	-2.393149	-0.000160
4	6	0	-1.004517	-1.009912	-0.000094
5	6	0	-2.389844	-0.641851	-0.000103
6	6	0	-3.369804	-1.670823	-0.000176
7	6	0	0.000041	-0.000023	-0.000002
8	6	0	-0.372462	1.374843	0.000037
9	6	0	-1.758299	1.741016	0.000022
10	6	0	-2.735134	0.724780	-0.000035
11	6	0	0.739816	-2.730847	-0.000119
12	6	0	1.750825	-1.748627	-0.000044
13	6	0	1.376922	-0.364864	0.000012
14	6	0	0.639089	2.390417	0.000105
15	6	0	0.237793	3.753558	0.000190
16	6	0	-1.110848	4.100448	0.000171
17	6	0	-2.099974	3.120280	0.000090
18	6	0	2.387094	0.652054	0.000091
19	6	0	1.995288	2.006096	0.000147
20	6	0	3.131997	-2.082659	0.000021
21	6	0	4.106831	-1.088294	0.000103
22	6	0	3.752435	0.258313	0.000138
23	1	0	-3.762303	-3.782810	-0.000276
24	1	0	-1.370542	-4.428286	-0.000257
25	1	0	-4.420922	-1.394354	-0.000183
26	1	0	-3.786528	1.003471	-0.000035
27	1	0	1.024088	-3.780768	-0.000154
28	1	0	1.002684	4.525750	0.000261
29	1	0	-1.394997	5.149466	0.000225
30	1	0	-3.150028	3.400802	0.000095
31	1	0	2.762267	2.777367	0.000230
32	1	0	3.418272	-3.131171	0.000045
33	1	0	5.157357	-1.366785	0.000162
34	1	0	4.520352	1.027464	0.000224

$C_{22}H_{10}$, M=5 (E = -844.23956 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.187083	4.015275	0.000005
2	6	0	2.157218	3.016174	0.000003
3	6	0	1.790109	1.643919	-0.000001

4	6	0	0.397089	1.304368	-0.000001
5	6	0	-0.595375	2.339947	-0.000002
6	6	0	-0.167767	3.694785	0.000002
7	6	0	-0.002015	-0.062384	-0.000004
8	6	0	-1.389439	-0.398839	-0.000007
9	6	0	-2.379002	0.637008	-0.000003
10	6	0	-1.958622	1.982692	-0.000002
11	6	0	2.750915	0.610916	-0.000002
12	6	0	2.385445	-0.748845	-0.000003
13	6	0	0.991436	-1.084103	-0.000002
14	6	0	-1.804828	-1.779091	0.000000
15	6	0	-3.189412	-2.087658	0.000005
16	6	0	-4.138244	-1.066105	0.000004
17	6	0	-3.752552	0.270629	0.000001
18	6	0	0.586476	-2.475262	-0.000015
19	6	0	-0.781262	-2.726914	-0.000003
20	6	0	3.354316	-1.795203	-0.000006
21	6	0	2.968965	-3.138634	0.000008
22	6	0	1.619995	-3.420967	0.000012
23	1	0	1.491608	5.058533	0.000008
24	1	0	3.212311	3.276918	0.000006
25	1	0	-0.917391	4.481648	0.000004
26	1	0	-2.710121	2.769004	0.000002
27	1	0	3.806202	0.874137	-0.000007
28	1	0	-3.494406	-3.129219	0.000007
29	1	0	-5.195214	-1.318338	0.000009
30	1	0	-4.503232	1.056565	0.000005
31	1	0	4.409579	-1.532944	0.000007
32	1	0	3.717494	-3.926548	0.000018

$C_{22}H_{10}$, M=3 (E = -844.22093 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.793811	3.794681	0.000055
2	6	0	2.600816	2.658996	0.000004
3	6	0	2.028950	1.356276	-0.000088
4	6	0	0.594894	1.232021	-0.000016
5	6	0	-0.228346	2.413654	-0.000007
6	6	0	0.406465	3.688635	0.000036
7	6	0	-0.005165	-0.048017	-0.000049
8	6	0	-1.423300	-0.180616	-0.000112
9	6	0	-2.236532	0.993017	0.000007
10	6	0	-1.623879	2.266634	0.000016
11	6	0	2.809429	0.188619	-0.000103
12	6	0	2.225699	-1.097800	-0.000018
13	6	0	0.800360	-1.223611	-0.000159
14	6	0	-2.014697	-1.485150	-0.000159
15	6	0	-3.418858	-1.568902	-0.000088
16	6	0	-4.230087	-0.423042	0.000181
17	6	0	-3.648395	0.833709	0.000136
18	6	0	0.161690	-2.518581	-0.000126

19	6	0	-1.276114	-2.734777	-0.000152
20	6	0	3.019436	-2.278542	0.000089
21	6	0	2.434553	-3.539630	0.000186
22	6	0	1.048850	-3.589255	0.000236
23	1	0	2.255406	4.778438	0.000161
24	1	0	3.683160	2.756181	0.000066
25	1	0	-0.212613	4.581734	0.000092
26	1	0	-2.249862	3.156396	0.000048
27	1	0	3.893540	0.278033	-0.000244
28	1	0	-3.850315	-2.565407	-0.000189
29	1	0	-5.312057	-0.520095	0.000295
30	1	0	-4.272796	1.724635	0.000158
31	1	0	4.103586	-2.181064	0.000163
32	1	0	3.044466	-4.438759	0.000230

$C_{22}H_{10}$, M=1 (E= -844.18767 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.176903	4.018691	-0.029917
2	6	0	2.148373	3.012580	-0.059514
3	6	0	1.784124	1.651255	-0.052007
4	6	0	0.392658	1.308737	-0.024457
5	6	0	-0.601011	2.347449	0.013071
6	6	0	-0.172577	3.702232	0.011266
7	6	0	-0.002375	-0.051891	-0.036354
8	6	0	-1.379622	-0.381842	-0.031494
9	6	0	-2.369413	0.646206	0.082593
10	6	0	-1.961335	1.990500	0.074105
11	6	0	2.739334	0.602600	-0.068480
12	6	0	2.366532	-0.739184	-0.033150
13	6	0	0.972366	-1.098134	-0.014193
14	6	0	-1.761107	-1.756013	-0.129290
15	6	0	-3.131492	-2.071301	-0.092572
16	6	0	-4.106756	-1.073836	0.082921
17	6	0	-3.737664	0.257721	0.150641
18	6	0	0.573845	-2.490629	-0.031479
19	6	0	-0.798036	-2.808283	-0.244931
20	6	0	3.333625	-1.783892	0.116297
21	6	0	2.935252	-3.098966	0.263846
22	6	0	1.621401	-3.458121	-0.070085
23	1	0	1.486116	5.060164	-0.029889
24	1	0	3.202407	3.276312	-0.087610
25	1	0	-0.920282	4.489274	0.061120
26	1	0	-2.713662	2.776288	0.083300
27	1	0	3.796185	0.860395	-0.061315
28	1	0	-3.409842	-3.117752	-0.172067
29	1	0	-5.156567	-1.347573	0.135744
30	1	0	-4.495547	1.031699	0.247191
31	1	0	4.390233	-1.518033	0.097108
32	1	0	3.682820	-3.866043	0.465517

$C_{22}H_8$, M=7 (E = -842.85429 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.087231	4.093738	0.000002
2	6	0	2.086555	3.156949	0.000000
3	6	0	1.747061	1.762924	-0.000001
4	6	0	0.362597	1.385400	-0.000001
5	6	0	-0.673035	2.390066	0.000001
6	6	0	-0.264590	3.737492	0.000003
7	6	0	0.000844	0.008543	-0.000002
8	6	0	-1.377326	-0.368134	-0.000003
9	6	0	-2.398907	0.635560	-0.000001
10	6	0	-2.026782	1.996010	0.000001
11	6	0	2.734565	0.761537	-0.000002
12	6	0	2.406312	-0.609557	-0.000001
13	6	0	1.023710	-0.983538	-0.000001
14	6	0	-1.750397	-1.760587	-0.000002
15	6	0	-3.124751	-2.111184	0.000000
16	6	0	-4.104738	-1.119964	0.000001
17	6	0	-3.760505	0.228029	0.000000
18	6	0	0.659455	-2.387165	-0.000002
19	6	0	-0.699844	-2.678137	-0.000001
20	6	0	3.405978	-1.625690	-0.000001
21	6	0	3.060096	-2.979739	0.000003
22	6	0	1.720171	-3.301387	0.000004
23	1	0	3.133936	3.452384	0.000000
24	1	0	-2.797658	2.761065	0.000003
25	1	0	3.782081	1.053000	-0.000008
26	1	0	-3.397480	-3.161666	0.000001
27	1	0	-5.153198	-1.405197	0.000003
28	1	0	-4.534210	0.991001	0.000001
29	1	0	4.452870	-1.332332	0.000008
30	1	0	3.831459	-3.745257	0.000004

$C_{22}H_8$, M=5 (E = -842.90221 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.136853	3.964630	0.000000
2	6	0	-2.224891	3.116932	0.000000
3	6	0	-1.797142	1.738266	0.000000
4	6	0	-0.390335	1.394759	-0.000001
5	6	0	0.655877	2.411601	-0.000001
6	6	0	0.083422	3.700008	0.000006
7	6	0	0.001473	0.024637	-0.000002
8	6	0	1.390322	-0.325029	-0.000004
9	6	0	2.397709	0.692300	-0.000002
10	6	0	2.005471	2.049152	-0.000001

11	6	0	-2.752257	0.701345	0.000001
12	6	0	-2.388612	-0.658962	-0.000001
13	6	0	-0.997246	-0.996372	-0.000004
14	6	0	1.792125	-1.710286	0.000001
15	6	0	3.172056	-2.036895	0.000004
16	6	0	4.135638	-1.030508	0.000003
17	6	0	3.765736	0.310312	0.000000
18	6	0	-0.601643	-2.390487	-0.000014
19	6	0	0.763127	-2.651467	0.000000
20	6	0	-3.364258	-1.698728	0.000000
21	6	0	-2.986698	-3.043911	0.000006
22	6	0	-1.639337	-3.331713	0.000002
23	1	0	-3.276381	3.383131	-0.000001
24	1	0	2.763674	2.826319	0.000001
25	1	0	-3.807715	0.962815	0.000002
26	1	0	3.461609	-3.082864	0.000007
27	1	0	5.188910	-1.297309	0.000005
28	1	0	4.524386	1.088264	0.000001
29	1	0	-4.417621	-1.429633	0.000005
30	1	0	-3.738975	-3.828211	0.000014

$C_{22}H_8$, M=3 (E = -842.88387 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.338643	3.910309	0.000081
2	6	0	2.385899	3.012729	0.000012
3	6	0	1.889955	1.653496	-0.000005
4	6	0	0.462226	1.377714	-0.000012
5	6	0	-0.534467	2.452453	-0.000025
6	6	0	0.106688	3.710388	0.000050
7	6	0	0.005066	0.039037	-0.000039
8	6	0	-1.394199	-0.253580	-0.000118
9	6	0	-2.343688	0.812011	-0.000016
10	6	0	-1.894677	2.154393	0.000008
11	6	0	2.781109	0.569439	-0.000007
12	6	0	2.335741	-0.770553	-0.000082
13	6	0	0.933454	-1.045906	-0.000125
14	6	0	-1.833976	-1.617522	-0.000061
15	6	0	-3.219103	-1.865358	0.000019
16	6	0	-4.159639	-0.824790	0.000126
17	6	0	-3.726873	0.490443	0.000098
18	6	0	0.441548	-2.402580	-0.000429
19	6	0	-0.962089	-2.776721	-0.000109
20	6	0	3.253850	-1.857401	-0.000159
21	6	0	2.810392	-3.174279	0.000257
22	6	0	1.438102	-3.371685	0.000294
23	1	0	3.449032	3.226912	0.000057
24	1	0	-2.616908	2.965400	0.000086
25	1	0	3.850154	0.769277	-0.000003
26	1	0	-3.528559	-2.906113	0.000000
27	1	0	-5.222827	-1.047220	0.000188

28	1	0	-4.449097	1.303845	0.000159
29	1	0	4.320738	-1.642020	0.000158
30	1	0	3.513694	-4.002293	0.000804

