

Electronic Supplementary Material (ESI) for Chemical Science.
This journal is © The Royal Society of Chemistry 2015

Electronic Supplementary Information

Repurposing of oxazolone chemistry gaining access to functionalized graphene nanosheets in a top-down approach from graphite

Giulia Neri,^a Angela Scala,^a Enza Fazio,^b Placido G. Mineo,^c Antonio Rescifina,^d
Anna Piperno*^a and Giovanni Grassi^a

^aDipartimento di Scienze Chimiche, Università di Messina, Viale Ferdinando Stagno D'Alcontres 31, 98166 Messina, Italy. Fax: +39090393897; Tel: +390906765173; E-mail: apiperno@unime.it

^bDipartimento di Fisica e di Scienze della Terra, Università di Messina, V.le F. Stagno d'Alcontres 31, 98166, Messina, Italy

^cDipartimento di Scienze Chimiche, Università di Catania, V.le A. Doria 6, 95125, Catania, Italy.

^dDipartimento di Scienze del Farmaco, Università di Catania, V.le A. Doria 6, 95125, Catania, Italy.

Table of Contents

1. FT-IR Analysis	S2
2. STEM Analysis	S3
3. Dispersibility	S4
4. Raman Analysis.....	S4
5. DFT-Computed Energies	S4
6. Cartesian Coordinates and Energies of DFT-Computed Stationary Points	S5

1. Fourier transform infrared spectroscopy (FT-IR) Analysis

FT-IR spectra of functionalized graphene materials (Fig S1) suggest the presence of functional groups covalently bonded on the graphene surface. However, the interpretation of the IR spectra of functionalized graphene materials and the assignment of the bands are difficult. In particular, the bands at 1520 cm^{-1} and 1350 cm^{-1} assigned as the asymmetric and symmetric stretching vibration of NO_2 are not clearly discriminable.

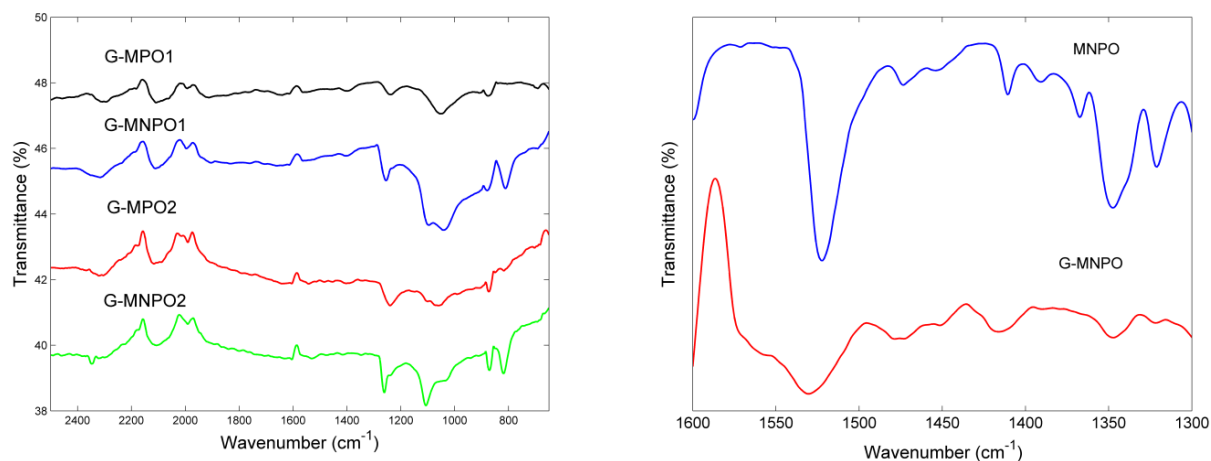


Figure S1. FT-IR spectra of functionalized graphene materials (left), and the comparison between the FT-IR spectra of MNPO and G-MNPO from 1300 cm^{-1} to 1600 cm^{-1} (right).

2. STEM Analysis

The thicknesses of 2-3 nm were estimated by STEM images of G-MNP01 and GMP02 samples.



Figure S2. STEM images of G-MNP01 (up) and G-MNP02 (down) samples.

3. Dispersibility

As expected an improved dispersibility in organic solvent of all functionalized graphene samples was found. Preliminary tests showed a good dispersibility in polar aprotic solvents such as THF and DMF. Dispersions with a concentration of 0.5 mg/mL are stable for some weeks under normal laboratory conditions. The dispersion in protic solvent such ethanol appears stable only for some days.

4. Raman Analysis

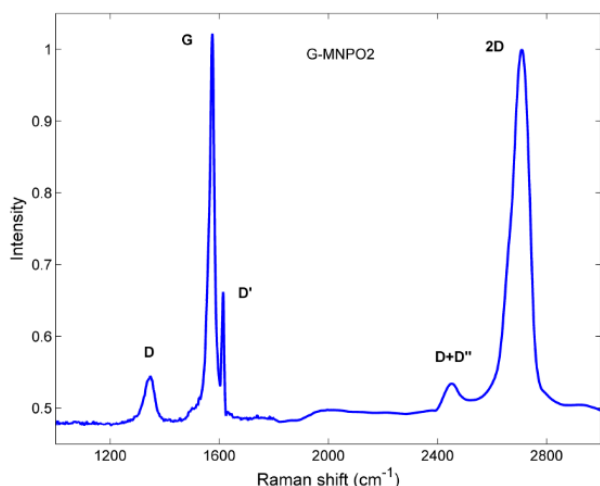


Figure S3. Raman spectrum of the G-MNPO2 sample.

5. DFT-Computed Energies

Table S1. Thermal Correction to Enthalpy (TCH), Thermal Correction to Free Energy (TCG), Electronic Energy (E), Enthalpy (H), and Free Energy (G). All values are in Hartree.

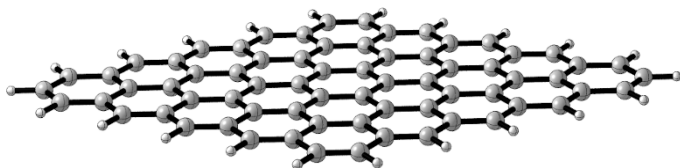
	TCH ^a	TCG ^a	E ^b	H	G
Reagents					
MPO	0.186223	0.137723	-591.606382	-591.420159	-591.468659
MPO-Mu	0.185571	0.135817	-591.573644	-591.388073	-591.437827
GF	0.720018	0.615958	-2680.622292	-2679.902274	-2680.006334
CO2	0.015525	-0.008735	-188.569864	-188.554339	-188.578599
Transition Structures					
TS-a1	0.906964	0.778234	-3272.197366	-3271.290402	-3271.419132
TS-a2	0.909384	0.781442	-3272.211956	-3271.302572	-3271.430514
TS-b	0.907722	0.784000	-3272.168188	-3271.260466	-3271.384188
TS-c1	0.906058	0.777017	-3272.200722	-3271.294664	-3271.423705
TS-c2	0.907723	0.780625	-3272.194318	-3271.286595	-3271.413693
TS-c3	0.908764	0.779991	-3272.181547	-3271.272783	-3271.401556
MPO_TS	0.180367	0.131449	-591.507789	-591.327422	-591.376340
Products					
I-a1	0.911391	0.785035	-3272.248606	-3271.337215	-3271.463571
I-c1	0.907248	0.778281	-3272.213788	-3271.306540	-3271.435507
I-c2	0.910497	0.783162	-3272.220998	-3271.310501	-3271.437836
I-b	0.910105	0.786569	-3272.178085	-3271.267980	-3271.391516
G-MPO-a	0.892927	0.770412	-3083.688615	-3082.795688	-3082.918203
G-MPO-c	0.892917	0.769151	-3083.662904	-3082.769987	-3082.893753

^aComputed at the (U)M06-2X/6-31G(d) level.

^bComputed at the (U)M06-2X/6-311G(d,p)//(U)M06-2X/6-31G(d) level.

6. Cartesian Coordinates and Energies of DFT-Computed Stationary Points

GF



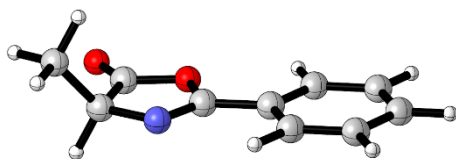
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-7.071072	0.000003	0.000334
2	6	0	-7.784433	-1.238067	0.000347
3	6	0	-4.945309	-1.231517	0.000526
4	6	0	-5.669615	-2.476092	-0.000227
5	6	0	-2.820485	-2.466362	0.000856
6	6	0	-7.784420	1.238080	0.000342
7	6	0	-4.945313	1.231515	0.000529
8	6	0	-5.669601	2.476090	-0.000222
9	6	0	-2.820492	2.466358	0.000869
10	6	0	-5.655660	0.000003	-0.000112
11	6	0	-2.825244	-0.000002	0.002269
12	6	0	-3.537608	-1.234221	-0.001299
13	6	0	-0.703697	-1.233120	0.003128
14	6	0	-3.537595	1.234221	-0.001290
15	6	0	-0.703704	1.233116	0.003135
16	6	0	-1.415458	-0.000002	-0.003121
17	6	0	1.415463	-0.000001	0.003105
18	6	0	-3.551229	-3.713178	-0.000690
19	6	0	-0.694244	-3.704140	0.000669
20	6	0	-1.433991	-4.952515	-0.000481
21	6	0	1.433997	-4.952511	0.000325
22	6	0	-1.420725	-2.468115	-0.001973
23	6	0	1.420725	-2.468117	0.001901
24	6	0	0.694246	-3.704137	-0.000793
25	6	0	3.551237	-3.713171	0.000610
26	6	0	0.703703	-1.233119	-0.003171
27	6	0	3.537598	-1.234222	0.001316
28	6	0	2.820491	-2.466359	-0.000908
29	6	0	5.669601	-2.476076	0.000305
30	6	0	-3.551223	3.713170	-0.000667
31	6	0	-0.694250	3.704132	0.000697
32	6	0	-1.433991	4.952508	-0.000440
33	6	0	1.433988	4.952507	0.000383
34	6	0	-1.420715	2.468114	-0.001944
35	6	0	1.420716	2.468112	0.001918
36	6	0	0.703705	1.233118	-0.003162
37	6	0	3.537602	1.234218	0.001294
38	6	0	0.694252	3.704133	-0.000745
39	6	0	3.551220	3.713170	0.000617
40	6	0	2.820494	2.466356	-0.000910
41	6	0	5.669594	2.476091	0.000200
42	6	0	2.825244	-0.000002	-0.002282
43	6	0	5.655668	0.000006	0.000202
44	6	0	4.945310	-1.231512	-0.000466
45	6	0	7.784416	-1.238076	-0.000075
46	6	0	4.945311	1.231521	-0.000511
47	6	0	7.784434	1.238085	-0.000334

48	6	0	7.071060	-0.000016	-0.000213
49	6	0	-0.673344	-6.189487	-0.000426
50	1	0	-1.227919	-7.124070	-0.000492
51	6	0	-2.798797	-4.937992	-0.000945
52	1	0	-3.347915	-5.877156	-0.001041
53	6	0	-4.927194	-3.695561	-0.000695
54	1	0	-5.475676	-4.634903	-0.000797
55	6	0	-7.056344	-2.452830	-0.000036
56	1	0	-7.605822	-3.391542	-0.000076
57	6	0	-9.192697	-1.208631	0.000523
58	1	0	-9.738412	-2.148065	0.000553
59	6	0	-9.878496	0.000015	0.000670
60	1	0	-10.964135	0.000003	0.000794
61	6	0	-9.192706	1.208640	0.000516
62	1	0	-9.738398	2.148088	0.000535
63	6	0	-7.056346	2.452826	-0.000037
64	1	0	-7.605808	3.391548	-0.000085
65	6	0	-4.927198	3.695552	-0.000682
66	1	0	-5.475670	4.634899	-0.000787
67	6	0	-2.798801	4.937981	-0.000915
68	1	0	-3.347915	5.877146	-0.001010
69	6	0	-0.673352	6.189480	-0.000378
70	1	0	-1.227928	7.124062	-0.000436
71	6	0	0.673354	-6.189486	0.000244
72	1	0	1.227931	-7.124068	0.000282
73	6	0	2.798801	-4.937983	0.000798
74	1	0	3.347923	-5.877146	0.000874
75	6	0	4.927207	-3.695546	0.000655
76	1	0	5.475691	-4.634884	0.000710
77	6	0	7.056350	-2.452808	0.000239
78	1	0	7.605770	-3.391554	0.000323
79	1	0	3.347919	5.877143	0.000931
80	1	0	1.227927	7.124060	0.000342
81	6	0	2.798800	4.937980	0.000856
82	6	0	0.673349	6.189479	0.000297
83	6	0	9.192689	1.208645	-0.000530
84	1	0	9.738395	2.148091	-0.000856
85	6	0	7.056345	2.452817	-0.000027
86	1	0	7.605808	3.391540	-0.000027
87	6	0	4.927201	3.695551	0.000632
88	1	0	5.475674	4.634895	0.000726
89	6	0	9.878487	0.000008	-0.000457
90	6	0	9.192700	-1.208614	-0.000111
91	1	0	10.964125	-0.000092	-0.000621
92	1	0	9.738386	-2.148062	-0.000033

