

Supporting Information for

Nature of Oxygen Adsorption on Defective Carbonaceous Materials

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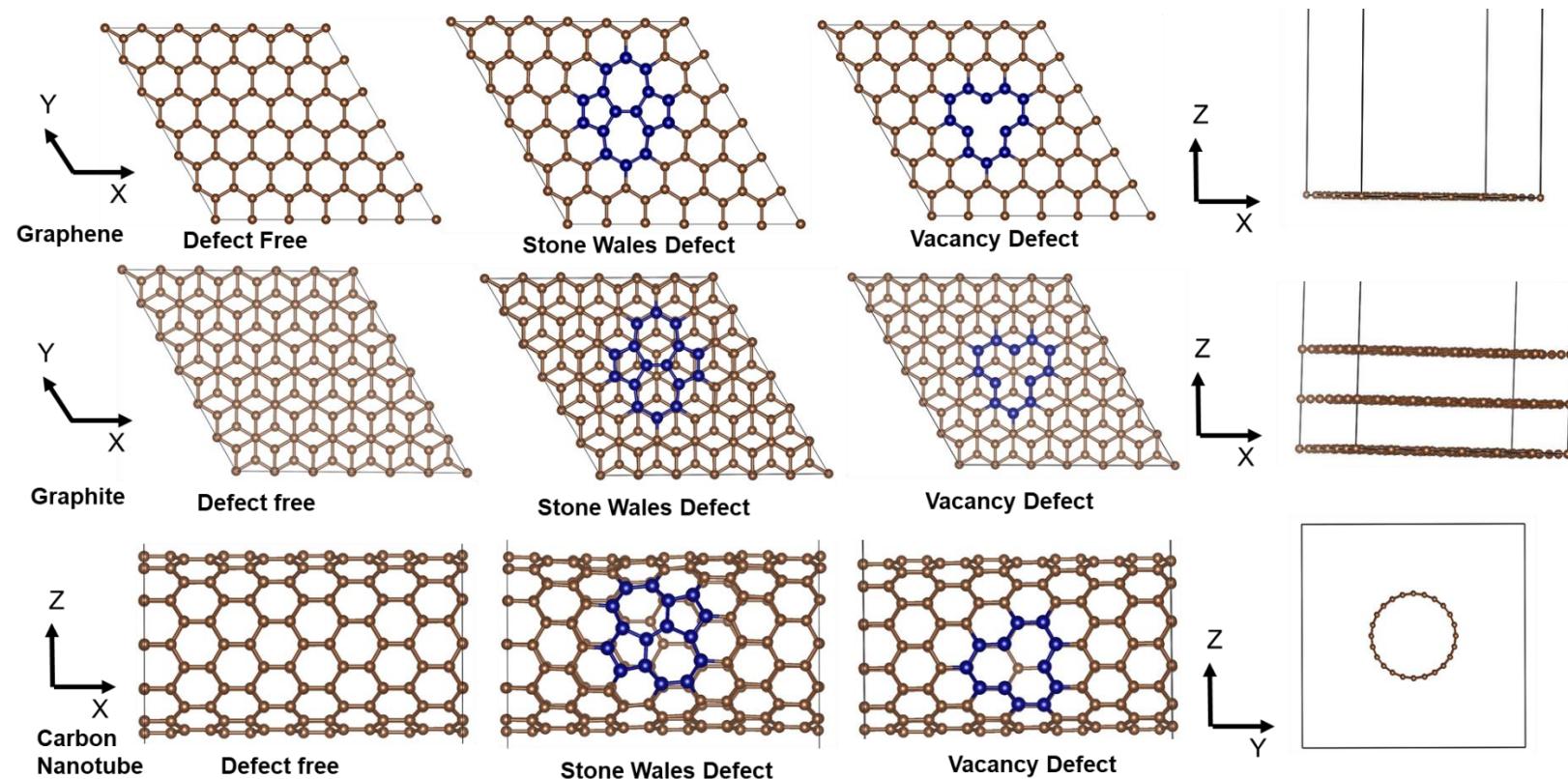


Figure S1 Top views of the basal planes of defect free, Stone-Wales (SW) defected, single vacancy defected graphene and graphite; Side views of defect free, SW defected, single vacancy defected (12,0) zigzag single-walled carbon nanotubes.

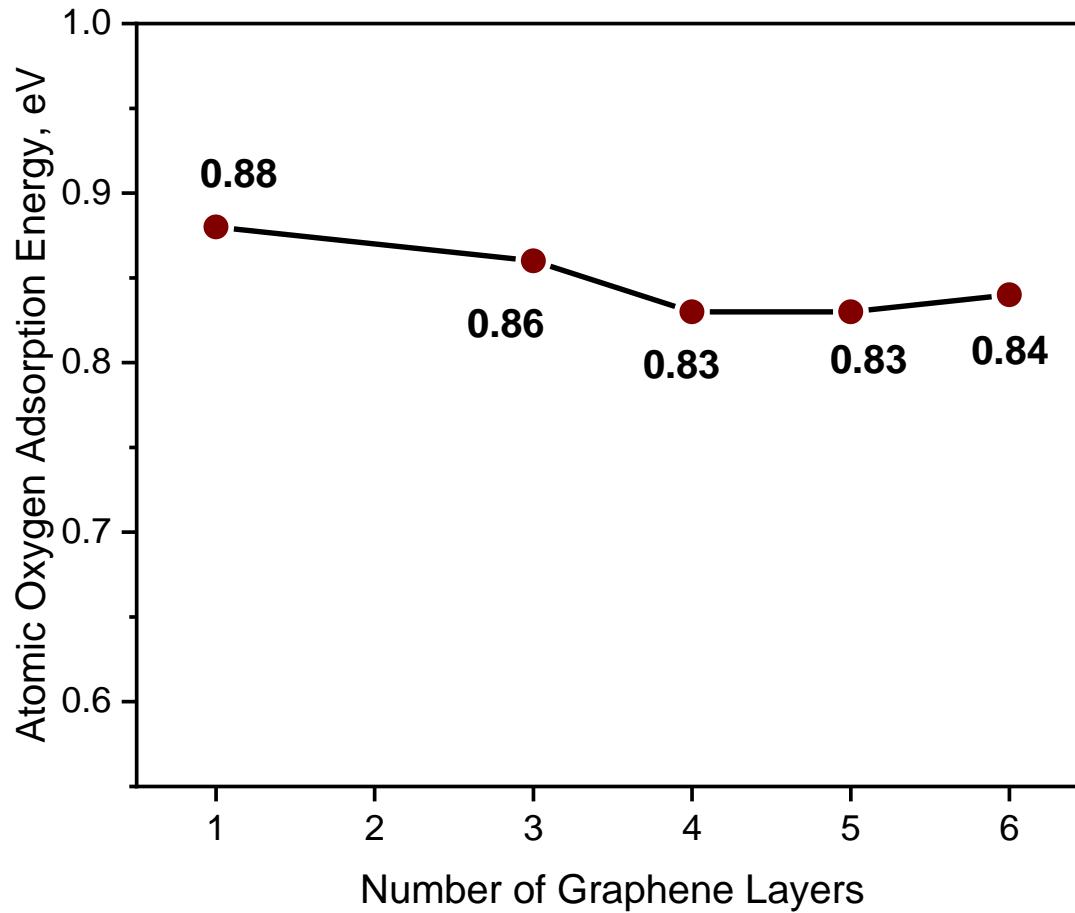


Figure S2. Adsorption energies in eV for atomic oxygen adsorption on different graphene layers with optPBE-vdw. The adsorption energy is predicted to be 0.94 eV with PBE on one-layer graphene.

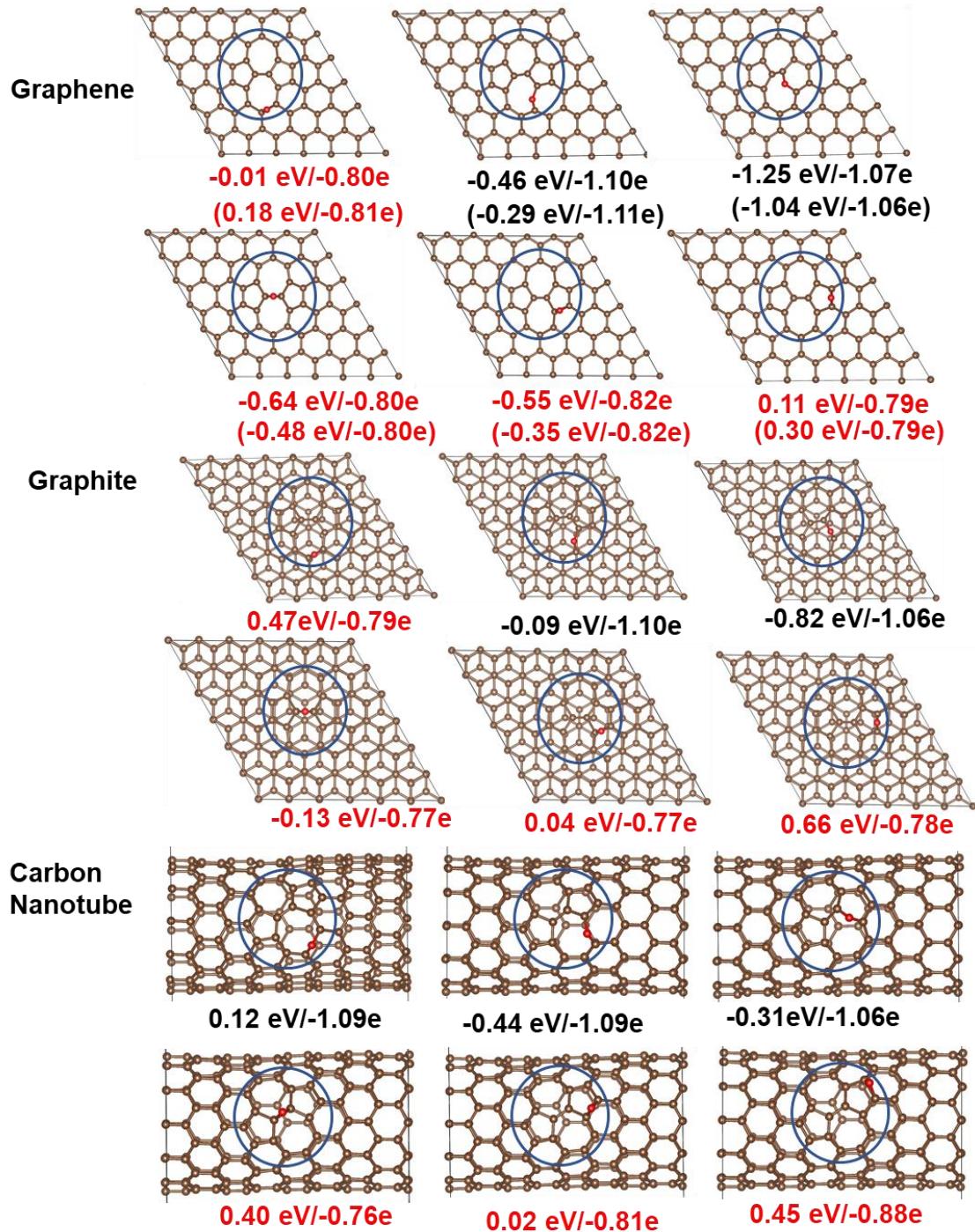


Figure S3. The adsorption energies in eV as well as the net Bader charge of O on various adsorption sites around a SW defect on studied graphene, graphite, and carbon nanotube. The energies are predicted at the optPBE-vdw level for graphene and graphite and with PBE for nanotube; The PBE values for graphene are shown in parenthesis. The energies and charges in black and in red are for the adsorption leading to the formation of an ether and an epoxide respectively.

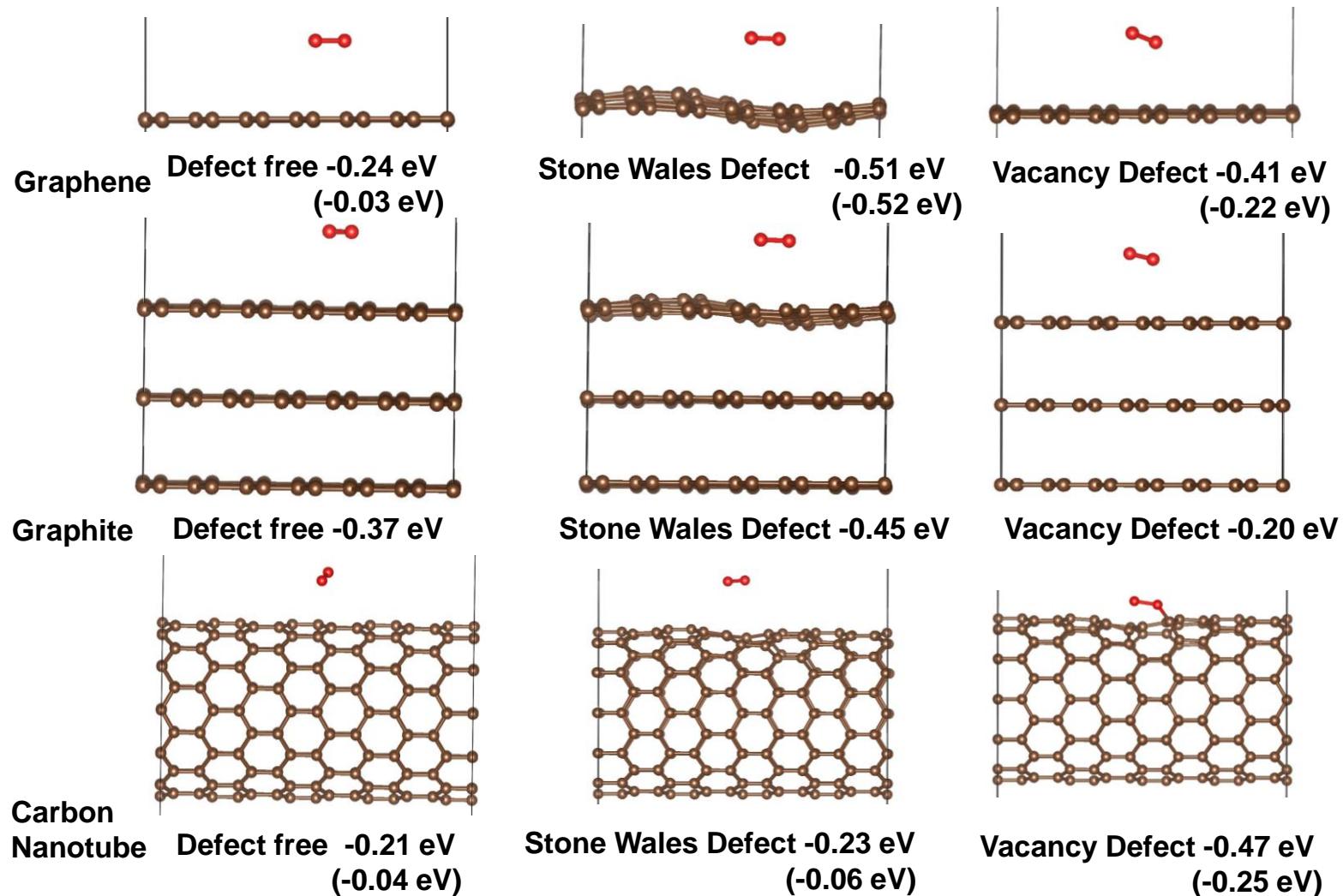
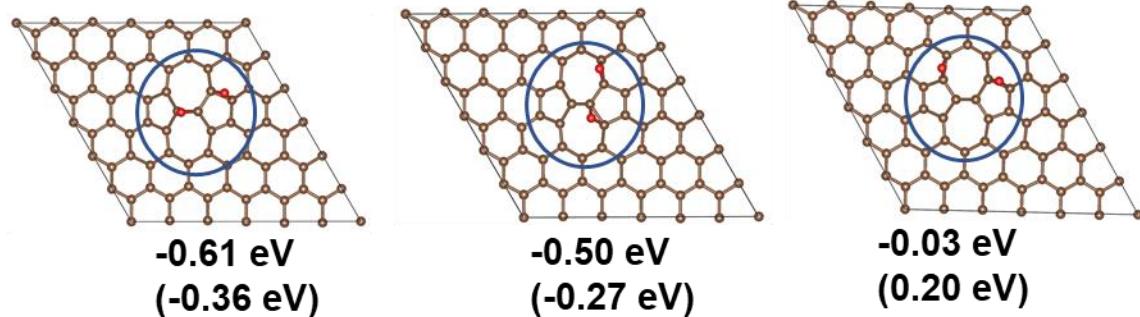
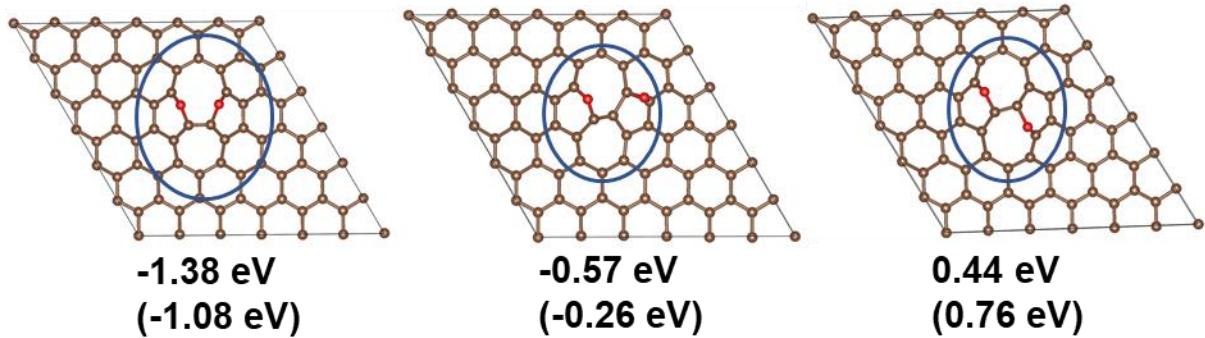
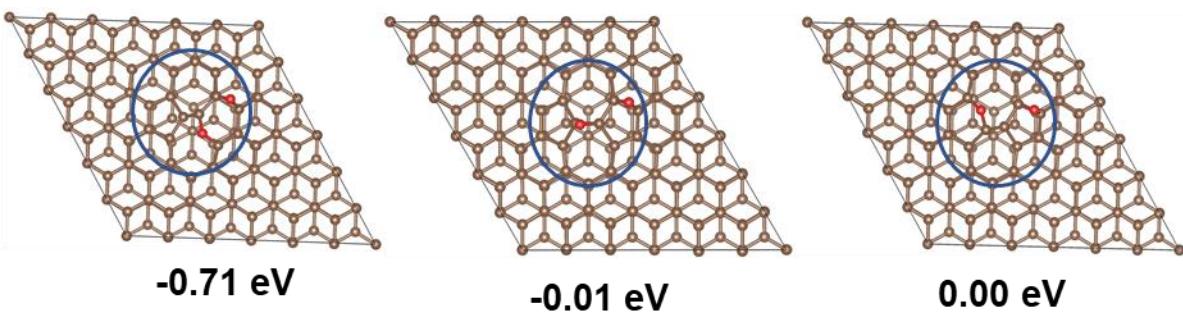


Figure S4. Side views of molecular oxygen adsorption on defect free, SW defected, and SV defected graphene, graphite, and carbon nanotubes and the adsorption energies in eV. The energies are predicted at the optPBE-vdw level; The PBE values for graphene and nanotubes are shown in parenthesis.

Graphene



Graphite



Carbon Nanotube

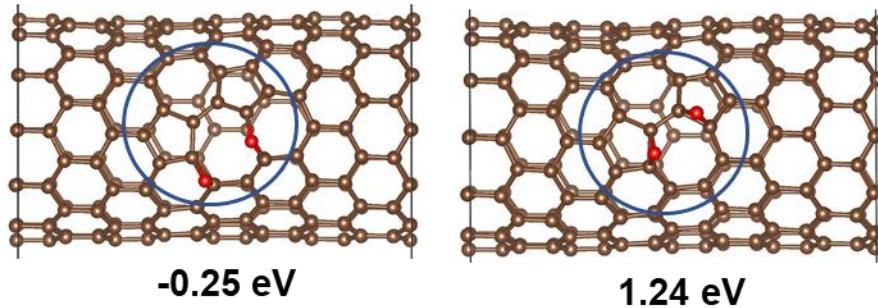


Figure S5. Additional structures and energetics for the chemisorption of O₂ on different binding site for graphene, graphite and carbon nanotube. The energies are predicted at the optPBE-vdw level for graphene and graphite and with PBE for nanotube; The PBE values for graphene are shown in parenthesis.