$C_{22}H_8$, M=1 (E = -842.84965 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.146559	3.959422	-0.016418
2	6	0	2.230788	3.102102	-0.044567
3	6	0	1.798414	1.739705	-0.061455
4	6	0	0.390916	1.397559	-0.030608
5	6	0	-0.652507	2.422601	0.014536
6	6	0	-0.072640	3.705830	-0.017119
7	6	0	-0.002872	0.035114	-0.042804
8	6	0	-1.383215	-0.301977	-0.032737
9	6	0	-2.386634	0.711126	0.086287
10	6	0	-2.002184	2.064800	0.077672
11	6	0	2.743671	0.682165	-0.073845
12	6	0	2.366684	-0.657517	-0.032232
13	6	0	0.974017	-1.013988	-0.017868
14	6	0	-1.757504	-1.678687	-0.134043
15	6	0	-3.124663	-2.010274	-0.094319
16	6	0	-4.108196	-1.025424	0.091675
17	6	0	-3.749681	0.309196	0.161435
18	6	0	0.579768	-2.408238	-0.031766
19	6	0	-0.789032	-2.720254	-0.258005
20	6	0	3.335861	-1.698478	0.123738
21	6	0	2.942000	-3.015391	0.265885
22	6	0	1.628599	-3.372984	-0.065241
23	1	0	3.283149	3.364996	-0.031460
24	1	0	-2.757847	2.844566	0.089108
25	1	0	3.801581	0.934306	-0.066857
26	1	0	-3.391128	-3.059101	-0.180604
27	1	0	-5.155127	-1.308863	0.148409
28	1	0	-4.513166	1.076706	0.263077
29	1	0	4.391643	-1.429426	0.108907
30	1	0	3.692015	-3.781634	0.460218

Figure 1b

$C_{19}H_{11}$, M=2 (E = -730.69409 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	2.435409	2.032997
2	6	0	0.000000	2.469374	0.603956

3	6	0	0.000000	1.235696	-0.108547
4	6	0	0.000000	0.000000	0.603026
5	6	0	0.000000	0.000000	2.029057
6	6	0	0.000000	1.247200	2.715888
7	6	0	0.000000	1.234440	-1.545342
8	6	0	0.000000	-1.235696	-0.108547
9	6	0	0.000000	-1.234440	-1.545342
10	6	0	0.000000	0.000000	-2.228967
11	6	0	0.000000	-2.478314	-2.223404
12	6	0	0.000000	-3.677392	-1.516482
13	6	0	0.000000	-3.682747	-0.122811
14	6	0	0.000000	-2.469374	0.603956
15	6	0	0.000000	-2.435409	2.032997
16	6	0	0.000000	-1.247200	2.715888
17	1	0	0.000000	-1.241709	3.803460
18	1	0	0.000000	-3.378207	2.574766
19	1	0	0.000000	3.378207	2.574766
20	1	0	0.000000	1.241709	3.803460
21	1	0	0.000000	-4.619659	-2.058137
22	1	0	0.000000	-4.623510	0.421932
23	6	0	0.000000	3.682747	-0.122811
24	6	0	0.000000	3.677392	-1.516482
25	6	0	0.000000	2.478314	-2.223404
26	1	0	0.000000	4.623510	0.421932
27	1	0	0.000000	4.619659	-2.058137
28	1	0	0.000000	0.000000	-3.316771
29	1	0	0.000000	2.484185	-3.310514
30	1	0	0.000000	-2.484185	-3.310514

$C_{19}H_{10}$, M=3 (E = -730.00855 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.687016	-1.543774	0.000004
2	6	0	3.687869	-0.150407	0.000004
3	6	0	2.474261	0.576425	0.000001
4	6	0	1.240862	-0.135304	-0.000002
5	6	0	1.250676	-1.579410	-0.000001
6	6	0	2.492052	-2.259727	0.000000
7	6	0	0.000000	0.571619	-0.000004
8	6	0	-1.240861	-0.135303	-0.000002
9	6	0	-1.250676	-1.579410	-0.000001
10	6	0	0.000000	-2.197487	-0.000011
11	6	0	-2.474260	0.576426	0.000001
12	6	0	-3.687870	-0.150408	0.000004
13	6	0	-3.687016	-1.543774	0.000005
14	6	0	-2.492052	-2.259727	0.000002
15	6	0	2.436745	2.005781	0.000001
16	6	0	1.247045	2.685478	0.000000
17	6	0	0.000000	1.997053	-0.000003
18	6	0	-1.247045	2.685478	-0.000002
19	6	0	-2.436745	2.005780	-0.000001

20	1	0	4.631792	-2.080618	0.000004
21	1	0	4.627792	0.395524	0.000007
22	1	0	2.496222	-3.345240	-0.000002
23	1	0	-4.627791	0.395525	0.000006
24	1	0	-4.631792	-2.080618	0.000006
25	1	0	-2.496223	-3.345239	0.000000
26	1	0	3.378306	2.549532	0.000005
27	1	0	1.239696	3.772878	0.000002
28	1	0	-1.239697	3.772878	-0.000001
29	1	0	-3.378306	2.549531	0.000000

$C_{19}H_{10}O$, M=1 (E = -805.33417 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.693454	-1.310331	0.000056
2	6	0	3.686329	0.074625	0.000049
3	6	0	2.470678	0.795936	0.000010
4	6	0	1.241229	0.075462	-0.000029
5	6	0	1.266027	-1.345596	-0.000070
6	6	0	2.482395	-2.019283	0.000022
7	6	0	-0.000038	0.792038	-0.000046
8	6	0	-1.241255	0.075384	-0.000032
9	6	0	-1.265965	-1.345700	-0.000068
10	6	0	0.000021	-2.127547	-0.000250
11	6	0	-2.470720	0.795828	0.000003
12	6	0	-3.686354	0.074497	0.000049
13	6	0	-3.693439	-1.310467	0.000067
14	6	0	-2.482377	-2.019373	0.000032
15	6	0	2.435941	2.226657	0.000016
16	6	0	1.248459	2.902246	0.000004
17	6	0	-0.000058	2.203671	-0.000019
18	6	0	-1.248592	2.902207	-0.000007
19	6	0	-2.436042	2.226557	0.000001
20	1	0	4.636106	-1.850147	0.000081
21	1	0	4.623128	0.627134	0.000094
22	1	0	2.465734	-3.104586	0.000001
23	1	0	-4.623162	0.626986	0.000091
24	1	0	-4.636075	-1.850312	0.000104
25	1	0	-2.465674	-3.104672	0.000016
26	1	0	3.377738	2.769899	0.000051
27	1	0	1.234886	3.989313	0.000029
28	1	0	-1.235049	3.989274	0.000011
29	1	0	-3.377870	2.769740	0.000024
30	8	0	0.000258	-3.357937	0.000096

Figure 2a

$C_{19}H_{10}OH$, M=2 (E = -805.90904 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.689471	-1.272249	-0.027516
2	6	0	-3.683677	0.118394	-0.001996
3	6	0	-2.462613	0.831751	0.007496
4	6	0	-1.231609	0.111549	0.003083
5	6	0	-1.244169	-1.326358	-0.006497
6	6	0	-2.495988	-1.989997	-0.033593
7	6	0	0.004205	0.822579	0.002484
8	6	0	1.236652	0.105770	-0.005812
9	6	0	1.242070	-1.326714	-0.000049
10	6	0	-0.000668	-2.013071	0.010645
11	6	0	2.473267	0.815688	-0.010792
12	6	0	3.685144	0.088622	-0.013815
13	6	0	3.677743	-1.303761	-0.006850
14	6	0	2.478736	-2.012507	0.002019
15	6	0	-2.423415	2.260270	0.016859
16	6	0	-1.233741	2.939768	0.016122
17	6	0	0.009205	2.247627	0.006763
18	6	0	1.258072	2.931714	0.000265
19	6	0	2.443192	2.245157	-0.009142
20	8	0	0.072480	-3.375939	0.029115
21	1	0	-4.634374	-1.808421	-0.048730
22	1	0	-4.619311	0.671219	0.002721
23	1	0	-2.553673	-3.075578	-0.083268
24	1	0	4.626302	0.632568	-0.019094
25	1	0	4.619134	-1.846822	-0.006999
26	1	0	2.479714	-3.096262	0.010161
27	1	0	-3.365317	2.803248	0.022229
28	1	0	-1.224329	4.027196	0.021094
29	1	0	1.255080	4.019180	0.002425
30	1	0	3.388216	2.782842	-0.013910
31	1	0	-0.808883	-3.747048	0.182394

$C_{19}H_{10}O_2$, M=1 (E = -880.43281 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.700329	-1.117530	-0.000023
2	6	0	-3.691632	0.265727	-0.000022
3	6	0	-2.474032	0.982253	-0.000003
4	6	0	-1.244244	0.259340	0.000013
5	6	0	-1.277298	-1.157977	0.000001
6	6	0	-2.490382	-1.831141	-0.000005

7	6	0	0.000000	0.975543	0.000013
8	6	0	1.244244	0.259340	0.000014
9	6	0	1.277299	-1.157977	0.000001
10	6	0	0.000000	-1.931942	-0.000002
11	6	0	2.474032	0.982253	-0.000003
12	6	0	3.691632	0.265728	-0.000022
13	6	0	3.700330	-1.117529	-0.000024
14	6	0	2.490383	-1.831140	-0.000005
15	6	0	-2.436016	2.412601	-0.000002
16	6	0	-1.247942	3.085669	0.000008
17	6	0	0.000000	2.385461	0.000013
18	6	0	1.247942	3.085670	0.000008
19	6	0	2.436015	2.412601	-0.000001
20	1	0	-4.642654	-1.657677	-0.000042
21	1	0	-4.626760	0.820679	-0.000034
22	1	0	-2.490664	-2.915823	-0.000013
23	8	0	0.000000	-3.132205	-0.749985
24	8	0	0.000000	-3.132190	0.750035
25	1	0	4.626760	0.820680	-0.000035
26	1	0	4.642655	-1.657677	-0.000043
27	1	0	2.490664	-2.915823	-0.000013
28	1	0	-3.377153	2.956843	-0.000005
29	1	0	-1.232106	4.172716	0.000018
30	1	0	1.232105	4.172716	0.000018
31	1	0	3.377152	2.956843	-0.000003

Figure 2b

$C_{18}H_{10}$, M=3 (E = -691.80664 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.840655	-1.583822	-0.000034
2	6	0	-3.753099	-0.206656	0.000132
3	6	0	-2.503077	0.462476	0.000125
4	6	0	-1.278659	-0.297445	0.000055
5	6	0	-1.471653	-1.682787	-0.000238
6	6	0	-2.653265	-2.359230	-0.000303
7	6	0	-2.435691	1.888506	0.000136
8	6	0	-1.232690	2.527613	0.000052
9	6	0	0.000000	1.802506	0.000000
10	6	0	0.000000	0.386118	-0.000001
11	6	0	1.232690	2.527614	-0.000051
12	6	0	2.435691	1.888506	-0.000136
13	6	0	2.503077	0.462476	-0.000125
14	6	0	1.278659	-0.297445	-0.000056
15	6	0	3.753099	-0.206656	-0.000132
16	6	0	3.840655	-1.583822	0.000034
17	6	0	2.653265	-2.359230	0.000304
18	6	0	1.471653	-1.682787	0.000238
19	1	0	-4.809940	-2.076299	-0.000023
20	1	0	-4.657636	0.396503	0.000260

21	1	0	-2.697001	-3.445592	-0.000536
22	1	0	-3.364608	2.453714	0.000118
23	1	0	-1.187530	3.613873	0.000019
24	1	0	1.187530	3.613874	-0.000018
25	1	0	3.364608	2.453714	-0.000117
26	1	0	4.657636	0.396503	-0.000260
27	1	0	4.809940	-2.076298	0.000023
28	1	0	2.697002	-3.445591	0.000537

$C_{18}H_{10}$, M=1 (E = -691.96060 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.134433	-1.884809	0.000029
2	6	0	-3.458539	-0.531004	-0.000062
3	6	0	-2.416481	0.437643	-0.000044
4	6	0	-1.133728	-0.102676	-0.000068
5	6	0	-0.752901	-1.473888	0.000008
6	6	0	-1.796444	-2.382316	0.000098
7	6	0	-2.463837	1.884862	0.000002
8	6	0	-1.323908	2.674493	0.000018
9	6	0	-0.000045	2.095019	0.000000
10	6	0	-0.000022	0.714643	-0.000014
11	6	0	1.323801	2.674532	0.000010
12	6	0	2.463747	1.884931	0.000001
13	6	0	2.416442	0.437708	0.000019
14	6	0	1.133709	-0.102672	0.000062
15	6	0	3.458551	-0.530877	0.000025
16	6	0	3.134529	-1.884706	-0.000047
17	6	0	1.796575	-2.382287	-0.000068
18	6	0	0.752973	-1.473917	0.000024
19	1	0	-3.943697	-2.610419	0.000036
20	1	0	-4.502970	-0.228210	-0.000058
21	1	0	-1.633513	-3.457169	0.000033
22	1	0	-3.434581	2.375460	0.000034
23	1	0	-1.438305	3.756049	0.000057
24	1	0	1.438166	3.756091	-0.000013
25	1	0	3.434478	2.375553	-0.000035
26	1	0	4.502964	-0.228022	0.000010
27	1	0	3.943839	-2.610265	-0.000058
28	1	0	1.633702	-3.457148	0.000035