0 imaginary frequencies

Zero-point correction=	0.680023 (Hartree/Particle)
Thermal correction to Energy=	0.719074
Thermal correction to Enthalpy=	0.720018
Thermal correction to Gibbs Free Energy=	0.615958
Sum of electronic and zero-point Energies=	-2679.393943
Sum of electronic and thermal Energies=	-2679.354892
Sum of electronic and thermal Enthalpies=	-2679.353948
Sum of electronic and thermal Free Energies=	-2679.458009

MPO

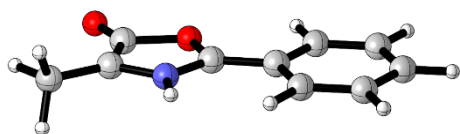


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.299816	-1.356568	0.707627
2	8	0	-3.203678	1.640848	-0.068160
3	8	0	-1.006959	1.099078	-0.044383
4	6	0	-2.352425	0.811653	-0.156045
5	6	0	1.852797	-1.232589	-0.150169
6	1	0	1.187786	2.087986	0.195353
7	1	0	3.664735	2.154798	0.364520
8	1	0	4.972787	0.054842	0.203796
9	1	0	3.810089	-2.111390	-0.124657
10	1	0	1.322504	-2.168379	-0.294658
11	1	0	-2.864223	-1.189220	1.696237
12	1	0	-4.306625	-0.932099	0.687611
13	6	0	3.236995	-1.192259	-0.055200
14	6	0	3.889930	0.026673	0.129892
15	1	0	-3.352878	-2.431893	0.527968
16	6	0	-2.440698	-0.694223	-0.366656
17	6	0	3.156784	1.206652	0.220570
18	6	0	1.768982	1.174691	0.126967
19	6	0	1.118554	-0.046497	-0.058696
20	7	0	-1.056329	-1.146682	-0.345220
21	6	0	-0.344290	-0.109423	-0.162275
22	1	0	-2.875662	-0.885928	-1.355386

0 imaginary frequencies

Zero-point correction=	0.174808 (Hartree/Particle)
Thermal correction to Energy=	0.185279
Thermal correction to Enthalpy=	0.186223
Thermal correction to Gibbs Free Energy=	0.137723
Sum of electronic and zero-point Energies=	-591.278060
Sum of electronic and thermal Energies=	-591.267590
Sum of electronic and thermal Enthalpies=	-591.266645
Sum of electronic and thermal Free Energies=	-591.315145

MPO_Mu

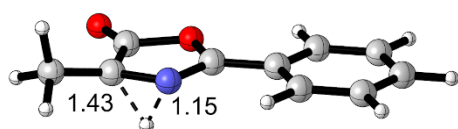


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	1	0	-0.867631	-1.988587	-0.000028
2	6	0	-3.648954	-1.455661	-0.000075
3	8	0	-3.215454	1.731042	0.000018
4	8	0	-0.974027	1.125637	0.000020
5	6	0	-2.413788	0.828612	0.000010
6	6	0	1.863237	-1.248155	0.000040
7	1	0	1.302355	2.105283	-0.000033
8	1	0	3.785334	2.111208	-0.000065
9	1	0	5.033318	-0.034932	-0.000047
10	1	0	3.790837	-2.183952	0.000024
11	1	0	1.337910	-2.200083	0.000085
12	1	0	-3.706673	-2.097859	0.887501
13	1	0	-4.528790	-0.807991	0.000941
14	6	0	3.250857	-1.242508	0.000012
15	6	0	3.948199	-0.035308	-0.000027
16	1	0	-3.707685	-2.096390	-0.888656
17	6	0	-2.453385	-0.574437	0.000029
18	6	0	3.247137	1.168731	-0.000039
19	6	0	1.858540	1.173887	-0.000021
20	6	0	1.155226	-0.038159	0.000018
21	7	0	-1.143596	-1.015889	0.000028
22	6	0	-0.293394	-0.001819	0.000016

0 imaginary frequencies

Zero-point correction=	0.173675 (Hartree/Particle)
Thermal correction to Energy=	0.184626
Thermal correction to Enthalpy=	0.185571
Thermal correction to Gibbs Free Energy=	0.135817
Sum of electronic and zero-point Energies=	-591.243911
Sum of electronic and thermal Energies=	-591.232960
Sum of electronic and thermal Enthalpies=	-591.232015
Sum of electronic and thermal Free Energies=	-591.281769

MPO_TS

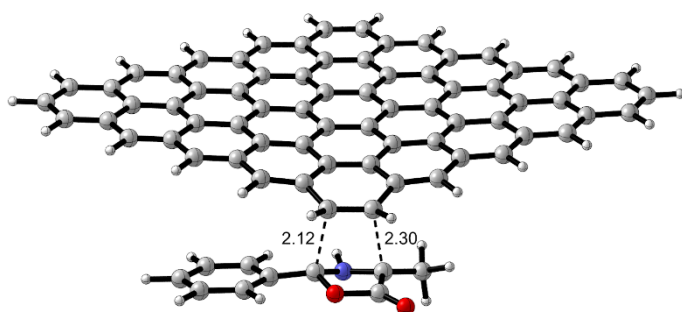


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.632630	-1.434920	0.129701
2	8	0	-3.189565	1.730659	-0.007951
3	8	0	-0.972434	1.108233	0.069386
4	6	0	-2.385006	0.838254	-0.028792
5	6	0	1.847821	-1.249281	0.029037
6	1	0	1.305457	2.113158	-0.003990
7	1	0	3.790051	2.104706	-0.015402
8	1	0	5.021654	-0.047462	-0.006852
9	1	0	3.774078	-2.191309	0.024052
10	1	0	1.288967	-2.179561	0.054013
11	1	0	-3.544734	-2.418355	-0.339938
12	1	0	-3.776179	-1.586804	1.206219
13	6	0	3.235249	-1.249223	0.015936
14	6	0	3.936212	-0.043188	0.000086
15	1	0	-4.521898	-0.938606	-0.265321
16	6	0	-2.440530	-0.582207	-0.144965
17	6	0	3.244850	1.166392	-0.003874
18	6	0	1.855453	1.177834	0.003321
19	6	0	1.153203	-0.032886	0.018129
20	1	0	-1.562019	-1.198429	-1.085597
21	6	0	-0.299278	-0.032889	0.024881
22	7	0	-1.081636	-1.102257	-0.045633

1 imaginary frequency

Zero-point correction=	0.168698 (Hartree/Particle)
Thermal correction to Energy=	0.179423
Thermal correction to Enthalpy=	0.180367
Thermal correction to Gibbs Free Energy=	0.131449
Sum of electronic and zero-point Energies=	-591.181234
Sum of electronic and thermal Energies=	-591.170509
Sum of electronic and thermal Enthalpies=	-591.169565
Sum of electronic and thermal Free Energies=	-591.218482

TS-a1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.418000	0.139293	-0.300896
2	6	0	7.898035	1.456847	-0.574058
3	6	0	5.106756	0.954707	-0.469159
4	6	0	5.595752	2.280536	-0.745153
5	6	0	2.795452	1.778301	-0.611917
6	6	0	8.340954	-0.928136	-0.077380
7	6	0	5.546761	-1.420470	0.012181
8	6	0	6.481527	-2.493345	0.232968
9	6	0	3.677360	-2.989988	0.294009
10	6	0	6.025591	-0.108502	-0.253615
11	6	0	3.240825	-0.605408	-0.161302
12	6	0	3.721011	0.711272	-0.419233
13	6	0	0.932810	0.209564	-0.345341
14	6	0	4.162307	-1.672481	0.046641
15	6	0	1.375197	-2.180129	0.079682
16	6	0	1.854101	-0.858404	-0.146810
17	6	0	-0.927181	-1.380153	-0.184384
18	6	0	3.290009	3.107636	-0.889188
19	6	0	0.479255	2.612555	-0.721498
20	1	0	-1.773938	-7.422770	0.843779
21	6	0	-1.402246	-6.412924	0.683644
22	6	0	1.416275	1.536946	-0.560390
23	6	0	-1.375967	1.010673	-0.611821
24	6	0	-0.890118	2.354755	-0.755817
25	6	0	-3.679189	1.789013	-1.020964
26	6	0	-0.449705	-0.051987	-0.377922
27	6	0	-3.227427	-0.596282	-0.528849
28	6	0	-2.744832	0.731619	-0.717612
29	6	0	-5.535655	0.189904	-0.907380
30	6	0	4.618804	-4.063472	0.517443
31	6	0	1.808099	-4.571688	0.528205
32	6	0	2.758222	-5.642600	0.765019
33	6	0	-0.059765	-6.171247	0.726412
34	6	0	2.301198	-3.245103	0.298873
35	6	0	-0.490635	-3.768437	0.262932
36	6	0	-0.007267	-2.441446	0.050011
37	6	0	-2.787671	-2.977650	-0.052626
38	6	0	0.443835	-4.828174	0.506409
39	6	0	-2.358898	-5.372862	0.420514
40	6	0	-1.864380	-4.031279	0.210883
41	6	0	-4.656179	-4.583557	0.078164
42	6	0	-2.309183	-1.650692	-0.254969
43	6	0	-5.082891	-2.194009	-0.411602
44	6	0	-4.605772	-0.870561	-0.616358
45	6	0	-7.387859	-1.410832	-0.782399

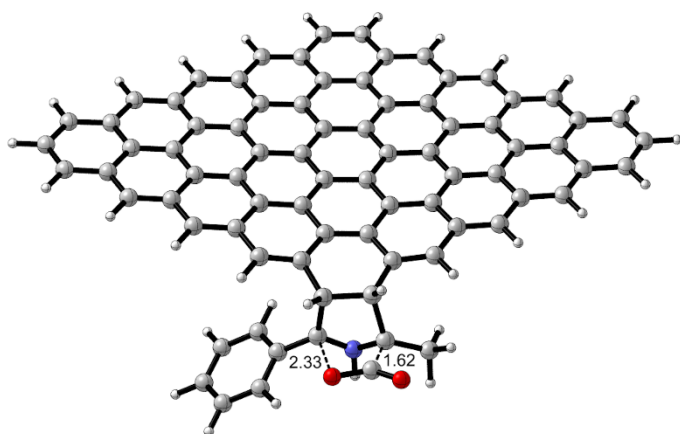
46	6	0	-4.167814	-3.244845	-0.128742
47	6	0	-6.948221	-3.796973	-0.286052
48	6	0	-6.469508	-2.466647	-0.492875
49	1	0	0.529325	-8.228574	1.147825
50	1	0	-4.081865	-6.628489	0.509138
51	6	0	2.329145	4.166694	-1.041628
52	1	0	2.702381	5.175042	-1.210802
53	6	0	4.646518	3.327071	-0.954003
54	1	0	5.018117	4.328329	-1.160466
55	6	0	6.964310	2.499607	-0.792346
56	1	0	7.337455	3.499962	-1.000282
57	6	0	9.288834	1.675157	-0.616573
58	1	0	9.657974	2.675660	-0.824317
59	6	0	10.180047	0.631501	-0.396694
60	1	0	11.248124	0.822186	-0.433750
61	6	0	9.721284	-0.652907	-0.130304
62	1	0	10.426221	-1.461992	0.039405
63	6	0	7.841813	-2.226767	0.187236
64	1	0	8.550112	-3.035032	0.354965
65	6	0	5.969209	-3.801230	0.488242
66	1	0	6.676738	-4.610018	0.656795
67	6	0	4.097635	-5.381167	0.759054
68	1	0	4.805569	-6.188387	0.934353
69	6	0	2.231341	-6.975897	0.996342
70	1	0	2.943436	-7.775719	1.181325
71	6	0	0.908004	-7.224100	0.978365
72	6	0	-3.711300	-5.617548	0.354586
73	6	0	-3.164608	3.124252	-1.163826
74	1	0	-3.879338	3.923434	-1.352551
75	6	0	-5.022803	1.508652	-1.106363
76	1	0	-5.723370	2.313779	-1.318008
77	6	0	-6.889553	-0.099960	-0.983449
78	1	0	-7.593867	0.698624	-1.206169
79	6	0	-8.761933	-1.710991	-0.859772
80	1	0	-9.463230	-0.911236	-1.081265
81	6	0	-9.218894	-3.007843	-0.657799
82	1	0	-10.282229	-3.217136	-0.722780
83	6	0	-8.332815	-4.040102	-0.374335
84	1	0	-8.700673	-5.050509	-0.219280
85	6	0	-6.019007	-4.827491	-0.002636
86	1	0	-6.390467	-5.838154	0.151226
87	1	0	-2.008049	5.556497	-1.407728
88	1	0	0.402072	6.023356	-1.249211
89	6	0	-1.843850	3.425091	-0.998087
90	6	0	0.985559	3.960826	-0.918400
91	6	0	-1.362381	4.807344	-0.957031
92	6	0	0.028298	5.062044	-0.906972
93	6	0	0.248958	5.459515	1.348708
94	6	0	-1.919077	5.421901	0.992842
95	6	0	-3.339698	5.131145	1.171338
96	7	0	-0.903965	4.790839	1.665985
97	6	0	-0.163263	6.811047	1.018473
98	8	0	-1.546867	6.728493	0.856072
99	8	0	0.455394	7.826604	0.837398
100	6	0	1.593891	5.101916	1.865233
101	1	0	1.819257	4.042605	1.707070
102	1	0	2.342276	5.694204	1.333363
103	1	0	1.676234	5.330616	2.933405
104	1	0	-0.908550	3.781075	1.766366
105	6	0	-3.763871	3.885547	1.645340
106	6	0	-4.287658	6.065370	0.738717
107	6	0	-5.640746	5.751836	0.783918