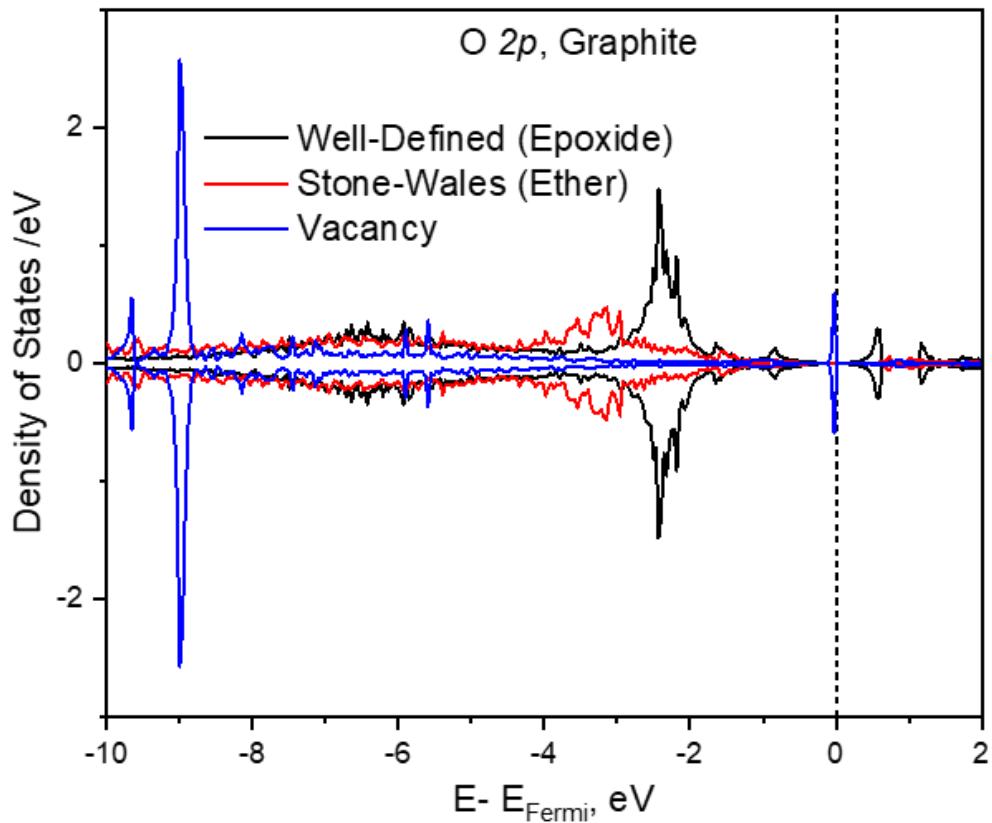
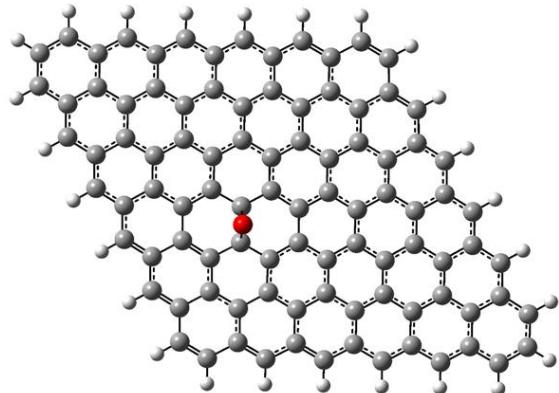
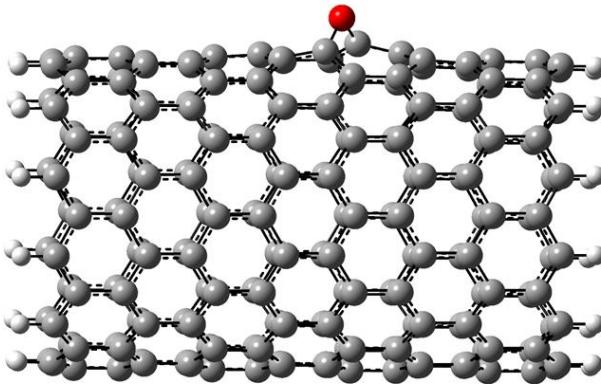


Figure S6. Projected density of states of O 2p orbitals in the products of atomic adsorption on defect free, SW defected, and single vacancy defected graphite at the optPBE-vdw level. The structures correspond to Figures 1d and 1f in the manuscript.



(a) Epoxide
Triplet 0.28



(b) Ether
Triplet -2.60

Figure 7. Optimized molecular structures and atomic oxygen adsorption energies (ΔH_{0K}) in eV for graphene (a) and nanotube (b) with cluster models at the M06-2X/6-311G(d,p) level using a larger model. For the graphene, there are 96 carbon atoms; For the nanotube, there are 192 carbon atoms. One half of the electronic energy of O_2 was selected for the adsorbate. T= Triplet in black.

Table S1. Calculated bond distances in Å and bond angles in degree for atomic oxygen adsorption with optPBE-vdw for graphene and graphite and with PBE for nanotubes.

Material		C1-O	C2-O	C3-O	\angle C-O-C
Graphene	Defect free	1.464	1.465		62.0
	Stone-Wales Defect	1.382	1.395		102.9
	Single vacancy ^a	1.478	1.478	1.478	120.0
Graphite	Defect free	1.485	1.486		60.7
	Stone-Wales Defect	1.389	1.403		102.5
	Single vacancy ^a	1.488	1.488	1.488	120.0
Nanotube	Defect free	1.390	1.390		95.3
	Stone-Wales Defect	1.384	1.403		102.3
	Single vacancy	1.492	1.518	1.518	112.7, 116.6, 116.6

^a The three \angle C-O-C are identical with 120°.

Table S2. Detailed hybridization properties on the alpha and beta spin orbitals to make the C-O bonds in the epoxide and the ether on graphene and nanotube from NBO analysis calculated at the M06-2X/6-311G(d,p) level.

Species	Bond	Hybrid ^a <i>h</i> _C (α, β)	% <i>p</i> ^b (α, β)	Hybrid ^a <i>h</i> _O (α, β)	% <i>p</i> ^b (α, β)	wt, <i>C</i> ^c (α, β)	wt, <i>O</i> ^c (α, β)
Graphene-Epoxide	C1-O	(sp ^{6.16} , sp ^{6.20})	(86.0%, 86.1%)	(sp ^{6.97} , sp ^{6.79})	(87.4%, 87.2%)	(35.6%, 35.0%)	(64.4%, 65.0%)
	C2-O	(sp ^{6.17} , sp ^{6.21})	(86.0%, 86.1%)	(sp ^{6.99} , sp ^{6.81})	(87.5%, 87.2%)	(35.6%, 35.0%)	(64.4%, 65.0%)
Graphene SW- Ether	C1-O	(sp ^{3.36} , sp ^{3.35})	(77.1%, 77.0%)	(sp ^{2.85} , sp ^{2.86})	(74.0%, 74.1%)	(32.8%, 32.8%)	(67.2%, 67.2%)
	C2-O	(sp ^{3.47} , sp ^{3.48})	(77.6%, 77.7%)	(sp ^{2.97} , sp ^{3.00})	(74.8%, 75.0%)	(33.0%, 33.0%)	(67.0%, 67.0%)
Nanotube Ether	C1-O	(sp ^{3.27} , sp ^{3.28})	(76.6%, 76.6%)	(sp ^{3.06} , sp ^{3.10})	(75.4%, 75.6%)	(33.5%, 33.4%)	(66.5%, 66.6%)
	C2-O	(sp ^{3.29} , sp ^{3.28})	(76.7%, 76.6%)	(sp ^{3.11} , sp ^{3.06})	(76.7%, 75.4%)	(33.4%, 33.5%)	(66.6%, 66.5%)
Nanotube SW-Ether	C1-O	(sp ^{3.52} , sp ^{3.51})	(77.9%, 77.8%)	(sp ^{3.07} , sp ^{3.10})	(75.4%, 75.6%)	(33.2%, 33.1%)	(66.8%, 66.9%)
	C2-O	(sp ^{3.37} , sp ^{3.36})	(77.1%, 77.1%)	(sp ^{2.79} , sp ^{2.77})	(73.6%, 73.4%)	(33.0%, 33.0%)	(67.0%, 67.0%)

^aComposition of the natural hybrids of C and O; ^b Percentage of *p* character of the natural hybrids of C and O; ^c Weights of the natural hybrid orbitals to make a C-O bond.

Table S3. Cartesian coordinates for the optimized geometries in Å, the ZPEs (a.u.) at the M06-2X/6-31G level and the total electronic energies at 0 K (E0K, a.u.) at the M06-2X/6-311G(d,p) level.

Figure 7a
Graphene ZPE= 0.690728 Ee=-2680.622128

C	9.897123	0.000000	-0.000047
C	3.557224	3.717486	0.000001
C	3.557226	-3.717486	-0.000017
C	-2.829626	0.000000	-0.000118
C	7.798609	1.240689	-0.000052
C	1.436693	4.957995	0.000112
C	1.422638	-2.471219	-0.000049
C	-4.953918	1.233227	-0.000062
C	5.679254	2.479394	-0.000046
C	-0.674997	6.195813	0.000223
C	-0.704804	-1.234847	-0.000159
C	-7.069567	2.456396	-0.000064
C	-0.674994	-6.195812	0.000235
C	-7.069565	-2.456398	-0.000046
C	5.679254	-2.479393	-0.000064
C	-0.704803	1.234845	-0.000136
C	-2.804657	-4.943421	0.000120
C	-9.209990	-1.211016	-0.000076
C	3.543791	-1.236006	-0.000050
C	-2.825787	2.469306	-0.000025
C	-4.936675	-3.699865	0.000009
C	1.418424	-0.000002	-0.000147
C	-4.936678	3.699864	-0.000009
C	1.436695	-4.957994	0.000109
C	-4.953916	-1.233228	-0.000059
C	7.798609	-1.240688	-0.000063
C	1.422636	2.471219	-0.000014
C	-0.696013	-3.708346	0.000038
C	-7.083448	-0.000001	-0.000074
C	5.666274	0.000001	-0.000053
C	-0.696015	3.708347	0.000057
C	-2.825785	-2.469306	-0.000030
C	-9.209991	1.211013	-0.000087
C	3.543791	1.236008	-0.000040
C	-2.804660	4.943422	0.000107
C	2.825790	-2.469313	-0.000004
C	-3.543792	1.236002	0.000013
C	0.704807	-1.234841	-0.000002
C	-5.679255	2.479380	-0.000046
C	-1.418417	0.000001	0.000010

C	-1.436671	-4.957990	0.000139
C	-7.798628	-1.240679	-0.000071
C	4.953913	-1.233234	-0.000054
C	-1.422634	2.471218	0.000062
C	-3.557211	-3.717475	0.000040
C	-9.897159	-0.000002	-0.000090
C	2.829625	0.000000	-0.000021
C	-3.557213	3.717475	0.000027
C	-5.679253	-2.479381	-0.000032
C	0.704807	1.234846	0.000005
C	0.696023	-3.708348	0.000082
C	-5.666284	-0.000001	-0.000050
C	7.083434	0.000000	-0.000061
C	0.696020	3.708348	0.000068
C	-1.422633	-2.471219	0.000085
C	-7.798629	1.240676	-0.000081
C	4.953913	1.233235	-0.000048
C	-1.436675	4.957991	0.000130
C	-3.543792	-1.236002	0.000020
C	2.825789	2.469313	-0.000007
C	9.209962	-1.211022	-0.000057
C	9.209961	1.211023	-0.000044
C	4.936680	3.699876	-0.000025
C	2.804670	4.943433	0.000071
C	4.936681	-3.699876	-0.000049
C	2.804673	-4.943432	0.000057
C	7.069555	2.456405	-0.000047
C	0.675017	6.195802	0.000210
C	0.675020	-6.195801	0.000215
C	7.069555	-2.456405	-0.000068
H	9.754519	-2.149253	-0.000058
H	9.754519	2.149253	-0.000034
H	5.484221	4.638062	-0.000009
H	3.353380	5.881095	0.000122
H	5.484225	-4.638061	-0.000042
H	3.353383	-5.881094	0.000106
H	7.617545	3.394277	-0.000040
H	1.229552	7.128561	0.000309
H	7.617546	-3.394276	-0.000074
H	1.229554	-7.128561	0.000320
H	10.980963	0.000001	-0.000033
H	-1.229534	7.128563	0.000319
H	-3.353373	5.881080	0.000146
H	-5.484210	4.638050	-0.000006
H	-7.617548	3.394268	-0.000071
H	-9.754547	2.149241	-0.000089
H	-10.981000	-0.000002	-0.000086

H	-9.754545	-2.149245	-0.000071
H	-7.617545	-3.394270	-0.000045
H	-5.484207	-4.638051	0.000019
H	-3.353369	-5.881079	0.000165
H	-1.229532	-7.128561	0.000341

SW Defected Graphene ZPE=0.690337 Ee=-2680.475359

C	5.242307	3.644823	0.004262
C	-5.361363	-3.727153	0.006685
C	-7.433013	-2.277077	0.015117
C	-0.928137	-6.031944	-0.002434
C	-3.090753	-4.938130	-0.000003
C	-9.418674	-0.794379	0.024674
C	-3.972901	-3.802624	-0.000037
C	-9.991472	0.483829	0.027511
C	-6.057756	-2.449584	0.007743
C	0.415400	-6.009830	-0.003039
C	-8.023935	-0.969601	0.017266
C	-1.710968	-4.811447	-0.004350
C	-3.246074	-2.583014	-0.006987
C	-9.200639	1.622931	0.023315
C	-5.270961	-1.235672	0.001806
C	1.160884	-4.766514	-0.006336
C	-0.982301	-3.514761	-0.010155
C	-7.202158	0.210421	0.012472
C	-1.882042	-2.393755	-0.011658
C	-7.788334	1.510934	0.015854
C	-3.909754	-1.332987	-0.005849
C	2.531322	-4.835150	-0.003269
C	0.439299	-3.492729	-0.011809
C	-5.795239	0.079293	0.004638
C	-1.713534	-0.925236	-0.015046
C	-6.927026	2.628968	0.012210
C	-2.993568	-0.266103	-0.010060
C	3.370221	-3.677338	-0.004980
C	1.271092	-2.287563	-0.018336
C	-4.909262	1.209474	0.000627
C	0.763762	-0.952809	-0.026920
C	-5.533095	2.505488	0.005348
C	-0.523563	-0.303059	-0.023381
C	2.710087	-2.395066	-0.014307
C	-3.462955	1.085019	-0.006788
C	1.669344	0.110502	-0.032634
C	-4.703474	3.652599	0.004366
C	-0.356560	1.170485	-0.026105

C	5.620261	-2.625628	0.004629
C	3.587995	-1.255580	-0.015935
C	-2.639247	2.290744	-0.008444
C	3.032015	0.036276	-0.025507
C	-3.323848	3.573467	-0.001223
C	1.007552	1.346482	-0.032456
C	4.992837	-1.335605	-0.004697
C	-1.202820	2.316907	-0.016233
C	3.779645	1.244154	-0.019185
C	-2.579653	4.804265	0.001260
C	1.714292	2.541429	-0.024698
C	7.816535	-1.516633	0.020313
C	5.778828	-0.136154	-0.000174
C	-0.475729	3.603579	-0.012206
C	5.168776	1.159805	-0.006020
C	-1.217289	4.844831	-0.002545
C	3.109010	2.503771	-0.019046
C	7.186834	-0.225064	0.013228
C	0.931664	3.710968	-0.014758
C	5.942405	2.378614	0.004481
C	-0.480364	6.104645	0.003545
C	9.984050	-0.401743	0.038647
C	3.854275	3.729961	-0.005626
C	7.971924	0.979971	0.020599
C	1.676023	4.962007	-0.004380
C	7.329398	2.253013	0.016682
C	9.377020	0.853574	0.033102
C	4.757123	-3.769982	0.002943
C	7.013139	-2.689859	0.015880
C	9.228121	-1.570451	0.032723
C	0.871007	6.171807	0.003301
C	3.059308	4.950010	-0.000823
H	0.986496	-6.932264	-0.000704
H	3.005220	-5.812838	0.001701
H	9.985335	1.751799	0.038650
H	5.212662	-4.756593	0.009724
H	7.507689	-3.656970	0.022536
H	9.717912	-2.538344	0.037939
H	1.375768	7.132320	0.009211
H	3.586819	5.900258	0.007855
H	7.952597	3.142665	0.024428
H	5.839872	4.552229	0.014324
H	11.066008	-0.467952	0.048174
H	-3.147879	5.730031	0.007750
H	-5.173440	4.631627	0.008990
H	-7.360857	3.624974	0.015407
H	-9.653165	2.608736	0.025808

H	-11.070863	0.580427	0.033202
H	-10.057890	-1.671040	0.028336
H	-8.095520	-3.137647	0.019793
H	-5.960640	-4.632239	0.012138
H	-3.509342	-5.940407	0.004194
H	-1.467611	-6.973135	0.000250
H	-1.070928	7.015406	0.009556

Graphene-O (Singlet) ZPE= 0.696920 Ee= -2755.747453

C	-7.061894	2.484174	-0.233158
C	5.674957	2.506405	-0.121434
C	-0.753706	-1.222900	0.564271
C	-2.801597	4.964238	0.042360
C	-9.193999	1.239092	-0.417460
C	3.545912	1.265498	0.059938
C	-2.828493	-2.461326	0.110926
C	-4.931384	3.725703	-0.074649
C	1.447034	0.044483	0.308318
C	-4.932219	-3.681355	-0.155575
C	1.435223	4.975481	0.095016
C	-4.956629	1.260745	-0.056170
C	7.783296	1.269974	-0.296701
C	1.451893	-2.480146	0.266164
C	-0.695155	3.725703	0.152734
C	-7.069062	0.030181	-0.243272
C	5.659821	0.030911	-0.116492
C	-0.705364	-3.690767	0.205559
C	-2.829759	2.489584	0.098113
C	-9.181031	-1.182581	-0.442961
C	3.552862	-1.214240	0.083111
C	-2.802172	-4.923825	-0.040647
C	3.556647	3.740490	0.022853
C	-2.836336	0.030879	0.156228
C	9.873076	0.032003	-0.487436
C	3.557631	-3.705482	-0.038319
C	1.422939	2.486818	0.182480
C	-4.940228	-1.209400	-0.060792
C	7.782547	-1.211165	-0.322284
C	1.433889	-4.935676	0.057394
C	-0.720422	1.250925	0.290814
C	-7.050071	-2.430780	-0.286984
C	5.670563	-2.458656	-0.166204
C	-0.674645	-6.173129	-0.002771
C	-1.435223	4.975481	0.095015
C	-7.783296	1.269974	-0.296705
C	4.956629	1.260745	-0.056173

C	-1.451894	-2.480145	0.266181
C	-3.556647	3.740491	0.022853
C	-9.873075	0.032003	-0.487444
C	2.836336	0.030879	0.156215
C	-3.557631	-3.705481	-0.038312
C	-5.674957	2.506405	-0.121435
C	0.753711	-1.222899	0.564245
C	0.695155	3.725703	0.152734
C	-5.659822	0.030911	-0.116488
C	7.069062	0.030180	-0.243271
C	0.705360	-3.690766	0.205551
C	-1.422939	2.486818	0.182481
C	-7.782547	-1.211165	-0.322286
C	4.940227	-1.209400	-0.060799
C	-1.433891	-4.935676	0.057400
C	-3.545911	1.265499	0.059943
C	2.828493	-2.461327	0.110912
C	2.829758	2.489584	0.098109
C	-3.552864	-1.214240	0.083125
C	9.181032	-1.182581	-0.442956
C	2.802170	-4.923825	-0.040653
C	0.720419	1.250925	0.290808
C	-5.670563	-2.458656	-0.166201
C	7.050071	-2.430780	-0.286983
C	0.674644	-6.173129	-0.002774
C	-1.447035	0.044481	0.308333
C	4.932220	-3.681355	-0.155578
C	0.674772	6.213448	0.081348
C	7.061894	2.484174	-0.233154
C	4.931383	3.725703	-0.074647
C	2.801597	4.964237	0.042361
C	9.194000	1.239092	-0.417452
H	7.608523	3.421820	-0.277274
H	5.474643	4.664818	-0.128082
H	9.736907	2.177473	-0.456203
C	-0.674772	6.213448	0.081348
H	-9.736906	2.177474	-0.456212
H	-7.608522	3.421820	-0.277280
H	-5.474644	4.664817	-0.128087
H	-3.346430	5.902987	-0.002793
H	-1.229986	7.145526	0.061391
H	1.229985	7.145527	0.061392
H	3.346430	5.902987	-0.002791
O	0.000006	-1.246192	1.855060
H	10.952840	0.027895	-0.580050
H	9.723089	-2.120458	-0.502999
H	7.596463	-3.366649	-0.362679

H	5.478528	-4.615749	-0.247162
H	3.340316	-5.862046	-0.142469
H	1.230530	-7.102696	-0.067758
H	-1.230532	-7.102695	-0.067754
H	-3.340320	-5.862045	-0.142463
H	-5.478526	-4.615749	-0.247162
H	-7.596462	-3.366649	-0.362683
H	-9.723088	-2.120458	-0.503006
H	-10.952839	0.027894	-0.580061

Graphene-O (Triplet) ZPE= 0.695011 Ee= -2755.764607

C	-7.072305	2.477183	-0.227983
C	5.674025	2.498949	-0.118444
C	-0.753939	-1.226162	0.564301
C	-2.803498	4.954626	0.031589
C	-9.210235	1.244802	-0.405343
C	3.546535	1.261182	0.060964
C	-2.847441	-2.463717	0.111030
C	-4.936007	3.715114	-0.077071
C	1.451121	0.040127	0.309555
C	-4.963264	-3.667145	-0.148957
C	1.436087	4.966628	0.082043
C	-4.963393	1.257210	-0.052942
C	7.788396	1.271742	-0.287099
C	1.447674	-2.483997	0.263221
C	-0.697269	3.717615	0.144243
C	-7.077202	0.029989	-0.232879
C	5.671395	0.027508	-0.108851
C	-0.725259	-3.678940	0.199012
C	-2.834784	2.482502	0.095691
C	-9.209133	-1.176389	-0.427551
C	3.559870	-1.222411	0.087523
C	-2.818128	-4.905002	-0.049740
C	3.557041	3.731170	0.018182
C	-2.836310	0.027065	0.159506
C	9.893934	0.041343	-0.471844
C	3.558748	-3.697325	-0.032752
C	1.419909	2.481312	0.179253
C	-4.951049	-1.216482	-0.053370
C	7.798957	-1.215276	-0.309508
C	1.435809	-4.915809	0.038599
C	-0.720123	1.249461	0.289012
C	-7.086496	-2.424298	-0.275356
C	5.674418	-2.461919	-0.155774
C	-0.675795	-6.149148	-0.041023
C	-1.436093	4.966625	0.082064