Figure 2c

$C_{14}H_{9}$, M=2 (two hexagons and one pentagon, E = -538.80121 hartrees):

Standard orientation:

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

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.730663	1.105959	-0.000006
2	6	0	-1.359277	1.264495	-0.000003
3	6	0	-3.271231	-0.213621	-0.000028
4	6	0	-2.470496	-1.342970	-0.000027
5	6	0	-1.050989	-1.208219	-0.000006
6	6	0	-0.553388	0.097188	0.000033
7	6	0	-0.069813	-2.242580	-0.000012
8	6	0	1.272481	-1.918913	-0.000010
9	6	0	1.764659	-0.570298	-0.000021
10	6	0	0.817369	0.451894	0.000075
11	6	0	3.221418	-0.365022	0.000092
12	6	0	3.879338	0.780065	-0.000438
13	6	0	0.853773	1.921754	0.000566
14	6	0	-0.424384	2.399875	-0.000287
15	1	0	-3.406127	1.958284	-0.000120
16	1	0	-4.351725	-0.330475	-0.000102
17	1	0	-2.922606	-2.331884	-0.000068
18	1	0	-0.375574	-3.286066	-0.000009
19	1	0	2.005592	-2.722452	0.000048
20	1	0	3.813854	-1.290355	0.000701
21	1	0	4.918241	1.083545	-0.000440
22	1	0	1.758539	2.516950	0.000954
23	1	0	-0.712972	3.444807	-0.000530

$C_{14}H_9$, M=2 (three hexagons, E = -538.85409 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.868964	-1.606596	0.000001
2	6	0	1.506198	-1.544664	0.000000
3	6	0	3.563090	-0.369962	0.000000
4	6	0	2.858791	0.820101	0.000000
5	6	0	1.443196	0.843463	0.000000
6	6	0	0.720113	-0.393523	0.000000
7	6	0	0.701783	2.073156	0.000000
8	6	0	-0.660042	2.078892	0.000000
9	6	0	-1.416389	0.857827	0.000000
10	6	0	-0.728730	-0.388800	-0.000001
11	6	0	-2.830641	0.861829	0.000000
12	6	0	-3.544029	-0.321841	0.000000
13	6	0	-1.479211	-1.584942	0.000000
14	6	0	-2.861628	-1.554677	0.000000
15	1	0	3.409803	-2.549171	0.000000
16	1	0	4.650314	-0.364091	-0.000001
17	1	0	3.393300	1.766906	0.000000
18	1	0	1.256209	3.008774	-0.000001
19	1	0	-1.203865	3.020621	0.000001
20	1	0	-3.351343	1.816705	0.000001
21	1	0	-4.630495	-0.303486	-0.000001
22	1	0	-0.948729	-2.533354	0.000000
23	1	0	-3.423993	-2.484480	0.000000

Figure 2d

$C_{24}H_{10}$, M=3 (E = -920.50947 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.847393	2.375172	-0.000040
2	6	0	-1.424461	2.404326	-0.000031
3	6	0	-0.713671	1.172983	0.000098
4	6	0	-1.428967	-0.062589	-0.000094
5	6	0	-2.850582	-0.061019	-0.000251
6	6	0	-3.534564	1.187043	-0.000199
7	6	0	-0.714180	-1.298324	0.000306
8	6	0	-1.439877	-2.530430	0.000438
9	6	0	-2.865842	-2.500762	0.000364
10	6	0	-3.540820	-1.307321	-0.000016
11	6	0	-0.685904	3.622102	-0.000073
12	6	0	0.685906	3.622102	-0.000040
13	6	0	1.424462	2.404324	0.000017
14	6	0	0.713673	1.172984	0.000010
15	6	0	1.428967	-0.062590	0.000147
16	6	0	0.714179	-1.298321	-0.000172
17	6	0	1.439876	-2.530432	-0.000364
18	6	0	0.686565	-3.721651	-0.000586
19	6	0	-0.686568	-3.721651	0.000055
20	6	0	2.847396	2.375169	0.000029
21	6	0	3.534566	1.187041	0.000136
22	6	0	2.850583	-0.061024	0.000188
23	6	0	3.540817	-1.307323	0.000134
24	6	0	2.865840	-2.500764	-0.000175
25	1	0	-3.387944	3.318604	0.000128
26	1	0	-4.621839	1.184725	-0.000101
27	1	0	-3.404569	-3.443316	0.001148
28	1	0	-4.628113	-1.299305	-0.000463
29	1	0	-1.232328	4.562164	-0.000086
30	1	0	1.232331	4.562164	-0.000100
31	1	0	3.387947	3.318601	-0.000123
32	1	0	4.621841	1.184721	0.000162
33	1	0	4.628111	-1.299310	0.000530
34	1	0	3.404569	-3.443317	-0.000395

$C_{24}H_{10}$, M=1 (E = -920.56278 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.846514	2.371020	0.000193
2	6	0	-1.422329	2.393605	0.000180
3	6	0	-0.713148	1.161002	0.000131

4	6	0	-1.430167	-0.076325	-0.000025
5	6	0	-2.855541	-0.065454	-0.000255
6	6	0	-3.535639	1.187080	-0.000112
7	6	0	-0.721263	-1.316103	0.000163
8	6	0	-1.489582	-2.540894	0.000219
9	6	0	-2.902721	-2.502838	-0.000031
10	6	0	-3.562933	-1.297263	-0.000117
11	6	0	-0.686018	3.610639	0.000104
12	6	0	0.686132	3.610617	-0.000071
13	6	0	1.422404	2.393560	-0.000150
14	6	0	0.713185	1.160979	0.000000
15	6	0	1.430167	-0.076368	0.000075
16	6	0	0.721224	-1.316123	-0.000076
17	6	0	1.489513	-2.540944	-0.000257
18	6	0	0.618905	-3.647822	-0.000692
19	6	0	-0.619049	-3.647853	0.000376
20	6	0	2.846590	2.370933	-0.000261
21	6	0	3.535679	1.186972	-0.000106
22	6	0	2.855541	-0.065540	0.000150
23	6	0	3.562891	-1.297370	0.000328
24	6	0	2.902647	-2.502926	0.000101
25	1	0	-3.382435	3.317020	0.000493
26	1	0	-4.622868	1.186245	-0.000143
27	1	0	-3.452708	-3.438582	0.000472
28	1	0	-4.649802	-1.272410	-0.000481
29	1	0	-1.233145	4.550245	0.000229
30	1	0	1.233289	4.550206	-0.000195
31	1	0	3.382537	3.316917	-0.000561
32	1	0	4.622908	1.186101	-0.000169
33	1	0	4.649760	-1.272558	0.000801
34	1	0	3.452617	-3.438681	0.000354

$C_{24}H_{10}(OH)_2$, M=1 (charge=0, E = -1072.32906 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.880063	2.865879	0.011641
2	6	0	2.918054	1.442138	0.014165
3	6	0	1.691859	0.722528	0.005264
4	6	0	0.450251	1.428201	-0.003499
5	6	0	0.444132	2.850599	-0.011436
6	6	0	1.687533	3.544172	-0.002146
7	6	0	-0.779149	0.705697	-0.008329
8	6	0	-2.014331	1.412672	-0.017026
9	6	0	-1.993793	2.836180	-0.048018
10	6	0	-0.807000	3.526656	-0.040720
11	6	0	4.140190	0.711765	0.023140
12	6	0	4.149081	-0.660604	0.021288
13	6	0	2.937081	-1.407403	0.010417
14	6	0	1.701049	-0.704687	0.003478
15	6	0	0.469672	-1.427175	-0.007320
16	6	0	-0.771146	-0.721649	-0.011291

17	6	0	-1.990735	-1.450150	-0.019571
18	6	0	-3.214584	-0.721848	0.001099
19	6	0	-3.217706	0.658769	0.007889
20	6	0	2.917373	-2.831145	0.005610
21	6	0	1.733914	-3.525341	-0.005288
22	6	0	0.480630	-2.849086	-0.011220
23	6	0	-0.761399	-3.544421	-0.020157
24	6	0	-1.958014	-2.871958	-0.023579
25	8	0	-4.472381	1.256382	0.002988
26	8	0	-4.386169	-1.414955	0.025119
27	1	0	3.820066	3.412359	0.018613
28	1	0	1.677024	4.631571	-0.007609
29	1	0	-2.931011	3.382875	-0.108860
30	1	0	-0.811847	4.613679	-0.069057
31	1	0	5.076849	1.264094	0.030747
32	1	0	5.093054	-1.200430	0.027435
33	1	0	3.864446	-3.365457	0.010387
34	1	0	1.737975	-4.612704	-0.009097
35	1	0	-0.749065	-4.631717	-0.024003
36	1	0	-2.897703	-3.413407	-0.028869
37	1	0	-4.472722	1.997807	0.628733
38	1	0	-5.096821	-0.748823	0.060377

$C_{24}H_{10}(OH)_2$, M=1 (charge = -2, E = -1072.20587 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.919499	-2.851484	0.056593
2	6	0	-2.966479	-1.438894	0.043095
3	6	0	-1.701330	-0.711055	0.006687
4	6	0	-0.471575	-1.422180	-0.024245
5	6	0	-0.454938	-2.874947	-0.018173
6	6	0	-1.736293	-3.553588	0.031693
7	6	0	0.772737	-0.698159	-0.065184
8	6	0	2.016843	-1.437679	-0.109114
9	6	0	2.001821	-2.830615	-0.126537
10	6	0	0.766577	-3.541827	-0.071577
11	6	0	-4.169197	-0.690273	0.061092
12	6	0	-4.185036	0.682360	0.047712
13	6	0	-2.950501	1.447783	0.018383
14	6	0	-1.701309	0.716356	-0.002666
15	6	0	-0.455229	1.437858	-0.029271
16	6	0	0.780753	0.723585	-0.046761
17	6	0	2.038989	1.465500	-0.044317
18	6	0	3.234778	0.708648	0.014118
19	6	0	3.231478	-0.662355	-0.088246
20	6	0	-2.916649	2.841671	0.010646
21	6	0	-1.692402	3.551083	-0.013343
22	6	0	-0.465749	2.885622	-0.031143
23	6	0	0.811489	3.573267	-0.051910
24	6	0	1.997477	2.878990	-0.054323
25	8	0	4.466556	-1.333375	0.092316

26	8	0	4.456742	1.353225	0.167001
27	1	0	-3.868498	-3.396023	0.087836
28	1	0	-1.739410	-4.644945	0.040291
29	1	0	2.937073	-3.375944	-0.249779
30	1	0	0.772534	-4.633690	-0.084108
31	1	0	-5.114427	-1.241561	0.085735
32	1	0	-5.129263	1.229199	0.060589
33	1	0	-3.860390	3.391573	0.026023
34	1	0	-1.698894	4.643183	-0.016349
35	1	0	0.808253	4.664363	-0.056878
36	1	0	2.944015	3.419564	-0.056670
37	1	0	4.279469	-2.019842	0.771980
38	1	0	5.082614	0.607338	0.237534

$C_{24}H_{10}O_2$, M=1 (E = -1071.11275 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.840104	-2.851282	0.000044
2	6	0	2.862683	-1.419115	0.000243
3	6	0	1.631993	-0.712955	0.000044
4	6	0	0.393114	-1.429136	-0.000215
5	6	0	0.403706	-2.857715	-0.000354
6	6	0	1.662898	-3.540878	-0.000353
7	6	0	-0.845877	-0.729213	-0.000066
8	6	0	-2.046080	-1.465280	-0.000034
9	6	0	-2.021645	-2.871541	-0.000314
10	6	0	-0.822136	-3.556408	-0.000268
11	6	0	4.077560	-0.687994	0.000457
12	6	0	4.077563	0.688000	0.000602
13	6	0	2.862682	1.419122	0.000201
14	6	0	1.631992	0.712957	0.000039
15	6	0	0.393112	1.429135	-0.000067
16	6	0	-0.845877	0.729210	-0.000055
17	6	0	-2.046080	1.465276	-0.000126
18	6	0	-3.355986	0.775335	0.000279
19	6	0	-3.355985	-0.775340	0.000185
20	6	0	2.840098	2.851287	-0.000097
21	6	0	1.662889	3.540879	-0.000288
22	6	0	0.403701	2.857713	-0.000267
23	6	0	-0.822141	3.556411	-0.000450
24	6	0	-2.021653	2.871539	-0.000328
25	8	0	-4.420714	-1.369158	0.000347
26	8	0	-4.420716	1.369152	0.000737
27	1	0	3.787878	-3.383977	0.000250
28	1	0	1.660825	-4.627732	-0.000795
29	1	0	-2.971980	-3.395315	-0.000636
30	1	0	-0.810282	-4.643291	-0.000044
31	1	0	5.017388	-1.234336	0.000427
32	1	0	5.017391	1.234341	0.001135
33	1	0	3.787869	3.383987	-0.000334
34	1	0	1.660814	4.627733	-0.000482