108	6	0	-5.118673	3.577262	1.688233
109	6	0	-6.059859	4.507240	1.253951
110	1	0	-3.952442	7.028916	0.368430
111	1	0	-6.371342	6.481522	0.448947
112	1	0	-3.040852	3.139663	1.966777
113	1	0	-5.435976	2.602186	2.043975
114	1	0	-7.117364	4.263576	1.281559

1 imaginary frequency

Zero-point correction=	0.856077 (Hartree/Particle)
Thermal correction to Energy=	0.906020
Thermal correction to Enthalpy=	0.906964
Thermal correction to Gibbs Free Energy=	0.778234
Sum of electronic and zero-point Energies=	-3270.635669
Sum of electronic and thermal Energies=	-3270.585726
Sum of electronic and thermal Enthalpies=	-3270.584782
Sum of electronic and thermal Free Energies=	-3270.713511

TS-a2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.382358	-0.048274	-0.207836
2	6	0	7.881698	1.263484	-0.473806
3	6	0	5.082426	0.798990	-0.373094
4	6	0	5.591990	2.117666	-0.642442
5	6	0	2.782176	1.654094	-0.508257
6	6	0	8.290305	-1.129537	0.011045
7	6	0	5.489683	-1.584663	0.092432
8	6	0	6.409355	-2.671510	0.307792
9	6	0	3.598836	-3.131653	0.350291
10	6	0	5.986815	-0.277743	-0.163254
11	6	0	3.195096	-0.737652	-0.081090
12	6	0	3.693400	0.573647	-0.324652
13	6	0	0.898481	0.114222	-0.270226
14	6	0	4.101838	-1.818403	0.119899
15	6	0	1.308833	-2.289230	0.123898
16	6	0	1.804887	-0.969567	-0.079019
17	6	0	-0.979678	-1.460941	-0.161767
18	6	0	3.300282	2.970446	-0.780140
19	6	0	0.477856	2.538421	-0.603525
20	1	0	-1.907310	-7.508532	0.768626
21	6	0	-1.522434	-6.500803	0.627877
22	6	0	1.397997	1.440993	-0.459876
23	6	0	-1.394571	0.942537	-0.554673
24	6	0	-0.892650	2.284891	-0.658239
25	6	0	-3.689018	1.742440	-0.988177
26	6	0	-0.485129	-0.134534	-0.325044
27	6	0	-3.264386	-0.650158	-0.537112
28	6	0	-2.765214	0.676326	-0.689216
29	6	0	-5.558525	0.160559	-0.957670
30	6	0	4.525033	-4.219194	0.569627
31	6	0	1.708819	-4.692184	0.546995
32	6	0	2.643280	-5.777079	0.783240
33	6	0	-0.178760	-6.273503	0.697938
34	6	0	2.219607	-3.368536	0.339814
35	6	0	-0.576090	-3.860270	0.258132
36	6	0	-0.075528	-2.535428	0.072272
37	6	0	-2.857939	-3.042462	-0.090236
38	6	0	0.342541	-4.933274	0.502938
39	6	0	-2.462849	-5.447891	0.358692
40	6	0	-1.950947	-4.108697	0.177331
41	6	0	-4.743817	-4.632177	-0.024096

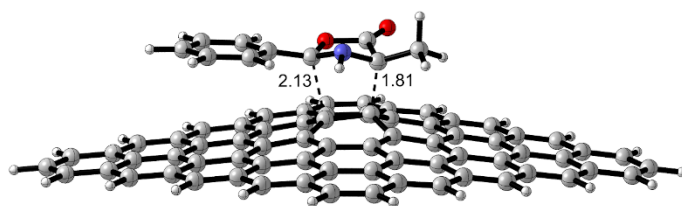
42	6	0	-2.362380	-1.717526	-0.261865
43	6	0	-5.136943	-2.232571	-0.489781
44	6	0	-4.643135	-0.910240	-0.661625
45	6	0	-7.425948	-1.424212	-0.907351
46	6	0	-4.238404	-3.295543	-0.200653
47	6	0	-7.018949	-3.820124	-0.433743
48	6	0	-6.523509	-2.491286	-0.609742
49	1	0	0.380599	-8.341523	1.106721
50	1	0	-4.198925	-6.687836	0.393484
51	6	0	2.351884	4.043956	-0.937426
52	1	0	2.749132	5.034811	-1.145168
53	6	0	4.655827	3.177433	-0.848859
54	1	0	5.038035	4.174943	-1.054170
55	6	0	6.962468	2.319915	-0.688266
56	1	0	7.348675	3.316265	-0.891493
57	6	0	9.275127	1.463489	-0.514146
58	1	0	9.658056	2.459900	-0.716444
59	6	0	10.151481	0.406534	-0.298573
60	1	0	11.222105	0.582401	-0.333651
61	6	0	9.674223	-0.872558	-0.038985
62	1	0	10.367842	-1.692041	0.127480
63	6	0	7.773176	-2.422783	0.267178
64	1	0	8.470256	-3.241449	0.431265
65	6	0	5.878821	-3.974370	0.550770
66	1	0	6.574831	-4.793703	0.716152
67	6	0	3.985677	-5.532328	0.794251
68	1	0	4.681862	-6.349898	0.968517
69	6	0	2.098519	-7.106543	0.993879
70	1	0	2.799125	-7.915980	1.180828
71	6	0	0.773042	-7.339743	0.953743
72	6	0	-3.815566	-5.678675	0.260383
73	6	0	-3.156657	3.079369	-1.080791
74	1	0	-3.858122	3.894854	-1.247073
75	6	0	-5.030093	1.479351	-1.115886
76	1	0	-5.718546	2.292656	-1.334364
77	6	0	-6.911763	-0.114709	-1.074944
78	1	0	-7.603024	0.693977	-1.301444
79	6	0	-8.799950	-1.710890	-1.024386
80	1	0	-9.488277	-0.901873	-1.252485
81	6	0	-9.272801	-3.006359	-0.852364
82	1	0	-10.335732	-3.205617	-0.947808
83	6	0	-8.402788	-4.049802	-0.560667
84	1	0	-8.782773	-5.058988	-0.428953
85	6	0	-6.106285	-4.862540	-0.141186
86	1	0	-6.490196	-5.871709	-0.010079
87	1	0	-1.992835	5.427204	-1.381072
88	1	0	0.317163	5.641348	-1.765547
89	6	0	-1.844424	3.351299	-0.877215
90	6	0	1.014218	3.875643	-0.788466
91	6	0	-1.408653	4.785863	-0.718516
92	6	0	0.113079	5.095154	-0.840135
93	6	0	0.325965	6.093165	0.349617
94	6	0	-1.722169	5.236740	0.706467
95	6	0	-3.020887	5.124390	1.401769
96	7	0	-0.623793	5.563462	1.321550
97	6	0	-0.368627	7.460389	-0.172319
98	8	0	-1.623807	7.416422	-0.109384
99	8	0	0.412553	8.294019	-0.616603
100	6	0	1.697066	6.348301	0.926089
101	1	0	2.210872	5.435166	1.233984
102	1	0	2.288315	6.886563	0.183770
103	1	0	1.601830	7.018229	1.787494

104	1	0	-0.665427	5.945107	2.263064
105	6	0	-3.463623	3.887694	1.885072
106	6	0	-3.795679	6.275308	1.572285
107	6	0	-5.023538	6.176642	2.221119
108	6	0	-4.689204	3.806084	2.536970
109	6	0	-5.470495	4.948026	2.700331
110	1	0	-3.425570	7.215450	1.176624
111	1	0	-5.632383	7.066063	2.349718
112	1	0	-2.853622	2.998789	1.751425
113	1	0	-5.034215	2.847710	2.911328
114	1	0	-6.430121	4.878168	3.203500

1 imaginary frequency

Zero-point correction=	0.859171 (Hartree/Particle)
Thermal correction to Energy=	0.908440
Thermal correction to Enthalpy=	0.909384
Thermal correction to Gibbs Free Energy=	0.781442
Sum of electronic and zero-point Energies=	-3270.645897
Sum of electronic and thermal Energies=	-3270.596628
Sum of electronic and thermal Enthalpies=	-3270.595684
Sum of electronic and thermal Free Energies=	-3270.723625

TS-b



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-7.320356	0.188585	-0.572041
2	6	0	-8.014723	-1.051655	-0.734688
3	6	0	-5.176212	-1.026552	-0.463878
4	6	0	-5.888456	-2.271810	-0.659031
5	6	0	-3.044153	-2.252860	-0.367394
6	6	0	-8.050329	1.415782	-0.544466
7	6	0	-5.226182	1.429377	-0.303106
8	6	0	-5.963943	2.663797	-0.279366
9	6	0	-3.126989	2.674591	-0.057796
10	6	0	-5.912333	0.200787	-0.443106
11	6	0	-3.084577	0.217710	-0.168027
12	6	0	-3.790949	-1.022704	-0.310203
13	1	0	0.851934	7.380435	0.213622
14	6	0	-3.815712	1.443912	-0.188511
15	6	0	-1.002714	1.455544	0.038624
16	6	0	-1.694012	0.231754	0.010269
17	6	0	1.155198	0.270534	-0.147430
18	6	0	-3.759952	-3.487445	-0.626692
19	6	0	-0.921733	-3.449522	-0.449541
20	6	0	-1.637346	-4.690240	-0.677982
21	6	0	1.212902	-4.636973	-0.831280
22	6	0	-1.668844	-2.259492	-0.203046
23	6	0	1.188385	-2.193983	-0.416801
24	6	0	0.475788	-3.426453	-0.532629
25	6	0	3.288772	-3.355230	-0.983967
26	6	0	0.309874	6.439489	0.170344
27	6	0	3.255373	-0.891608	-0.680595
28	6	0	2.551794	-2.141822	-0.699082
29	6	0	5.375353	-2.070716	-1.116282
30	6	0	-3.872983	3.914711	-0.036937
31	6	0	-1.018188	3.933718	0.071705
32	6	0	-1.775883	5.171973	0.123340
33	6	0	1.085580	5.217934	0.054036
34	6	0	-1.725985	2.685515	0.020045
35	6	0	1.111207	2.730512	-0.063907
36	6	0	0.432778	1.480207	-0.010114
37	6	0	3.218453	1.568634	-0.468331
38	6	0	0.367119	3.955799	0.036911
39	6	0	3.209833	4.030836	-0.235941
40	6	0	2.503116	2.770420	-0.245180
41	6	0	5.325127	2.853869	-0.613254
42	6	0	2.529744	0.318552	-0.446168
43	6	0	5.334532	0.395994	-0.859602
44	6	0	4.636660	-0.849857	-0.888631
45	6	0	7.464007	-0.791159	-1.229667
46	6	0	4.619620	1.600555	-0.654242
47	6	0	7.436642	1.673756	-0.978717
48	6	0	6.739704	0.426615	-1.023033
49	6	0	-0.867795	-5.905618	-0.868002