C	-7.788396	1.271737	-0.287099
C	4.963385	1.257215	-0.052971
C	-1.447678	-2.483981	0.263255
C	-3.557042	3.731159	0.018217
C	-9.893935	0.041334	-0.471879
C	2.836312	0.027079	0.159441
C	-3.558747	-3.697304	-0.032802
C	-5.674030	2.498949	-0.118419
C	0.754020	-1.226154	0.563907
C	0.697263	3.717619	0.144238
C	-5.671398	0.027503	-0.108824
C	7.077200	0.029995	-0.232885
C	0.725261	-3.678965	0.199022
C	-1.419921	2.481305	0.179253
C	-7.798962	-1.215273	-0.309521
C	4.951061	-1.216484	-0.053387
C	-1.435812	-4.915794	0.038542
C	-3.546543	1.261158	0.061006
C	2.847446	-2.463731	0.111029
C	2.834787	2.482516	0.095652
C	-3.559868	-1.222415	0.087559
C	9.209130	-1.176381	-0.427518
C	2.818138	-4.905019	-0.049666
C	0.720118	1.249489	0.288981
C	-5.674418	-2.461910	-0.155786
C	7.086500	-2.424300	-0.275334
C	0.675791	-6.149154	-0.040988
C	-1.451126	0.040122	0.309651
C	4.963268	-3.667155	-0.148909
C	0.674911	6.204061	0.062619
C	7.072306	2.477186	-0.227995
C	4.936009	3.715121	-0.077109
C	2.803490	4.954634	0.031553
C	9.210241	1.244811	-0.405322
H	7.614891	3.417067	-0.272469
H	5.479098	4.654200	-0.132277
H	9.746650	2.186767	-0.443616
C	-0.674921	6.204060	0.062630
H	-9.746652	2.186754	-0.443643
H	-7.614893	3.417063	-0.272467
H	-5.479086	4.654200	-0.132237
H	-3.348604	5.893070	-0.016347
H	-1.229677	7.136331	0.038846
H	1.229666	7.136331	0.038813
H	3.348595	5.893077	-0.016409
O	-0.000032	-1.245534	1.853929
H	10.974042	0.041866	-0.561707

H	9.754588	-2.112237	-0.484662
H	7.630837	-3.361405	-0.345646
H	5.505918	-4.603284	-0.242430
H	3.353262	-5.844643	-0.153740
H	1.229251	-7.079096	-0.119772
H	-1.229254	-7.079091	-0.119822
H	-3.353238	-5.844629	-0.153841
H	-5.505921	-4.603268	-0.242493
H	-7.630833	-3.361402	-0.345691
H	-9.754578	-2.112252	-0.484709
H	-10.974041	0.041875	-0.561757

SW Defected Graphene-O (Singlet) ZPE= 0.694797 Ee= -2755.633532

C	-5.013742	3.665528	0.285681
C	5.093883	-3.721368	0.491972
C	7.148673	-2.329747	1.009665
C	0.841855	-5.989836	-0.695190
C	2.915005	-4.893503	-0.168265
C	9.125275	-0.893059	1.450729
C	3.760591	-3.766095	0.106314
C	9.721391	0.368105	1.525634
C	5.813569	-2.465909	0.666993
C	-0.498809	-6.003975	-0.751396
C	7.766479	-1.036918	1.108309
C	1.588713	-4.754293	-0.525321
C	3.080848	-2.535320	-0.115722
C	8.994778	1.523668	1.260613
C	5.090938	-1.240270	0.439706
C	-1.253404	-4.769661	-0.675785
C	0.871581	-3.451568	-0.708483
C	7.015795	0.156828	0.842922
C	1.792690	-2.315557	-0.576963
C	7.628153	1.442219	0.911796
C	3.768646	-1.310817	0.087320
C	-2.595246	-4.839481	-0.395187
C	-0.543218	-3.491093	-0.833728
C	5.644519	0.054964	0.498386
C	1.734521	-0.832668	-0.697831
C	6.830729	2.580484	0.624946
C	2.953044	-0.221113	-0.201761
C	-3.420773	-3.680820	-0.194464
C	-1.466035	-2.349650	-0.955753
C	4.836908	1.202276	0.196140
C	-1.106716	-1.105190	-1.454841
C	5.483916	2.483414	0.277862
C	0.866072	-0.125556	-1.422074

C	-2.813788	-2.412013	-0.491808
C	3.447183	1.100814	-0.183407
C	-1.735967	0.088885	-1.138482
C	4.694039	3.634680	0.020167
C	0.427908	1.238091	-1.190010
C	-5.527065	-2.553355	0.419825
C	-3.594824	-1.229704	-0.342254
C	2.651977	2.304977	-0.461736
C	-3.018025	0.041025	-0.593645
C	3.350698	3.573421	-0.296894
C	-0.970812	1.316105	-1.152873
C	-4.923063	-1.280539	0.144479
C	1.258648	2.353107	-0.790996
C	-3.698365	1.251379	-0.302836
C	2.636516	4.812178	-0.416530
C	-1.643811	2.510729	-0.783282
C	-7.586239	-1.395728	1.095484
C	-5.638392	-0.073658	0.374974
C	0.540409	3.625655	-0.699697
C	-5.014337	1.197968	0.163363
C	1.283501	4.860668	-0.550989
C	-3.001411	2.493654	-0.439380
C	-6.968527	-0.126159	0.854933
C	-0.858998	3.695030	-0.677331
C	-5.719758	2.424518	0.449806
C	0.559296	6.121092	-0.500711
C	-9.612760	-0.235456	1.791485
C	-3.689373	3.717804	-0.114141
C	-7.682989	1.092316	1.106103
C	-1.571496	4.944050	-0.443391
C	-7.032208	2.343841	0.897568
C	-9.008214	1.005510	1.571306
C	-4.737677	-3.734900	0.222600
C	-6.844296	-2.583634	0.875903
C	-8.922614	-1.418189	1.564474
C	-0.787192	6.165698	-0.437203
C	-2.922266	4.936972	-0.197835
H	-1.051814	-6.935565	-0.805690
H	-3.048743	-5.818583	-0.269733
H	-9.559702	1.919974	1.762525
H	-5.196318	-4.700184	0.418077
H	-7.318064	-3.539505	1.080723
H	-9.399017	-2.375534	1.746911
H	-1.312109	7.111508	-0.354283
H	-3.431190	5.878063	-0.008431
H	-7.583204	3.254790	1.112694
H	-5.538397	4.587565	0.519583

H	-10.634939	-0.272620	2.150012
O	0.051410	-0.938903	-2.217643
H	3.203518	5.732951	-0.315659
H	5.162611	4.610611	0.107983
H	7.287846	3.564466	0.679518
H	9.470442	2.496910	1.317555
H	10.769180	0.444821	1.791963
H	9.712453	-1.782063	1.655789
H	7.761504	-3.205626	1.201949
H	5.642798	-4.645384	0.647985
H	3.316708	-5.898003	-0.073901
H	1.409005	-6.914477	-0.708579
H	1.148140	7.032006	-0.471437

SW Defected Graphene-O (Triplet) ZPE= 0.693608 Ee= -2755.654192

C	-5.047124	3.650756	0.276030
C	5.107102	-3.709830	0.501915
C	7.174108	-2.320556	0.989673
C	0.842711	-5.980699	-0.640995
C	2.920790	-4.883734	-0.135625
C	9.167669	-0.897225	1.400174
C	3.769347	-3.756213	0.125852
C	9.767246	0.356551	1.458893
C	5.828027	-2.454812	0.662196
C	-0.498262	-5.993790	-0.697353
C	7.792660	-1.036998	1.071316
C	1.591981	-4.745056	-0.487583
C	3.091093	-2.526748	-0.098114
C	9.040863	1.517697	1.193577
C	5.111756	-1.232863	0.437738
C	-1.252162	-4.758626	-0.638998
C	0.876771	-3.442985	-0.679046
C	7.046031	0.155193	0.807582
C	1.797864	-2.309252	-0.557197
C	7.667354	1.444023	0.860264
C	3.777433	-1.302637	0.096561
C	-2.598284	-4.827859	-0.370344
C	-0.541612	-3.483315	-0.804773
C	5.669786	0.056599	0.480352
C	1.742579	-0.829272	-0.680499
C	6.879916	2.578553	0.576843
C	2.965380	-0.219005	-0.190652
C	-3.427873	-3.671213	-0.185673
C	-1.462813	-2.343544	-0.933070
C	4.858631	1.208584	0.177022
C	-1.109461	-1.106679	-1.437340

C	5.503835	2.487261	0.239684
C	0.869742	-0.122860	-1.398048
C	-2.823479	-2.405376	-0.477414
C	3.464611	1.108137	-0.186481
C	-1.744620	0.092280	-1.129520
C	4.730627	3.624117	-0.011208
C	0.432884	1.241333	-1.174611
C	-5.541267	-2.547315	0.401760
C	-3.603497	-1.226516	-0.340844
C	2.677443	2.305561	-0.462322
C	-3.027150	0.043988	-0.595767
C	3.359070	3.559912	-0.314006
C	-0.977753	1.317841	-1.140272
C	-4.941937	-1.278854	0.131634
C	1.248960	2.350891	-0.774954
C	-3.712031	1.256907	-0.308936
C	2.646015	4.792737	-0.397426
C	-1.640027	2.507449	-0.770308
C	-7.614995	-1.395605	1.052290
C	-5.665229	-0.070524	0.351244
C	0.547672	3.609694	-0.659632
C	-5.039686	1.202590	0.145199
C	1.283777	4.839567	-0.498964
C	-3.025671	2.491385	-0.436693
C	-6.996866	-0.124211	0.815684
C	-0.871063	3.681752	-0.639469
C	-5.737287	2.423490	0.421878
C	0.560410	6.096512	-0.408140
C	-9.662136	-0.235797	1.725356
C	-3.699671	3.707192	-0.114054
C	-7.718527	1.097202	1.058703
C	-1.574411	4.924771	-0.386506
C	-7.081331	2.336022	0.861387
C	-9.061843	1.004435	1.511902
C	-4.754373	-3.724523	0.219365
C	-6.875687	-2.576061	0.846044
C	-8.964511	-1.418164	1.507842
C	-0.786920	6.141861	-0.341937
C	-2.934649	4.919813	-0.161506
H	-1.051877	-6.925631	-0.740023
H	-3.050435	-5.807088	-0.241560
H	-9.616031	1.918914	1.694173
H	-5.212510	-4.689891	0.414757
H	-7.348356	-3.533447	1.045696
H	-9.439775	-2.376863	1.685483
H	-1.309028	7.086443	-0.232146
H	-3.440406	5.859614	0.041318

H	-7.632167	3.249582	1.065182
H	-5.569510	4.574043	0.509802
H	-10.688426	-0.277606	2.071423
O	0.052556	-0.939025	-2.188243
H	3.210227	5.714813	-0.293340
H	5.193611	4.603361	0.066509
H	7.337939	3.562488	0.617514
H	9.522660	2.488478	1.238794
H	10.818321	0.432599	1.712564
H	9.749332	-1.789844	1.604662
H	7.783876	-3.199039	1.180237
H	5.656485	-4.633515	0.659014
H	3.320480	-5.888459	-0.034724
H	1.408054	-6.906580	-0.642460
H	1.149459	7.006199	-0.355038

Figure 7b

Nanotube ZPE= 1.184520 Ee= -5501.434128

C	5.684729	-3.713167	2.962508
C	5.002610	-2.813344	3.806246
C	5.676336	-1.735005	4.417962
C	4.994149	-0.535797	4.709919
C	5.674432	0.699677	4.693921
C	4.998121	1.887392	4.345029
C	5.681276	2.950751	3.719874
C	5.010062	3.799021	2.813318
C	5.689316	4.419387	1.745408
C	5.017808	4.691662	0.534489
C	5.691202	4.700180	-0.704946
C	5.014723	4.331904	-1.885660
C	5.685331	3.712767	-2.962532
C	5.003211	2.812716	-3.806105
C	5.676725	1.734424	-4.417917
C	4.994361	0.535158	-4.709795
C	5.674470	-0.700273	-4.693634
C	4.997887	-1.888021	-4.344915
C	5.680985	-2.951150	-3.719451
C	5.009514	-3.799587	-2.813159
C	5.688811	-4.419630	-1.745099
C	5.017094	-4.692173	-0.534340
C	5.690579	-4.700448	0.705058
C	5.013961	-4.332468	1.885785
C	3.558043	-2.804117	3.799516
C	2.847499	-1.727754	4.397887
C	3.550926	-0.534314	4.704117
C	2.845867	0.697434	4.676039

C	3.554188	1.881963	4.338707
C	2.851818	2.933840	3.697086
C	3.564774	3.784696	2.807171
C	2.859536	4.380591	1.729492
C	3.572253	4.671463	0.533050
C	2.861426	4.655645	-0.698109
C	3.569138	4.314207	-1.881107
C	2.855582	3.685968	-2.940082
C	3.558569	2.803430	-3.799360
C	2.847845	1.727262	-4.397816
C	3.551133	0.533682	-4.704060
C	2.845925	-0.697919	-4.676038
C	3.554038	-1.882630	-4.338783
C	2.851535	-2.934382	-3.697121
C	3.564292	-3.785385	-2.807194
C	2.858969	-4.381159	-1.729480
C	3.571564	-4.672119	-0.533000
C	2.860731	-4.656214	0.698162
C	3.568419	-4.314888	1.881211
C	2.854972	-3.686516	2.940174
C	1.417646	-1.729039	4.390811
C	0.706390	-0.534362	4.686632
C	1.416164	0.697963	4.667452
C	0.708753	1.884576	4.326105
C	1.421575	2.937761	3.692912
C	0.716115	3.799214	2.806110
C	1.428453	4.390296	1.729048
C	0.721241	4.697007	0.533687
C	1.430076	4.666929	-0.698132
C	0.719142	4.334889	-1.882310
C	1.424946	3.692486	-2.938093
C	0.711855	2.810150	-3.792329
C	1.418015	1.728773	-4.390758
C	0.706595	0.534183	-4.686576
C	1.416205	-0.698213	-4.667496
C	0.708618	-1.884722	-4.326129
C	1.421276	-2.938115	-3.693014
C	0.715681	-3.799363	-2.806139
C	1.427876	-4.390715	-1.729090
C	0.720609	-4.697040	-0.533698
C	1.429372	-4.667327	0.698141
C	0.718477	-4.334986	1.882288
C	1.424315	-3.692832	2.938156
C	0.711339	-2.810320	3.792385
C	-0.723254	-0.534133	4.680022
C	-1.431150	0.698732	4.658362
C	-0.720651	1.884784	4.321294

C	-1.425016	2.944710	3.691067
C	-0.712080	3.803439	2.805881
C	-1.416746	4.409112	1.731502
C	-0.705954	4.705625	0.534016
C	-1.414706	4.689019	-0.699459
C	-0.708536	4.341529	-1.882984
C	-1.421025	3.704566	-2.939328
C	-0.717075	2.811605	-3.789767
C	-1.429132	1.731231	-4.384161
C	-0.723060	0.534159	-4.680031
C	-1.431125	-0.698530	-4.658315
C	-0.720737	-1.884714	-4.321428
C	-1.425276	-2.944455	-3.691058
C	-0.712481	-3.803401	-2.805983
C	-1.417355	-4.408634	-1.731459
C	-0.706638	-4.705444	-0.534059
C	-1.415460	-4.688475	0.699354
C	-0.709212	-4.341391	1.882938
C	-1.421624	-3.704239	2.939199
C	-0.717553	-2.811529	3.789802
C	-1.429485	-1.731028	4.384139
C	-2.860788	0.698886	4.645808
C	-3.565259	1.888175	4.309029
C	-2.855569	2.947173	3.684032
C	-3.555143	3.821036	2.805843
C	-2.848325	4.417510	1.730115
C	-3.548079	4.737889	0.535202
C	-2.846584	4.699211	-0.699104
C	-3.551054	4.366949	-1.885318
C	-2.852059	3.709503	-2.935273
C	-3.561074	2.819741	-3.783165
C	-2.859024	1.731806	-4.373487
C	-3.568249	0.534947	-4.663009
C	-2.860829	-0.698423	-4.645827
C	-3.565478	-1.887580	-4.309091
C	-2.855739	-2.946669	-3.684063
C	-3.555692	-3.820238	-2.805971
C	-2.848929	-4.416793	-1.730101
C	-3.548819	-4.736565	-0.535261
C	-2.847358	-4.698394	0.698970
C	-3.551790	-4.365926	1.885191
C	-2.852618	-3.708925	2.935123
C	-3.561658	-2.819090	3.783132
C	-2.859433	-1.731325	4.373434
C	-3.568479	-0.534314	4.663030
C	-5.011294	1.884161	4.305089
C	-5.689653	2.949768	3.679007

C	-4.998040	3.811996	2.802081
C	-4.987870	4.725577	0.534263
C	-4.992290	4.356021	-1.882502
C	-5.685041	3.708710	-2.927696
C	-5.005968	2.813539	-3.779188
C	-5.694523	1.735614	-4.372889
C	-5.014986	0.533767	-4.659344
C	-5.696858	-0.699990	-4.648136
C	-5.011491	-1.883876	-4.305253
C	-5.690101	-2.949339	-3.679580
C	-4.998568	-3.811619	-2.802338
C	-5.680421	-4.410658	-1.723858
C	-4.988931	-4.724802	-0.534443
C	-5.678086	-4.689197	0.695924
C	-4.993170	-4.355462	1.882316
C	-5.685705	-3.708200	2.928084
C	-5.006472	-2.813228	3.779120
C	-5.694818	-1.734855	4.373277
C	-5.015184	-0.533467	4.659315
C	-5.677561	4.689342	-0.695748
H	-6.763876	4.673390	-0.691886
C	-5.680014	4.410739	1.723477
H	-6.766218	4.397345	1.713556
C	-5.697092	0.700838	4.648003
H	-6.782488	0.699715	4.629830
H	6.767083	2.941789	3.716642
H	6.774665	4.409108	1.744930
H	6.776450	4.689750	-0.704666
H	6.770917	3.703051	-2.960963
H	6.760622	0.696844	4.686199
H	6.762793	1.728131	-4.411951
H	6.762409	-1.728912	4.411875
H	6.760663	-0.697658	-4.685736
H	6.770321	-3.703491	2.960815
H	6.766798	-2.942215	-3.715976
H	6.775830	-4.690011	0.704777
H	6.774163	-4.409320	-1.744514
H	-6.766901	-4.398049	-1.714703
H	-6.764680	-4.674213	0.691976
H	-6.776114	-2.943898	-3.664184
H	-6.771926	-3.699587	2.914264
H	-6.782528	-0.698925	-4.630934
H	-6.780579	-1.732152	4.356232
H	-6.780292	1.732782	-4.355678
H	-6.771287	3.699839	-2.913759
H	-6.775657	2.943988	3.662946

SW Defected Nanotube ZPE= 1.186688 Ee= -5501.322377
 C -5.714189 -4.769254 -0.046535
 C -6.009659 -3.814479 2.205243
 C -6.209116 -1.855383 3.684344
 C -6.290720 0.571603 4.037292
 C -6.308942 2.836672 3.142997
 C -4.993171 1.835042 -4.929563
 C -5.396851 -4.423388 -2.461900
 C -4.883071 -4.740400 -1.184187
 C -5.198409 -4.417513 1.217811
 C -5.451037 -2.914464 3.132207
 C -5.588234 -0.652664 4.071485
 C -5.622370 1.788927 3.797084
 C -5.605003 3.753166 2.335714
 C -5.370340 4.689858 0.067091
 C -4.742855 4.362273 -2.287397
 C -4.397387 2.877502 -4.189678
 C -4.309629 0.622217 -5.130276
 C -4.379225 -1.809783 -4.855319
 C -4.585459 -3.780135 -3.414606
 C -3.450141 -4.726689 -0.998495
 C -3.764793 -4.393800 1.396218
 C -4.016968 -2.884117 3.296331
 C -4.152437 -0.614958 4.201064
 C -4.174897 1.819305 3.905489
 C -4.166980 3.808904 2.528988
 C -3.977865 4.755806 0.309230
 C -3.299800 4.325796 -1.991307
 C -2.976983 2.831964 -3.909062
 C -2.881562 0.603938 -4.919788
 C -2.946621 -1.824564 -4.673251
 C -3.152729 -3.784088 -3.229718
 C -2.590637 -4.411610 -2.088286
 C -2.904858 -4.724604 0.313314
 C -3.198755 -3.759415 2.537148
 C -3.400075 -1.791689 3.967607
 C -3.475966 0.634295 4.249045
 C -3.448679 2.912278 3.370124
 C -3.407691 4.470803 1.578571
 C -2.969159 4.686326 -0.667233
 C -2.391522 3.680122 -2.935975
 C -2.211023 1.766565 -4.478748
 C -2.194594 -0.639176 -4.872178
 C -2.333514 -2.909024 -3.994221
 C -1.171355 -4.422358 -1.904038
 C -1.484073 -4.727212 0.499127
 C -1.779008 -3.750783 2.717169