35	1	0	-0.810288	4.643293	-0.000727
36	1	0	-2.971988	3.395313	-0.000327

Figure 2e

$C_{25}H_{10}O$, M=5 (E = -1033.80367 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.932936	-1.785108	0.000044
2	6	0	-4.934139	-0.394420	0.000157
3	6	0	-3.718174	0.335223	0.000130
4	6	0	-2.482963	-0.376119	0.000012
5	6	0	-2.495095	-1.820322	-0.000012
6	6	0	-3.734492	-2.500003	-0.000038
7	6	0	-1.245325	0.337369	-0.000064
8	6	0	0.000011	-0.368727	-0.000033
9	6	0	-0.000042	-1.818292	-0.000056
10	6	0	-1.245924	-2.443477	0.000049
11	6	0	1.245377	0.337381	0.000038
12	6	0	2.482996	-0.376093	0.000144
13	6	0	2.495075	-1.820327	-0.000111
14	6	0	1.245907	-2.443522	-0.000143
15	6	0	3.718182	0.335249	0.000295
16	6	0	4.934177	-0.394407	0.000233
17	6	0	4.932953	-1.785081	-0.000040
18	6	0	3.734523	-2.500001	-0.000293
19	6	0	-3.686498	1.759160	0.000188
20	6	0	-2.491093	2.443885	0.000082
21	6	0	-1.260852	1.754512	-0.000099
22	6	0	-0.000056	2.523694	-0.000262
23	6	0	1.260854	1.754482	-0.000101
24	6	0	2.491069	2.443887	0.000122
25	6	0	3.686487	1.759166	0.000315
26	8	0	-0.000022	3.763103	-0.000536
27	1	0	-5.876358	-2.323836	0.000001
28	1	0	-5.873256	0.152451	0.000315
29	1	0	-3.738039	-3.585450	-0.000138
30	1	0	5.873288	0.152472	0.000350
31	1	0	5.876365	-2.323829	0.000041
32	1	0	3.738101	-3.585446	-0.000737
33	1	0	-4.628630	2.301657	0.000314
34	1	0	-2.460055	3.528413	0.000139
35	1	0	2.460020	3.528415	0.000157
36	1	0	4.628608	2.301685	0.000496

$C_{25}H_{10}O_3$, M=1 (E = -1184.42141 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.967562	-1.406089	-0.011373
2	6	0	-4.955239	-0.026184	-0.048488
3	6	0	-3.731035	0.689598	-0.040299
4	6	0	-2.503666	-0.041574	-0.002442
5	6	0	-2.540225	-1.457174	0.040852
6	6	0	-3.756638	-2.122373	0.039191
7	6	0	-1.257377	0.653363	0.003384
8	6	0	0.000015	-0.102126	0.000162
9	6	0	0.000006	-1.484232	0.000141
10	6	0	-1.278213	-2.247162	0.121522
11	6	0	1.257396	0.653357	-0.003112
12	6	0	2.503683	-0.041591	0.002422
13	6	0	2.540226	-1.457173	-0.041096
14	6	0	1.278140	-2.247233	-0.120968
15	6	0	3.731059	0.689584	0.040037
16	6	0	4.955266	-0.026197	0.047639
17	6	0	4.967581	-1.406088	0.010118
18	6	0	3.756640	-2.122370	-0.040081
19	6	0	-3.688003	2.109738	-0.062678
20	6	0	-2.485184	2.771122	-0.046033
21	6	0	-1.267259	2.050029	-0.014117
22	6	0	-0.000013	2.823193	0.000173
23	6	0	1.267287	2.050012	0.014480
24	6	0	2.485201	2.771109	0.046356
25	6	0	3.688026	2.109719	0.062706
26	8	0	0.000001	4.051549	0.000100
27	8	0	-1.318409	-3.457046	0.307042
28	8	0	1.318312	-3.457257	-0.305585
29	1	0	-5.911287	-1.943713	-0.018154
30	1	0	-5.886925	0.533010	-0.081942
31	1	0	-3.746165	-3.206808	0.081116
32	1	0	5.886965	0.532990	0.080908
33	1	0	5.911312	-1.943707	0.016395
34	1	0	3.746141	-3.206797	-0.082192
35	1	0	-4.622308	2.664751	-0.089698
36	1	0	-2.429215	3.854014	-0.058599
37	1	0	2.429237	3.853999	0.059050
38	1	0	4.622335	2.664729	0.089692

Figure 5b

$C_{19}H_{10}O_2$, M=1 (E = -880.41644 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.435731	1.813209	-0.000275
2	6	0	3.716639	0.455502	-0.000191

3	6	0	2.674202	-0.494039	-0.000080
4	6	0	1.321439	-0.043164	-0.000081
5	6	0	1.047291	1.353240	-0.000148
6	6	0	2.111598	2.263068	-0.000245
7	6	0	0.254115	-0.994924	0.000041
8	6	0	-1.104107	-0.546264	-0.000026
9	6	0	-1.434268	0.851984	-0.000224
10	6	0	-0.341855	1.802219	-0.000013
11	6	0	-2.150968	-1.512370	0.000003
12	6	0	-3.496868	-1.077636	-0.000206
13	6	0	-3.803368	0.268725	-0.000478
14	6	0	-2.786376	1.235055	-0.000460
15	6	0	2.934965	-1.901481	0.000056
16	6	0	1.913144	-2.806277	0.000195
17	6	0	0.548090	-2.380467	0.000186
18	6	0	-0.522319	-3.321956	0.000290
19	6	0	-1.823082	-2.902625	0.000199
20	8	0	-0.452659	3.099412	0.000405
21	8	0	-1.658599	3.740348	0.000845
22	1	0	4.245545	2.536881	-0.000352
23	1	0	4.746511	0.107214	-0.000212
24	1	0	1.900005	3.325830	-0.000297
25	1	0	-4.287506	-1.824355	-0.000167
26	1	0	-4.839959	0.592863	-0.000664
27	1	0	-3.010294	2.291002	-0.000597
28	1	0	3.968808	-2.237332	0.000057
29	1	0	2.122563	-3.872938	0.000304
30	1	0	-0.284646	-4.382601	0.000419
31	1	0	-2.634983	-3.625442	0.000253

Figure 5d

$C_{19}H_{10}O$(O1), M=1 (E = -880.48366 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.809272	2.021517	0.060723
2	6	0	2.672681	0.593178	0.012995
3	6	0	1.370932	0.017685	-0.001760
4	6	0	0.211956	0.881052	0.027349
5	6	0	0.388037	2.292407	0.036761
6	6	0	1.715529	2.833537	0.066962
7	6	0	1.244699	-1.395523	-0.080048
8	6	0	-1.094665	0.341127	0.028409
9	6	0	-1.282802	-1.121629	0.125972
10	6	0	-0.093859	-2.035225	-0.093798
11	6	0	-2.669358	-1.676132	-0.092131
12	6	0	-3.741984	-0.717920	-0.412837
13	6	0	-3.535737	0.610330	-0.300969
14	6	0	-2.217581	1.179859	-0.062931
15	6	0	-2.022392	2.583092	-0.056171
16	6	0	-0.757297	3.123838	0.012677

17	1	0	-0.623416	4.202590	0.027488
18	1	0	-2.890782	3.234535	-0.115662
19	1	0	3.810474	2.444546	0.078983
20	1	0	1.832210	3.914160	0.089798
21	1	0	-4.703637	-1.110740	-0.731156
22	1	0	-4.350924	1.306444	-0.485814
23	6	0	3.799486	-0.257468	-0.035231
24	6	0	3.657431	-1.633855	-0.108964
25	6	0	2.377406	-2.202596	-0.135398
26	1	0	4.791032	0.188963	-0.020260
27	1	0	4.535759	-2.271646	-0.147515
28	1	0	2.238754	-3.277329	-0.194609
29	1	0	-2.739431	-2.698767	-0.456419
30	8	0	-0.252015	-3.240612	-0.221349
31	8	0	-2.109306	-1.578938	1.222037

Figure 6a: see Figure 5d

Figure 6b

$C_{19}H_{10}O$(O2), M=1 (E = -880.45672 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.735727	-1.368921	0.005294
2	6	0	3.768193	0.011879	-0.013658
3	6	0	2.571934	0.770118	-0.018417
4	6	0	1.316013	0.087578	0.034976
5	6	0	1.304461	-1.343522	0.007985
6	6	0	2.501036	-2.043834	-0.009242
7	6	0	0.118957	0.852519	0.050756
8	6	0	-1.174734	0.178053	0.267392
9	6	0	-1.250354	-1.367727	0.160672
10	6	0	0.033741	-2.109639	-0.123737
11	6	0	-2.418864	0.930352	0.000353
12	6	0	-3.600818	0.244309	-0.134080
13	6	0	-3.646544	-1.181177	-0.283717
14	6	0	-2.523763	-1.948879	-0.250644
15	6	0	2.579247	2.192645	-0.105076
16	6	0	1.408289	2.902839	-0.159530
17	6	0	0.146656	2.243149	-0.079332
18	6	0	-1.099422	2.984453	-0.132618
19	6	0	-2.307076	2.361297	-0.120666
20	1	0	4.661091	-1.937507	0.004478
21	1	0	4.719609	0.538007	-0.039381
22	1	0	2.460367	-3.127682	-0.052541
23	1	0	-4.523570	0.807514	-0.254272
24	1	0	-4.600609	-1.636411	-0.536788
25	1	0	-2.522284	-2.988316	-0.560489
26	1	0	3.535806	2.707479	-0.148450
27	1	0	1.427407	3.985692	-0.253210

28	1	0	-1.043861	4.065737	-0.227476
29	1	0	-3.223732	2.937717	-0.220010
30	8	0	0.006383	-3.286786	-0.458585
31	8	0	-1.214669	-0.678863	1.422070

Figure 6c

$C_{19}H_{10}O_2$, M=1 (E = -880.52214 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.963043	-0.820233	-0.222292
2	6	0	3.735820	0.518032	-0.003272
3	6	0	2.424025	1.038761	0.112313
4	6	0	1.268012	0.180916	0.071641
5	6	0	1.558322	-1.215592	-0.106843
6	6	0	2.859205	-1.677758	-0.284595
7	6	0	-0.059249	0.801640	0.093557
8	6	0	-1.341307	0.099113	0.065670
9	6	0	-1.524975	-1.278828	0.349984
10	6	0	0.568844	-2.314104	-0.025637
11	6	0	-2.553400	0.824962	-0.202929
12	6	0	-3.800742	0.163957	-0.290651
13	6	0	-3.903833	-1.192315	-0.071718
14	6	0	-2.751222	-1.914111	0.267895
15	6	0	2.285879	2.452808	0.219338
16	6	0	1.056527	3.024416	0.172477
17	6	0	-0.118135	2.224712	0.058907
18	6	0	-1.352913	2.917144	-0.137151
19	6	0	-2.517946	2.245513	-0.318966
20	8	0	-0.490563	-2.060656	0.831036
21	8	0	0.699556	-3.410750	-0.507366
22	1	0	4.970345	-1.208807	-0.336718
23	1	0	4.566974	1.216198	0.057919
24	1	0	2.995615	-2.742052	-0.441180
25	1	0	-4.683145	0.758253	-0.511980
26	1	0	-4.863610	-1.696515	-0.134591
27	1	0	-2.787899	-2.973244	0.497860
28	1	0	3.184780	3.059747	0.285537
29	1	0	0.942621	4.104901	0.195517
30	1	0	-1.326795	4.002915	-0.175205
31	1	0	-3.446552	2.775651	-0.512891

Figure 7a

$C_{16}H_{10}$(O1), M=1 (E = -690.88769 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.416357	0.166300	-0.369490
2	6	0	-2.826261	-1.064032	-0.380731
3	6	0	-1.462412	-1.245359	0.092564
4	6	0	-0.620544	0.112470	0.286036
5	6	0	-1.316419	1.380780	0.026965
6	6	0	-2.682086	1.372771	-0.139365
7	6	0	-0.669979	-2.443913	-0.226590
8	6	0	0.829000	0.032833	0.090997
9	6	0	1.469738	-1.225517	0.006247
10	6	0	0.678384	-2.437779	-0.160954
11	6	0	2.871492	-1.258122	-0.088047
12	1	0	3.376543	-2.218932	-0.150710
13	6	0	3.610801	-0.076982	-0.132677
14	6	0	2.966829	1.158754	-0.121758
15	6	0	1.567192	1.234075	-0.023955
16	6	0	0.857250	2.500626	-0.050957
17	6	0	-0.499645	2.566537	-0.056092
18	1	0	-1.002391	3.527598	-0.136586
19	1	0	1.447659	3.411084	-0.116637
20	1	0	-1.206275	-3.342497	-0.522589
21	1	0	-4.457466	0.257856	-0.669120
22	1	0	-3.343580	-1.924851	-0.797546
23	1	0	-3.203580	2.321389	-0.245893
24	1	0	1.227084	-3.357275	-0.352933
25	1	0	4.694247	-0.120833	-0.202373
26	1	0	3.544649	2.077056	-0.192281
27	8	0	-1.152349	-0.658906	1.359189