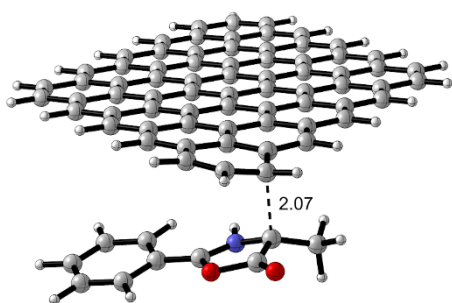
50	1	0	-1.415153	-6.838180	-0.975459
51	6	0	-3.000405	-4.694359	-0.735355
52	1	0	-3.532564	-5.628932	-0.897539
53	6	0	-5.130008	-3.476502	-0.740319
54	1	0	-5.659306	-4.412287	-0.904914
55	6	0	-7.263949	-2.258252	-0.781178
56	1	0	-7.794502	-3.196616	-0.926420
57	6	0	-9.409965	-1.035627	-0.857392
58	1	0	-9.938389	-1.976677	-0.982209
59	6	0	-10.118093	0.167475	-0.823532
60	1	0	-11.199259	0.154366	-0.920753
61	6	0	-9.457903	1.373630	-0.671364
62	1	0	-10.014273	2.306570	-0.649330
63	6	0	-7.347017	2.630256	-0.395198
64	1	0	-7.906555	3.562821	-0.375026
65	6	0	-5.242651	3.887002	-0.139779
66	1	0	-5.801518	4.820034	-0.125345
67	6	0	-3.138489	5.143760	0.079277
68	1	0	-3.698576	6.075845	0.110394
69	6	0	-1.035553	6.418141	0.201221
70	1	0	-1.604627	7.341444	0.269596
71	6	0	0.474843	-5.881604	-0.938836
72	1	0	1.040625	-6.794236	-1.105829
73	6	0	2.565038	-4.589657	-1.024340
74	1	0	3.113067	-5.505241	-1.235120
75	6	0	4.651581	-3.299227	-1.166495
76	1	0	5.203087	-4.218335	-1.353133
77	6	0	6.747509	-2.017136	-1.276752
78	1	0	7.300712	-2.938154	-1.447399
79	6	0	8.856856	-0.733661	-1.385482
80	1	0	9.407469	-1.656583	-1.544834
81	6	0	9.529061	0.487546	-1.340630
82	1	0	10.607572	0.508240	-1.464955
83	6	0	8.840341	1.672277	-1.141608
84	1	0	9.372739	2.618777	-1.109160
85	6	0	6.704186	2.863766	-0.773065
86	1	0	7.238500	3.810567	-0.740593
87	6	0	4.573651	4.049699	-0.406295
88	1	0	5.103738	4.999505	-0.392708
89	6	0	2.444467	5.234221	-0.059759
90	1	0	2.975423	6.183775	-0.047249
91	6	0	0.522682	-1.014419	0.109274
92	6	0	-0.979867	-1.041838	0.334214
93	6	0	-1.150309	-1.101172	2.130589
94	6	0	1.033396	-1.278297	2.156975
95	6	0	2.463586	-1.087232	2.360093
96	7	0	0.025736	-0.440143	2.596959
97	6	0	-0.791217	-2.527437	2.408359
98	8	0	0.584640	-2.567491	2.330970
99	8	0	-1.471163	-3.490245	2.587830
100	6	0	-2.464573	-0.647669	2.704862
101	1	0	-2.655386	0.406138	2.488825
102	1	0	-3.276757	-1.251178	2.294935
103	1	0	-2.445652	-0.792014	3.788487
104	6	0	3.011664	0.191814	2.510331
105	6	0	3.308761	-2.203291	2.276528
106	6	0	4.685515	-2.032104	2.315550
107	6	0	4.390685	0.354987	2.545818
108	6	0	5.228974	-0.753779	2.433445
109	1	0	2.877025	-3.191404	2.154422
110	1	0	5.337177	-2.895719	2.227886
111	1	0	2.366952	1.067050	2.559267

112	1	0	4.811662	1.351858	2.633932
113	1	0	6.306405	-0.618249	2.430389
114	1	0	0.120390	0.546843	2.362516

1 imaginary frequency

Zero-point correction=	0.857835 (Hartree/Particle)
Thermal correction to Energy=	0.906778
Thermal correction to Enthalpy=	0.907722
Thermal correction to Gibbs Free Energy=	0.784000
Sum of electronic and zero-point Energies=	-3270.600925
Sum of electronic and thermal Energies=	-3270.551982
Sum of electronic and thermal Enthalpies=	-3270.551038
Sum of electronic and thermal Free Energies=	-3270.674759

TS-c1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-8.640274	0.322198	0.584310
2	6	0	-9.422291	-0.870657	0.739511
3	6	0	-6.605738	-1.043755	0.357869
4	6	0	-7.398304	-2.236258	0.511005
5	6	0	-4.573393	-2.409000	0.136677
6	6	0	-9.275505	1.607744	0.621953
7	6	0	-6.461409	1.413308	0.238290
8	6	0	-7.107595	2.699790	0.273286
9	6	0	-4.285406	2.503351	-0.109421
10	6	0	-7.238172	0.230584	0.392660
11	6	0	-4.433049	0.047671	0.019871
12	6	0	-5.212745	-1.137825	0.168859
13	6	0	-2.403339	-1.318287	-0.192253
14	6	0	-5.068059	1.324882	0.046714
15	6	0	-2.260078	1.139350	-0.321205
16	6	0	-3.038282	-0.043896	-0.171763
17	6	0	-0.231303	-0.226083	-0.524278
18	6	0	-5.368344	-3.601168	0.285940
19	6	0	-2.540872	-3.777294	-0.078328
20	6	0	-3.344494	-4.972376	0.068262
21	6	0	-0.502915	-5.157684	-0.285060
22	6	0	-3.185385	-2.501958	-0.047685
23	6	0	-0.373123	-2.685989	-0.396435
24	6	0	-1.160191	-3.868143	-0.253318
25	6	0	1.669636	-4.061846	-0.585730
26	6	0	-1.009360	-1.410928	-0.377080
27	6	0	1.798078	-1.593518	-0.707552
28	6	0	1.021709	-2.775314	-0.564997
29	6	0	3.840986	-2.964047	-0.854267
30	6	0	-4.933911	3.789019	-0.079055
31	6	0	-2.110469	3.596089	-0.462090
32	6	0	-2.766778	4.885167	-0.434743
33	6	0	0.069280	4.700014	-0.823774
34	6	0	-2.897844	2.414568	-0.300532
35	6	0	-0.088672	2.232671	-0.670614
36	6	0	-0.866609	1.049499	-0.511834
37	6	0	1.938091	0.868461	-0.865859
38	6	0	-0.731081	3.506451	-0.650936
39	6	0	2.091915	3.332973	-1.035262
40	6	0	1.303981	2.140668	-0.858559
41	6	0	4.110801	1.965861	-1.239467
42	6	0	1.162963	-0.316915	-0.701707
43	6	0	3.974290	-0.497796	-1.011772
44	6	0	3.199428	-1.682302	-0.854433
45	6	0	6.023536	-1.859240	-1.032614

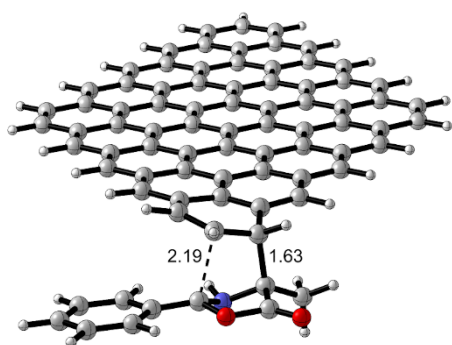
46	6	0	3.336250	0.777515	-1.039871
47	6	0	6.139467	0.606301	-1.362043
48	6	0	5.379946	-0.584039	-1.125936
49	6	0	-2.665373	-6.253382	0.024438
50	1	0	-3.269311	-7.151111	0.129733
51	6	0	-4.697385	-4.868280	0.241839
52	1	0	-5.294974	-5.771380	0.351474
53	6	0	-6.732423	-3.495168	0.466446
54	1	0	-7.326872	-4.399632	0.579369
55	6	0	-8.769957	-2.125092	0.696458
56	1	0	-9.365052	-3.028185	0.812106
57	6	0	-10.813470	-0.748965	0.929587
58	1	0	-11.407946	-1.650467	1.046730
59	6	0	-11.413754	0.503010	0.964953
60	1	0	-12.488062	0.573525	1.112479
61	6	0	-10.670743	1.666739	0.815172
62	1	0	-11.155865	2.638056	0.845789
63	6	0	-8.481588	2.767535	0.463618
64	1	0	-8.966912	3.740394	0.492624
65	6	0	-6.299270	3.861679	0.109643
66	1	0	-6.783281	4.835872	0.135296
67	6	0	-4.120238	4.958144	-0.247901
68	1	0	-4.607467	5.931165	-0.225398
69	6	0	-1.944367	6.067104	-0.609670
70	1	0	-2.438288	7.035259	-0.588689
71	6	0	-1.330522	-6.341792	-0.141101
72	1	0	-0.838639	-7.310438	-0.172314
73	6	0	0.854594	-5.232023	-0.446341
74	1	0	1.341116	-6.204744	-0.470422
75	6	0	3.047082	-4.127907	-0.730721
76	1	0	3.535984	-5.099636	-0.741089
77	6	0	5.247416	-3.012820	-0.936788
78	1	0	5.738572	-3.984336	-0.916985
79	1	0	2.015449	5.499487	-1.146750
80	1	0	-0.011676	6.877963	-0.925192
81	6	0	1.422276	4.597671	-1.009852
82	6	0	-0.611603	5.981225	-0.793529
83	6	0	7.562100	0.477512	-1.525439
84	1	0	8.131006	1.364778	-1.793636
85	6	0	5.502237	1.838718	-1.425125
86	1	0	6.094921	2.735194	-1.598577
87	6	0	3.462242	3.220175	-1.226649
88	1	0	4.055997	4.119456	-1.378976
89	6	0	8.193855	-0.717662	-1.368366
90	6	0	7.471961	-1.887234	-0.928344
91	1	0	9.271122	-0.790498	-1.490868
92	1	0	7.963193	-2.851862	-1.052534
93	6	0	7.768823	-1.857424	1.124965
94	6	0	7.913505	0.348331	1.534595
95	6	0	7.567912	1.740437	1.673344
96	7	0	7.089062	-0.683642	1.485578
97	6	0	9.172750	-1.483270	1.244558
98	8	0	9.172138	-0.068833	1.455853
99	8	0	10.193170	-2.090888	1.118832
100	6	0	7.297610	-3.188195	1.622415
101	1	0	6.277488	-3.390711	1.283949
102	1	0	7.963244	-3.963085	1.233425
103	1	0	7.320853	-3.234219	2.715850
104	6	0	6.226067	2.144234	1.595360
105	6	0	8.583823	2.694019	1.843874
106	6	0	8.249318	4.035441	1.949032
107	6	0	5.904297	3.490617	1.695255

108	6	0	6.913500	4.435273	1.873719
109	1	0	9.618329	2.370232	1.891619
110	1	0	9.030890	4.775147	2.086020
111	1	0	5.428032	1.424630	1.432056
112	1	0	4.866198	3.797320	1.616457
113	1	0	6.660163	5.487857	1.950536
114	1	0	6.079636	-0.591602	1.424305

1 imaginary frequency

Zero-point correction=	0.854927 (Hartree/Particle)
Thermal correction to Energy=	0.905114
Thermal correction to Enthalpy=	0.906058
Thermal correction to Gibbs Free Energy=	0.777017
Sum of electronic and zero-point Energies=	-3270.639786
Sum of electronic and thermal Energies=	-3270.589600
Sum of electronic and thermal Enthalpies=	-3270.588656
Sum of electronic and thermal Free Energies=	-3270.717696