C	-1.982918	-1.766109	4.123540
C	-2.054629	0.670214	4.346286
C	-2.001055	2.927674	3.370670
C	-1.994990	4.414802	1.482524
C	-0.483153	4.633957	-0.474560
C	-0.934964	3.714359	-2.858062
C	-0.791401	1.761469	-4.349862
C	-0.779518	-0.654720	-4.705440
C	-0.916585	-2.923960	-3.815736
C	-0.329296	-3.811053	-2.868419
C	-0.620757	-4.741103	-0.628651
C	-0.933645	-4.387470	1.766214
C	-1.192004	-2.845275	3.639122
C	-1.334213	-0.549129	4.459437
C	-1.334882	1.861921	4.027876
C	-1.220050	3.776865	2.480923
C	-1.707163	4.618924	0.082927
C	-0.187283	4.404611	-1.874882
C	-0.139797	2.855629	-3.716433
C	-0.061177	0.570474	-4.621293
C	-0.127885	-1.859484	-4.326328
C	1.087089	-3.818996	-2.688754
C	0.795817	-4.738224	-0.444523
C	0.483018	-4.372027	1.948370
C	0.223327	-2.820766	3.813248
C	0.078725	-0.520733	4.615570
C	0.085321	1.879038	4.140250
C	0.240317	3.764157	2.552367
C	0.776118	4.758613	0.270497
C	1.212799	4.499183	-1.977969
C	1.303530	2.859469	-3.700303
C	1.361785	0.549000	-4.497945
C	1.289323	-1.875925	-4.160307
C	1.905635	-2.952629	-3.467462
C	1.653125	-4.428934	-1.538729
C	1.342655	-4.707488	0.866978
C	1.047567	-3.706987	3.073630
C	0.836255	-1.707087	4.453546
C	0.760803	0.726331	4.615299
C	0.846452	2.929700	3.541730
C	1.137803	4.407083	1.599731
C	1.764897	4.847077	-0.716686
C	1.992656	3.803536	-2.898759
C	2.055912	1.742492	-4.176563
C	2.045936	-0.698697	-4.407195
C	3.322576	-2.967905	-3.300139
C	3.072329	-4.426895	-1.358916

C	2.763830	-4.687085	1.049122
C	2.468087	-3.674279	3.250559
C	2.252260	-1.676061	4.631915
C	2.169783	0.752572	4.821310
C	2.260036	2.970845	3.801489
C	2.578513	4.438379	1.878744
C	3.135016	4.784742	-0.478877
C	3.413387	3.754282	-2.687443
C	3.490520	1.716924	-4.034041
C	3.465750	-0.724261	-4.260459
C	4.108127	-1.921811	-3.848641
C	3.909245	-3.835830	-2.337941
C	3.624914	-4.713902	-0.078136
C	3.316025	-4.313745	2.306620
C	3.050851	-2.752437	4.160582
C	2.889165	-0.460471	4.985824
C	2.879868	1.950451	4.576796
C	3.089548	3.853599	3.067940
C	3.550198	4.745107	0.864415
C	3.995053	4.372890	-1.536840
C	4.178281	2.792330	-3.386612
C	4.193718	0.499076	-4.220688
C	5.542041	-1.952787	-3.690324
C	5.342151	-3.856530	-2.159917
C	5.057940	-4.723340	0.111733
C	4.748690	-4.307523	2.501769
C	4.482905	-2.732924	4.357291
C	4.315160	-0.438362	5.206585
C	4.295264	1.987740	4.853939
C	4.511453	3.902508	3.355015
C	4.975360	4.715127	1.107359
C	5.408262	4.284601	-1.281271
C	5.609303	2.743863	-3.175090
C	5.632123	0.467337	-4.065566
C	5.880190	-4.459620	-1.006108
C	5.571056	-4.698606	1.423756
C	5.272386	-3.651947	3.637033
C	5.048231	-1.631548	5.038785
C	4.945388	0.819300	5.306707
C	5.037865	3.078499	4.369568
C	5.399470	4.480376	2.426910
C	5.866113	4.642120	0.012061
C	6.204226	3.609247	-2.230417
C	6.315998	1.640832	-3.699358
H	-6.063774	1.872568	-5.104342
H	-7.085970	-3.818651	2.065563
H	-6.789939	-4.759613	-0.189069

H	-6.473721	-4.406133	-2.597220
H	-7.288204	-1.870530	3.564170
H	-7.371637	0.546903	3.933340
H	-7.386303	2.757126	3.033992
H	6.349293	-3.626212	3.768005
H	6.647541	-4.677694	1.559153
H	6.956979	-4.453116	-0.868446
H	7.390567	1.592639	-3.552559
H	6.123789	-1.606691	5.182874
H	7.272346	3.526698	-2.057107
H	6.016599	0.856268	5.480179
H	6.929647	4.582879	0.219887
H	6.105669	3.113823	4.563593
H	6.462097	4.472756	2.649826
C	-6.185743	4.335830	1.178192
H	-7.257008	4.235812	1.037509
C	-5.715322	4.669104	-1.296554
H	-6.758597	4.597353	-1.585160
C	-5.195388	3.793339	-3.494194
H	-6.258742	3.823336	-3.708739
C	-4.997176	-0.600872	-5.246525
H	-6.073871	-0.584719	-5.387051
C	-5.139330	-2.884948	-4.359031
H	-6.217374	-2.866845	-4.487499
C	6.277524	-0.784651	-3.966952
H	7.355661	-0.802902	-3.837544
C	6.130119	-3.017673	-2.976527
H	7.208072	-3.024641	-2.844873

Nanotube-O (Singlet) ZPE= 1.187321 Ee= -5576.585329

C	-5.864601	-3.689359	-2.854450
C	-5.182715	-2.798523	-3.707401
C	-5.856355	-1.694680	-4.271546
C	-5.167455	-0.492751	-4.532500
C	-5.830572	0.749805	-4.475403
C	-5.136804	1.916620	-4.089882
C	-5.786852	2.986924	-3.441311
C	-5.077659	3.820533	-2.551564
C	-5.688031	4.481862	-1.462743
C	-4.949594	4.805037	-0.304396
C	-5.552630	4.866180	0.969805
C	-4.807918	4.512642	2.112686
C	-5.443287	3.889276	3.203314
C	-4.747536	2.939127	3.978397
C	-5.444325	1.868145	4.571643
C	-4.812261	0.622973	4.775532

C	-5.544793	-0.581050	4.769999
C	-4.937166	-1.791948	4.371209
C	-5.673779	-2.841366	3.784342
C	-5.059113	-3.724391	2.871564
C	-5.781411	-4.346034	1.830272
C	-5.142665	-4.672689	0.616926
C	-5.844507	-4.666386	-0.607931
C	-5.179486	-4.342653	-1.807919
C	-3.740069	-2.822371	-3.728939
C	-3.027558	-1.734889	-4.298687
C	-3.722370	-0.519710	-4.546409
C	-2.999422	0.699012	-4.499531
C	-3.689531	1.884660	-4.115572
C	-2.952448	2.928201	-3.501904
C	-3.636124	3.786749	-2.596679
C	-2.883547	4.413397	-1.574164
C	-3.507099	4.783747	-0.362365
C	-2.713001	4.820037	0.830515
C	-3.363445	4.471199	2.037990
C	-2.612377	3.775857	3.019466
C	-3.308181	2.877802	3.878360
C	-2.628239	1.744753	4.379106
C	-3.372576	0.571370	4.689819
C	-2.724469	-0.685833	4.621698
C	-3.494161	-1.840734	4.312070
C	-2.847920	-2.935672	3.678059
C	-3.614666	-3.772960	2.824635
C	-2.952983	-4.426396	1.746919
C	-3.698319	-4.713749	0.574635
C	-3.015878	-4.729604	-0.674236
C	-3.736618	-4.372817	-1.841984
C	-3.036642	-3.736672	-2.903012
C	-1.598363	-1.751845	-4.314948
C	-0.877000	-0.554442	-4.582880
C	-1.569235	0.681992	-4.521750
C	-0.836888	1.857055	-4.182894
C	-1.518884	2.922056	-3.548241
C	-0.773588	3.815931	-2.727452
C	-1.464341	4.444691	-1.658581
C	-0.721271	4.947488	-0.574457
C	-1.278372	4.882572	0.762067
C	-0.497589	4.480627	1.905497
C	-1.182026	3.734160	2.924137
C	-0.477711	2.748496	3.688830
C	-1.203321	1.684009	4.286236
C	-0.537941	0.451178	4.553943
C	-1.296646	-0.746356	4.572054

C	-0.649976	-1.970893	4.246530
C	-1.418734	-3.005589	3.651942
C	-0.767179	-3.914915	2.775014
C	-1.523528	-4.492554	1.719078
C	-0.851816	-4.828296	0.512484
C	-1.586180	-4.774123	-0.704926
C	-0.891737	-4.437117	-1.898595
C	-1.606950	-3.760221	-2.925935
C	-0.895916	-2.858809	-3.765014
C	0.552704	-0.572792	-4.597862
C	1.277207	0.647454	-4.558463
C	0.591214	1.839205	-4.198136
C	1.326549	2.895527	-3.596725
C	0.654101	3.810013	-2.754412
C	1.396097	4.587596	-1.801120
C	0.631267	5.210584	-0.817887
C	1.763359	5.119612	1.014290
C	0.964678	4.458293	1.942885
C	1.670898	3.588400	2.841342
C	0.951274	2.666959	3.634819
C	1.632284	1.551156	4.190756
C	0.885376	0.386187	4.513471
C	1.539515	-0.873138	4.509194
C	0.774288	-2.035809	4.218932
C	1.422446	-3.140900	3.603341
C	0.658866	-3.980922	2.747685
C	1.320206	-4.618591	1.659964
C	0.575448	-4.881110	0.479074
C	1.259074	-4.860665	-0.770999
C	0.536674	-4.468109	-1.928385
C	1.239887	-3.807850	-2.976514
C	0.533468	-2.877701	-3.783637
C	1.249317	-1.786406	-4.349373
C	2.705168	0.637153	-4.578584
C	3.427394	1.828307	-4.270953
C	2.758233	2.905031	-3.639019
C	3.494193	3.831585	-2.834960
C	2.856727	4.538780	-1.765661
C	3.646679	4.844882	-0.601075
C	3.104180	4.808749	0.741345
C	3.825434	4.190456	1.778999
C	3.102223	3.518753	2.802739
C	3.797970	2.542164	3.570515
C	3.061022	1.486550	4.161230
C	3.723648	0.260430	4.458846
C	2.968137	-0.938180	4.480539
C	3.612889	-2.168649	4.176297

C	2.852046	-3.206601	3.578429
C	3.498685	-4.117433	2.701417
C	2.750418	-4.677353	1.631395
C	3.417219	-4.989702	0.417696
C	2.689620	-4.898856	-0.800344
C	3.381481	-4.527727	-1.983887
C	2.670247	-3.826015	-2.995863
C	3.379592	-2.908135	-3.817636
C	2.678488	-1.798297	-4.360535
C	3.395516	-0.598897	-4.632478
C	4.868230	1.799144	-4.333435
C	5.580269	2.873433	-3.771255
C	4.932187	3.787572	-2.913286
C	5.083091	4.706861	-0.671943
C	5.260700	4.080458	1.687971
C	5.952093	3.344725	2.663600
C	5.245897	2.469497	3.519243
C	5.893498	1.365475	4.100181
C	5.165972	0.201636	4.428710
C	5.795820	-1.057758	4.429468
C	5.052743	-2.222773	4.142135
C	5.679943	-3.317549	3.513381
C	4.937838	-4.163827	2.662991
C	5.580162	-4.770227	1.562515
C	4.858479	-5.025827	0.379385
C	5.521868	-4.971759	-0.865894
C	4.826016	-4.552684	-2.016345
C	5.504835	-3.877901	-3.054828
C	4.826308	-2.928966	-3.841810
C	5.513539	-1.837678	-4.418519
C	4.842035	-0.625496	-4.663061
C	5.865861	4.522799	0.496991
H	6.945586	4.464885	0.397151
C	5.698165	4.378314	-1.892679
H	6.782018	4.325735	-1.945092
C	5.535691	0.603166	-4.668216
H	6.621310	0.596039	-4.695351
H	-6.871210	2.988494	-3.404797
H	-6.771315	4.482139	-1.400052
H	-6.635939	4.878843	1.037170
H	-6.526930	3.922152	3.265954
H	-6.915530	0.758010	-4.444955
H	-6.527752	1.918593	4.625912
H	-6.941751	-1.676888	-4.243011
H	-6.628432	-0.530893	4.808211
H	-6.949823	-3.657432	-2.826799
H	-6.757465	-2.790015	3.806038

H	-6.929060	-4.622625	-0.585568
H	-6.865259	-4.294824	1.848639
H	6.665885	-4.792484	1.533335
H	6.607622	-4.985866	-0.883361
H	6.765064	-3.352765	3.476342
H	6.590384	-3.888120	-3.063559
H	6.880182	-1.102873	4.392362
H	6.599040	-1.849014	-4.429498
H	6.976672	1.309757	4.054380
H	7.033130	3.265865	2.606894
H	6.666194	2.864343	-3.803280
O	1.215700	6.061828	0.129191

Nanotube-O (Triplet) ZPE= 1.185847 Ee= -5576.678988

C	-5.877317	-3.717002	-2.760575
C	-5.192906	-2.866679	-3.636577
C	-5.868033	-1.765173	-4.245999
C	-5.170216	-0.580609	-4.521716
C	-5.829241	0.669209	-4.504070
C	-5.116840	1.846055	-4.135098
C	-5.766591	2.902179	-3.488362
C	-5.040840	3.779953	-2.636370
C	-5.660717	4.432398	-1.548393
C	-4.918686	4.816922	-0.418972
C	-5.538059	4.901351	0.863539
C	-4.798124	4.572762	2.005357
C	-5.438467	3.991760	3.126809
C	-4.744516	3.038986	3.907492
C	-5.443205	1.984446	4.524539
C	-4.804601	0.743531	4.759327
C	-5.543588	-0.462675	4.767369
C	-4.928150	-1.680474	4.417628
C	-5.675372	-2.741083	3.844546
C	-5.056391	-3.652773	2.959680
C	-5.788720	-4.285332	1.938819
C	-5.146065	-4.647802	0.718046
C	-5.854908	-4.643781	-0.487726
C	-5.186701	-4.362228	-1.708233
C	-3.756919	-2.894208	-3.660070
C	-3.034919	-1.815098	-4.264650
C	-3.720950	-0.607103	-4.535197
C	-2.991612	0.611802	-4.527985
C	-3.672604	1.817031	-4.171937
C	-2.935159	2.863766	-3.580804
C	-3.614134	3.760958	-2.698709
C	-2.863981	4.395729	-1.681612
C	-3.487191	4.806180	-0.483968

C	-2.694792	4.858384	0.718313
C	-3.351234	4.524199	1.927135
C	-2.603200	3.852562	2.926439
C	-3.307812	2.966910	3.805133
C	-2.629213	1.848771	4.332403
C	-3.374864	0.682345	4.681215
C	-2.726730	-0.582079	4.638745
C	-3.492109	-1.741673	4.369260
C	-2.848096	-2.859395	3.753237
C	-3.611800	-3.714228	2.921600
C	-2.956703	-4.392451	1.857471
C	-3.706401	-4.702663	0.682391
C	-3.030397	-4.738037	-0.559601
C	-3.757813	-4.405740	-1.742316
C	-3.055106	-3.785708	-2.815393
C	-1.610173	-1.843252	-4.285229
C	-0.883312	-0.659548	-4.575113
C	-1.568566	0.585310	-4.549071
C	-0.827485	1.764490	-4.226867
C	-1.502539	2.846260	-3.620430
C	-0.752328	3.754946	-2.812346
C	-1.441694	4.412313	-1.759726
C	-0.701483	4.939689	-0.687427
C	-1.264903	4.913804	0.654369
C	-0.486895	4.528402	1.807089
C	-1.176646	3.811538	2.841716
C	-0.474972	2.836653	3.634426
C	-1.202292	1.787287	4.248044
C	-0.537818	0.559548	4.549873
C	-1.297941	-0.642695	4.590514
C	-0.652945	-1.868771	4.293953
C	-1.425090	-2.926889	3.723792
C	-0.775470	-3.846819	2.860457
C	-1.535664	-4.457159	1.824946
C	-0.864867	-4.814240	0.614348
C	-1.600465	-4.787321	-0.595261
C	-0.906928	-4.481215	-1.805637
C	-1.621830	-3.819368	-2.843619
C	-0.910837	-2.947470	-3.705872
C	0.547974	-0.684888	-4.591462
C	1.281053	0.532978	-4.577321
C	0.600907	1.737846	-4.236599
C	1.342012	2.795182	-3.653386
C	0.671870	3.738499	-2.833568
C	1.416059	4.529744	-1.896214
C	0.650895	5.188607	-0.935781
C	1.783566	5.138079	0.906138

C	0.977520	4.505138	1.852043
C	1.678937	3.661060	2.773850
C	0.951440	2.752705	3.589939
C	1.628311	1.649584	4.164954
C	0.878487	0.491279	4.515135
C	1.533019	-0.773028	4.528069
C	0.769204	-1.935411	4.265508
C	1.419058	-3.059141	3.667273
C	0.654096	-3.912225	2.830119
C	1.313233	-4.577638	1.760018
C	0.562135	-4.868180	0.579818
C	1.241051	-4.877768	-0.663497
C	0.513879	-4.519049	-1.837155
C	1.218195	-3.882366	-2.899847
C	0.514392	-2.975188	-3.729206
C	1.238006	-1.894332	-4.323890
C	2.702428	0.512200	-4.599504
C	3.437400	1.702482	-4.301909
C	2.772149	2.791833	-3.691416
C	3.519939	3.728367	-2.900080
C	2.877132	4.469255	-1.852226
C	3.670837	4.796296	-0.697369
C	3.119875	4.816292	0.650313
C	3.833779	4.218976	1.703956
C	3.104496	3.588002	2.744724
C	3.797540	2.625865	3.545278
C	3.059316	1.585456	4.146483
C	3.722795	0.365049	4.474868
C	2.963067	-0.839048	4.503138
C	3.609529	-2.062940	4.217165
C	2.841416	-3.122585	3.638383
C	3.490118	-4.033258	2.769002
C	2.735035	-4.634127	1.727996
C	3.404317	-4.973469	0.510425
C	2.672249	-4.921420	-0.696916
C	3.365129	-4.594143	-1.902495
C	2.651221	-3.910699	-2.927434
C	3.360460	-3.027448	-3.776686
C	2.662057	-1.916380	-4.343216
C	3.385167	-0.731506	-4.632233
C	4.875904	1.679232	-4.381400
C	5.588389	2.767632	-3.855379
C	4.953465	3.691954	-2.987735
C	5.105771	4.668309	-0.769244
C	5.271164	4.120868	1.620385
C	5.953902	3.425524	2.625449
C	5.237470	2.552891	3.501447

C	5.880124	1.458830	4.085199
C	5.149686	0.300181	4.447985
C	5.781571	-0.967256	4.459184
C	5.045916	-2.128170	4.196020
C	5.671585	-3.267698	3.607679
C	4.937528	-4.103533	2.745890
C	5.567560	-4.776624	1.680670
C	4.843721	-5.028968	0.476420
C	5.496520	-5.010200	-0.759109
C	4.794727	-4.625834	-1.932583
C	5.474415	-3.966186	-2.982596
C	4.797497	-3.054121	-3.802527
C	5.492788	-1.967859	-4.414433
C	4.830688	-0.760920	-4.675961
C	5.880305	4.549676	0.422270
H	6.960617	4.494975	0.330937
C	5.715063	4.323783	-1.987177
H	6.797816	4.260411	-2.034837
C	5.529816	0.470808	-4.723306
H	6.614555	0.457463	-4.768525
H	-6.851500	2.907012	-3.443291
H	-6.744572	4.421229	-1.481798
H	-6.621811	4.923438	0.922252
H	-6.520681	4.041214	3.196917
H	-6.914610	0.690694	-4.490499
H	-6.526538	2.034701	4.578566
H	-6.953477	-1.747181	-4.227797
H	-6.627793	-0.411065	4.799502
H	-6.961570	-3.671433	-2.721715
H	-6.759710	-2.692544	3.873721
H	-6.938896	-4.584793	-0.462984
H	-6.873337	-4.241258	1.961617
H	6.651720	-4.828039	1.656548
H	6.582070	-5.022566	-0.782659
H	6.756068	-3.316116	3.591997
H	6.560330	-3.972393	-2.985559
H	6.865906	-1.008832	4.418117
H	6.578168	-1.991207	-4.434887
H	6.963209	1.397042	4.036507
H	7.036787	3.358170	2.591812
H	6.673433	2.756690	-3.894386
O	1.244336	6.055636	-0.007261

SW Defected Nanotube-O (Singlet) ZPE= 1.184872 Ee= -5576.502223
C -5.665986 -4.819143 -1.025018
C -5.973630 -4.400457 1.380050
C -6.203044 -2.784952 3.222624