Figure 7b

$C_{16}H_{10}(O)$, TS, M=1 (E = -690.83216 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.453292	0.001671	-0.285335
2	6	0	-2.800863	-1.218578	-0.176531
3	6	0	-1.400921	-1.252978	-0.063385
4	6	0	-0.693380	0.027356	0.245020
5	6	0	-1.409154	1.297402	-0.134384
6	6	0	-2.776391	1.247317	-0.300880
7	6	0	-0.652324	-2.458872	-0.138976
8	6	0	0.775977	0.003165	-0.015653
9	6	0	1.478456	-1.230777	-0.112608
10	6	0	0.716931	-2.444801	-0.189668
11	6	0	2.882070	-1.211534	-0.168514
12	1	0	3.419892	-2.153618	-0.245206
13	6	0	3.583145	-0.007606	-0.133373
14	6	0	2.893822	1.204460	-0.079438
15	6	0	1.491590	1.231746	-0.034535

16	6	0	0.731601	2.453207	-0.078637
17	6	0	-0.638127	2.490409	-0.153317
18	1	0	-1.148685	3.446262	-0.244467
19	1	0	1.287072	3.389040	-0.092181
20	1	0	-1.191433	-3.401074	-0.198260
21	1	0	-4.535467	0.005668	-0.397259
22	1	0	-3.366063	-2.146005	-0.215805
23	1	0	-3.346344	2.161479	-0.446985
24	1	0	1.260919	-3.383113	-0.274714
25	1	0	4.668521	-0.011495	-0.170417
26	1	0	3.442198	2.143635	-0.093485
27	8	0	-0.608181	-0.105038	1.662508

Figure 7c

$C_{16}H_{10}$(O2), M=1 (E = -690.90622 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.366016	0.000001	-0.865423
2	6	0	2.752718	1.219648	-0.560108
3	6	0	1.533415	1.243067	0.140109
4	6	0	1.059828	0.000000	0.587250
5	6	0	1.533416	-1.243066	0.140110
6	6	0	2.752719	-1.219647	-0.560107
7	6	0	0.681928	2.427159	0.290556
8	6	0	-1.059823	0.000000	0.587308
9	6	0	-1.533425	1.243060	0.140132
10	6	0	-0.681939	2.427159	0.290565
11	6	0	-2.752709	1.219645	-0.560118
12	1	0	-3.196544	2.151511	-0.901574
13	6	0	-3.366001	-0.000001	-0.865450
14	6	0	-2.752708	-1.219646	-0.560118
15	6	0	-1.533423	-1.243061	0.140132
16	6	0	-0.681937	-2.427159	0.290564
17	6	0	0.681930	-2.427158	0.290556
18	1	0	1.184237	-3.392674	0.268550
19	1	0	-1.184246	-3.392674	0.268584
20	1	0	1.184234	3.392675	0.268551
21	1	0	4.307484	0.000001	-1.407562
22	1	0	3.196560	2.151513	-0.901555
23	1	0	3.196562	-2.151512	-0.901552
24	1	0	-1.184248	3.392674	0.268586
25	1	0	-4.307454	-0.000002	-1.407616
26	1	0	-3.196542	-2.151513	-0.901573
27	8	0	-0.000009	0.000000	1.473925

Figure 8b

$C_{19}H_{10}O_2$, M=1 (E = -880.49304 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.835659	0.523564	-0.025657
2	6	0	-0.226099	-0.445644	-0.020056
3	6	0	-0.007380	-1.904761	-0.083983
4	6	0	1.157065	-2.600573	-0.131319
5	6	0	0.458714	1.928834	-0.047674
6	6	0	-1.587188	-0.005927	0.013439
7	6	0	-1.915914	1.394762	0.040253
8	6	0	-0.880859	2.318678	-0.005797
9	6	0	-3.277317	1.826368	0.095073
10	6	0	-4.299568	0.916282	0.114202
11	6	0	-4.004410	-0.464792	0.068774
12	6	0	-2.700779	-0.929024	0.014465
13	6	0	-2.430938	-2.342474	-0.056831
14	6	0	-1.166199	-2.790738	-0.115195
15	1	0	-0.972110	-3.857975	-0.174007
16	1	0	-3.269495	-3.033449	-0.069423
17	1	0	1.119103	-3.680829	-0.215965
18	1	0	-5.333841	1.246105	0.156957
19	1	0	-4.815592	-1.188367	0.070533
20	6	0	3.166293	1.334882	-0.060728
21	6	0	2.768032	2.681931	-0.139793
22	6	0	1.434738	2.966554	-0.116362
23	1	0	4.220657	1.093851	-0.025932
24	1	0	3.515593	3.467172	-0.196125
25	1	0	1.079354	3.993338	-0.148055
26	1	0	-1.115058	3.380420	-0.012721
27	1	0	-3.476256	2.894495	0.118763
28	8	0	2.456263	-2.243538	-0.063344
29	8	0	4.210560	-1.048845	0.371204
30	6	0	2.269268	0.275719	-0.003806
31	6	0	3.025727	-1.012924	0.133177

$C_{18}H_{10}$, M=3 (E = -691.76837 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.379536	0.282971	-0.006002
2	6	0	0.040899	0.782371	0.011788
3	6	0	-0.274487	2.230586	0.040941
4	6	0	0.614427	3.228698	0.172592
5	6	0	1.627641	-1.147782	0.023130
6	6	0	-1.032039	-0.145057	0.005611
7	6	0	-0.776834	-1.565353	0.029279
8	6	0	0.540201	-2.027787	0.048465
9	6	0	-1.875356	-2.479743	0.032102
10	6	0	-3.169526	-2.027515	0.002308
11	6	0	-3.433102	-0.638358	-0.033303

12	6	0	-2.406656	0.291908	-0.030812
13	6	0	-2.682067	1.709382	-0.075261
14	6	0	-1.686634	2.617830	-0.048093
15	1	0	-1.908950	3.680792	-0.070681
16	1	0	-3.719912	2.030251	-0.125865
17	1	0	0.520159	4.307231	0.218535
18	1	0	-3.997585	-2.730917	0.002292
19	1	0	-4.461733	-0.287499	-0.064567
20	6	0	3.835001	0.624162	-0.081779
21	6	0	4.048953	-0.787947	-0.033204
22	6	0	2.971976	-1.635564	0.015313
23	1	0	4.677423	1.309747	-0.132502
24	1	0	5.063062	-1.179701	-0.040355
25	1	0	3.121764	-2.711873	0.044198
26	1	0	0.726650	-3.099478	0.072792
27	1	0	-1.658963	-3.544717	0.054967
28	6	0	2.551082	1.058227	-0.066210

Figure 9a

$C_{15}H_8O$, M=1 (E = -651.57941 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.511049	-0.096270	0.000344
2	6	0	-2.861658	1.137490	0.000323
3	6	0	-1.455532	1.220677	0.000186
4	6	0	-0.724793	0.003592	0.000072
5	6	0	-1.376260	-1.256780	0.000093
6	6	0	-2.776923	-1.287285	0.000230
7	6	0	-0.717950	2.456518	0.000156
8	6	0	0.694084	0.027700	-0.000067
9	6	0	1.413724	1.254215	-0.000097
10	6	0	0.647524	2.472122	0.000021
11	6	0	2.820187	1.198089	-0.000240
12	1	0	3.392029	2.122369	-0.000265
13	6	0	3.478494	-0.028640	-0.000347
14	6	0	2.769311	-1.239622	-0.000317
15	6	0	1.383860	-1.193967	-0.000176
16	6	0	-0.661791	-2.536271	-0.000021
17	1	0	-1.273068	3.391538	0.000243
18	1	0	-4.596891	-0.128868	0.000449
19	1	0	-3.445523	2.055378	0.000413
20	1	0	-3.267519	-2.256328	0.000243
21	1	0	1.181709	3.418959	-0.000002
22	1	0	4.564592	-0.052757	-0.000457
23	1	0	3.275738	-2.199152	-0.000401
24	8	0	0.680197	-2.392569	-0.000149

$C_{14}H_8$, M=3 (E = -538.16528 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.563124	-0.372777	0.000339
2	6	0	-2.848100	0.811038	0.000311
3	6	0	-1.432485	0.820722	0.000171
4	6	0	-0.724845	-0.424603	0.000057
5	6	0	-1.517279	-1.569453	0.000095
6	6	0	-2.881173	-1.615754	0.000228
7	6	0	-0.681033	2.044533	0.000140
8	6	0	0.724849	-0.424666	-0.000086
9	6	0	1.432453	0.820704	-0.000113
10	6	0	0.680933	2.044487	0.000005
11	6	0	2.848084	0.811081	-0.000254
12	1	0	3.373493	1.762896	-0.000273
13	6	0	3.563186	-0.372740	-0.000366
14	6	0	2.881230	-1.615648	-0.000342
15	6	0	1.517309	-1.569424	-0.000205
16	1	0	-1.229237	2.983729	0.000228
17	1	0	-4.650219	-0.356341	0.000447
18	1	0	-3.373606	1.762811	0.000397
19	1	0	-3.431607	-2.552735	0.000248
20	1	0	1.229138	2.983689	-0.000017
21	1	0	4.650286	-0.356416	-0.000473
22	1	0	3.431723	-2.552628	-0.000429

Figure 9b

$C_{18}H_{10}O$, M=1 (E = -767.20990 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.365684	-2.225271	0.000002
2	6	0	-1.194464	-1.490307	-0.000008
3	6	0	-1.222923	-0.077260	-0.000004
4	6	0	1.194464	-1.490307	-0.000009
5	6	0	1.222923	-0.077260	-0.000003
6	6	0	0.000000	0.653827	-0.000002
7	6	0	2.471131	0.604091	0.000002
8	6	0	3.660896	-0.161408	0.000003
9	6	0	3.598919	-1.543980	0.000005
10	6	0	2.365684	-2.225271	-0.000001
11	1	0	4.621199	0.347130	0.000007
12	1	0	4.517056	-2.124999	0.000009
13	6	0	-3.598919	-1.543981	0.000010
14	6	0	-3.660896	-0.161408	0.000004
15	6	0	-2.471131	0.604091	0.000000
16	1	0	-4.517057	-2.124999	0.000016
17	1	0	-4.621199	0.347130	0.000005
18	6	0	-2.443340	2.037517	-0.000001

19	6	0	-1.262942	2.732295	-0.000004
20	6	0	0.000000	2.059523	-0.000001
21	1	0	-3.389888	2.572296	-0.000002
22	1	0	-1.272978	3.819805	-0.000003
23	6	0	2.443340	2.037517	0.000004
24	1	0	3.389888	2.572295	0.000009
25	6	0	1.262942	2.732295	0.000002
26	1	0	1.272978	3.819805	0.000006
27	1	0	-2.317985	-3.309316	0.000005
28	1	0	2.317985	-3.309316	0.000002
29	8	0	0.000000	-2.174755	-0.000005

$C_{17}H_{10}$, M=5 (E = -653.55931 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.779821	0.259326	-0.000004
2	6	0	2.500386	-0.384625	-0.000002
3	6	0	1.260889	0.240671	-0.000005
4	6	0	3.249104	2.705558	0.000015
5	6	0	4.082481	1.640172	0.000002
6	6	0	0.009842	-0.356124	-0.000004
7	6	0	-1.355069	1.760549	-0.000011
8	6	0	-1.245332	0.373136	-0.000004
9	6	0	-2.510714	2.486222	-0.000019
10	1	0	4.634917	-0.412755	-0.000009
11	1	0	5.156342	1.870412	-0.000004
12	6	0	2.430532	-1.822654	0.000001
13	6	0	1.227765	-2.486251	0.000001
14	6	0	-0.011052	-1.789260	-0.000002
15	1	0	3.362650	-2.384207	0.000005
16	1	0	1.210249	-3.573353	0.000003
17	6	0	-1.269328	-2.468382	0.000000
18	6	0	-2.450029	-1.782812	0.000003
19	6	0	-2.483332	-0.348472	0.000000
20	1	0	-1.268053	-3.555956	-0.000002
21	1	0	-3.395585	-2.319768	0.000007
22	6	0	-3.725376	1.754686	0.000007
23	1	0	-4.673305	2.287192	0.000023
24	6	0	-3.702539	0.372205	0.000011
25	1	0	-4.635153	-0.186615	0.000025
26	1	0	-2.515357	3.572965	-0.000008
27	1	0	3.395008	3.778417	0.000023