TS-c2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-8.892671	0.326786	0.473428
2	6	0	-9.670543	-0.873188	0.553541
3	6	0	-6.847121	-1.019162	0.266892
4	6	0	-7.634135	-2.220875	0.345400
5	6	0	-4.801072	-2.364076	0.065246
6	6	0	-9.535814	1.605196	0.538800
7	6	0	-6.710613	1.441439	0.247305
8	6	0	-7.364490	2.722524	0.309691
9	6	0	-4.532814	2.557744	0.016731
10	6	0	-7.485958	0.249125	0.328538
11	6	0	-4.669731	0.095937	0.047708
12	6	0	-5.445568	-1.098764	0.123945
13	6	0	-2.628437	-1.249169	-0.145588
14	6	0	-5.313420	1.367817	0.101471
15	6	0	-2.493303	1.213451	-0.176657
16	6	0	-3.269993	0.019621	-0.098010
17	6	0	-0.452021	-0.132407	-0.360246
18	6	0	-5.591957	-3.566732	0.140544
19	6	0	-2.751978	-3.711392	-0.132708
20	6	0	-3.552120	-4.916563	-0.059905
21	6	0	-0.697852	-5.070087	-0.327448
22	6	0	-3.404705	-2.441904	-0.074052
23	6	0	-0.584225	-2.594338	-0.334552
24	6	0	-1.366031	-3.786397	-0.264945
25	6	0	1.474278	-3.947486	-0.518178
26	6	0	-1.226238	-1.326483	-0.285377
27	6	0	1.587496	-1.478720	-0.529831
28	6	0	0.818152	-2.668285	-0.461838
29	6	0	3.641304	-2.824286	-0.686825
30	6	0	-5.190873	3.839581	0.074057
31	6	0	-2.355746	3.677254	-0.223524
32	6	0	-3.022682	4.962310	-0.169296
33	6	0	-0.175966	4.807893	-0.478295
34	6	0	-3.141374	2.484111	-0.130681
35	6	0	-0.318829	2.332393	-0.415071
36	6	0	-1.096936	1.138322	-0.322638
37	6	0	1.723588	0.987388	-0.590078
38	6	0	-0.973692	3.602660	-0.371985
39	6	0	1.860663	3.459262	-0.679560
40	6	0	1.074486	2.255538	-0.562024
41	6	0	3.897249	2.113758	-0.870014
42	6	0	0.946878	-0.208926	-0.493106
43	6	0	3.768940	-0.361889	-0.723581
44	6	0	2.996922	-1.553601	-0.639608

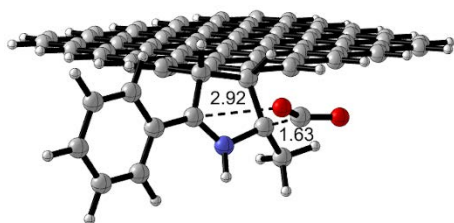
45	6	0	5.815890	-1.706315	-0.763773
46	6	0	3.120227	0.910207	-0.723649
47	6	0	5.936611	0.766778	-1.044394
48	6	0	5.175519	-0.441248	-0.806537
49	6	0	-2.861137	-6.190959	-0.130614
50	1	0	-3.461256	-7.095745	-0.079825
51	6	0	-4.909919	-4.828208	0.071163
52	1	0	-5.504667	-5.737848	0.125313
53	6	0	-6.961749	-3.474872	0.276606
54	1	0	-7.555101	-4.384949	0.333586
55	6	0	-9.014267	-2.121802	0.485824
56	1	0	-9.608918	-3.030539	0.544845
57	6	0	-11.071047	-0.763844	0.698255
58	1	0	-11.664098	-1.671972	0.758064
59	6	0	-11.680710	0.480341	0.761441
60	1	0	-12.759475	0.541133	0.873111
61	6	0	-10.935257	1.652708	0.684214
62	1	0	-11.426206	2.620265	0.736161
63	6	0	-8.743612	2.776140	0.454494
64	1	0	-9.236443	3.744440	0.505025
65	6	0	-6.560277	3.897026	0.219364
66	1	0	-7.052942	4.865940	0.266705
67	6	0	-4.380012	5.020806	-0.023218
68	1	0	-4.875211	5.988813	0.021122
69	6	0	-2.203262	6.155781	-0.273011
70	1	0	-2.704472	7.119249	-0.228767
71	6	0	-1.521401	-6.263895	-0.256300
72	1	0	-1.021709	-7.227613	-0.308899
73	6	0	0.663522	-5.128513	-0.450387
74	1	0	1.158179	-6.096254	-0.499147
75	6	0	2.855307	-3.997939	-0.631430
76	1	0	3.352087	-4.964863	-0.672573
77	6	0	5.055158	-2.858999	-0.751200
78	1	0	5.549804	-3.828881	-0.756835
79	1	0	1.771657	5.629162	-0.714532
80	1	0	-0.267428	6.987588	-0.496537
81	6	0	1.179764	4.720254	-0.630133
82	6	0	-0.865986	6.083722	-0.419697
83	6	0	7.305385	0.644944	-1.349807
84	1	0	7.835328	1.524281	-1.710396
85	6	0	5.276110	2.006602	-1.061934
86	1	0	5.860943	2.908606	-1.233769
87	6	0	3.230011	3.364844	-0.839748
88	1	0	3.819051	4.273283	-0.945587
89	6	0	8.026528	-0.513695	-1.091061
90	6	0	7.315509	-1.768189	-0.624357
91	1	0	9.014225	-0.621812	-1.531418
92	1	0	7.703793	-2.660624	-1.127896
93	6	0	7.702337	-1.955721	0.948626
94	6	0	8.766216	-0.028340	0.907432
95	6	0	9.126987	1.374459	0.999666
96	7	0	7.684284	-0.620309	1.517185
97	6	0	9.197805	-2.198267	0.918639
98	8	0	9.785066	-0.950086	0.870241
99	8	0	9.814764	-3.215457	0.863333
100	6	0	6.946575	-3.010314	1.719234
101	1	0	5.879364	-2.783725	1.755884
102	1	0	7.085264	-3.981975	1.237819
103	1	0	7.338996	-3.071205	2.736879
104	6	0	8.139880	2.343422	1.235395
105	6	0	10.452656	1.769353	0.777323
106	6	0	10.785541	3.117253	0.804684

107	6	0	8.483375	3.688898	1.253684
108	6	0	9.804394	4.079622	1.040052
109	1	0	11.210726	1.015597	0.592915
110	1	0	11.815199	3.418642	0.641291
111	1	0	7.105891	2.054920	1.401585
112	1	0	7.717214	4.434732	1.439947
113	1	0	10.068568	5.132126	1.058269
114	1	0	6.800682	-0.118806	1.433639

1 imaginary frequency

Zero-point correction=	0.857514 (Hartree/Particle)
Thermal correction to Energy=	0.906778
Thermal correction to Enthalpy=	0.907723
Thermal correction to Gibbs Free Energy=	0.780625
Sum of electronic and zero-point Energies=	-3270.632469
Sum of electronic and thermal Energies=	-3270.583205
Sum of electronic and thermal Enthalpies=	-3270.582260
Sum of electronic and thermal Free Energies=	-3270.709358

TS-c3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.056584	0.095335	0.304995
2	6	0	-9.778415	-1.136142	0.344070
3	6	0	-6.949186	-1.152706	0.165025
4	6	0	-7.679382	-2.391404	0.203307
5	6	0	-4.840176	-2.402288	0.024912
6	6	0	-9.757857	1.338766	0.356336
7	6	0	-6.923970	1.310515	0.176792
8	6	0	-7.636732	2.561369	0.227620
9	6	0	-4.794841	2.530911	0.048636
10	6	0	-7.645405	0.083342	0.214899
11	6	0	-4.820186	0.062552	0.039847
12	6	0	-5.541017	-1.166551	0.073709
13	6	0	-2.716559	-1.185336	-0.097905
14	6	0	-5.522242	1.302407	0.085693
15	6	0	-2.691064	1.281652	-0.086348
16	6	0	-3.415086	0.051870	-0.055416
17	6	0	-0.587498	0.032290	-0.222193
18	6	0	-5.576371	-3.643807	0.061758
19	6	0	-2.725995	-3.653084	-0.117130
20	6	0	-3.471850	-4.896100	-0.080270
21	6	0	-0.607762	-4.913752	-0.261067
22	6	0	-3.438001	-2.414062	-0.067065
23	6	0	-0.607849	-2.432246	-0.239057
24	6	0	-1.336629	-3.661753	-0.206584
25	6	0	1.512859	-3.687696	-0.382436
26	6	0	-1.307921	-1.195842	-0.193110
27	6	0	1.514557	-1.215925	-0.357635
28	6	0	0.797947	-2.439692	-0.328301
29	6	0	3.628266	-2.464659	-0.493833
30	6	0	-5.514361	3.783905	0.098046
31	6	0	-2.664652	3.753841	-0.082153
32	6	0	-3.393328	5.007907	-0.032633
33	6	0	-0.532896	4.987087	-0.216892
34	6	0	-3.399707	2.522589	-0.043577
35	6	0	-0.561385	2.502368	-0.217684
36	6	0	-1.291445	1.271123	-0.182335
37	6	0	1.546492	1.252535	-0.351948
38	6	0	-1.279393	3.743843	-0.172845
39	6	0	1.570497	3.732832	-0.356034
40	6	0	0.831758	2.491020	-0.310047
41	6	0	3.679934	2.483652	-0.496361
42	6	0	0.816633	0.020535	-0.314031
43	6	0	3.652903	-0.000398	-0.473955
44	6	0	2.929849	-1.225019	-0.439158
45	6	0	5.741602	-1.252701	-0.562114
46	6	0	2.941102	1.239011	-0.439999
47	6	0	5.803992	1.238531	-0.644439
48	6	0	5.061469	-0.021698	-0.541518

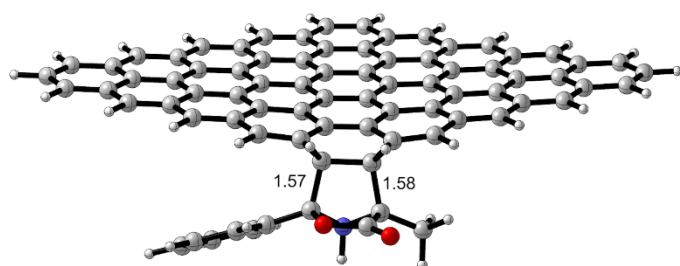
49	6	0	-2.719956	-6.137225	-0.137281
50	1	0	-3.278821	-7.068749	-0.109127
51	6	0	-4.834727	-4.872968	0.006248
52	1	0	-5.388894	-5.808561	0.035065
53	6	0	-6.951757	-3.615484	0.149362
54	1	0	-7.506544	-4.550487	0.178887
55	6	0	-9.067075	-2.355194	0.291860
56	1	0	-9.623537	-3.289275	0.322012
57	6	0	-11.187302	-1.092929	0.434186
58	1	0	-11.739904	-2.027928	0.464449
59	6	0	-11.859813	0.118716	0.483441
60	1	0	-12.942957	0.129802	0.552789
61	6	0	-11.160734	1.323066	0.445696
62	1	0	-11.696731	2.267335	0.485555
63	6	0	-9.019800	2.549178	0.315779
64	1	0	-9.560557	3.492224	0.355665
65	6	0	-6.887519	3.776195	0.185658
66	1	0	-7.428093	4.719277	0.224923
67	6	0	-4.755339	5.003514	0.054482
68	1	0	-5.296521	5.946402	0.093187
69	6	0	-2.625816	6.239762	-0.077930
70	1	0	-3.172514	7.178160	-0.039446
71	6	0	-1.375714	-6.145285	-0.222511
72	1	0	-0.829121	-7.083603	-0.264655
73	6	0	0.755891	-4.907028	-0.346373
74	1	0	1.297894	-5.849321	-0.388672
75	6	0	2.892791	-3.676164	-0.466250
76	1	0	3.437031	-4.616901	-0.508133
77	6	0	5.036075	-2.442599	-0.561976
78	1	0	5.588180	-3.381694	-0.594190
79	1	0	1.383151	5.898145	-0.341103
80	1	0	-0.721679	7.160026	-0.198435
81	6	0	0.828654	4.962730	-0.305829
82	6	0	-1.282186	6.229561	-0.164889
83	6	0	7.154797	1.246107	-0.824567
84	1	0	7.667324	2.197573	-0.944519
85	6	0	5.052816	2.459811	-0.601270
86	1	0	5.598394	3.398715	-0.662244
87	6	0	2.941947	3.707382	-0.448759
88	1	0	3.493615	4.644072	-0.489127
89	6	0	8.002721	0.003678	-0.835879
90	6	0	7.250669	-1.329491	-0.559370
91	1	0	8.584795	-0.072416	-1.763410
92	1	0	7.531703	-2.043772	-1.336066
93	6	0	7.860118	-1.874213	0.784859
94	6	0	8.954756	0.128689	0.330597
95	6	0	9.973728	1.166274	0.488857
96	7	0	8.685573	-0.759715	1.223625
97	6	0	8.887614	-3.037932	0.283750
98	8	0	9.938925	-2.572152	-0.176063
99	8	0	8.388225	-4.162997	0.353508
100	6	0	6.933719	-2.337579	1.888586
101	1	0	6.135881	-1.619563	2.102593
102	1	0	6.507549	-3.297940	1.599704
103	1	0	7.514969	-2.512878	2.801231
104	6	0	10.415468	1.560593	1.758820
105	6	0	10.518301	1.773088	-0.648831
106	6	0	11.504519	2.743456	-0.517481
107	6	0	11.394846	2.535419	1.885637
108	6	0	11.943538	3.125127	0.747605
109	1	0	10.186592	1.468011	-1.636172
110	1	0	11.932024	3.199166	-1.404379