C	-6.326962	-0.462768	4.000651
C	-6.384518	1.919373	3.498910
C	-4.936261	2.785750	-4.461985
C	-5.350800	-3.908940	-3.285362
C	-4.833469	-4.522245	-2.120822
C	-5.153901	-4.760758	0.288953
C	-5.428079	-3.699436	2.473262
C	-5.601992	-1.661298	3.820656
C	-5.680558	0.787560	3.973509
C	-5.690959	2.985054	2.892464
C	-5.422567	4.433992	0.901158
C	-4.708269	4.771091	-1.422200
C	-4.340018	3.693664	-3.562789
C	-4.257658	1.618919	-4.850870
C	-4.335496	-0.823891	-5.035682
C	-4.540171	-3.064237	-4.063421
C	-3.400501	-4.546750	-1.936618
C	-3.720611	-4.757719	0.469935
C	-3.994350	-3.673225	2.635813
C	-4.166457	-1.620153	3.950978
C	-4.233460	0.823070	4.106033
C	-4.261114	3.029010	3.131712
C	-4.039454	4.481852	1.189870
C	-3.261194	4.732522	-1.115869
C	-2.920642	3.615430	-3.281925
C	-2.830911	1.558613	-4.627687
C	-2.902704	-0.878103	-4.858231
C	-3.106982	-3.112315	-3.888662
C	-2.543057	-3.985725	-2.923086
C	-2.856486	-4.835271	-0.656546
C	-3.162793	-4.365743	1.718117
C	-3.393529	-2.716720	3.501682
C	-3.511245	-0.386430	4.228769
C	-3.524671	2.014412	3.800096
C	-3.508236	3.898645	2.372642
C	-2.993942	4.773622	0.291543
C	-2.342315	4.344919	-2.206859
C	-2.157071	2.628941	-4.002877
C	-2.149734	0.319481	-4.809868
C	-2.290173	-2.086918	-4.434910
C	-1.123537	-4.035801	-2.745348
C	-1.436204	-4.864731	-0.470522
C	-1.743041	-4.368788	1.898216
C	-1.974790	-2.691167	3.654568
C	-2.088071	-0.339488	4.326094
C	-2.078652	2.065693	3.825559
C	-2.101323	3.918186	2.337041

C	-0.596328	5.145500	0.810702
C	-0.866628	4.414665	-2.225971
C	-0.736954	2.571932	-3.865781
C	-0.735093	0.260746	-4.652718
C	-0.872599	-2.145307	-4.270276
C	-0.283486	-3.222653	-3.547909
C	-0.572218	-4.627839	-1.571694
C	-0.890203	-4.789382	0.842196
C	-1.168017	-3.645464	2.977480
C	-1.345532	-1.544215	4.205040
C	-1.390623	0.902421	4.242043
C	-1.312011	3.112279	3.153818
C	-1.780554	4.624485	1.119294
C	-0.104539	5.176180	-1.355387
C	-0.079997	3.558401	-3.093952
C	-0.013212	1.441098	-4.330824
C	-0.084102	-0.997042	-4.538322
C	1.133722	-3.271064	-3.378091
C	0.844674	-4.657439	-1.387728
C	0.526690	-4.791419	1.028281
C	0.246624	-3.626735	3.151640
C	0.066395	-1.514959	4.356780
C	0.032871	0.934145	4.346151
C	0.165519	3.146532	3.209382
C	0.723471	4.821469	1.281858
C	1.252204	4.982722	-1.107747
C	1.353283	3.526080	-3.021099
C	1.410092	1.390956	-4.213727
C	1.335015	-1.051656	-4.386383
C	1.951614	-2.255766	-3.948223
C	1.701186	-4.118784	-2.389510
C	1.390382	-4.895800	-0.096899
C	1.083030	-4.346845	2.259736
C	0.842608	-2.637036	3.981276
C	0.726582	-0.274471	4.587862
C	0.776388	2.111488	3.990181
C	1.059956	4.028432	2.451772
C	1.699005	5.037311	0.272981
C	2.029916	4.285714	-2.033606
C	2.105398	2.492521	-3.665125
C	2.093110	0.147722	-4.377727
C	3.369297	-2.310921	-3.791521
C	3.120011	-4.154824	-2.212370
C	2.810465	-4.900231	0.089831
C	2.503534	-4.324756	2.440564
C	2.260023	-2.615137	4.162281
C	2.134765	-0.268116	4.810506

C	2.182387	2.116200	4.283519
C	2.488350	3.978309	2.744694
C	3.066768	4.816600	0.525494
C	3.431895	4.151583	-1.792577
C	3.535071	2.424143	-3.505282
C	3.513070	0.087966	-4.237439
C	4.155749	-1.168528	-4.094878
C	3.955471	-3.367979	-3.044234
C	3.670953	-4.699297	-1.018361
C	3.357524	-4.767155	1.398396
C	3.075147	-3.573456	3.505161
C	2.876791	-1.479350	4.742323
C	2.818589	0.962977	4.834989
C	2.996383	3.153441	3.784397
C	3.465383	4.510254	1.838068
C	3.972607	4.577769	-0.552780
C	4.212654	3.339947	-2.642199
C	4.242791	1.272464	-3.926801
C	5.590850	-1.226823	-3.945691
C	5.387722	-3.419283	-2.872943
C	5.103092	-4.731112	-0.827079
C	4.789809	-4.773894	1.598202
C	4.506113	-3.566543	3.708780
C	4.300180	-1.479274	4.978972
C	4.228240	0.966285	5.142541
C	4.408787	3.171650	4.114019
C	4.886488	4.450039	2.104311
C	5.382025	4.450924	-0.297153
C	5.638812	3.259842	-2.425923
C	5.681491	1.215144	-3.766796
C	5.927185	-4.240946	-1.863742
C	5.617246	-4.945946	0.466856
C	5.307174	-4.328524	2.832363
C	5.052474	-2.606121	4.589664
C	4.900629	-0.255346	5.348162
C	4.944597	2.158835	4.930869
C	5.293538	3.961838	3.358139
C	5.808112	4.594670	1.046013
C	6.202634	3.948913	-1.328221
C	6.356173	2.289523	-3.157024
H	-6.005355	2.858171	-4.635756
H	-7.049927	-4.392582	1.240959
H	-6.741777	-4.788359	-1.164617
H	-6.427856	-3.865246	-3.414139
H	-7.281837	-2.796015	3.101134
H	-7.406594	-0.488958	3.886288
H	-7.458370	1.836823	3.361509

H	6.383862	-4.312031	2.966441
H	6.693743	-4.941878	0.605389
H	7.003990	-4.258172	-1.725212
H	7.428866	2.212970	-3.011484
H	6.127114	-2.591631	4.740007
H	7.266525	3.842336	-1.144275
H	5.968412	-0.233459	5.542617
H	6.866926	4.517970	1.270681
H	6.006309	2.181571	5.157290
H	6.351661	3.939320	3.600235
C	-6.251682	3.792032	1.868761
H	-7.317126	3.711318	1.678967
C	-5.725050	4.779405	-0.423190
H	-6.754397	4.765045	-0.764741
C	-5.143993	4.473525	-2.727549
H	-6.205660	4.538091	-2.941772
C	-4.948989	0.440073	-5.185791
H	-6.024253	0.486932	-5.331282
C	-5.096784	-1.976667	-4.777581
H	-6.174716	-1.932764	-4.902568
C	6.326725	-0.026246	-3.952879
H	7.403699	-0.074650	-3.823623
C	6.177440	-2.422648	-3.484210
H	7.254997	-2.457546	-3.353294
O	-0.688112	5.949759	-0.347728

SW Defected Nanotube-O (Triplet) ZPE= 1.184872 Ee= -5576.607424

C	-5.660890	-4.817411	-1.014004
C	-5.973732	-4.390013	1.380660
C	-6.206212	-2.768272	3.213182
C	-6.330696	-0.442899	3.991060
C	-6.385065	1.941372	3.492964
C	-4.925136	2.777281	-4.506748
C	-5.338358	-3.914176	-3.271728
C	-4.816902	-4.531407	-2.123331
C	-5.145598	-4.761476	0.293085
C	-5.425578	-3.686064	2.478216
C	-5.601577	-1.640727	3.817057
C	-5.677996	0.806911	3.967518
C	-5.682334	3.007302	2.887505
C	-5.403070	4.446554	0.888321
C	-4.686129	4.766804	-1.435235
C	-4.328575	3.677098	-3.574627
C	-4.250924	1.596915	-4.871572
C	-4.320738	-0.851885	-5.050655
C	-4.519452	-3.082186	-4.068804

C	-3.390643	-4.570593	-1.936514
C	-3.714352	-4.770911	0.480182
C	-3.997024	-3.667669	2.645811
C	-4.174348	-1.602603	3.950376
C	-4.237742	0.843634	4.100438
C	-4.254899	3.060979	3.132507
C	-4.032482	4.525022	1.186571
C	-3.255282	4.755351	-1.129559
C	-2.912158	3.610891	-3.291858
C	-2.821130	1.539125	-4.631491
C	-2.895774	-0.902931	-4.863854
C	-3.100382	-3.137271	-3.894549
C	-2.535648	-4.007986	-2.915331
C	-2.850933	-4.854894	-0.644892
C	-3.163306	-4.370751	1.726667
C	-3.399038	-2.706894	3.501116
C	-3.516679	-0.366094	4.221295
C	-3.523190	2.042562	3.794177
C	-3.500461	3.937689	2.376531
C	-2.992093	4.794705	0.281517
C	-2.337719	4.345949	-2.223012
C	-2.147409	2.618778	-4.013619
C	-2.139256	0.307968	-4.814775
C	-2.282439	-2.102860	-4.432472
C	-1.117146	-4.052481	-2.734556
C	-1.438183	-4.879234	-0.457205
C	-1.750418	-4.371353	1.910197
C	-1.982716	-2.681295	3.659440
C	-2.092746	-0.321752	4.324002
C	-2.080744	2.088718	3.821307
C	-2.101594	3.948873	2.338112
C	-0.594506	5.158657	0.797703
C	-0.862914	4.414044	-2.242553
C	-0.734175	2.563222	-3.877696
C	-0.729311	0.249495	-4.656539
C	-0.862415	-2.158958	-4.263819
C	-0.273409	-3.237313	-3.542514
C	-0.568580	-4.638890	-1.562967
C	-0.894524	-4.793455	0.855726
C	-1.176937	-3.637585	2.990011
C	-1.353325	-1.529121	4.210999
C	-1.393107	0.918220	4.243150
C	-1.311929	3.129341	3.152388
C	-1.777637	4.642233	1.109445
C	-0.100446	5.180034	-1.368556
C	-0.077082	3.555997	-3.104237
C	-0.009249	1.427777	-4.334419

C	-0.075088	-1.014156	-4.536420
C	1.137222	-3.284214	-3.369327
C	0.845910	-4.667254	-1.375198
C	0.521747	-4.796387	1.044621
C	0.235535	-3.622030	3.167408
C	0.054033	-1.501912	4.365925
C	0.024400	0.949235	4.348083
C	0.162328	3.159022	3.206093
C	0.725529	4.832467	1.274586
C	1.251541	4.986166	-1.119808
C	1.354447	3.522707	-3.031146
C	1.415999	1.378585	-4.217822
C	1.340150	-1.067458	-4.382303
C	1.956431	-2.266717	-3.937911
C	1.703641	-4.131667	-2.373085
C	1.388148	-4.909066	-0.077459
C	1.074302	-4.354347	2.279878
C	0.830848	-2.634855	3.996444
C	0.717013	-0.264486	4.591855
C	0.771674	2.124967	3.984483
C	1.060994	4.043890	2.441958
C	1.701118	5.048062	0.261845
C	2.029597	4.283810	-2.046511
C	2.110377	2.487150	-3.678005
C	2.100218	0.138541	-4.380670
C	3.374287	-2.319999	-3.776285
C	3.120535	-4.166392	-2.190804
C	2.802339	-4.914741	0.113836
C	2.488151	-4.336235	2.465866
C	2.242810	-2.617559	4.182214
C	2.123100	-0.262391	4.816643
C	2.178509	2.124928	4.275814
C	2.486986	3.988774	2.731355
C	3.066245	4.830309	0.509889
C	3.431274	4.159662	-1.810329
C	3.534242	2.424007	-3.518755
C	3.515648	0.081592	-4.237958
C	4.162134	-1.181442	-4.085081
C	3.961327	-3.379515	-3.026438
C	3.667950	-4.713868	-0.999033
C	3.343168	-4.784979	1.423687
C	3.054129	-3.582892	3.534739
C	2.858935	-1.474499	4.762097
C	2.811515	0.972548	4.836288
C	2.997614	3.159340	3.774237
C	3.463868	4.519199	1.824831
C	3.969870	4.600914	-0.572938

C	4.209106	3.351059	-2.662771
C	4.243198	1.266508	-3.934262
C	5.592042	-1.242446	-3.935105
C	5.386681	-3.429883	-2.856516
C	5.094148	-4.737539	-0.809453
C	4.770696	-4.776891	1.617618
C	4.480606	-3.562245	3.728615
C	4.276759	-1.467158	4.992792
C	4.214661	0.979420	5.144798
C	4.405248	3.178174	4.107770
C	4.880290	4.455140	2.097553
C	5.367420	4.457230	-0.309364
C	5.625533	3.254809	-2.434739
C	5.677213	1.201188	-3.766923
C	5.926524	-4.249025	-1.839221
C	5.609322	-4.937458	0.493272
C	5.293580	-4.310192	2.846157
C	5.037193	-2.592018	4.592803
C	4.888902	-0.246144	5.349174
C	4.939141	2.169659	4.932647
C	5.294254	3.971002	3.352092
C	5.803636	4.584150	1.035386
C	6.192417	3.925413	-1.326168
C	6.352539	2.270588	-3.144354
H	-5.989730	2.865143	-4.699560
H	-7.050554	-4.388625	1.241588
H	-6.736748	-4.791158	-1.157884
H	-6.415823	-3.861059	-3.395895
H	-7.284854	-2.778296	3.088506
H	-7.409919	-0.467665	3.873123
H	-7.459041	1.861752	3.354684
H	6.370609	-4.294010	2.983563
H	6.685724	-4.932521	0.635903
H	7.002757	-4.264730	-1.696021
H	7.425090	2.195254	-2.992849
H	6.112507	-2.578073	4.743366
H	7.256465	3.815833	-1.139153
H	5.957544	-0.227131	5.540563
H	6.863503	4.504122	1.256583
H	6.000724	2.188668	5.159104
H	6.352569	3.946431	3.592122
C	-6.245465	3.795636	1.854664
H	-7.309342	3.709107	1.656317
C	-5.708590	4.741205	-0.446126
H	-6.737582	4.704048	-0.789741
C	-5.137076	4.429440	-2.740737
H	-6.200289	4.491585	-2.950236

C	-4.935879	0.429443	-5.229341
H	-6.007496	0.474513	-5.397590
C	-5.081032	-1.990356	-4.783717
H	-6.159704	-1.946200	-4.901131
C	6.330972	-0.037619	-3.946901
H	7.408064	-0.083325	-3.817313
C	6.182199	-2.436413	-3.472201
H	7.259260	-2.470786	-3.338704
O	-0.683628	5.959703	-0.364445

Figure 7c

Graphene-2O (Singlet) ZPE= 0.698871 Ee= -2830.893490

C	-6.958686	2.433023	-0.848933
C	5.653686	2.381703	0.269962
C	-0.523358	-1.593637	1.212235
C	-2.672569	4.905617	-0.826751
C	-9.094831	1.199593	-0.850758
C	3.518632	1.147535	0.587847
C	-2.804908	-2.405383	0.609261
C	-4.824371	3.670142	-0.862128
C	1.644047	-0.383279	1.210789
C	-4.931946	-3.597703	0.304040
C	1.515690	4.919450	-0.120843
C	-4.903807	1.288915	-0.198568
C	7.747616	1.182299	-0.153632
C	1.447024	-2.614266	0.246530
C	-0.660525	3.764741	-0.043244
C	-7.009714	0.042566	-0.269950
C	5.616439	-0.063622	-0.030011
C	-0.722476	-3.742320	0.157102
C	-2.810649	2.551117	-0.078807
C	-9.146099	-1.167687	-0.358242
C	3.535046	-1.337980	0.098011
C	-2.865948	-4.856590	0.064816
C	3.552518	3.621850	0.359447
C	-2.878447	0.171980	0.643163
C	9.803632	-0.011058	-0.692909
C	3.469168	-3.723352	-0.607940
C	1.370426	2.565600	0.673155
C	-4.912547	-1.145331	0.302598
C	7.697224	-1.243881	-0.654797
C	1.326072	-4.940439	-0.575981
C	-0.844278	1.525886	0.941302
C	-7.038927	-2.371993	0.098579
C	5.582758	-2.479567	-0.647862
C	-0.825348	-6.112062	-0.585425

C	-1.326073	4.940440	-0.575987
C	-7.697222	1.243878	-0.654812
C	4.912546	1.145331	0.302600
C	-1.370427	-2.565598	0.673159
C	-3.469167	3.723350	-0.607949
C	-9.803630	0.011055	-0.692927
C	2.878446	-0.171979	0.643164
C	-3.552519	-3.621849	0.359450
C	-5.582757	2.479565	-0.647875
C	0.844278	-1.525884	0.941304
C	0.722474	3.742322	0.157098
C	-5.616438	0.063621	-0.030018
C	7.009715	-0.042567	-0.269940
C	0.660525	-3.764740	-0.043239
C	-1.447024	2.614267	0.246525
C	-7.747615	-1.182300	-0.153641
C	4.903808	-1.288916	-0.198561
C	-1.515691	-4.919448	-0.120840
C	-3.535046	1.337979	0.098006
C	2.810650	-2.551117	-0.078800
C	2.804906	2.405384	0.609255
C	-3.518634	-1.147535	0.587851
C	9.094834	-1.199596	-0.850739
C	2.672569	-4.905618	-0.826742
C	0.523356	1.593639	1.212233
C	-5.653686	-2.381703	0.269961
C	6.958688	-2.433026	-0.848917
C	0.507492	-6.119779	-0.809316
C	-1.644049	0.383281	1.210788
C	4.824373	-3.670144	-0.862115
C	0.825347	6.112065	-0.585427
C	7.038927	2.371993	0.098583
C	4.931946	3.597704	0.304037
C	2.865948	4.856591	0.064814
C	9.146100	1.167685	-0.358229
H	7.577694	3.314867	0.112094
H	5.477093	4.528932	0.181425
H	9.698589	2.096027	-0.260390
C	-0.507493	6.119780	-0.809320
H	-9.611254	2.110722	-1.133344
H	-7.483218	3.330386	-1.163855
H	-5.339895	4.551760	-1.231457
H	-3.169545	5.789767	-1.215812
H	-1.001457	7.014393	-1.174081
H	1.421511	7.000605	-0.765740
H	3.477061	5.738670	-0.103804
O	-1.128000	-0.629766	2.028033

O	1.128000	0.629770	2.028033
H	10.876489	-0.002691	-0.845793
H	9.611258	-2.110725	-1.133321
H	7.483220	-3.330390	-1.163835
H	5.339896	-4.551763	-1.231441
H	3.169545	-5.789768	-1.215802
H	1.001456	-7.014391	-1.174077
H	-1.421512	-7.000603	-0.765739
H	-3.477061	-5.738669	-0.103803
H	-5.477093	-4.528932	0.181428
H	-7.577695	-3.314868	0.112091
H	-9.698589	-2.096028	-0.260402
H	-10.876487	0.002688	-0.845815

Graphene-2O (Triplet) ZPE= 0.697354 Ee= -2830.918999

C	6.979049	-2.422834	-0.849574
C	-5.654158	-2.378133	0.281107
C	0.521788	1.596238	1.220994
C	2.677575	-4.888842	-0.840776
C	9.117527	-1.196629	-0.852771
C	-3.524469	-1.147378	0.597776
C	2.815227	2.400588	0.616877
C	4.837114	-3.656732	-0.862600
C	-1.651727	0.386923	1.224909
C	4.943297	3.585303	0.312616
C	-1.518207	-4.897704	-0.146916
C	4.916277	-1.290299	-0.190398
C	-7.758723	-1.185669	-0.144786
C	-1.447374	2.612748	0.256492
C	0.666829	-3.751986	-0.052023
C	7.018876	-0.043562	-0.259999
C	-5.630260	0.066126	-0.016802
C	0.726222	3.726070	0.144125
C	2.823173	-2.547325	-0.072505
C	9.165728	1.168799	-0.352577
C	-3.539918	1.339555	0.107872
C	2.869599	4.838715	0.052254
C	-3.551706	-3.610488	0.367391
C	2.884033	-0.176055	0.658444
C	-9.823280	0.010972	-0.692631
C	-3.473296	3.712838	-0.607219
C	-1.363162	-2.560508	0.673590
C	4.922047	1.145966	0.317683
C	-7.705928	1.244841	-0.652960
C	-1.327014	4.921801	-0.596760
C	0.851241	-1.531574	0.956040

C	7.059723	2.366083	0.108613
C	-5.585624	2.473439	-0.643152
C	0.830060	6.083867	-0.630040
C	1.327001	-4.921795	-0.596756
C	7.705945	-1.244873	-0.652917
C	-4.922028	-1.145942	0.317706
C	1.363190	2.560420	0.673681
C	3.473268	-3.712867	-0.607115
C	9.823262	-0.010892	-0.692717
C	-2.884070	0.176109	0.658357
C	3.551763	3.610439	0.367429
C	5.585578	-2.473466	-0.643039
C	-0.851302	1.531544	0.956032
C	-0.726267	-3.726135	0.144149
C	5.630271	-0.066111	-0.016794
C	-7.018898	0.043592	-0.259990
C	-0.666748	3.751942	-0.052042
C	1.447357	-2.612802	0.256493
C	7.758672	1.185705	-0.144912
C	-4.916330	1.290283	-0.190475
C	1.518243	4.897701	-0.146843
C	3.539902	-1.339542	0.107916
C	-2.823157	2.547301	-0.072548
C	-2.815217	-2.400647	0.616801
C	3.524459	1.147382	0.597835
C	-9.117534	1.196642	-0.852800
C	-2.677522	4.888849	-0.840831
C	-0.521723	-1.596211	1.220875
C	5.654163	2.378095	0.281033
C	-6.979018	2.422824	-0.849690
C	-0.503899	6.093151	-0.850890
C	1.651756	-0.386919	1.225049
C	-4.837046	3.656729	-0.862737
C	-0.830078	-6.083827	-0.630209
C	-7.059767	-2.366065	0.108795
C	-4.943332	-3.585280	0.312666
C	-2.869632	-4.838681	0.052176
C	-9.165728	-1.168740	-0.352393
H	-7.595407	-3.310424	0.132133
H	-5.485834	-4.518303	0.192003
H	-9.717592	-2.097032	-0.251946
C	0.503909	-6.093103	-0.851025
H	9.631251	-2.108406	-1.137697
H	7.499355	-3.321360	-1.167963
H	5.350911	-4.537165	-1.237060
H	3.172422	-5.770116	-1.238930
H	0.994611	-6.984240	-1.228475