Figure 9d

$C_{16}H_8O$, M=3 (E = -689.67753 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.302814	-0.970876	0.000535
2	6	0	2.358035	-1.985373	0.000430
3	6	0	0.977852	-1.690535	0.000120
4	6	0	0.562982	-0.325989	-0.000099
5	6	0	1.547800	0.701628	-0.000114
6	6	0	2.898612	0.372256	0.000293
7	6	0	-0.020481	-2.721219	0.000045
8	6	0	-0.836519	-0.019282	-0.000262
9	6	0	-1.801082	-1.057870	-0.000250
10	6	0	-1.350212	-2.420825	-0.000147
11	6	0	-3.175362	-0.720643	-0.000294
12	1	0	-3.911219	-1.520794	-0.000304
13	6	0	-3.591440	0.608263	-0.000256
14	6	0	-2.658452	1.643638	-0.000165
15	6	0	-1.273696	1.358234	-0.000162
16	6	0	-0.279073	2.334925	-0.000076
17	6	0	1.145514	2.147153	-0.000738
18	1	0	0.307766	-3.757696	0.000173
19	1	0	4.361460	-1.214973	0.000749
20	1	0	2.672653	-3.026259	0.000614
21	1	0	3.623429	1.179999	0.000256
22	1	0	-2.094831	-3.212799	-0.000158
23	1	0	-4.652458	0.840680	-0.000258
24	1	0	-2.980262	2.680292	-0.000114
25	8	0	1.978714	3.063829	0.000736

$C_{15}H_8$, M=5 (E = -576.12146 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.634638	-0.362279	0.000356
2	6	0	-2.957442	0.842384	0.000330
3	6	0	-1.543613	0.904114	0.000187
4	6	0	-0.766164	-0.309986	0.000066
5	6	0	-1.540885	-1.474218	0.000102
6	6	0	-2.900588	-1.572980	0.000234
7	6	0	-0.867399	2.165105	0.000160
8	6	0	0.682245	-0.242479	-0.000081
9	6	0	1.300417	1.043652	-0.000103
10	6	0	0.490000	2.228099	0.000021
11	6	0	2.710015	1.174888	-0.000243
12	1	0	3.138178	2.173663	-0.000253
13	6	0	3.530931	0.057946	-0.000359
14	6	0	2.969068	-1.215352	-0.000338
15	6	0	1.559994	-1.402522	-0.000204
16	6	0	1.094654	-2.730971	-0.000173
17	1	0	-1.465030	3.073556	0.000255
18	1	0	-4.721592	-0.385149	0.000467
19	1	0	-3.511671	1.777658	0.000422

20	1	0	-3.408764	-2.534129	0.000251
21	1	0	0.996746	3.189903	0.000002
22	1	0	4.611847	0.169360	-0.000464
23	1	0	3.600722	-2.097279	-0.000422

Figure 9e

$C_{16}H_8O_2$, M=1 (E = -764.99523 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.467465	0.796413	-0.000185
2	6	0	0.722558	-0.413638	-0.000171
3	6	0	-0.722552	-0.413644	-0.000157
4	6	0	-1.467472	0.796399	-0.000192
5	6	0	-0.775679	2.109555	-0.000501
6	6	0	0.775659	2.109561	-0.000369
7	6	0	-1.422056	-1.652332	0.000012
8	6	0	-2.836188	-1.643107	0.000160
9	6	0	-3.545503	-0.454244	0.000183
10	6	0	-2.858209	0.767851	0.000019
11	6	0	1.422073	-1.652320	-0.000063
12	6	0	0.680535	-2.881546	-0.000003
13	6	0	-0.680507	-2.881551	0.000051
14	6	0	2.858202	0.767875	0.000001
15	6	0	3.545508	-0.454214	0.000085
16	6	0	2.836204	-1.643084	0.000033
17	8	0	1.368291	3.173858	0.000608
18	8	0	-1.368326	3.173844	0.000065
19	1	0	-3.363538	-2.594010	0.000296
20	1	0	-4.631445	-0.466323	0.000338
21	1	0	-3.390709	1.713517	-0.000017
22	1	0	1.232377	-3.817954	0.000073
23	1	0	-1.232341	-3.817965	0.000159
24	1	0	3.390693	1.713546	0.000029
25	1	0	4.631451	-0.466284	0.000202
26	1	0	3.363562	-2.593983	0.000132

$C_{15}H_8O$, M=5 (E = -651.42176 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.678477	0.819943	-0.037549
2	6	0	-3.273071	-0.483543	0.092874
3	6	0	-1.888469	-0.844253	0.071242
4	6	0	-0.869955	0.192052	-0.051479
5	6	0	-1.390456	1.478290	-0.222463

6	6	0	-2.699815	1.845083	-0.226276
7	6	0	-1.480337	-2.178001	0.150953
8	6	0	0.528732	-0.153022	-0.021206
9	6	0	0.882266	-1.541069	-0.001064
10	6	0	-0.117977	-2.514068	0.093267
11	6	0	2.273767	-1.945810	-0.062540
12	1	0	2.502367	-3.006889	-0.063628
13	6	0	3.301879	-0.981906	-0.167140
14	6	0	2.994567	0.347480	-0.153186
15	6	0	1.589448	0.808462	0.003500
16	6	0	1.383301	2.216417	0.251223
17	1	0	-2.227204	-2.961668	0.249430
18	1	0	-4.733698	1.078702	-0.020860
19	1	0	-4.005094	-1.278903	0.206780
20	1	0	-3.005024	2.876717	-0.382409
21	1	0	0.172943	-3.560268	0.139499
22	1	0	4.334550	-1.307753	-0.261447
23	1	0	3.752433	1.118369	-0.233085
24	8	0	2.234539	3.080670	0.255598

Figure 10

$C_{22}H_{10}O_3$, M=1 (E = -1070.03557 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.344110	-2.435264	-0.152310
2	6	0	2.137660	-3.008760	-0.313880
3	6	0	0.901977	-2.255917	-0.240953
4	6	0	0.924224	-0.793900	-0.092189
5	6	0	2.175228	-0.234739	0.112594
6	6	0	3.450357	-0.998011	0.097341
7	6	0	-0.272352	-2.949304	-0.253645
8	6	0	-1.529823	-2.308528	-0.081299
9	6	0	-1.567751	-0.872403	0.009582
10	6	0	-0.386693	-0.075985	-0.081195
11	6	0	-2.869502	-0.283269	0.186569
12	6	0	-2.987345	1.100156	0.247931
13	6	0	-1.883756	1.935253	0.067358
14	6	0	-0.563799	1.363601	-0.123845
15	6	0	-2.693976	-3.066917	-0.002174
16	6	0	-3.953452	-2.469786	0.193346
17	6	0	-4.033428	-1.102633	0.290358
18	6	0	-2.102479	3.345000	0.029893
19	6	0	-1.074712	4.210523	-0.227520
20	6	0	0.216868	3.688841	-0.445150
21	6	0	0.454231	2.331449	-0.408563
22	6	0	2.341185	1.209949	0.327834
23	8	0	1.730074	1.933716	-0.719402
24	8	0	4.540504	-0.443626	0.244344
25	8	0	2.915079	1.772694	1.213319
26	1	0	4.273068	-2.994916	-0.191701

27	1	0	2.047550	-4.079996	-0.481095
28	1	0	-0.252247	-4.032055	-0.355230
29	1	0	-3.966999	1.546775	0.399942
30	1	0	-2.616894	-4.147813	-0.088180
31	1	0	-4.844525	-3.085993	0.262880
32	1	0	-4.991846	-0.612012	0.438486
33	1	0	-3.114013	3.707643	0.188996
34	1	0	-1.240381	5.282889	-0.265613
35	1	0	1.060386	4.337072	-0.655078

$C_{22}H_{10}O_3$, TS, M=1 (E = -1069.93802 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.953629	-3.208658	0.000000
2	6	0	1.744790	-1.772642	0.000000
3	6	0	0.386688	-1.227643	0.000000
4	6	0	-0.608301	-2.193753	0.000000
5	6	0	-0.443927	-3.642270	0.000000
6	6	0	0.943641	-4.104998	0.000000
7	6	0	0.186526	0.265358	0.000000
8	6	0	-2.411113	0.436162	0.000000
9	6	0	-1.083371	0.993057	0.000000
10	6	0	-3.588421	1.132518	0.000000
11	1	0	2.987984	-3.545854	0.000000
12	1	0	1.114086	-5.176875	0.000000
13	6	0	2.830328	-0.946594	0.000000
14	6	0	2.694299	0.468807	0.000000
15	6	0	1.376411	1.056000	0.000000
16	1	0	3.831137	-1.372195	0.000000
17	6	0	1.330276	2.496045	0.000000
18	6	0	0.098700	3.143906	0.000000
19	6	0	-1.104553	2.440324	0.000000
20	1	0	0.070153	4.230871	0.000000
21	6	0	-3.536969	2.546484	0.000000
22	1	0	-4.466554	3.108094	0.000000
23	6	0	-2.326992	3.184918	0.000000
24	1	0	-2.264406	4.268521	0.000000
25	6	0	3.837291	1.266045	0.000000
26	6	0	2.528463	3.268332	0.000000
27	6	0	3.764832	2.669342	0.000000
28	1	0	4.808201	0.777038	0.000000
29	1	0	4.672956	3.264134	0.000000
30	1	0	2.437345	4.351369	0.000000
31	8	0	-1.423838	-4.396455	0.000000
32	1	0	-4.526873	0.591745	0.000000
33	6	0	-1.912471	-1.540282	0.000000
34	8	0	-2.326992	-0.981748	1.067712
35	8	0	-2.326992	-0.981748	-1.067712

Figure 11b

$C_{42}H_{22}O$, M=1 (E = -1688.91336 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-12.244183	0.490753	0.000423
2	6	0	-12.210787	-0.938307	0.000370
3	6	0	-11.016317	-1.604556	0.000240
4	6	0	-9.774587	-0.889952	0.000160
5	6	0	-9.808494	0.560276	0.000214
6	6	0	-11.082902	1.213843	0.000346
7	6	0	-8.541828	-1.541322	0.000040
8	6	0	-7.326177	-0.829813	-0.000029
9	6	0	-7.359948	0.622578	0.000026
10	6	0	-8.608219	1.271729	0.000145
11	6	0	-6.074321	-1.481229	-0.000139
12	6	0	-4.877695	-0.767651	-0.000173
13	6	0	-4.911587	0.685935	-0.000124
14	6	0	-6.139268	1.336241	-0.000033
15	6	0	-3.608573	-1.416175	-0.000243
16	6	0	-2.408588	-0.719905	-0.000280
17	6	0	-2.468132	0.738977	-0.000226
18	6	0	-3.668665	1.395998	-0.000156
19	6	0	-1.194426	-1.515275	-0.000284
20	6	0	0.011257	-0.708954	-0.000250
21	6	0	0.057350	0.752707	-0.000231
22	6	0	-1.209404	1.533378	-0.000247
23	6	0	1.216802	-1.393545	-0.000189
24	6	0	2.481272	-0.733462	-0.000168
25	6	0	2.502063	0.723851	-0.000179
26	6	0	1.250245	1.421144	-0.000210
27	6	0	3.680575	-1.435919	-0.000142
28	6	0	4.931695	-0.774040	-0.000092
29	6	0	4.952748	0.683668	-0.000079
30	6	0	3.719734	1.385178	-0.000141
31	6	0	6.144630	-1.474685	-0.000046
32	6	0	7.382951	-0.813159	0.000017
33	6	0	7.404417	0.642950	0.000053
34	6	0	6.186174	1.343472	0.000000
35	6	0	8.610970	-1.512772	0.000059
36	6	0	9.833398	-0.850641	0.000148
37	6	0	9.854938	0.603407	0.000198
38	6	0	8.653079	1.303207	0.000146
39	6	0	11.084457	-1.553435	0.000197
40	6	0	12.271131	-0.876778	0.000292
41	6	0	12.292323	0.555185	0.000347
42	6	0	11.126614	1.267644	0.000304
43	8	0	-1.216327	2.763890	-0.000284
44	1	0	-13.203853	1.000176	0.000529
45	1	0	-13.145301	-1.492422	0.000437