111	1	0	9.971186	1.130158	2.652276
112	1	0	11.726557	2.841378	2.872260
113	1	0	12.710769	3.885915	0.849705
114	1	0	9.265958	-0.877182	2.049636

1 imaginary frequency

Zero-point correction=	0.858149 (Hartree/Particle)
Thermal correction to Energy=	0.907820
Thermal correction to Enthalpy=	0.908764
Thermal correction to Gibbs Free Energy=	0.779991
Sum of electronic and zero-point Energies=	-3270.616171
Sum of electronic and thermal Energies=	-3270.566499
Sum of electronic and thermal Enthalpies=	-3270.565555
Sum of electronic and thermal Free Energies=	-3270.694328

I-a1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.425971	0.296635	-0.216660
2	6	0	7.865733	1.635504	-0.450749
3	6	0	5.089274	1.044792	-0.356551
4	6	0	5.539634	2.390571	-0.595916
5	6	0	2.751704	1.798939	-0.469986
6	6	0	8.382166	-0.748415	-0.027564
7	6	0	5.603857	-1.328488	0.051249
8	6	0	6.571992	-2.378134	0.236257
9	6	0	3.784532	-2.961984	0.284770
10	6	0	6.041723	0.004620	-0.174544
11	6	0	3.272624	-0.579830	-0.092454
12	6	0	3.711268	0.756997	-0.310057
13	6	0	0.938902	0.173622	-0.249561
14	6	0	4.227645	-1.623498	0.080092
15	6	0	1.457558	-2.215422	0.098220
16	6	0	1.893645	-0.872408	-0.084667
17	6	0	-0.868699	-1.478892	-0.139419
18	6	0	3.211935	3.142485	-0.712712
19	6	0	0.408698	2.577588	-0.548794
20	1	0	-1.521855	-7.579317	0.685128
21	6	0	-1.182495	-6.553457	0.558657
22	6	0	1.377907	1.522628	-0.422437
23	6	0	-1.391945	0.912439	-0.494975
24	6	0	-0.952296	2.278271	-0.597636
25	6	0	-3.721046	1.612440	-0.885919
26	6	0	-0.434393	-0.129408	-0.290096
27	6	0	-3.191695	-0.761398	-0.457829
28	6	0	-2.750654	0.585250	-0.608541
29	6	0	-5.526457	-0.039409	-0.809316
30	6	0	4.759336	-4.012284	0.472174
31	6	0	1.966533	-4.606663	0.466585
32	6	0	2.949796	-5.654835	0.667668
33	6	0	0.151332	-6.270317	0.610024
34	6	0	2.416691	-3.258364	0.281873
35	6	0	-0.356143	-3.867261	0.228327
36	6	0	0.083993	-2.518635	0.060654
37	6	0	-2.676782	-3.140814	-0.059413
38	6	0	0.611181	-4.905092	0.435748
39	6	0	-2.171459	-5.535890	0.331255
40	6	0	-1.720609	-4.172829	0.167753
41	6	0	-4.492785	-4.809146	0.018541
42	6	0	-2.240768	-1.793552	-0.217332
43	6	0	-4.996505	-2.419666	-0.389612
44	6	0	-4.561442	-1.076117	-0.552683
45	6	0	-7.327095	-1.698610	-0.728435
46	6	0	-4.047899	-3.449493	-0.143279

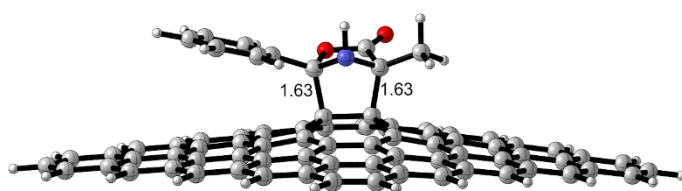
47	6	0	-6.809789	-4.083876	-0.313131
48	6	0	-6.374158	-2.733070	-0.476858
49	1	0	0.804339	-8.320943	0.963850
50	1	0	-3.853257	-6.848333	0.378932
51	6	0	2.215409	4.174159	-0.844448
52	1	0	2.565790	5.190704	-1.013852
53	6	0	4.556689	3.411461	-0.776787
54	1	0	4.893730	4.429512	-0.959133
55	6	0	6.899696	2.654497	-0.638448
56	1	0	7.240589	3.671534	-0.818805
57	6	0	9.249056	1.897825	-0.487446
58	1	0	9.586799	2.915002	-0.665281
59	6	0	10.172141	0.875798	-0.299948
60	1	0	11.233909	1.099937	-0.331735
61	6	0	9.753355	-0.429653	-0.073453
62	1	0	10.482688	-1.221855	0.070488
63	6	0	7.923397	-2.069053	0.196833
64	1	0	8.656012	-2.860442	0.338129
65	6	0	6.100929	-3.708261	0.450379
66	1	0	6.832902	-4.500159	0.592239
67	6	0	4.280264	-5.352295	0.670876
68	1	0	5.012889	-6.142527	0.819662
69	6	0	2.466077	-7.010960	0.854664
70	1	0	3.203281	-7.793306	1.013800
71	6	0	1.151434	-7.300184	0.827414
72	6	0	-3.515302	-5.821536	0.257984
73	6	0	-3.244077	2.964162	-1.018047
74	1	0	-3.985360	3.736977	-1.211495
75	6	0	-5.054811	1.298923	-0.975619
76	1	0	-5.779302	2.087560	-1.166902
77	6	0	-6.870908	-0.367502	-0.890294
78	1	0	-7.600290	0.415794	-1.084217
79	6	0	-8.691601	-2.038483	-0.809636
80	1	0	-9.418689	-1.254025	-1.000335
81	6	0	-9.106631	-3.354927	-0.648789
82	1	0	-10.163286	-3.595324	-0.715067
83	6	0	-8.186546	-4.367381	-0.404231
84	1	0	-8.521673	-5.393434	-0.280949
85	6	0	-5.847459	-5.093469	-0.067645
86	1	0	-6.186255	-6.119921	0.053495
87	1	0	-2.045175	5.278955	-1.641620
88	1	0	0.232325	5.788116	-1.501875
89	6	0	-1.945946	3.308009	-0.825314
90	6	0	0.887216	3.934790	-0.709445
91	6	0	-1.583498	4.772492	-0.789584
92	6	0	-0.061226	5.107458	-0.696176
93	6	0	0.000432	5.904004	0.668306
94	6	0	-2.114494	5.478166	0.512182
95	6	0	-3.494449	5.170172	1.002905
96	7	0	-1.037114	5.197464	1.432664
97	6	0	-0.702781	7.216060	0.307644
98	8	0	-2.020664	6.910966	0.219959
99	8	0	-0.239235	8.299625	0.094138
100	6	0	1.315918	6.110617	1.374119
101	1	0	1.798961	5.160044	1.604427
102	1	0	1.980615	6.718501	0.754756
103	1	0	1.146111	6.661675	2.304627
104	1	0	-1.211847	5.654001	2.330559
105	6	0	-3.706465	4.043607	1.799696
106	6	0	-4.575991	5.957756	0.607697
107	6	0	-5.866344	5.608904	0.997907
108	6	0	-4.997159	3.697993	2.185864

109	6	0	-6.079211	4.477930	1.781853
110	1	0	-4.401166	6.839517	-0.000046
111	1	0	-6.706199	6.224368	0.690526
112	1	0	-2.857746	3.430238	2.089741
113	1	0	-5.158918	2.814730	2.795777
114	1	0	-7.086711	4.205815	2.081368

0 imaginary frequencies

Zero-point correction=	0.861364 (Hartree/Particle)
Thermal correction to Energy=	0.910447
Thermal correction to Enthalpy=	0.911391
Thermal correction to Gibbs Free Energy=	0.785035
Sum of electronic and zero-point Energies=	-3270.684064
Sum of electronic and thermal Energies=	-3270.634981
Sum of electronic and thermal Enthalpies=	-3270.634037
Sum of electronic and thermal Free Energies=	-3270.760393

I-b



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-7.311262	0.217657	-0.534032
2	6	0	-8.012877	-1.017988	-0.702692
3	6	0	-5.169937	-1.008339	-0.443846
4	6	0	-5.890763	-2.247094	-0.661110
5	6	0	-3.044303	-2.245953	-0.373908
6	6	0	-8.035350	1.447690	-0.496984
7	6	0	-5.209788	1.445871	-0.276579
8	6	0	-5.940477	2.683582	-0.253649
9	6	0	-3.100682	2.678409	-0.062550
10	6	0	-5.902624	0.222770	-0.411727
11	6	0	-3.071447	0.223714	-0.134435
12	6	0	-3.787595	-1.012517	-0.285152
13	1	0	0.897693	7.370362	0.054935
14	6	0	-3.796602	1.452797	-0.169384
15	6	0	-0.983603	1.445865	0.047983
16	6	0	-1.682098	0.231383	0.054252
17	6	0	1.183607	0.263705	-0.098943
18	6	0	-3.766770	-3.466516	-0.678767
19	6	0	-0.928459	-3.443361	-0.490828
20	6	0	-1.648234	-4.667306	-0.785929
21	6	0	1.193651	-4.627639	-0.950145
22	6	0	-1.672932	-2.264951	-0.197206
23	6	0	1.208595	-2.224749	-0.381356
24	6	0	0.474424	-3.424632	-0.578019
25	6	0	3.286152	-3.373323	-1.025823
26	6	0	0.350424	6.431653	0.038411
27	6	0	3.278265	-0.920322	-0.626545
28	6	0	2.558736	-2.168892	-0.674637
29	6	0	5.384724	-2.109453	-1.099255
30	6	0	-3.840452	3.922955	-0.052121
31	6	0	-0.986323	3.927435	0.010546
32	6	0	-1.737349	5.170284	0.049805
33	6	0	1.118454	5.204288	-0.060146
34	6	0	-1.697313	2.678984	-0.002025
35	6	0	1.133741	2.712457	-0.126413
36	6	0	0.458043	1.461810	-0.024863
37	6	0	3.240427	1.541770	-0.483478
38	6	0	0.396560	3.943573	-0.046196
39	6	0	3.238156	4.008597	-0.320915
40	6	0	2.527877	2.747376	-0.301458
41	6	0	5.350939	2.818657	-0.651771
42	6	0	2.547411	0.296582	-0.417076
43	6	0	5.357105	0.359849	-0.835088
44	6	0	4.649473	-0.885868	-0.848364
45	6	0	7.479231	-0.837342	-1.208079
46	6	0	4.645433	1.566867	-0.661919
47	6	0	7.459868	1.628162	-0.985368
48	6	0	6.759566	0.383721	-1.006628
49	6	0	-0.892607	-5.877672	-1.045317