H	-1.428068	-6.967993	-0.825351
H	-3.480378	-5.719721	-0.122891
O	1.126785	0.629226	2.030841
O	-1.126766	-0.629229	2.030525
H	-10.896043	0.000612	-0.846638
H	-9.631210	2.108424	-1.137797
H	-7.499373	3.321297	-1.168149
H	-5.350843	4.537128	-1.237286
H	-3.172372	5.770125	-1.238984
H	-0.994637	6.984313	-1.228236
H	1.428074	6.968053	-0.825024
H	3.480423	5.719710	-0.122749
H	5.485824	4.518297	0.191849
H	7.595300	3.310482	0.131844
H	9.717513	2.097144	-0.252202
H	10.896023	-0.000577	-0.846760

Graphene-2O (Quintet) ZPE=0.695079 Ee= -2830.881658

C	7.016048	-2.460084	-0.743098
C	-5.718492	-2.394756	0.192806
C	0.551167	1.554131	1.102213
C	2.697763	-4.866831	-0.707842
C	9.158853	-1.231692	-0.769863
C	-3.569004	-1.159254	0.427845
C	2.846575	2.417380	0.606396
C	4.866395	-3.674293	-0.732235
C	-1.468834	0.097000	0.908668
C	4.988419	3.586508	0.287336
C	-1.520460	-4.869027	-0.106835
C	4.953173	-1.287167	-0.156333
C	-7.817300	-1.145854	-0.136744
C	-1.391003	2.514724	0.134685
C	0.648110	-3.697613	-0.079285
C	7.068581	-0.058937	-0.234539
C	-5.657174	0.061116	-0.045163
C	0.766632	3.717589	0.128284
C	2.803652	-2.511071	-0.073125
C	9.207016	1.145992	-0.335547
C	-3.523490	1.266549	0.070811
C	2.901098	4.837766	0.041811
C	-3.597464	-3.642137	0.255700
C	2.927828	-0.158789	0.620629
C	-9.880122	0.094949	-0.553386
C	-3.441990	3.677352	-0.528410
C	-1.453890	-2.482040	0.475657
C	4.956829	1.142980	0.306824

C	-7.751666	1.295143	-0.524172
C	-1.309816	4.884810	-0.539968
C	0.783495	-1.376424	0.734712
C	7.098850	2.360845	0.091853
C	-5.595701	2.492504	-0.519165
C	0.830251	6.083428	-0.581837
C	1.304667	-4.879652	-0.493385
C	7.751015	-1.267928	-0.580307
C	-4.974375	-1.155770	0.202357
C	1.410858	2.566534	0.627997
C	3.463715	-3.708038	-0.518063
C	9.866634	-0.042209	-0.638790
C	-2.870490	0.064677	0.451289
C	3.579642	3.618851	0.344736
C	5.623064	-2.497620	-0.555755
C	-0.752212	1.380242	0.724067
C	-0.778757	-3.673858	0.113473
C	5.659842	-0.073578	-0.003631
C	-7.076047	0.070665	-0.230963
C	-0.643656	3.699278	-0.080538
C	1.407587	-2.520344	0.152434
C	7.802426	1.166301	-0.139367
C	-4.918681	1.267190	-0.164250
C	1.535725	4.896359	-0.140675
C	3.562809	-1.316919	0.116510
C	-2.785460	2.489382	-0.111671
C	-2.857204	-2.427699	0.448471
C	3.565488	1.143549	0.592483
C	-9.162557	1.280925	-0.676123
C	-2.676646	4.856674	-0.742047
C	-0.685764	-1.302265	0.916989
C	5.693216	2.382501	0.258341
C	-6.998696	2.477021	-0.674974
C	-0.511058	6.075570	-0.768003
C	1.622268	-0.354591	1.103629
C	-4.845716	3.661034	-0.707347
C	-0.820755	-6.070776	-0.483072
C	-7.121874	-2.355238	0.066420
C	-5.018711	-3.604448	0.233900
C	-2.910556	-4.840845	0.028581
C	-9.226887	-1.106066	-0.293363
H	-7.677577	-3.287899	0.090472
H	-5.565753	-4.539968	0.168910
H	-9.787775	-2.031097	-0.214165
C	0.523190	-6.075766	-0.677373
H	9.673509	-2.152150	-1.023717
H	7.539658	-3.369522	-1.022541

H	5.371781	-4.584013	-1.042209
H	3.189149	-5.780034	-1.030338
H	1.036332	-6.983284	-0.977431
H	-1.403992	-6.974253	-0.627001
H	-3.478475	-5.756174	-0.109852
O	1.141939	0.631509	1.962439
O	-1.221101	-0.676416	2.135656
H	-10.957494	0.105283	-0.670192
H	-9.673721	2.212554	-0.893390
H	-7.510121	3.402022	-0.923836
H	-5.352654	4.576515	-0.996712
H	-3.188874	5.754545	-1.075252
H	-1.025750	6.970641	-1.101601
H	1.409220	6.982499	-0.764657
H	3.503943	5.725040	-0.128655
H	5.530542	4.520037	0.170064
H	7.639613	3.302355	0.102612
H	9.759073	2.076058	-0.254313
H	10.940421	-0.037576	-0.784926

SW Defected Graphene-2O (Singlet) ZPE= 0.698813 Ee= -2830.805741

C	-4.904551	3.667814	0.383377
C	4.836398	-3.716942	0.455396
C	6.746507	-2.419183	1.385419
C	0.720883	-6.110513	-0.690103
C	2.800402	-4.917303	-0.322907
C	8.593713	-1.090821	2.363080
C	3.608207	-3.739723	-0.168410
C	9.175524	0.140812	2.657576
C	5.549961	-2.490499	0.701027
C	-0.621527	-6.099133	-0.686914
C	7.377788	-1.166526	1.656392
C	1.476476	-4.871302	-0.672033
C	3.035958	-2.530049	-0.704546
C	8.556874	1.326499	2.272852
C	4.966927	-1.263946	0.213920
C	-1.354827	-4.847666	-0.646903
C	0.775986	-3.603163	-0.952658
C	6.754628	0.047611	1.231549
C	1.713998	-2.484069	-1.158349
C	7.338600	1.301408	1.565042
C	3.816917	-1.306545	-0.571250
C	-2.684205	-4.883783	-0.312725
C	-0.637445	-3.588063	-0.902712
C	5.538372	0.004328	0.485219
C	1.373772	-1.228693	-1.768668
C	6.637448	2.485755	1.208067

C	3.325363	-0.120224	-1.127611
C	-3.481462	-3.704866	-0.124695
C	-1.509832	-2.400995	-0.945901
C	4.864670	1.202845	0.091587
C	-1.072892	-1.133229	-1.356823
C	5.430123	2.455190	0.535483
C	0.178273	-0.622258	-1.866243
C	-2.854795	-2.452070	-0.461246
C	3.669740	1.176888	-0.711640
C	-1.839440	0.004120	-1.130954
C	4.680707	3.649398	0.311844
C	0.072214	0.824861	-1.937064
C	-5.549191	-2.547657	0.594591
C	-3.635826	-1.269434	-0.265656
C	2.838907	2.427982	-0.816939
C	-3.087622	-0.009983	-0.569963
C	3.425032	3.641164	-0.234732
C	-1.122316	1.211008	-1.412087
C	-4.937447	-1.287852	0.281902
C	1.542219	2.569336	-1.293451
C	-3.699606	1.234403	-0.290217
C	2.668277	4.858569	-0.273833
C	-1.632590	2.475816	-0.981281
C	-7.535304	-1.336724	1.377554
C	-5.606421	-0.058074	0.533497
C	0.638098	3.676181	-0.959775
C	-4.975137	1.206719	0.265757
C	1.336008	4.895594	-0.568996
C	-2.953180	2.465517	-0.497101
C	-6.907435	-0.080983	1.092247
C	-0.781326	3.655838	-0.895666
C	-5.638221	2.446680	0.594592
C	0.591742	6.135384	-0.452063
C	-9.491567	-0.128666	2.186014
C	-3.610720	3.691559	-0.103563
C	-7.581036	1.153174	1.378134
C	-1.495399	4.888286	-0.537531
C	-6.914962	2.395356	1.124342
C	-8.873407	1.099448	1.921857
C	-4.777760	-3.737994	0.357996
C	-6.837014	-2.546860	1.123117
C	-8.841985	-1.325407	1.925451
C	-0.752394	6.133430	-0.456140
C	-2.830054	4.891328	-0.216128
H	-1.192722	-7.020584	-0.650883
H	-3.146842	-5.849660	-0.129116
H	-9.392738	2.026401	2.141240

H	-5.231247	-4.697767	0.590226
H	-7.323407	-3.488427	1.361508
H	-9.327338	-2.271181	2.142090
H	-1.316582	7.051496	-0.330695
H	-3.303325	5.836232	0.036163
H	-7.433591	3.316631	1.374325
H	-5.384379	4.604166	0.655050
H	-10.490885	-0.141379	2.605385
O	2.411553	-0.383749	-2.137328
O	1.101685	1.671783	-2.273655
H	3.169638	5.771121	0.034171
H	5.099621	4.589540	0.657815
H	7.049791	3.445187	1.506860
H	9.002607	2.283830	2.521158
H	10.112456	0.174963	3.200953
H	9.072347	-2.010376	2.682942
H	7.221335	-3.327803	1.743934
H	5.265251	-4.643431	0.825436
H	3.243164	-5.879912	-0.083815
H	1.278045	-7.040377	-0.652881
H	1.155997	7.052440	-0.320429

SW Defected Graphene-2O (Triplet) ZPE= 0.694442 Ee= -2830.812640

C	5.027990	-3.649771	0.317190
C	-4.944307	3.691923	0.415562
C	-6.906995	2.401151	1.226641
C	-0.736983	6.059859	-0.412925
C	-2.841152	4.874279	-0.198617
C	-8.811636	1.077941	2.081909
C	-3.653782	3.717972	-0.146934
C	-9.413304	-0.152147	2.332980
C	-5.654331	2.479381	0.609096
C	0.609690	6.055463	-0.429544
C	-7.544918	1.154912	1.450864
C	-1.485596	4.829385	-0.498840
C	-3.073500	2.523616	-0.665369
C	-8.775150	-1.337931	1.983022
C	-5.046569	1.253474	0.159031
C	1.345646	4.815931	-0.497786
C	-0.800703	3.584607	-0.825374
C	-6.896814	-0.059170	1.061153
C	-1.717533	2.482347	-1.074602
C	-7.506272	-1.316200	1.352443
C	-3.850517	1.298987	-0.562418
C	2.709012	4.861129	-0.210316
C	0.652142	3.578044	-0.781745

C	-5.634029	-0.014483	0.392206
C	-1.364247	1.226640	-1.673656
C	-6.798834	-2.494107	1.040312
C	-3.335966	0.115167	-1.098910
C	3.512171	3.701220	-0.084111
C	1.518343	2.398411	-0.839307
C	-4.937982	-1.212868	0.033301
C	1.078056	1.124949	-1.232981
C	-5.523909	-2.467447	0.440183
C	-0.172184	0.616250	-1.743180
C	2.884950	2.449106	-0.399436
C	-3.696581	-1.186731	-0.699965
C	1.850173	-0.005989	-1.025938
C	-4.775613	-3.635510	0.283065
C	-0.062319	-0.827869	-1.830517
C	5.629488	2.548249	0.534658
C	3.677220	1.265805	-0.236242
C	-2.866772	-2.432060	-0.771231
C	3.122304	0.010630	-0.517214
C	-3.445657	-3.620113	-0.194629
C	1.135147	-1.210527	-1.314444
C	5.009416	1.285359	0.248954
C	-1.523718	-2.577318	-1.209349
C	3.756660	-1.236751	-0.286453
C	-2.681088	-4.794200	-0.092008
C	1.652511	-2.482404	-0.912011
C	7.659590	1.340962	1.209817
C	5.695330	0.060618	0.457483
C	-0.654520	-3.649265	-0.833217
C	5.058172	-1.207441	0.208240
C	-1.315324	-4.819324	-0.336189
C	3.018411	-2.468408	-0.477664
C	7.027476	0.088396	0.950126
C	0.833833	-3.640387	-0.803110
C	5.736252	-2.451112	0.490241
C	-0.573446	-6.038121	-0.102588
C	9.669990	0.147318	1.908249
C	3.669233	-3.681329	-0.118902
C	7.727002	-1.147688	1.190705
C	1.521250	-4.845867	-0.412021
C	7.069536	-2.385970	0.962785
C	9.049286	-1.084690	1.667216
C	4.847556	3.734268	0.343687
C	6.944462	2.549267	0.998297
C	8.997734	1.338195	1.690422
C	0.771641	-6.059877	-0.173464
C	2.893261	-4.857598	-0.151135

H	1.174150	6.975909	-0.326652
H	3.157496	5.829410	-0.007289
H	9.586687	-2.009104	1.850549
H	5.304196	4.695402	0.562339
H	7.438395	3.491951	1.215520
H	9.484328	2.287752	1.886415
H	1.327754	-6.970454	0.022245
H	3.356362	-5.800110	0.126773
H	7.605414	-3.307213	1.171476
H	5.515840	-4.589810	0.558982
H	10.689867	0.166032	2.274677
O	-2.387994	0.376550	-2.071657
O	-1.070253	-1.690562	-2.199320
H	-3.166076	-5.695904	0.268741
H	-5.191697	-4.580198	0.619103
H	-7.229606	-3.455757	1.302731
H	-9.237886	-2.295558	2.196074
H	-10.383436	-0.186056	2.814743
H	-9.306152	1.998681	2.372417
H	-7.402062	3.310427	1.554370
H	-5.384610	4.619805	0.767874
H	-3.273458	5.830271	0.082544
H	-1.294239	6.982364	-0.291177
H	-1.137391	-6.928941	0.152379

SW Defected Graphene-2O (Quintet) ZPE= 0.694509 Ee= -2830.819329

C	5.037246	-3.648791	0.318306
C	-4.980434	3.689097	0.399212
C	-6.951227	2.401713	1.185492
C	-0.734733	6.039046	-0.326837
C	-2.849932	4.859763	-0.158440
C	-8.860217	1.075660	2.017548
C	-3.661759	3.714934	-0.146715
C	-9.460256	-0.155881	2.264812
C	-5.680877	2.485418	0.581857
C	0.612130	6.037992	-0.357437
C	-7.584207	1.156385	1.403354
C	-1.483214	4.812267	-0.446370
C	-3.085526	2.527243	-0.660605
C	-8.812699	-1.340033	1.927658
C	-5.065416	1.256645	0.141350
C	1.349719	4.803800	-0.467269
C	-0.812291	3.579398	-0.799260
C	-6.925311	-0.058540	1.026204
C	-1.715527	2.486495	-1.058822
C	-7.534623	-1.315519	1.313582
C	-3.862454	1.302462	-0.564788

C	2.727739	4.853175	-0.194050
C	0.669165	3.576207	-0.761140
C	-5.653244	-0.012493	0.373007
C	-1.360482	1.227075	-1.654798
C	-6.820935	-2.492671	1.014726
C	-3.339610	0.116033	-1.094145
C	3.522317	3.702105	-0.090229
C	1.521143	2.403919	-0.822056
C	-4.951061	-1.209450	0.026254
C	1.079459	1.124262	-1.208594
C	-5.538883	-2.465255	0.430038
C	-0.169428	0.617300	-1.724550
C	2.899609	2.454147	-0.396372
C	-3.701999	-1.183638	-0.696311
C	1.848599	-0.003279	-1.000066
C	-4.787460	-3.631745	0.284735
C	-0.060795	-0.826245	-1.812256
C	5.649960	2.553171	0.506874
C	3.691270	1.267332	-0.234191
C	-2.870536	-2.430113	-0.759516
C	3.129277	0.010580	-0.501559
C	-3.449874	-3.615520	-0.181739
C	1.135409	-1.207185	-1.289594
C	5.025816	1.287240	0.234395
C	-1.524770	-2.574723	-1.190174
C	3.760886	-1.232159	-0.277038
C	-2.684866	-4.785524	-0.065679
C	1.654884	-2.478954	-0.888429
C	7.694735	1.339895	1.166056
C	5.713007	0.059766	0.441684
C	-0.656232	-3.644258	-0.806534
C	5.073060	-1.203769	0.205930
C	-1.315757	-4.810264	-0.303997
C	3.021356	-2.464543	-0.460922
C	7.052692	0.083667	0.919196
C	0.835648	-3.637223	-0.777941
C	5.750914	-2.447062	0.482547
C	-0.574529	-6.026799	-0.060468
C	9.710111	0.135089	1.846893
C	3.674253	-3.678941	-0.105349
C	7.746609	-1.149227	1.155508
C	1.520660	-4.839895	-0.385495
C	7.087017	-2.383368	0.940440
C	9.084318	-1.089646	1.619666
C	4.884721	3.728438	0.327190
C	6.985619	2.546713	0.958154
C	9.037057	1.332592	1.630191

C	0.770877	-6.050573	-0.135074
C	2.896871	-4.852655	-0.130554
H	1.174850	6.957132	-0.235248
H	3.171440	5.821758	0.016638
H	9.617574	-2.017227	1.799085
H	5.342140	4.690494	0.539399
H	7.484458	3.489508	1.163174
H	9.530928	2.280405	1.816264
H	1.326288	-6.960412	0.066112
H	3.359317	-5.795526	0.147360
H	7.622836	-3.305509	1.145946
H	5.526553	-4.588694	0.557293
H	10.734224	0.153553	2.201210
O	-2.381857	0.376514	-2.055281
O	-1.068883	-1.689598	-2.179537
H	-3.169482	-5.686091	0.298383
H	-5.204577	-4.576368	0.619516
H	-7.253011	-3.454386	1.274725
H	-9.274280	-2.298927	2.137394
H	-10.436697	-0.191987	2.733473
H	-9.362209	1.995509	2.297825
H	-7.452885	3.310901	1.502855
H	-5.422891	4.619544	0.741354
H	-3.276562	5.812411	0.141835
H	-1.291707	6.957150	-0.174515
H	-1.138330	-6.915083	0.203502

Figure 7d

Nanotube-2O (Singlet) ZPE= 1.189528 Ee= -5651.804943

C	-5.812384	-4.410088	-2.057854
C	-5.197724	-3.630396	-3.060233
C	-5.926550	-2.665020	-3.783374
C	-5.296085	-1.482264	-4.222827
C	-6.002031	-0.268074	-4.345643
C	-5.346176	0.961523	-4.145770
C	-6.029167	2.084813	-3.627925
C	-5.337979	3.076248	-2.911429
C	-5.968390	3.836791	-1.898078
C	-5.214220	4.419297	-0.862789
C	-5.734307	4.698087	0.413293
C	-4.895088	4.660184	1.557996
C	-5.452200	4.202409	2.759851
C	-4.677560	3.393829	3.611643
C	-5.310050	2.401905	4.389348
C	-4.642675	1.206157	4.700203
C	-5.333690	-0.008949	4.910604

C	-4.703019	-1.243441	4.674269
C	-5.423731	-2.396727	4.290241
C	-4.803615	-3.415066	3.539817
C	-5.542702	-4.215805	2.643072
C	-4.928605	-4.760311	1.496299
C	-5.677341	-4.974520	0.320217
C	-5.066773	-4.851186	-0.945113
C	-3.753898	-3.598912	-3.112281
C	-3.098888	-2.584845	-3.858571
C	-3.851967	-1.444986	-4.253914
C	-3.173655	-0.203835	-4.402162
C	-3.901459	0.995067	-4.190676
C	-3.195645	2.158522	-3.765658
C	-3.897329	3.130701	-3.018173
C	-3.155501	3.998269	-2.171473
C	-3.787884	4.521310	-1.021721
C	-2.984886	4.971638	0.054188
C	-3.452037	4.739734	1.413673
C	-2.612364	4.219417	2.443558
C	-3.244775	3.365027	3.419480
C	-2.513216	2.306271	4.025727
C	-3.209736	1.173993	4.528816
C	-2.521593	-0.068522	4.641048
C	-3.260901	-1.272569	4.564474
C	-2.599591	-2.451462	4.113713
C	-3.360323	-3.449787	3.458798
C	-2.716421	-4.268185	2.490201
C	-3.487054	-4.782990	1.416605
C	-2.850859	-4.986465	0.163583
C	-3.624648	-4.844758	-1.019146
C	-2.984932	-4.360182	-2.189273
C	-1.670978	-2.553739	-3.923445
C	-1.006417	-1.377029	-4.371745
C	-1.743832	-0.170979	-4.456016
C	-1.051626	1.064166	-4.300352
C	-1.761504	2.194760	-3.828057
C	-1.035960	3.241877	-3.190193
C	-1.741327	4.090028	-2.300913
C	-1.014826	4.917901	-1.404044
C	-1.678294	5.345681	-0.236995
C	-0.388115	5.055452	1.603800
C	-1.136515	4.228056	2.425822
C	-0.395863	3.271340	3.226394
C	-1.080896	2.257125	3.918674
C	-0.372330	1.097873	4.348101
C	-1.094477	-0.102752	4.564315
C	-0.419314	-1.342927	4.430168