46	1	0	-10.987720	-2.691468	0.000201
47	1	0	-11.107067	2.300833	0.000388
48	1	0	-8.514249	-2.628932	-0.000009
49	1	0	-8.635390	2.359291	0.000178
50	1	0	-6.044621	-2.568591	-0.000190
51	1	0	-6.166473	2.423571	0.000002
52	1	0	-3.553018	-2.501548	-0.000273
53	1	0	-3.671942	2.483113	-0.000125
54	1	0	1.171439	-2.479409	-0.000178
55	1	0	1.242742	2.508282	-0.000219
56	1	0	3.660547	-2.523502	-0.000143
57	1	0	3.736672	2.472705	-0.000141
58	1	0	6.126647	-2.562387	-0.000066
59	1	0	6.203972	2.431115	0.000016
60	1	0	8.593751	-2.600623	0.000029
61	1	0	8.670198	2.391022	0.000183
62	1	0	11.065784	-2.640594	0.000156
63	1	0	13.210957	-1.421888	0.000327
64	1	0	13.248029	1.072013	0.000427
65	1	0	11.141189	2.354847	0.000347

$C_{42}H_{22}O$ (zigzag), M=3 (E = -1688.92653 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	12.268440	0.614602	0.000487
2	6	0	12.267438	-0.813164	0.000437
3	6	0	11.087596	-1.507786	0.000313
4	6	0	9.830261	-0.823721	0.000230
5	6	0	9.831860	0.625350	0.000283
6	6	0	11.088320	1.309217	0.000413
7	6	0	8.611032	-1.505312	0.000102
8	6	0	7.378612	-0.825328	0.000029
9	6	0	7.382427	0.627178	0.000083
10	6	0	8.611668	1.306987	0.000209
11	6	0	6.140888	-1.505821	-0.000091
12	6	0	4.922240	-0.823912	-0.000163
13	6	0	4.931514	0.632241	-0.000123
14	6	0	6.142561	1.310342	0.000007
15	6	0	3.673049	-1.499645	-0.000255
16	6	0	2.463108	-0.805486	-0.000320
17	6	0	2.483402	0.658739	-0.000336
18	6	0	3.678574	1.323392	-0.000239
19	6	0	1.202000	-1.410163	-0.000335
20	6	0	-0.050178	-0.803850	-0.000360
21	6	0	-0.067313	0.662081	-0.000368
22	6	0	1.208906	1.434246	-0.000455
23	6	0	-1.268614	-1.494874	-0.000329
24	6	0	-2.511621	-0.816926	-0.000254
25	6	0	-2.516742	0.642527	-0.000201
26	6	0	-1.260455	1.329369	-0.000290
27	6	0	-3.734166	-1.494714	-0.000210

28	6	0	-4.972702	-0.811371	-0.000106
29	6	0	-4.970975	0.646855	-0.000036
30	6	0	-3.722373	1.324201	-0.000084
31	6	0	-6.200471	-1.485917	-0.000065
32	6	0	-7.430077	-0.799600	0.000044
33	6	0	-7.425053	0.655296	0.000117
34	6	0	-6.187481	1.331098	0.000076
35	6	0	-8.668791	-1.473191	0.000088
36	6	0	-9.882621	-0.786051	0.000195
37	6	0	-9.876441	0.664882	0.000269
38	6	0	-8.655483	1.340424	0.000229
39	6	0	-11.144511	-1.463607	0.000237
40	6	0	-12.320291	-0.763476	0.000344
41	6	0	-12.313910	0.665510	0.000420
42	6	0	-11.131301	1.354348	0.000385
43	8	0	1.210597	2.664905	-0.000588
44	1	0	13.215521	1.147044	0.000585
45	1	0	13.214179	-1.346379	0.000500
46	1	0	11.085431	-2.595160	0.000274
47	1	0	11.086007	2.396612	0.000450
48	1	0	8.611458	-2.593343	0.000062
49	1	0	8.611591	2.395064	0.000251
50	1	0	6.140528	-2.593650	-0.000127
51	1	0	6.142434	2.398182	0.000046
52	1	0	3.660554	-2.586067	-0.000275
53	1	0	3.662658	2.410200	-0.000251
54	1	0	-1.258649	-2.581321	-0.000366
55	1	0	-1.241574	2.416164	-0.000295
56	1	0	-3.736994	-2.582509	-0.000248
57	1	0	-3.718233	2.412037	-0.000028
58	1	0	-6.205610	-2.573800	-0.000110
59	1	0	-6.183088	2.419059	0.000136
60	1	0	-8.674366	-2.561246	0.000039
61	1	0	-8.650576	2.428515	0.000288
62	1	0	-11.147610	-2.551013	0.000182
63	1	0	-13.269895	-1.291558	0.000370
64	1	0	-13.258559	1.202325	0.000511
65	1	0	-11.123946	2.441744	0.000443

10,0-CNT $C_{40}H_{18}O$, M=1 (E = -1610.09865 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.434217	3.586784	-1.422955
2	6	0	-2.535224	3.104274	-0.673951
3	6	0	-3.490749	2.288209	-1.300661
4	6	0	-4.059233	1.213833	-0.581673
5	6	0	-4.309333	-0.000005	-1.251031
6	6	0	-4.059230	-1.213843	-0.581674
7	6	0	-3.490741	-2.288217	-1.300662
8	6	0	-2.535215	-3.104279	-0.673952
9	6	0	-1.434206	-3.586787	-1.422956

10	6	0	-0.183943	-3.722324	-0.811442
11	6	0	1.000644	-3.479130	-1.560296
12	6	0	2.135676	-2.974162	-0.936585
13	6	0	3.062460	-2.157919	-1.662275
14	6	0	3.789618	-1.172386	-1.005396
15	6	0	4.055659	0.000001	-1.787359
16	6	0	3.789608	1.172391	-1.005400
17	6	0	3.062446	2.157921	-1.662278
18	6	0	2.135666	2.974167	-0.936587
19	6	0	1.000633	3.479135	-1.560297
20	6	0	-0.183953	3.722325	-0.811442
21	6	0	-2.450373	3.108156	0.785707
22	6	0	-3.324084	2.293706	1.521346
23	6	0	-3.971537	1.214354	0.878478
24	6	0	-4.140379	-0.000005	1.571582
25	6	0	-3.971534	-1.214365	0.878477
26	6	0	-3.324078	-2.293716	1.521345
27	6	0	-2.450365	-3.108162	0.785706
28	6	0	-1.270073	-3.603707	1.397459
29	6	0	-0.100620	-3.735021	0.647210
30	6	0	1.170493	-3.518031	1.258278
31	6	0	2.224228	-3.001458	0.521959
32	6	0	3.228681	-2.190564	1.162246
33	6	0	3.886547	-1.222158	0.453644
34	6	0	4.351654	0.000006	1.183764
35	6	0	3.886540	1.222165	0.453640
36	6	0	3.228674	2.190573	1.162243
37	6	0	2.224219	3.001465	0.521957
38	6	0	1.170484	3.518037	1.258276
39	6	0	-0.100629	3.735022	0.647209
40	6	0	-1.270082	3.603703	1.397459
41	1	0	-1.487943	3.550426	-2.508752
42	1	0	-3.528462	2.265654	-2.387447
43	1	0	-4.339361	-0.000004	-2.338243
44	1	0	-3.528453	-2.265661	-2.387448
45	1	0	-1.487932	-3.550430	-2.508752
46	1	0	0.929956	-3.436024	-2.644877
47	1	0	3.016119	-2.120630	-2.747172
48	1	0	3.016101	2.120630	-2.747174
49	1	0	0.929944	3.436029	-2.644878
50	1	0	-3.231504	2.272938	2.604827
51	1	0	-4.037965	-0.000005	2.654327
52	1	0	-3.231499	-2.272947	2.604826
53	1	0	-1.198837	-3.578080	2.482521
54	1	0	1.225580	-3.504188	2.344546
55	1	0	3.281801	-2.178525	2.248385
56	1	0	3.281798	2.178536	2.248381
57	1	0	1.225572	3.504197	2.344544
58	1	0	-1.198845	3.578074	2.482521
59	8	0	4.809893	0.000009	2.318148

Figure 12

$C_{16}H_8O$, M=3 (E = -689.67753 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.302814	-0.970876	0.000535
2	6	0	2.358035	-1.985373	0.000430
3	6	0	0.977852	-1.690535	0.000120
4	6	0	0.562982	-0.325989	-0.000099
5	6	0	1.547800	0.701628	-0.000114
6	6	0	2.898612	0.372256	0.000293
7	6	0	-0.020481	-2.721219	0.000045
8	6	0	-0.836519	-0.019282	-0.000262
9	6	0	-1.801082	-1.057870	-0.000250
10	6	0	-1.350212	-2.420825	-0.000147
11	6	0	-3.175362	-0.720643	-0.000294
12	1	0	-3.911219	-1.520794	-0.000304
13	6	0	-3.591440	0.608263	-0.000256
14	6	0	-2.658452	1.643638	-0.000165
15	6	0	-1.273696	1.358234	-0.000162
16	6	0	-0.279073	2.334925	-0.000076
17	6	0	1.145514	2.147153	-0.000738
18	1	0	0.307766	-3.757696	0.000173
19	1	0	4.361460	-1.214973	0.000749
20	1	0	2.672653	-3.026259	0.000614
21	1	0	3.623429	1.179999	0.000256
22	1	0	-2.094831	-3.212799	-0.000158
23	1	0	-4.652458	0.840680	-0.000258
24	1	0	-2.980262	2.680292	-0.000114
25	8	0	1.978714	3.063829	0.000736

$C_{42}H_{22}O$ (armchair), M=3 (E = -1688.95004 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	10.414873	0.735375	-0.000013
2	6	0	11.146983	-0.433598	-0.000074
3	6	0	10.476198	-1.672674	-0.000064
4	6	0	9.095239	-1.722896	0.000022
5	6	0	8.312436	-0.541466	0.000096
6	6	0	8.999700	0.708766	0.000067
7	6	0	6.858670	-0.550050	0.000206
8	6	0	6.137427	0.672887	0.000134
9	6	0	6.876487	1.901256	0.000093
10	6	0	8.239289	1.917631	0.000066
11	6	0	6.116013	-1.762953	0.000476
12	6	0	4.747456	-1.775560	0.000463
13	6	0	3.985717	-0.573180	0.000141
14	6	0	4.690321	0.657984	0.000064
15	6	0	2.533270	-0.581250	-0.000035
16	6	0	1.797651	0.644644	-0.000112
17	6	0	2.552737	1.861728	-0.000180

18	6	0	3.918168	1.858781	-0.000129
19	6	0	1.801676	-1.792785	-0.000128
20	6	0	0.431508	-1.809957	-0.000221
21	6	0	-0.336063	-0.616853	-0.000233
22	6	0	0.355561	0.621472	-0.000192
23	6	0	-1.802081	-0.703403	-0.000221
24	6	0	-2.584690	0.495096	-0.000012
25	6	0	-1.868893	1.672252	-0.000028
26	6	0	-0.453912	1.885681	-0.000262
27	6	0	-2.514342	-1.923202	-0.000364
28	6	0	-3.894019	-1.969944	-0.000293
29	6	0	-4.701669	-0.797255	-0.000063
30	6	0	-4.031388	0.450947	0.000096
31	6	0	-6.148931	-0.834476	0.000019
32	6	0	-6.883371	0.382083	0.000192
33	6	0	-6.160807	1.610203	0.000310
34	6	0	-4.791514	1.646552	0.000285
35	6	0	-6.868595	-2.071992	-0.000062
36	6	0	-8.231546	-2.106137	-0.000181
37	6	0	-9.007020	-0.907369	-0.000012
38	6	0	-8.337136	0.352770	0.000148
39	6	0	-10.421858	-0.954388	0.000080
40	6	0	-11.170025	0.204018	0.000180
41	6	0	-10.516585	1.452445	0.000138
42	6	0	-9.136687	1.522992	0.000189
43	8	0	0.007403	3.042580	-0.000520
44	1	0	10.916687	1.700223	-0.000027
45	1	0	12.233019	-0.401741	-0.000156
46	1	0	11.047501	-2.597027	-0.000118
47	1	0	8.614090	-2.694591	0.000007
48	1	0	6.349074	2.847164	0.000109
49	1	0	8.772512	2.865293	0.000026
50	1	0	6.636605	-2.713576	0.000782
51	1	0	4.249279	-2.737649	0.000803
52	1	0	2.016982	2.798058	-0.000333
53	1	0	4.418450	2.819882	-0.000272
54	1	0	2.320255	-2.743817	-0.000150
55	1	0	-0.062983	-2.773385	-0.000250
56	1	0	-1.982146	-2.866745	-0.000553
57	1	0	-4.361772	-2.947482	-0.000417
58	1	0	-6.699305	2.550517	0.000401
59	1	0	-4.269036	2.598761	0.000359
60	1	0	-6.326687	-3.010372	0.000035
61	1	0	-8.752584	-3.060463	-0.000405
62	1	0	-10.909850	-1.926206	0.000069
63	1	0	-12.255407	0.157132	0.000433
64	1	0	-11.100845	2.368514	-0.000056
65	1	0	-8.670563	2.501821	0.000335