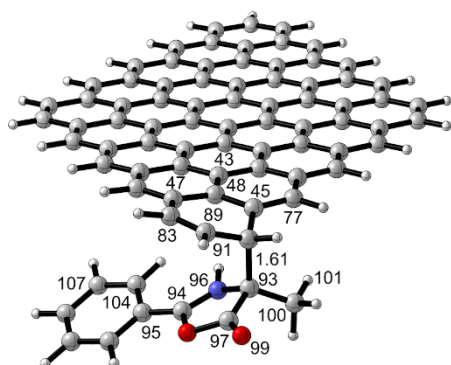
50	1	0	-1.449688	-6.797528	-1.200659
51	6	0	-3.011792	-4.667065	-0.839732
52	1	0	-3.545182	-5.592689	-1.043576
53	6	0	-5.137362	-3.450457	-0.782054
54	1	0	-5.669387	-4.379645	-0.972733
55	6	0	-7.265910	-2.226846	-0.772810
56	1	0	-7.800344	-3.160643	-0.932419
57	6	0	-9.407429	-0.995338	-0.814596
58	1	0	-9.940779	-1.933022	-0.943795
59	6	0	-10.111180	0.211345	-0.766064
60	1	0	-11.193128	0.202813	-0.854786
61	6	0	-9.445181	1.412710	-0.612598
62	1	0	-9.996619	2.348328	-0.581698
63	6	0	-7.325098	2.657690	-0.354762
64	1	0	-7.878877	3.593639	-0.331630
65	6	0	-5.211018	3.903291	-0.134588
66	1	0	-5.763553	4.840118	-0.123945
67	6	0	-3.099934	5.149847	0.031117
68	1	0	-3.654923	6.085138	0.055325
69	6	0	-0.993827	6.415717	0.089658
70	1	0	-1.560067	7.341449	0.147708
71	6	0	0.448387	-5.859280	-1.124578
72	1	0	1.008748	-6.763643	-1.345133
73	6	0	2.547080	-4.590568	-1.132688
74	1	0	3.082920	-5.502832	-1.385198
75	6	0	4.650187	-3.327636	-1.195576
76	1	0	5.192245	-4.244671	-1.415701
77	6	0	6.754353	-2.061019	-1.260369
78	1	0	7.301974	-2.982525	-1.445612
79	6	0	8.868144	-0.785871	-1.368074
80	1	0	9.415371	-1.711690	-1.522986
81	6	0	9.548997	0.434710	-1.335317
82	1	0	10.627178	0.448249	-1.461792
83	6	0	8.865488	1.621594	-1.150069
84	1	0	9.399680	2.567516	-1.131509
85	6	0	6.731360	2.822355	-0.806500
86	1	0	7.267140	3.768968	-0.793654
87	6	0	4.602145	4.020859	-0.482456
88	1	0	5.133796	4.969834	-0.490627
89	6	0	2.476236	5.216878	-0.177390
90	1	0	3.009090	6.165292	-0.186732
91	6	0	0.583454	-1.053801	0.334348
92	6	0	-1.002402	-1.063386	0.439148
93	6	0	-1.195497	-1.181041	2.051422
94	6	0	0.962126	-1.240938	1.909168
95	6	0	2.377564	-1.005881	2.331759
96	7	0	-0.043015	-0.398320	2.500157
97	6	0	-0.757572	-2.609113	2.376213
98	8	0	0.593936	-2.603089	2.251294
99	8	0	-1.406865	-3.567626	2.675998
100	6	0	-2.512170	-0.815003	2.690056
101	1	0	-2.761000	0.233708	2.519658
102	1	0	-3.312061	-1.452840	2.308224
103	1	0	-2.440573	-0.992800	3.768098
104	6	0	2.825970	0.294346	2.570637
105	6	0	3.271853	-2.076152	2.406335
106	6	0	4.615911	-1.839346	2.675090
107	6	0	4.172344	0.527039	2.832673
108	6	0	5.070558	-0.537548	2.872681
109	1	0	2.913358	-3.084956	2.229549
110	1	0	5.311270	-2.672065	2.712836
111	1	0	2.124903	1.123365	2.502116

112	1	0	4.522471	1.543314	2.986772
113	1	0	6.123995	-0.351341	3.058601
114	1	0	0.038110	-0.405106	3.518823

0 imaginary frequencies

Zero-point correction=	0.860513 (Hartree/Particle)
Thermal correction to Energy=	0.909161
Thermal correction to Enthalpy=	0.910105
Thermal correction to Gibbs Free Energy=	0.786569
Sum of electronic and zero-point Energies=	-3270.608480
Sum of electronic and thermal Energies=	-3270.559833
Sum of electronic and thermal Enthalpies=	-3270.558889
Sum of electronic and thermal Free Energies=	-3270.682424

I-c1



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	8.609702	-0.317497	0.608767
2	6	0	9.390921	0.875173	0.790997
3	6	0	6.575049	1.051659	0.381351
4	6	0	7.365833	2.241515	0.561655
5	6	0	4.542381	2.417143	0.159817
6	6	0	9.247288	-1.605907	0.633791
7	6	0	6.432346	-1.403336	0.224098
8	6	0	7.079335	-2.689444	0.247124
9	6	0	4.259755	-2.487509	-0.158928
10	6	0	7.208409	-0.223001	0.403802
11	6	0	4.404021	-0.035379	0.004861
12	6	0	5.182073	1.148112	0.179419
13	6	0	2.374189	1.331498	-0.206895
14	6	0	5.040312	-1.312888	0.020538
15	6	0	2.233102	-1.122778	-0.370911
16	6	0	3.010222	0.057944	-0.197911
17	6	0	0.203359	0.243643	-0.572243
18	6	0	5.332409	3.605098	0.336366
19	6	0	2.509209	3.784406	-0.051840
20	6	0	3.307227	4.975724	0.122268
21	6	0	0.466977	5.163578	-0.247908
22	6	0	3.152195	2.512402	-0.036278
23	6	0	0.344444	2.699363	-0.405087
24	6	0	1.124137	3.877095	-0.236012
25	6	0	-1.702625	4.072613	-0.575213
26	6	0	0.979599	1.426362	-0.400982
27	6	0	-1.826079	1.611577	-0.745199
28	6	0	-1.056114	2.790552	-0.578706
29	6	0	-3.870370	2.978608	-0.858519
30	6	0	4.905771	-3.770746	-0.140208
31	6	0	2.088244	-3.574230	-0.542991
32	6	0	2.741920	-4.861425	-0.527464
33	6	0	-0.091644	-4.672153	-0.933510
34	6	0	2.870080	-2.397023	-0.360535
35	6	0	0.065523	-2.212115	-0.750025
36	6	0	0.839884	-1.031677	-0.570634
37	6	0	-1.963446	-0.847608	-0.942092
38	6	0	0.704060	-3.482824	-0.740888
39	6	0	-2.114136	-3.306305	-1.140710
40	6	0	-1.331874	-2.118555	-0.946108
41	6	0	-4.132103	-1.940575	-1.342243
42	6	0	-1.189689	0.335788	-0.756280
43	6	0	-4.003594	0.519103	-1.071491

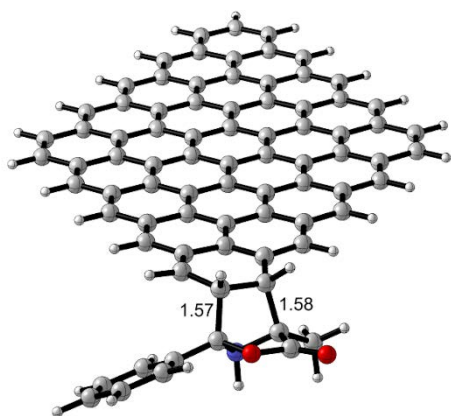
44	6	0	-3.230474	1.702196	-0.890938
45	6	0	-6.050780	1.873492	-1.013927
46	6	0	-3.362974	-0.756202	-1.121928
47	6	0	-6.164188	-0.584420	-1.452488
48	6	0	-5.408648	0.604477	-1.174129
49	6	0	2.626544	6.255167	0.095430
50	1	0	3.227666	7.152270	0.221381
51	6	0	4.661371	4.869455	0.306919
52	1	0	5.255759	5.771974	0.438167
53	6	0	6.698513	3.496745	0.529835
54	1	0	7.289026	4.400963	0.664113
55	6	0	8.737739	2.127377	0.760346
56	1	0	9.329682	3.029465	0.897106
57	6	0	10.781161	0.748452	0.994045
58	1	0	11.374416	1.647634	1.132287
59	6	0	11.378614	-0.504347	1.015851
60	1	0	12.451808	-0.576564	1.173744
61	6	0	10.640741	-1.667691	0.840672
62	1	0	11.126043	-2.638994	0.861217
63	6	0	8.453924	-2.760461	0.450058
64	1	0	8.937290	-3.734526	0.468960
65	6	0	6.274111	-3.845306	0.059970
66	1	0	6.756649	-4.820622	0.075864
67	6	0	4.097073	-4.935710	-0.330827
68	1	0	4.584132	-5.909163	-0.317870
69	6	0	1.922038	-6.040103	-0.724061
70	1	0	2.415857	-7.008568	-0.713537
71	6	0	1.291726	6.345139	-0.077947
72	1	0	0.799317	7.313914	-0.094860
73	6	0	-0.893647	5.238604	-0.412872
74	1	0	-1.380852	6.211276	-0.419087
75	6	0	-3.089722	4.136064	-0.713991
76	1	0	-3.580445	5.106800	-0.696282
77	6	0	-5.297123	3.016740	-0.904651
78	1	0	-5.789207	3.984232	-0.816345
79	1	0	-2.037949	-5.468702	-1.280069
80	1	0	-0.008319	-6.848044	-1.064823
81	6	0	-1.447391	-4.567818	-1.126742
82	6	0	0.589430	-5.952519	-0.915964
83	6	0	-7.600855	-0.440892	-1.668982
84	1	0	-8.137636	-1.293286	-2.079481
85	6	0	-5.535784	-1.802652	-1.546982
86	1	0	-6.120706	-2.693710	-1.767668
87	6	0	-3.492077	-3.188909	-1.339901
88	1	0	-4.082711	-4.086774	-1.510797
89	6	0	-8.244524	0.708347	-1.417111
90	6	0	-7.541667	1.868043	-0.763042
91	1	0	-9.308966	0.807075	-1.613619
92	1	0	-8.002934	2.820588	-1.046445
93	6	0	-7.759254	1.762261	0.824161
94	6	0	-7.752919	-0.401703	1.597049
95	6	0	-7.333957	-1.745571	1.868273
96	7	0	-6.989672	0.633662	1.324374
97	6	0	-9.161401	1.265019	1.133985
98	8	0	-9.047014	-0.066418	1.591097
99	8	0	-10.210604	1.801603	1.029452
100	6	0	-7.469950	3.061329	1.564103
101	1	0	-6.443047	3.378022	1.370271
102	1	0	-8.160509	3.830895	1.209740
103	1	0	-7.607294	2.932299	2.640527
104	6	0	-5.994871	-2.118647	1.643842
105	6	0	-8.274351	-2.694277	2.307242

106	6	0	-7.867242	-3.999191	2.531072
107	6	0	-5.606090	-3.430795	1.857928
108	6	0	-6.538656	-4.368523	2.306276
109	1	0	-9.305202	-2.396211	2.467681
110	1	0	-8.584879	-4.734709	2.878206
111	1	0	-5.262818	-1.407797	1.268634
112	1	0	-4.579119	-3.720264	1.659652
113	1	0	-6.229602	-5.394887	2.476889
114	1	0	-5.993254	0.553394	1.135707

0 imaginary frequencies

Zero-point correction=	0.856082 (Hartree/Particle)
Thermal correction to Energy=	0.906304
Thermal correction to Enthalpy=	0.907248
Thermal correction to Gibbs Free Energy=	0.778281
Sum of electronic and zero-point Energies=	-3270.651701
Sum of electronic and thermal Energies=	-3270.601479
Sum of electronic and thermal Enthalpies=	-3270.600535
Sum of electronic and thermal Free Energies=	-3270.729501

I-c2



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-9.009533	0.200980	0.360886
2	6	0	-9.758116	-1.014946	0.420296
3	6	0	-6.930284	-1.093311	0.209016
4	6	0	-7.687610	-2.314842	0.267451
5	6	0	-4.849767	-2.388994	0.058349
6	6	0	-9.683426	1.460694	0.408348
7	6	0	-6.851543	1.368956	0.194283
8	6	0	-7.537501	2.635149	0.240162
9	6	0	-4.697243	2.541131	0.024300
10	6	0	-7.599310	0.157790	0.254101
11	6	0	-4.776720	0.074313	0.046516
12	6	0	-5.523866	-1.138542	0.101944
13	6	0	-2.701715	-1.220052	-0.099899
14	6	0	-5.451621	1.329522	0.085796
15	6	0	-2.622738	1.245546	-0.120722
16	6	0	-3.372949	0.032126	-0.064853
17	6	0	-0.548261	-0.050310	-0.262627
18	6	0	-5.612914	-3.613055	0.114694
19	6	0	-2.765137	-3.686803	-0.093724
20	6	0	-3.537904	-4.912648	-0.038424
21	6	0	-0.676844	-4.995003	-0.248690
22	6	0	-3.449739	-2.432213	-0.048252
23	6	0	-0.622152	-2.514102	-0.248707
24	6	0	-1.377587	-3.726917	-0.197205
25	6	0	1.469160	-3.816915	-0.401994
26	6	0	-1.294689	-1.262383	-0.209365
27	6	0	1.524551	-1.344927	-0.400711
28	6	0	0.782007	-2.552917	-0.351147
29	6	0	3.608747	-2.638931	-0.542326
30	6	0	-5.389757	3.809083	0.067352
31	6	0	-2.543406	3.716334	-0.153577
32	6	0	-3.244908	4.985962	-0.111258
33	6	0	-0.389487	4.902711	-0.342363
34	6	0	-3.304704	2.501713	-0.086650
35	6	0	-0.469188	2.418815	-0.300237
36	6	0	-1.225126	1.203894	-0.233935
37	6	0	1.609998	1.121838	-0.439515
38	6	0	-1.160772	3.675833	-0.265669
39	6	0	1.683805	3.602961	-0.498817
40	6	0	0.921362	2.376511	-0.413883
41	6	0	3.761754	2.307280	-0.653810