C	-1.172181	-2.486864	4.049845
C	-0.518067	-3.516621	3.322768
C	-1.288283	-4.295914	2.416770
C	-0.645466	-4.814784	1.258477
C	-1.422561	-4.990903	0.081194
C	-0.782276	-4.826951	-1.179581
C	-1.556896	-4.341047	-2.266804
C	-0.909569	-3.545929	-3.254316
C	0.419146	-1.342407	-4.430314
C	1.094448	-0.102150	-4.564288
C	0.372509	1.098335	-4.348009
C	1.081172	2.257668	-3.918455
C	0.396303	3.271712	-3.226029
C	1.137046	4.228414	-2.425399
C	0.388806	5.055649	-1.603124
C	1.679024	5.345747	0.237574
C	1.015411	4.917697	1.404820
C	1.741789	4.089536	2.301282
C	1.036297	3.241308	3.190605
C	1.761734	2.193998	3.828193
C	1.051743	1.063534	4.300462
C	1.743809	-0.171796	4.455980
C	1.006299	-1.377637	4.371608
C	1.670712	-2.554499	3.923331
C	0.909173	-3.546490	3.253977
C	1.556383	-4.341604	2.266477
C	0.781688	-4.827251	1.179038
C	1.421963	-4.991023	-0.081670
C	0.644894	-4.814578	-1.259037
C	1.287785	-4.295623	-2.417142
C	0.517636	-3.516123	-3.323142
C	1.171860	-2.486321	-4.049978
C	2.521650	-0.068014	-4.640991
C	3.209878	1.174196	-4.528817
C	2.513501	2.306786	-4.025535
C	3.245062	3.365221	-3.419437
C	2.612884	4.219760	-2.443252
C	3.452393	4.739881	-1.413497
C	2.985252	4.971415	-0.053839
C	3.788326	4.520421	1.021997
C	3.155950	3.997387	2.171589
C	3.897829	3.129566	3.018237
C	3.195934	2.157524	3.765736
C	3.901724	0.994055	4.190685
C	3.173655	-0.204954	4.402138
C	3.851731	-1.445944	4.253903
C	3.098542	-2.585922	3.858462

C	3.753279	-3.599907	3.112150
C	2.984392	-4.360980	2.188986
C	3.623985	-4.845485	1.018754
C	2.850289	-4.986727	-0.163968
C	3.486512	-4.782958	-1.417024
C	2.715948	-4.268006	-2.490438
C	3.360068	-3.449395	-3.458937
C	2.599400	-2.451045	-4.113727
C	3.260920	-1.272269	-4.564521
C	4.642781	1.206049	-4.700017
C	5.310427	2.401598	-4.388624
C	4.677888	3.393689	-3.611185
C	4.895511	4.659976	-1.557421
C	5.214718	4.418552	0.863251
C	5.968905	3.836168	1.898618
C	5.338503	3.075316	2.911795
C	6.029593	2.084130	3.628779
C	5.346351	0.960628	4.146006
C	6.002040	-0.269168	4.345801
C	5.295833	-1.483137	4.222662
C	5.926190	-2.665788	3.782696
C	5.197122	-3.631219	3.059708
C	5.811752	-4.410238	2.057074
C	5.066077	-4.851738	0.944421
C	5.676681	-4.974748	-0.320778
C	4.928125	-4.760514	-1.496918
C	5.542271	-4.216454	-2.643853
C	4.803428	-3.415172	-3.540305
C	5.423533	-2.397135	-4.291117
C	4.702961	-1.243529	-4.674527
C	5.734665	4.697456	-0.412839
H	6.808740	4.652022	-0.565627
C	5.452684	4.201744	-2.759139
H	6.532744	4.180985	-2.863661
C	5.333750	-0.008979	-4.910827
H	6.415230	0.018906	-4.996303
H	-7.110908	2.042180	-3.551012
H	-7.047693	3.777575	-1.797023
H	-6.808359	4.652709	0.566169
H	-6.532252	4.181640	2.864282
H	-7.085474	-0.291301	-4.290598
H	-6.389843	2.439802	4.490421
H	-7.010244	-2.684688	-3.729340
H	-6.415178	0.018954	4.996095
H	-6.896122	-4.414380	-1.993544
H	-6.507743	-2.375187	4.345058
H	-6.761551	-4.956250	0.380210

H	-6.627326	-4.189850	2.691334
H	6.895513	-4.414447	1.992924
H	6.760905	-4.956565	-0.380720
H	7.009892	-2.685399	3.728670
H	6.626879	-4.190781	-2.692365
H	7.085467	-0.292450	4.290697
H	6.507514	-2.375639	-4.346222
H	7.111302	2.041236	3.551947
H	7.048212	3.776855	1.797812
H	6.390245	2.439180	-4.489611
O	-1.027458	6.023465	0.813230
O	1.027972	6.023758	-0.812561

Nanotube-2O (Triplet) ZPE= 1.189528 Ee= -5651.862351

C	-5.799275	4.413864	2.057238
C	-5.183340	3.650653	3.051891
C	-5.923506	2.676190	3.780771
C	-5.287803	1.493760	4.216077
C	-6.003435	0.285818	4.313429
C	-5.341013	-0.955449	4.133819
C	-6.035534	-2.058364	3.594572
C	-5.343454	-3.066637	2.897317
C	-5.985765	-3.830231	1.883967
C	-5.231349	-4.414322	0.849125
C	-5.755617	-4.728580	-0.418136
C	-4.899439	-4.659031	-1.572448
C	-5.454037	-4.169224	-2.751918
C	-4.664542	-3.374887	-3.610979
C	-5.303917	-2.359744	-4.364279
C	-4.622539	-1.190206	-4.700422
C	-5.320023	0.037957	-4.909944
C	-4.681920	1.266556	-4.683567
C	-5.405667	2.424155	-4.315761
C	-4.782478	3.444946	-3.544468
C	-5.522520	4.236866	-2.660628
C	-4.905834	4.780707	-1.496130
C	-5.657160	4.981351	-0.324875
C	-5.044582	4.868384	0.937634
C	-3.741203	3.615839	3.118808
C	-3.090877	2.595617	3.873976
C	-3.844419	1.452621	4.266414
C	-3.176499	0.213423	4.411338
C	-3.907881	-0.995512	4.203020
C	-3.209770	-2.152742	3.765049
C	-3.914459	-3.125773	3.017399
C	-3.172428	-3.991046	2.159308

C	-3.803377	-4.507658	1.010609
C	-2.998675	-4.978726	-0.062544
C	-3.464003	-4.740614	-1.429998
C	-2.618843	-4.211163	-2.452686
C	-3.242904	-3.361273	-3.435792
C	-2.506802	-2.293303	-4.041400
C	-3.193597	-1.167263	-4.546538
C	-2.504258	0.084504	-4.657468
C	-3.237579	1.287952	-4.577925
C	-2.577898	2.465796	-4.127142
C	-3.339766	3.468688	-3.462347
C	-2.697240	4.277339	-2.495884
C	-3.473997	4.797724	-1.414638
C	-2.837368	4.991654	-0.161184
C	-3.614628	4.861876	1.020462
C	-2.973906	4.367852	2.199903
C	-1.672088	2.559766	3.936369
C	-1.011186	1.375542	4.374269
C	-1.750751	0.174586	4.462225
C	-1.061720	-1.070437	4.300661
C	-1.772987	-2.194896	3.825657
C	-1.051189	-3.247371	3.187750
C	-1.760682	-4.096288	2.295441
C	-1.038668	-4.928288	1.404111
C	-1.703900	-5.360938	0.232361
C	-0.396201	-5.056832	-1.613313
C	-1.140356	-4.225642	-2.434202
C	-0.394703	-3.272039	-3.234454
C	-1.075509	-2.248229	-3.928491
C	-0.364179	-1.095458	-4.354349
C	-1.083894	0.114729	-4.575962
C	-0.406721	1.351292	-4.432966
C	-1.157567	2.498522	-4.058439
C	-0.501712	3.527980	-3.320205
C	-1.270481	4.303818	-2.419006
C	-0.627298	4.823712	-1.252917
C	-1.405040	4.994146	-0.077383
C	-0.766932	4.834461	1.183048
C	-1.546743	4.345133	2.275911
C	-0.904241	3.551004	3.256876
C	0.417237	1.336871	4.433840
C	1.086524	0.097311	4.573269
C	0.359175	-1.109123	4.349601
C	1.063116	-2.264510	3.919377
C	0.375717	-3.282186	3.223631
C	1.114504	-4.238551	2.420774
C	0.364286	-5.064522	1.599069

C	1.669616	-5.370710	-0.246609
C	1.007783	-4.931302	-1.418127
C	1.735216	-4.100834	-2.306169
C	1.031882	-3.246129	-3.197327
C	1.761092	-2.195194	-3.831654
C	1.057652	-1.065509	-4.303797
C	1.754331	0.175536	-4.462886
C	1.020744	1.381596	-4.371872
C	1.687627	2.560043	-3.928956
C	0.925367	3.554192	-3.249256
C	1.572354	4.343918	-2.265427
C	0.794867	4.832713	-1.171445
C	1.433342	4.987891	0.088594
C	0.653955	4.818343	1.264566
C	1.294869	4.290659	2.428435
C	0.523359	3.516904	3.327207
C	1.174255	2.482104	4.063743
C	2.507248	0.058363	4.653296
C	3.189615	-1.195893	4.540292
C	2.495003	-2.319036	4.031023
C	3.222869	-3.387496	3.426217
C	2.592350	-4.234109	2.438924
C	3.432211	-4.765341	1.417799
C	2.966851	-4.999708	0.049127
C	3.773785	-4.527949	-1.022254
C	3.147757	-4.004674	-2.167986
C	3.896974	-3.140184	-3.023429
C	3.197911	-2.161261	-3.768613
C	3.904002	-1.006444	-4.201233
C	3.179017	0.206387	-4.409952
C	3.854916	1.442404	-4.260468
C	3.107864	2.587838	-3.865080
C	3.763174	3.603864	-3.109996
C	2.998501	4.359477	-2.188688
C	3.640212	4.846892	-1.008722
C	2.864869	4.979134	0.172257
C	3.500666	4.778910	1.427214
C	2.722810	4.257222	2.504510
C	3.361235	3.442766	3.469488
C	2.593458	2.441363	4.131209
C	3.247509	1.258211	4.577192
C	4.616473	-1.226940	4.688779
C	5.290927	-2.402863	4.349340
C	4.644931	-3.412402	3.602508
C	4.871909	-4.699163	1.562810
C	5.204309	-4.446894	-0.861520
C	5.959886	-3.864336	-1.879483

C	5.322215	-3.086596	-2.899087
C	6.019871	-2.077343	-3.577219
C	5.334356	-0.973673	-4.122548
C	6.004820	0.269472	-4.291217
C	5.296616	1.473202	-4.203700
C	5.938581	2.660966	-3.759115
C	5.204631	3.632261	-3.044543
C	5.825323	4.409216	-2.045671
C	5.074491	4.853739	-0.927882
C	5.687416	4.974175	0.336507
C	4.933913	4.759252	1.510390
C	5.547583	4.211670	2.665852
C	4.802779	3.409934	3.550908
C	5.421626	2.386257	4.306315
C	4.690855	1.226589	4.676800
C	5.725855	-4.787819	0.412532
H	6.799999	-4.781269	0.566706
C	5.428791	-4.221302	2.745468
H	6.508683	-4.202199	2.854894
C	5.322554	-0.002897	4.890432
H	6.404668	-0.036833	4.973423
H	-7.116975	-2.006533	3.511217
H	-7.065481	-3.770931	1.787967
H	-6.829315	-4.702796	-0.574175
H	-6.534058	-4.136236	-2.857075
H	-7.087532	0.311123	4.257972
H	-6.385454	-2.389054	-4.455788
H	-7.007921	2.704827	3.737639
H	-6.401453	0.010963	-5.003183
H	-6.882954	4.418342	1.989502
H	-6.488820	2.412708	-4.389615
H	-6.740956	4.950960	-0.385047
H	-6.606974	4.214630	-2.710990
H	6.909276	4.415468	-1.983359
H	6.771326	4.951773	0.397493
H	7.023025	2.680501	-3.710867
H	6.631881	4.186018	2.718130
H	7.088414	0.288082	-4.224370
H	6.505075	2.365493	4.374056
H	7.100345	-2.026402	-3.481520
H	7.039841	-3.810481	-1.783001
H	6.372556	-2.437265	4.437849
O	-1.039214	-6.019202	-0.822541
O	1.001928	-6.029685	0.806522

Nanotube-2O (Quintet) ZPE= 1.189901 Ee= -5651.871980

C	-5.803670	4.403611	2.047264
C	-5.187724	3.647815	3.046138
C	-5.930065	2.667189	3.773497
C	-5.295425	1.489874	4.207353
C	-6.009647	0.278649	4.312179
C	-5.344903	-0.961964	4.126924
C	-6.036206	-2.063814	3.586915
C	-5.341032	-3.073656	2.891618
C	-5.981676	-3.838545	1.876987
C	-5.226247	-4.422863	0.845064
C	-5.749986	-4.749222	-0.420846
C	-4.892147	-4.669864	-1.576745
C	-5.446394	-4.177059	-2.752273
C	-4.656886	-3.379687	-3.611887
C	-5.298041	-2.365995	-4.362874
C	-4.617722	-1.193483	-4.699117
C	-5.316462	0.032189	-4.906670
C	-4.678549	1.262247	-4.684312
C	-5.404303	2.419877	-4.314785
C	-4.782907	3.440952	-3.548833
C	-5.524887	4.238643	-2.667254
C	-4.910203	4.778866	-1.500084
C	-5.661579	4.980642	-0.332332
C	-5.048837	4.865544	0.934639
C	-3.749112	3.615880	3.116045
C	-3.097708	2.592128	3.871106
C	-3.849146	1.450013	4.258769
C	-3.180056	0.211355	4.408754
C	-3.910765	-1.000357	4.197006
C	-3.211686	-2.153621	3.760660
C	-3.914922	-3.130601	3.013303
C	-3.169722	-3.992591	2.153711
C	-3.797258	-4.509967	1.006805
C	-2.990441	-4.986811	-0.065029
C	-3.456336	-4.747156	-1.432934
C	-2.611513	-4.213665	-2.452364
C	-3.236140	-3.364146	-3.436287
C	-2.500501	-2.295542	-4.040917
C	-3.189027	-1.169168	-4.546092
C	-2.501097	0.081960	-4.657059
C	-3.236410	1.285433	-4.579468
C	-2.577751	2.464458	-4.126614
C	-3.340005	3.465606	-3.465141
C	-2.697845	4.278439	-2.498056
C	-3.475421	4.795604	-1.416714
C	-2.840448	4.992824	-0.165218
C	-3.620499	4.861147	1.019158

C	-2.981227	4.365664	2.195531
C	-1.678606	2.557931	3.935136
C	-1.017756	1.376756	4.372040
C	-1.757420	0.173603	4.461452
C	-1.066058	-1.070879	4.297617
C	-1.774016	-2.194316	3.822114
C	-1.049552	-3.248562	3.186351
C	-1.756996	-4.098593	2.292442
C	-1.034326	-4.931692	1.404889
C	-1.698320	-5.369200	0.230199
C	-0.388259	-5.060065	-1.612058
C	-1.133208	-4.224811	-2.430569
C	-0.389160	-3.271777	-3.230901
C	-1.071040	-2.249107	-3.926832
C	-0.360556	-1.094393	-4.352240
C	-1.080690	0.113246	-4.575091
C	-0.403671	1.352168	-4.433996
C	-1.156072	2.498499	-4.057525
C	-0.501655	3.528193	-3.322051
C	-1.273156	4.305855	-2.419922
C	-0.631530	4.823433	-1.253319
C	-1.410130	4.996109	-0.079804
C	-0.772356	4.835264	1.183975
C	-1.551624	4.344172	2.273021
C	-0.909564	3.553290	3.257439
C	0.411187	1.339697	4.433541
C	1.082194	0.098390	4.575908
C	0.356184	-1.107572	4.348654
C	1.062003	-2.261753	3.921409
C	0.375033	-3.282407	3.223914
C	1.116612	-4.235585	2.421647
C	0.368197	-5.065741	1.601530
C	1.677503	-5.370840	-0.246245
C	1.014630	-4.930780	-1.417238
C	1.741857	-4.098703	-2.305827
C	1.038091	-3.244437	-3.194625
C	1.767532	-2.194331	-3.831687
C	1.061989	-1.062669	-4.301928
C	1.756761	0.175789	-4.461328
C	1.021139	1.383892	-4.372062
C	1.686310	2.561583	-3.925519
C	0.924122	3.555185	-3.250209
C	1.570910	4.348277	-2.263486
C	0.792808	4.833315	-1.170868
C	1.430426	4.992905	0.089078
C	0.648232	4.819975	1.266919
C	1.287788	4.293226	2.428062

C	0.514900	3.519861	3.329446
C	1.165988	2.482811	4.064225
C	2.500593	0.059569	4.658253
C	3.183663	-1.190512	4.542067
C	2.491064	-2.314831	4.034527
C	3.221144	-3.383685	3.425060
C	2.594529	-4.228432	2.443501
C	3.439085	-4.758737	1.416110
C	2.973711	-4.991788	0.052025
C	3.783898	-4.527734	-1.022052
C	3.155441	-4.002070	-2.170094
C	3.901206	-3.139465	-3.022964
C	3.201135	-2.159931	-3.770315
C	3.905334	-1.001249	-4.199820
C	3.181624	0.206792	-4.408157
C	3.857802	1.447890	-4.260495
C	3.109439	2.590113	-3.860555
C	3.763296	3.606652	-3.109507
C	2.995230	4.364275	-2.184935
C	3.635142	4.846688	-1.005915
C	2.858272	4.984399	0.174095
C	3.493863	4.780125	1.432160
C	2.716667	4.261089	2.505359
C	3.355708	3.447665	3.476188
C	2.587536	2.443329	4.133730
C	3.241757	1.264803	4.582852
C	4.614333	-1.221240	4.699669
C	5.288443	-2.405787	4.372913
C	4.646877	-3.410011	3.607935
C	4.875968	-4.685397	1.561267
C	5.207879	-4.437891	-0.857106
C	5.966676	-3.849622	-1.884940
C	5.330765	-3.085668	-2.898825
C	6.029509	-2.078282	-3.594061
C	5.341228	-0.967999	-4.127383
C	6.008252	0.268594	-4.299391
C	5.296088	1.480707	-4.203739
C	5.936591	2.656900	-3.749200
C	5.201699	3.634264	-3.041053
C	5.822579	4.409885	-2.039305
C	5.071960	4.853589	-0.923560
C	5.683271	4.978499	0.340795
C	4.928034	4.759290	1.515883
C	5.540054	4.208998	2.666761
C	4.792597	3.412507	3.555742
C	5.412096	2.380359	4.305776
C	4.682279	1.234476	4.683232

C	5.729120	-4.745476	0.417935
H	6.802633	-4.713423	0.574806
C	5.430378	-4.213201	2.758099
H	6.510100	-4.195734	2.869480
C	5.315575	-0.005964	4.906845
H	6.397001	-0.037024	4.999200
H	-7.117627	-2.014514	3.501822
H	-7.061592	-3.782155	1.781454
H	-6.823784	-4.734180	-0.577173
H	-6.526367	-4.143586	-2.858302
H	-7.093977	0.302253	4.261611
H	-6.379498	-2.396912	-4.454757
H	-7.014349	2.696654	3.727115
H	-6.398018	0.003856	-4.998258
H	-6.887127	4.401208	1.975145
H	-6.487540	2.405702	-4.387526
H	-6.745415	4.951167	-0.392148
H	-6.609203	4.218869	-2.720769
H	6.906480	4.414092	-1.975615
H	6.767094	4.958430	0.403530
H	7.020814	2.673676	-3.693275
H	6.624310	4.177770	2.717330
H	7.092107	0.289816	-4.237456
H	6.495995	2.357473	4.366912
H	7.111094	-2.032940	-3.509230
H	7.045919	-3.790528	-1.783292
H	6.368621	-2.446005	4.475243
O	-1.029438	-6.023894	-0.824238
O	1.010580	-6.030497	0.808053

SW Defected Nanotube-2O (Singlet) ZPE= 1.189013 Ee= -5651.718293

C	-5.123384	-5.551006	-0.405855
C	-5.453339	-4.863887	1.926879
C	-5.830532	-3.049535	3.550755
C	-6.169585	-0.660352	4.037934
C	-6.439022	1.652257	3.304404
C	-5.271885	1.638906	-4.533426
C	-4.928220	-4.892967	-2.756422
C	-4.332606	-5.316138	-1.549539
C	-4.607040	-5.285841	0.879859
C	-4.975563	-3.973100	2.908809
C	-5.339275	-1.805075	3.981158
C	-5.639786	0.625518	3.875294
C	-5.846681	2.750923	2.674770
C	-5.721314	4.181055	0.639929
C	-5.201101	4.146174	-1.854600