5,5-CNT $C_{40}H_{18}O$, M=3 (E = -1610.13173 hartrees):

Standard orientation:

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

1	6	0	1.483074	-3.145614	-1.836615
2	6	0	2.592036	-2.352542	-1.918910
3	6	0	3.502725	0.438209	-1.999948
4	6	0	3.058818	1.729617	-1.983528
5	6	0	0.626202	3.362044	-1.845906
6	6	0	-0.739705	3.346584	-1.754603
7	6	0	-3.681035	0.369253	-1.562855
8	6	0	-2.576653	-2.381927	-1.561377
9	6	0	-1.454110	-3.154828	-1.626632
10	6	0	3.102679	-1.704367	-0.743969
11	6	0	3.546205	-0.323439	-0.783770
12	6	0	2.632393	2.327204	-0.749787
13	6	0	1.432592	3.142819	-0.681635
14	6	0	-1.361311	3.124574	-0.489816
15	6	0	-2.557495	2.300934	-0.394684
16	6	0	-3.426633	-0.388608	-0.288660
17	6	0	-2.915139	-1.726961	-0.323864
18	6	0	-0.618861	-3.338161	-0.470214
19	6	0	0.826775	-3.339137	-0.574623
20	6	0	3.616825	0.400330	0.429591
21	6	0	3.140486	1.771376	0.447135
22	6	0	0.835960	3.370979	0.584080
23	6	0	-0.609446	3.358351	0.680162
24	6	0	-2.929147	1.745474	0.882119
25	6	0	-3.364885	0.346704	0.915141
26	6	0	-2.388701	-2.284732	0.877572
27	6	0	-1.207172	-3.122766	0.797841
28	6	0	1.593484	-3.119309	0.595415
29	6	0	2.768265	-2.272488	0.507750
30	6	0	2.782544	2.419291	1.677440
31	6	0	1.663994	3.200472	1.743997
32	6	0	-1.287443	3.190528	1.936874
33	6	0	-2.412248	2.405728	2.033564
34	6	0	-3.271067	-0.402882	2.127809
35	6	0	-2.800708	-1.691295	2.107515
36	6	0	-0.400093	-3.389538	1.953471
37	6	0	0.962626	-3.389885	1.855183
38	6	0	3.333030	-1.661824	1.678222
39	6	0	3.744391	-0.359760	1.640821
40	1	0	1.026150	-3.513874	-2.749385
41	1	0	2.994615	-2.104605	-2.895766
42	1	0	3.690727	-0.045976	-2.952900
43	1	0	2.904294	2.249160	-2.923734
44	1	0	1.087219	3.386651	-2.827728
45	1	0	-1.349561	3.347192	-2.653565
46	1	0	-3.136272	-2.137011	-2.454644
47	1	0	-1.128951	-3.529127	-2.592221
48	1	0	3.319831	2.184784	2.590859
49	1	0	1.334885	3.574440	2.708399
50	1	0	-0.838552	3.573401	2.847883
51	1	0	-2.805890	2.173515	3.018428
52	1	0	-3.431158	0.085051	3.084072
53	1	0	-2.600412	-2.191546	3.049400
54	1	0	-0.860313	-3.462024	2.933872
55	1	0	1.559352	-3.460449	2.758965
56	1	0	3.306380	-2.181971	2.630421

57	1	0	4.036806	0.131219	2.563688
58	6	0	-3.142939	1.699283	-1.488564
59	8	0	-4.213879	-0.134624	-2.560810

Figure S1b

$C_{19}H_{10}O_2$, TS, M=1 (E = -880.38594 hartrees)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.753394	-0.728504	-0.117062
2	6	0	3.609112	0.652959	-0.082606
3	6	0	2.330169	1.240227	-0.022757
4	6	0	1.176603	0.400007	-0.014865
5	6	0	1.338167	-1.019148	-0.036956
6	6	0	2.633284	-1.558585	-0.070687
7	6	0	-0.121165	1.003605	0.008696
8	6	0	-1.285011	0.181318	-0.019108
9	6	0	-1.162007	-1.235895	-0.092235
10	6	0	0.144398	-1.850308	-0.137306
11	6	0	-2.579554	0.771173	0.012465
12	6	0	-3.713267	-0.072402	-0.018409
13	6	0	-3.581678	-1.452748	-0.072830
14	6	0	-2.310809	-2.038238	-0.102875
15	6	0	2.157843	2.661338	0.020378
16	6	0	0.915002	3.225902	0.064257
17	6	0	-0.259571	2.411817	0.055871
18	6	0	-1.568583	2.982658	0.088804
19	6	0	-2.687180	2.195372	0.070352
20	1	0	2.726110	-2.636512	-0.005035
21	1	0	4.744986	-1.170437	-0.147927
22	1	0	4.485038	1.297178	-0.087905
23	1	0	3.045689	3.288679	0.014823
24	1	0	-3.676921	2.643960	0.096148
25	1	0	-4.702133	0.379316	0.008641
26	1	0	-4.465938	-2.082830	-0.080818
27	1	0	-2.189959	-3.115223	-0.117691
28	8	0	0.845241	-3.565054	0.801023
29	8	0	0.174549	-3.134774	-0.439394
30	1	0	0.801065	4.306237	0.099294
31	1	0	-1.661134	4.064972	0.128680

Figure S2

$C_{15}H_8O$, M=3 (E = -651.56363 hartrees):

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	3.378643	0.090277	0.000495
2	6	0	2.804043	-1.257462	0.000470
3	6	0	1.404796	-1.415631	0.000277
4	6	0	0.676430	-0.223374	0.000232
5	6	0	1.203806	1.126597	0.000171
6	6	0	2.635129	1.244811	0.000495
7	6	0	0.602955	-2.617634	0.000032
8	6	0	-0.695329	-0.178556	-0.000276
9	6	0	-1.508366	-1.345756	-0.000367
10	6	0	-0.783948	-2.582840	-0.000178
11	6	0	-2.893413	-1.096814	-0.000372
12	1	0	-3.607194	-1.916304	-0.000483
13	6	0	-3.359612	0.227732	-0.000256
14	6	0	-2.512590	1.373536	-0.000214
15	6	0	-1.146625	1.180741	-0.000337
16	6	0	0.071368	2.063868	-0.000052
17	1	0	1.103567	-3.582961	-0.000023
18	1	0	4.463186	0.161568	0.000506
19	1	0	3.473803	-2.112273	0.000846
20	1	0	3.110544	2.220451	0.000556
21	1	0	-1.334238	-3.520415	-0.000192
22	1	0	-4.434561	0.389712	-0.000285
23	1	0	-2.946762	2.369325	-0.000145
24	8	0	0.113491	3.306740	-0.000186

$C_{17}H_{10}$, M=3 (E = -653.73395 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.676494	-1.026159	-0.000239
2	6	0	-2.700282	0.053046	-0.000149
3	6	0	-1.406397	-0.538220	-0.000223
4	6	0	-1.607169	-1.975224	0.000102
5	6	0	-2.989032	-2.240008	0.000440
6	6	0	-0.244787	0.261905	-0.000080
7	6	0	1.436184	-1.619735	-0.000166
8	6	0	1.107806	-0.265687	-0.000073
9	6	0	2.686573	-2.168891	-0.000155
10	1	0	-4.752665	-0.893493	-0.000230
11	1	0	-3.438861	-3.225197	0.000998
12	6	0	-2.858787	1.438988	-0.000093
13	6	0	-1.722356	2.242350	-0.000020
14	6	0	-0.424573	1.688621	0.000024
15	1	0	-3.848933	1.887930	-0.000098
16	1	0	-1.823258	3.324751	0.000026
17	6	0	0.728452	2.544090	0.000135
18	6	0	1.993387	2.043959	0.000154
19	6	0	2.231364	0.627538	0.000051
20	1	0	0.565548	3.619241	0.000203
21	1	0	2.851872	2.711287	0.000242

22	6	0	3.776708	-1.266101	-0.000038
23	1	0	4.794272	-1.648980	-0.000024
24	6	0	3.542483	0.098208	0.000064
25	1	0	4.379814	0.791649	0.000157
26	1	0	2.850913	-3.243113	-0.000234
27	1	0	-0.817175	-2.716161	0.000552

$C_{15}H_8$, M=3 (E = -576.31373 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.383993	-0.409517	0.000297
2	6	0	-2.866834	0.887161	0.000311
3	6	0	-1.457876	1.086998	0.000191
4	6	0	-0.700750	-0.080084	0.000071
5	6	0	-1.192173	-1.422437	0.000055
6	6	0	-2.578635	-1.575937	0.000170
7	6	0	-0.689844	2.312102	0.000173
8	6	0	0.700759	-0.080162	-0.000063
9	6	0	1.457938	1.086906	-0.000092
10	6	0	0.690013	2.312040	0.000038
11	6	0	2.866887	0.887121	-0.000248
12	1	0	3.545463	1.736515	-0.000282
13	6	0	3.383985	-0.409614	-0.000360
14	6	0	2.578525	-1.575993	-0.000325
15	6	0	1.192017	-1.422567	-0.000168
16	6	0	-0.000068	-2.232243	-0.000064
17	1	0	-1.217378	3.263165	0.000264
18	1	0	-4.463511	-0.535050	0.000388
19	1	0	-3.545398	1.736552	0.000410
20	1	0	-3.047550	-2.555729	0.000166
21	1	0	1.217715	3.263026	0.000026
22	1	0	4.463455	-0.535371	-0.000478
23	1	0	3.047502	-2.555762	-0.000414

Figure S3

5,5-CNT $C_{40}H1_8O$, M=1 (E = -1610.11549 hartrees):

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.085583	-2.805957	1.841478
2	6	0	-3.023817	-1.815180	1.908846
3	6	0	-3.369786	1.098955	1.963012
4	6	0	-2.675807	2.275106	1.945621
5	6	0	0.029194	3.392095	1.838383
6	6	0	1.366118	3.108043	1.767513

7	6	0	3.655787	-0.276386	1.519925
8	6	0	2.057297	-2.820199	1.583864
9	6	0	0.804192	-3.363270	1.647106
10	6	0	-3.390652	-1.090594	0.725042
11	6	0	-3.550117	0.351857	0.750762
12	6	0	-2.123620	2.766128	0.714651
13	6	0	-0.785858	3.329800	0.659345
14	6	0	1.955532	2.801590	0.507085
15	6	0	2.954839	1.766464	0.412251
16	6	0	3.336621	-1.058456	0.305702
17	6	0	2.517515	-2.242597	0.350493
18	6	0	-0.046400	-3.397027	0.491396
19	6	0	-1.469744	-3.131000	0.586419
20	6	0	-3.460581	1.064905	-0.467364
21	6	0	-2.716301	2.311387	-0.486213
22	6	0	-0.142570	3.435502	-0.601525
23	6	0	1.276461	3.162475	-0.678181
24	6	0	3.224092	1.131754	-0.844929
25	6	0	3.387568	-0.322888	-0.894741
26	6	0	1.889904	-2.688114	-0.849429
27	6	0	0.577398	-3.301091	-0.773889
28	6	0	-2.174515	-2.782791	-0.590162
29	6	0	-3.163576	-1.723398	-0.519176
30	6	0	-2.221547	2.862557	-1.716137
31	6	0	-0.972185	3.411575	-1.772035
32	6	0	1.954050	2.891414	-1.916866
33	6	0	2.933881	1.930448	-1.997759
34	6	0	3.119614	-1.015154	-2.110545
35	6	0	2.397823	-2.182938	-2.081910
36	6	0	-0.259253	-3.432123	-1.932493
37	6	0	-1.599045	-3.181142	-1.843112
38	6	0	-3.584750	-1.022367	-1.699622
39	6	0	-3.725378	0.336157	-1.675490
40	1	0	-1.712560	-3.245823	2.760765
41	1	0	-3.377841	-1.486165	2.880563
42	1	0	-3.661438	0.669108	2.915956
43	1	0	-2.432711	2.760490	2.885247
44	1	0	-0.435030	3.508512	2.811814
45	1	0	1.956368	2.967937	2.670044
46	1	0	2.637072	-2.673250	2.484140
47	1	0	0.410482	-3.657097	2.615125
48	1	0	-2.781649	2.726132	-2.635664
49	1	0	-0.562198	3.701916	-2.734384
50	1	0	1.614482	3.367121	-2.831987
51	1	0	3.347341	1.675565	-2.969256
52	1	0	3.337721	-0.550176	-3.066548
53	1	0	2.084275	-2.625172	-3.021952
54	1	0	0.182887	-3.605369	-2.908598
55	1	0	-2.195807	-3.154620	-2.749332
56	1	0	-3.654164	-1.545699	-2.647935
57	1	0	-3.904391	0.867670	-2.604762
58	6	0	3.767580	1.194264	1.380824
59	8	0	3.645110	-0.689991	2.682242