C	-4.765335	2.699561	-3.759458
C	-4.470013	0.536359	-4.841010
C	-4.282862	-1.901273	-4.817895
C	-4.223666	-4.049949	-3.641671
C	-2.903162	-5.178867	-1.393914
C	-3.179178	-5.124529	1.027192
C	-3.549615	-3.790246	3.032891
C	-3.913319	-1.612955	4.075674
C	-4.202281	0.814979	3.992433
C	-4.430338	2.972848	2.933185
C	-4.394090	4.546455	1.055086
C	-3.798625	4.507794	-1.851832
C	-3.345315	2.850803	-3.553392
C	-3.051241	0.664240	-4.628728
C	-2.854106	-1.774888	-4.641957
C	-2.792503	-3.926253	-3.484914
C	-2.125861	-4.633743	-2.451613
C	-2.322900	-5.253021	-0.102784
C	-2.657185	-4.518730	2.197168
C	-3.037895	-2.681409	3.756685
C	-3.370514	-0.302249	4.217850
C	-3.605088	2.054504	3.625005
C	-3.788797	3.958887	2.225729
C	-3.408651	5.155558	0.347363
C	-2.831850	3.889917	-2.665203
C	-2.490017	1.873217	-4.129512
C	-2.238285	-0.501825	-4.705360
C	-2.103789	-2.868916	-4.131770
C	-0.710305	-4.505070	-2.299742
C	-0.907708	-5.106300	0.055423
C	-1.244046	-4.356558	2.350675
C	-1.626583	-2.504950	3.892717
C	-1.955716	-0.113319	4.311053
C	-2.173419	2.249649	3.649876
C	-2.395331	4.177085	2.233937
C	-0.983610	5.222154	0.446731
C	-1.336207	4.057323	-2.639279
C	-1.056613	1.998277	-4.034803
C	-0.822780	-0.384590	-4.579967
C	-0.689776	-2.750468	-3.993492
C	0.024049	-3.682546	-3.195726
C	-0.084957	-4.903063	-1.084659
C	-0.361284	-4.815735	1.337952
C	-0.736666	-3.453236	3.325371
C	-1.106137	-1.252339	4.312354
C	-1.377622	1.174977	4.134226
C	-1.523101	3.361534	2.974975

C	-2.155684	4.998761	1.055975
C	-0.609464	4.877318	-1.788585
C	-0.487159	3.135478	-3.408622
C	-0.228898	0.899585	-4.401253
C	-0.038867	-1.545144	-4.379498
C	1.439877	-3.560071	-3.055194
C	1.328653	-4.756130	-0.929253
C	1.050452	-4.649937	1.492872
C	0.670593	-3.282676	3.475926
C	0.295605	-1.081998	4.458766
C	0.033845	1.345659	4.251214
C	-0.045283	3.482262	2.977816
C	0.347925	4.905836	0.842705
C	0.776832	4.793296	-1.575503
C	0.950871	3.225745	-3.378438
C	1.195484	0.999145	-4.347602
C	1.380685	-1.441079	-4.273750
C	2.131529	-2.527587	-3.743424
C	2.109119	-4.237468	-2.001091
C	1.909864	-4.791664	0.366315
C	1.568314	-4.017839	2.653741
C	1.172562	-2.163614	4.188807
C	0.838237	0.227352	4.579944
C	0.666367	2.558294	3.806407
C	0.772168	4.315493	2.090521
C	1.265047	5.021578	-0.234912
C	1.588918	4.120518	-2.474629
C	1.788487	2.215271	-3.941263
C	2.003713	-0.178319	-4.413410
C	3.548958	-2.420838	-3.623289
C	3.524146	-4.100024	-1.853269
C	3.323190	-4.623625	0.519901
C	2.980503	-3.838491	2.803466
C	2.582801	-1.997275	4.354176
C	2.242547	0.379410	4.794806
C	2.076344	2.701502	4.058525
C	2.206054	4.387368	2.319178
C	2.649023	4.964028	-0.010998
C	3.005105	4.149003	-2.275431
C	3.228337	2.305943	-3.838082
C	3.428216	-0.082932	-4.327552
C	4.203851	-1.241791	-4.074377
C	4.256446	-3.321285	-2.786626
C	4.142778	-4.451902	-0.623893
C	3.863999	-4.297917	1.795836
C	3.482144	-2.932892	3.781747
C	3.093928	-0.761135	4.825979

C	2.817478	1.661653	4.701922
C	2.800388	3.732681	3.431682
C	3.108182	4.861877	1.314522
C	3.537950	4.718348	-1.097298
C	3.839617	3.355420	-3.092605
C	4.042091	1.195243	-4.175257
C	5.642754	-1.138579	-3.980744
C	5.687864	-3.195247	-2.649707
C	5.569611	-4.294051	-0.463250
C	5.290286	-4.125967	1.964282
C	4.906519	-2.768963	3.967128
C	4.510553	-0.611574	5.057427
C	4.224804	1.817854	4.986121
C	4.215099	3.890864	3.704816
C	4.535192	4.944377	1.533852
C	4.960851	4.753666	-0.884869
C	5.273293	3.438971	-2.932963
C	5.485149	1.299855	-4.084015
C	6.323896	-3.824746	-1.561218
C	6.119306	-4.303992	0.833506
C	5.773298	-3.517689	3.138811
C	5.362871	-1.696136	4.759700
C	4.998882	0.687623	5.312581
C	4.840010	3.033431	4.626212
C	5.015671	4.638975	2.818846
C	5.407946	5.046411	0.427572
C	5.796103	4.262925	-1.905935
C	6.063362	2.495446	-3.616009
H	-6.347427	1.558629	-4.652353
H	-6.525905	-4.980118	1.807592
H	-6.198078	-5.648360	-0.525749
H	-6.004762	-4.983231	-2.866513
H	-6.903346	-3.177079	3.447806
H	-7.241147	-0.796463	3.930669
H	-7.495270	1.452153	3.152367
H	6.844138	-3.380912	3.250748
H	7.190563	-4.168003	0.947105
H	7.397514	-3.708283	-1.445075
H	7.141941	2.540051	-3.507223
H	6.431814	-1.567383	4.894635
H	6.870906	4.280402	-1.758552
H	6.061661	0.820923	5.487482
H	6.475952	5.086106	0.617587
H	5.900746	3.160260	4.819595
H	6.079295	4.721602	3.020847
C	-6.471172	3.436334	1.594155
H	-7.497082	3.168680	1.356363

C	-6.089427	4.237566	-0.713950
H	-7.116499	3.957710	-0.938276
C	-5.663395	3.409120	-2.936691
H	-6.719773	3.172111	-3.006188
C	-5.026877	-0.742209	-5.081591
H	-6.101531	-0.821972	-5.210745
C	-4.902325	-3.118353	-4.451018
H	-5.978036	-3.210271	-4.566064
C	6.249182	0.116235	-4.171098
H	7.328261	0.191509	-4.081498
C	6.358262	-2.206339	-3.399375
H	7.435699	-2.115563	-3.298512
O	-1.141801	5.756664	-0.840098
O	-3.545260	5.590069	-0.974191

SW Defected Nanotube-2O (Triplet) ZPE= 1.189013 Ee= -5651.801772

C	-5.078673	-5.595263	-0.431208
C	-5.420513	-4.907614	1.897697
C	-5.810287	-3.089589	3.502181
C	-6.158559	-0.706725	3.984222
C	-6.446198	1.616354	3.285319
C	-5.273065	1.587633	-4.485936
C	-4.881397	-4.933218	-2.785109
C	-4.281882	-5.354029	-1.575877
C	-4.563122	-5.325563	0.854351
C	-4.945032	-4.008084	2.885825
C	-5.319150	-1.837641	3.960778
C	-5.632086	0.587048	3.866424
C	-5.862978	2.715063	2.681318
C	-5.756801	4.164210	0.646742
C	-5.215228	4.136585	-1.848949
C	-4.763320	2.670410	-3.729653
C	-4.457139	0.514262	-4.827045
C	-4.252046	-1.928051	-4.829199
C	-4.177354	-4.084563	-3.664841
C	-2.862236	-5.206008	-1.414846
C	-3.140518	-5.158386	1.011404
C	-3.522001	-3.825712	3.028143
C	-3.905836	-1.647306	4.084429
C	-4.214331	0.780569	4.005422
C	-4.451273	2.936965	2.939105
C	-4.421569	4.516465	1.056686
C	-3.827879	4.511352	-1.857141
C	-3.354850	2.852708	-3.555296
C	-3.039528	0.659851	-4.634721
C	-2.826414	-1.787619	-4.657163

C	-2.755630	-3.946663	-3.504915
C	-2.086205	-4.646102	-2.466658
C	-2.283639	-5.274333	-0.113249
C	-2.625917	-4.549174	2.192413
C	-3.021998	-2.717894	3.757678
C	-3.374425	-0.336604	4.223526
C	-3.622443	2.028271	3.628254
C	-3.811649	3.933664	2.228548
C	-3.443351	5.137908	0.351406
C	-2.852520	3.891686	-2.672413
C	-2.490520	1.869219	-4.138345
C	-2.218892	-0.503748	-4.721786
C	-2.071304	-2.873668	-4.148947
C	-0.671445	-4.506643	-2.311077
C	-0.871840	-5.117812	0.046431
C	-1.221367	-4.379010	2.347005
C	-1.619009	-2.532514	3.895515
C	-1.960203	-0.137640	4.316967
C	-2.191968	2.232518	3.655583
C	-2.428755	4.163171	2.243038
C	-1.020539	5.217139	0.455279
C	-1.358531	4.063622	-2.642948
C	-1.065502	2.003998	-4.045146
C	-0.813208	-0.378121	-4.594989
C	-0.660919	-2.746133	-4.006750
C	0.059909	-3.680409	-3.205166
C	-0.045521	-4.906241	-1.096473
C	-0.330515	-4.828021	1.327484
C	-0.722211	-3.470057	3.321405
C	-1.106550	-1.268661	4.317316
C	-1.389253	1.160215	4.144381
C	-1.547550	3.347855	2.985190
C	-2.189935	4.986578	1.062515
C	-0.635908	4.886540	-1.781827
C	-0.504572	3.150734	-3.409415
C	-0.229593	0.910537	-4.406517
C	-0.018746	-1.539859	-4.387325
C	1.468396	-3.547072	-3.060843
C	1.361227	-4.750245	-0.938007
C	1.077197	-4.654547	1.485935
C	0.683970	-3.292200	3.475800
C	0.291581	-1.090662	4.465585
C	0.014207	1.338768	4.260619
C	-0.074647	3.477276	2.989264
C	0.319422	4.911276	0.856807
C	0.744054	4.810677	-1.565231
C	0.929600	3.247852	-3.374691

C	1.195051	1.019864	-4.350575
C	1.397305	-1.424977	-4.277064
C	2.154856	-2.503358	-3.747636
C	2.140749	-4.220091	-2.004668
C	1.940139	-4.786580	0.364767
C	1.588488	-4.024221	2.658405
C	1.177497	-2.175011	4.199122
C	0.826709	0.217626	4.588556
C	0.641833	2.553332	3.811150
C	0.742463	4.320490	2.098579
C	1.233573	5.044125	-0.223508
C	1.560436	4.140428	-2.468225
C	1.778243	2.240739	-3.946277
C	2.012494	-0.152272	-4.421359
C	3.568927	-2.384764	-3.624685
C	3.553159	-4.070349	-1.851742
C	3.349032	-4.609142	0.524013
C	2.992883	-3.839540	2.815204
C	2.578762	-2.004040	4.371050
C	2.227061	0.374421	4.806968
C	2.052874	2.699953	4.063712
C	2.175157	4.394413	2.325026
C	2.614744	4.993357	-0.004123
C	2.975796	4.184074	-2.275198
C	3.211022	2.344016	-3.845505
C	3.429605	-0.045301	-4.335481
C	4.216190	-1.205705	-4.077093
C	4.285069	-3.285551	-2.782988
C	4.174017	-4.425544	-0.622131
C	3.884096	-4.292296	1.801890
C	3.482456	-2.936475	3.799591
C	3.078356	-0.758766	4.846154
C	2.795419	1.668029	4.713744
C	2.775631	3.737488	3.438040
C	3.075873	4.879032	1.323222
C	3.503458	4.763278	-1.095715
C	3.811369	3.405097	-3.100643
C	4.031042	1.237457	-4.185240
C	5.648621	-1.099155	-3.974424
C	5.709658	-3.156349	-2.645473
C	5.593449	-4.261937	-0.463648
C	5.302622	-4.107217	1.963745
C	4.901415	-2.755587	3.971734
C	4.489781	-0.595445	5.064362
C	4.194857	1.834749	4.992450
C	4.183550	3.906743	3.713861
C	4.498714	4.970388	1.549080

C	4.916676	4.794064	-0.872372
C	5.235194	3.481308	-2.922027
C	5.467687	1.341000	-4.076019
C	6.351718	-3.789529	-1.559182
C	6.141616	-4.269847	0.840488
C	5.782370	-3.482743	3.140496
C	5.358583	-1.669466	4.751729
C	4.983081	0.702628	5.304728
C	4.814111	3.049312	4.633352
C	4.984668	4.669561	2.833936
C	5.374077	5.077612	0.441745
C	5.761483	4.286077	-1.882027
C	6.043142	2.527567	-3.580876
H	-6.349594	1.494851	-4.590583
H	-6.492150	-5.035683	1.779457
H	-6.152185	-5.702395	-0.553897
H	-5.957091	-5.030066	-2.897298
H	-6.882663	-3.217772	3.389832
H	-7.227214	-0.848729	3.852675
H	-7.498826	1.402749	3.124987
H	6.852492	-3.340406	3.257686
H	7.211368	-4.125965	0.958974
H	7.424116	-3.667196	-1.440577
H	7.121610	2.579273	-3.466720
H	6.427116	-1.535505	4.891037
H	6.836867	4.305007	-1.732641
H	6.046071	0.840293	5.477975
H	6.442682	5.122682	0.628357
H	5.874349	3.177898	4.828052
H	6.046930	4.759587	3.038301
C	-6.509125	3.433883	1.601581
H	-7.536948	3.168045	1.371863
C	-6.129993	4.267668	-0.706838
H	-7.164673	4.031265	-0.944691
C	-5.670392	3.359640	-2.899197
H	-6.724618	3.110148	-2.965110
C	-5.010505	-0.771781	-5.081640
H	-6.084184	-0.857938	-5.217180
C	-4.866191	-3.150166	-4.476687
H	-5.940429	-3.251668	-4.597606
C	6.249630	0.165220	-4.153458
H	7.328420	0.250407	-4.064995
C	6.377362	-2.161193	-3.398044
H	7.454253	-2.063652	-3.299193
O	-1.175811	5.759548	-0.829809
O	-3.577055	5.579930	-0.965029

SW Defected Nanotube-2O (Quintet) ZPE= 1.189557 Ee= -5651.796547

C	-5.084203	-5.568987	-0.434818
C	-5.430568	-4.905994	1.901704
C	-5.819802	-3.091138	3.508124
C	-6.167154	-0.708625	3.989909
C	-6.452248	1.613262	3.291232
C	-5.264154	1.594927	-4.500625
C	-4.881266	-4.906588	-2.790172
C	-4.281711	-5.339969	-1.585370
C	-4.569377	-5.318426	0.839287
C	-4.955167	-4.008503	2.877276
C	-5.327512	-1.838397	3.961002
C	-5.639750	0.589310	3.865199
C	-5.866399	2.717534	2.676222
C	-5.752516	4.160550	0.641372
C	-5.209225	4.132099	-1.850268
C	-4.755955	2.674931	-3.736801
C	-4.448625	0.522636	-4.842178
C	-4.246822	-1.922681	-4.842602
C	-4.174464	-4.076456	-3.671451
C	-2.867459	-5.201409	-1.424538
C	-3.146020	-5.154617	0.999831
C	-3.527618	-3.822564	3.018434
C	-3.912884	-1.646866	4.080481
C	-4.219248	0.780417	4.002758
C	-4.454098	2.937560	2.937304
C	-4.420493	4.515965	1.055009
C	-3.823358	4.510412	-1.857112
C	-3.348014	2.855844	-3.559254
C	-3.030785	0.666286	-4.643113
C	-2.818162	-1.781582	-4.664093
C	-2.753421	-3.941564	-3.511574
C	-2.087764	-4.638059	-2.474868
C	-2.289843	-5.268160	-0.120071
C	-2.631534	-4.549182	2.186604
C	-3.029232	-2.719610	3.749588
C	-3.381646	-0.338789	4.218177
C	-3.626677	2.027501	3.627040
C	-3.812840	3.934605	2.228725
C	-3.439618	5.135804	0.350338
C	-2.847217	3.891213	-2.672959
C	-2.483102	1.872166	-4.142922
C	-2.210664	-0.499674	-4.729470
C	-2.065211	-2.867803	-4.158611
C	-0.670434	-4.500496	-2.316375
C	-0.875306	-5.113119	0.041379

C	-1.229349	-4.380647	2.342215
C	-1.625732	-2.535511	3.889393
C	-1.965033	-0.140565	4.312995
C	-2.195971	2.230872	3.655408
C	-2.429713	4.163319	2.245001
C	-1.018869	5.213317	0.457764
C	-1.352779	4.062644	-2.640187
C	-1.056800	2.006401	-4.045828
C	-0.805166	-0.374987	-4.598861
C	-0.656473	-2.742184	-4.013203
C	0.062157	-3.677305	-3.207939
C	-0.046527	-4.904329	-1.101721
C	-0.336493	-4.827311	1.320148
C	-0.730536	-3.470573	3.315387
C	-1.112822	-1.271234	4.315564
C	-1.394099	1.156225	4.144086
C	-1.550820	3.344207	2.986626
C	-2.188302	4.983640	1.064418
C	-0.632571	4.884607	-1.779565
C	-0.497242	3.151025	-3.408163
C	-0.220914	0.914195	-4.408208
C	-0.012659	-1.535821	-4.389796
C	1.471657	-3.544752	-3.060950
C	1.358602	-4.750262	-0.941108
C	1.072567	-4.655113	1.481262
C	0.678472	-3.293624	3.472018
C	0.284509	-1.094414	4.465533
C	0.008957	1.333843	4.262080
C	-0.076821	3.472438	2.991334
C	0.318214	4.906817	0.859755
C	0.747994	4.809566	-1.561243
C	0.936840	3.248914	-3.371655
C	1.203180	1.022819	-4.349054
C	1.404960	-1.421566	-4.276071
C	2.160739	-2.501155	-3.747777
C	2.140568	-4.217715	-2.005836
C	1.935367	-4.786077	0.363422
C	1.583127	-4.027675	2.657362
C	1.170939	-2.180322	4.197322
C	0.820138	0.212382	4.587840
C	0.637791	2.549326	3.813593
C	0.740705	4.316651	2.102599
C	1.234192	5.039695	-0.218962
C	1.566048	4.141862	-2.463726
C	1.785796	2.242427	-3.941872
C	2.020521	-0.150361	-4.418695
C	3.573811	-2.383608	-3.622164

C	3.554543	-4.069613	-1.850460
C	3.346223	-4.610172	0.525023
C	2.986250	-3.844429	2.816163
C	2.572358	-2.009962	4.370964
C	2.222445	0.368652	4.807756
C	2.048877	2.695171	4.067399
C	2.172682	4.391013	2.331047
C	2.615845	4.990576	0.002854
C	2.981037	4.185413	-2.268572
C	3.219458	2.345369	-3.838336
C	3.437792	-0.043843	-4.329600
C	4.222608	-1.203883	-4.070551
C	4.287927	-3.285909	-2.778826
C	4.173426	-4.428578	-0.620587
C	3.879148	-4.296281	1.801799
C	3.475082	-2.940582	3.799691
C	3.072076	-0.763962	4.848622
C	2.790532	1.661938	4.717961
C	2.772075	3.732052	3.443336
C	3.074735	4.876387	1.330425
C	3.506260	4.763002	-1.087601
C	3.818106	3.406141	-3.092701
C	4.039523	1.239370	-4.177596
C	5.655988	-1.098138	-3.965220
C	5.712892	-3.157576	-2.638866
C	5.591548	-4.266112	-0.459756
C	5.298318	-4.112819	1.966407
C	4.895929	-2.761115	3.974657
C	4.483029	-0.601569	5.068101
C	4.189527	1.827908	4.997483
C	4.180551	3.901296	3.721410
C	4.497329	4.968382	1.558733
C	4.919392	4.794318	-0.862022
C	5.241683	3.482102	-2.911453
C	5.475790	1.342205	-4.065454
C	6.352129	-3.790787	-1.553051
C	6.137846	-4.273713	0.845716
C	5.777004	-3.490975	3.146566
C	5.352174	-1.677180	4.755774
C	4.977215	0.695393	5.307011
C	4.809723	3.043381	4.639727
C	4.981823	4.667393	2.844142
C	5.374268	5.076601	0.452920
C	5.766062	4.287100	-1.870402
C	6.050533	2.528061	-3.568361
H	-6.340385	1.504122	-4.610142
H	-6.501482	-5.041230	1.785908

H	-6.158599	-5.662459	-0.561060
H	-5.958611	-4.991285	-2.896591
H	-6.892648	-3.223119	3.405107
H	-7.236898	-0.849823	3.866184
H	-7.506806	1.404710	3.136961
H	6.847180	-3.351551	3.266511
H	7.207454	-4.129650	0.965458
H	7.424240	-3.668464	-1.431721
H	7.128751	2.579308	-3.451701
H	6.420516	-1.543690	4.896937
H	6.841176	4.306524	-1.719165
H	6.040430	0.832284	5.479642
H	6.442559	5.121674	0.641413
H	5.869759	3.171501	4.835863
H	6.043767	4.758166	3.049756
C	-6.508959	3.427043	1.606300
H	-7.538980	3.168020	1.378524
C	-6.121839	4.245033	-0.705687
H	-7.152500	3.990786	-0.943312
C	-5.662992	3.358728	-2.904759
H	-6.716981	3.108353	-2.971832
C	-5.001604	-0.761184	-5.107968
H	-6.073819	-0.846005	-5.254882
C	-4.861373	-3.136774	-4.496402
H	-5.934809	-3.240227	-4.622260
C	6.257561	0.165727	-4.142259
H	7.336215	0.250561	-4.051952
C	6.382913	-2.161761	-3.390640
H	7.459832	-2.065885	-3.290644
O	-1.173774	5.753865	-0.826785
O	-3.574444	5.581295	-0.965453