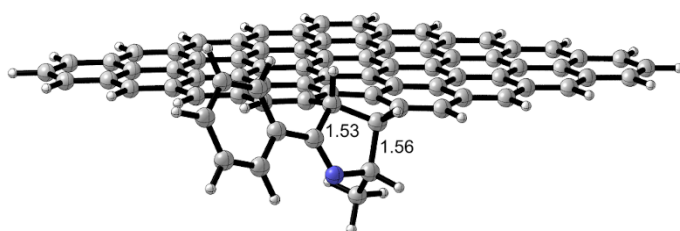
42	6	0	0.854353	-0.093425	-0.368475
43	6	0	3.689581	-0.178145	-0.554802
44	6	0	2.938628	-1.384834	-0.492719
45	6	0	5.756956	-1.473741	-0.626820
46	6	0	3.002638	1.077419	-0.545798
47	6	0	5.853344	1.013454	-0.799645
48	6	0	5.097222	-0.229174	-0.628703
49	6	0	-2.814310	-6.170361	-0.093451
50	1	0	-3.393158	-7.089243	-0.052992
51	6	0	-4.898828	-4.858649	0.062098
52	1	0	-5.472804	-5.781879	0.104014
53	6	0	-6.986014	-3.554490	0.216798
54	1	0	-7.559899	-4.477493	0.260260
55	6	0	-9.072662	-2.248839	0.371282
56	1	0	-9.647816	-3.170955	0.415887
57	6	0	-11.164676	-0.940876	0.526583
58	1	0	-11.736551	-1.863525	0.571513
59	6	0	-11.808383	0.285946	0.572400
60	1	0	-12.890346	0.321549	0.654538
61	6	0	-11.084948	1.475224	0.514904
62	1	0	-11.600432	2.430856	0.552520
63	6	0	-8.918606	2.654025	0.346242
64	1	0	-9.438109	3.608984	0.383344
65	6	0	-6.760928	3.832331	0.174173
66	1	0	-7.280045	4.787611	0.209670
67	6	0	-4.604989	5.011406	-0.003225
68	1	0	-5.125397	5.966212	0.031013
69	6	0	-2.452884	6.200710	-0.186119
70	1	0	-2.979387	7.150799	-0.151190
71	6	0	-1.471537	-6.209145	-0.192576
72	1	0	-0.946444	-7.159781	-0.233806
73	6	0	0.685627	-5.019084	-0.348443
74	1	0	1.205766	-5.973763	-0.389649
75	6	0	2.847989	-3.834558	-0.500040
76	1	0	3.369861	-4.788156	-0.541280
77	6	0	5.016559	-2.643484	-0.620281
78	1	0	5.529572	-3.602377	-0.664713
79	1	0	1.541934	5.771661	-0.517511
80	1	0	-0.532449	7.079388	-0.351205
81	6	0	0.968960	4.848836	-0.456598
82	6	0	-1.111531	6.161435	-0.295626
83	6	0	7.197128	0.986900	-1.007855
84	1	0	7.717010	1.921218	-1.206673
85	6	0	5.128799	2.251067	-0.796603
86	1	0	5.694161	3.174242	-0.903318
87	6	0	3.051228	3.547274	-0.620976
88	1	0	3.621383	4.470736	-0.694564
89	6	0	8.040262	-0.235344	-0.909204
90	6	0	7.267151	-1.565140	-0.624162
91	1	0	8.693157	-0.320664	-1.785664
92	1	0	7.556746	-2.339657	-1.342379
93	6	0	7.857626	-1.963466	0.786361
94	6	0	8.967725	-0.157775	0.353883
95	6	0	9.665426	1.137176	0.635739
96	7	0	8.065018	-0.633082	1.377771
97	6	0	9.289663	-2.378804	0.431608
98	8	0	9.953378	-1.222371	0.173909
99	8	0	9.770562	-3.471714	0.340971
100	6	0	7.131458	-2.964474	1.646173
101	1	0	6.112255	-2.635443	1.856217
102	1	0	7.105694	-3.936293	1.146059
103	1	0	7.667729	-3.097481	2.591050

104	6	0	8.991370	2.143710	1.332263
105	6	0	10.960324	1.360431	0.169105
106	6	0	11.579379	2.586085	0.399873
107	6	0	9.615603	3.366432	1.560574
108	6	0	10.909067	3.589805	1.093980
109	1	0	11.481009	0.570070	-0.361206
110	1	0	12.588913	2.754733	0.038111
111	1	0	7.980204	1.959749	1.685341
112	1	0	9.090961	4.145596	2.104901
113	1	0	11.393979	4.544610	1.272769
114	1	0	8.554024	-0.700175	2.273198

0 imaginary frequencies

Zero-point correction=	0.860266 (Hartree/Particle)
Thermal correction to Energy=	0.909553
Thermal correction to Enthalpy=	0.910497
Thermal correction to Gibbs Free Energy=	0.783162
Sum of electronic and zero-point Energies=	-3270.657867
Sum of electronic and thermal Energies=	-3270.608580
Sum of electronic and thermal Enthalpies=	-3270.607636
Sum of electronic and thermal Free Energies=	-3270.734970

G-MPO-a



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	7.322983	1.388923	-0.078259
2	6	0	7.588156	2.792935	-0.076210
3	6	0	4.908998	1.848230	-0.070613
4	6	0	5.183992	3.261031	-0.064084
5	6	0	2.493579	2.310651	-0.070164
6	6	0	8.405614	0.456217	-0.083191
7	6	0	5.723348	-0.475597	-0.074485
8	6	0	6.818585	-1.410526	-0.075107
9	6	0	4.127152	-2.342868	-0.063342
10	6	0	5.987070	0.921358	-0.074224
11	6	0	3.314375	-0.014255	-0.075435
12	6	0	3.578516	1.385599	-0.068885
13	6	0	0.902301	0.451112	-0.090641
14	6	0	4.395669	-0.942960	-0.068035
15	6	0	1.721290	-1.878313	-0.062199
16	6	0	1.983166	-0.478127	-0.068851
17	6	0	-0.686456	-1.416521	-0.057280
18	6	0	2.778870	3.724835	-0.053501
19	6	0	0.071642	2.786684	-0.108382
20	1	0	-0.555798	-7.606132	0.051605
21	6	0	-0.350640	-6.537930	0.032632
22	6	0	1.167150	1.855586	-0.084594
23	6	0	-1.512500	0.914860	-0.120969
24	6	0	-1.244865	2.328677	-0.170047
25	6	0	-3.934207	1.357838	-0.105425
26	6	0	-0.425792	-0.014152	-0.081162
27	6	0	-3.095809	-0.964501	-0.039353
28	6	0	-2.829097	0.435070	-0.088120
29	6	0	-5.520227	-0.504693	0.001048
30	6	0	5.229362	-3.277800	-0.059830
31	6	0	2.532356	-4.214147	-0.035735
32	6	0	3.643586	-5.147611	-0.033616
33	6	0	0.940388	-6.097807	0.006865
34	6	0	2.807116	-2.806709	-0.049443
35	6	0	0.128303	-3.748686	-0.019833
36	6	0	0.394019	-2.344403	-0.038662
37	6	0	-2.276289	-3.290504	0.005671
38	6	0	1.223218	-4.674170	-0.014628
39	6	0	-1.466238	-5.632555	0.037998
40	6	0	-1.191175	-4.213604	0.010110
41	6	0	-3.873795	-5.170882	0.078028
42	6	0	-2.014053	-1.889532	-0.025607
43	6	0	-4.683508	-2.832147	0.044362
44	6	0	-4.422636	-1.434927	0.004043
45	6	0	-7.102250	-2.372616	0.088592
46	6	0	-3.604117	-3.756455	0.043552
47	6	0	-6.278983	-4.707064	0.123797
48	6	0	-6.017791	-3.302340	0.085930

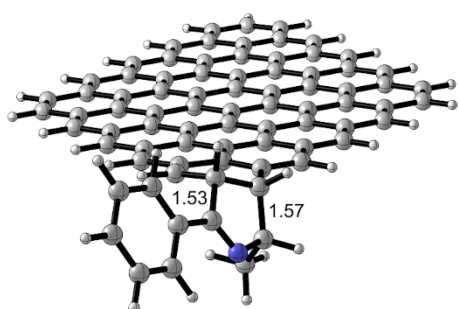
49	1	0	1.853720	-8.078534	0.017394
50	1	0	-2.972185	-7.142134	0.095193
51	6	0	1.658909	4.632238	-0.028840
52	1	0	1.869707	5.699581	0.010925
53	6	0	4.078166	4.165821	-0.051869
54	1	0	4.282638	5.234135	-0.039853
55	6	0	6.498844	3.698372	-0.067666
56	1	0	6.705683	4.766238	-0.063827
57	6	0	8.926701	3.230626	-0.081292
58	1	0	9.130617	4.297768	-0.079966
59	6	0	9.973339	2.316473	-0.087783
60	1	0	10.998003	2.675159	-0.091833
61	6	0	9.724919	0.949073	-0.088397
62	1	0	10.550130	0.242442	-0.092707
63	6	0	8.119541	-0.930821	-0.081141
64	1	0	8.947887	-1.635752	-0.083329
65	6	0	6.521667	-2.806725	-0.068424
66	1	0	7.349708	-3.512073	-0.068216
67	6	0	4.926028	-4.682500	-0.047312
68	1	0	5.755304	-5.386648	-0.046889
69	6	0	3.337325	-6.566893	-0.016245
70	1	0	4.170895	-7.264118	-0.018315
71	6	0	2.067354	-7.013097	0.002986
72	6	0	-2.768684	-6.073874	0.071405
73	6	0	-3.638717	2.765621	-0.209128
74	1	0	-4.486285	3.442158	-0.255907
75	6	0	-5.223682	0.892095	-0.055352
76	1	0	-6.050465	1.598839	-0.067094
77	6	0	-6.819079	-0.985060	0.045287
78	1	0	-7.648435	-0.281350	0.045125
79	6	0	-8.419866	-2.867758	0.131938
80	1	0	-9.246608	-2.162932	0.134979
81	6	0	-8.664775	-4.235395	0.170161
82	1	0	-9.688214	-4.596056	0.203202
83	6	0	-7.616227	-5.147152	0.165802
84	1	0	-7.817345	-6.214427	0.195042
85	6	0	-5.188507	-5.610216	0.117382
86	1	0	-5.392939	-6.678192	0.144801
87	1	0	-2.131559	4.899943	-1.603684
88	1	0	-0.465462	6.100077	-0.483239
89	6	0	-2.372867	3.245215	-0.274475
90	6	0	0.373751	4.204332	-0.046993
91	6	0	-2.092987	4.721048	-0.522351
92	6	0	-0.751827	5.187893	0.053198
93	6	0	-1.158220	5.640264	1.486159
94	6	0	-3.028234	5.658247	0.248344
95	6	0	-4.389330	6.028063	-0.206538
96	7	0	-2.528147	6.139395	1.320281
97	6	0	-1.122770	4.552978	2.558355
98	1	0	-1.773166	3.714549	2.292156
99	1	0	-0.103648	4.177407	2.690918
100	1	0	-1.472451	4.965817	3.508078
101	1	0	-0.523112	6.471583	1.813135
102	6	0	-5.206109	6.809006	0.621083
103	6	0	-4.865867	5.642936	-1.463381
104	6	0	-6.136265	6.025558	-1.885807
105	6	0	-6.472907	7.188697	0.199096
106	6	0	-6.941893	6.798670	-1.055667
107	1	0	-4.249362	5.028954	-2.114377
108	1	0	-6.494322	5.717683	-2.863224
109	1	0	-4.821895	7.107593	1.590922
110	1	0	-7.099642	7.791802	0.848903

111	1	0	-7.932994	7.097226	-1.383391
-----	---	---	-----------	----------	-----------

0 imaginary frequencies

Zero-point correction=	0.844736 (Hartree/Particle)
Thermal correction to Energy=	0.891983
Thermal correction to Enthalpy=	0.892927
Thermal correction to Gibbs Free Energy=	0.770412
Sum of electronic and zero-point Energies=	-3082.197239
Sum of electronic and thermal Energies=	-3082.149993
Sum of electronic and thermal Enthalpies=	-3082.149049
Sum of electronic and thermal Free Energies=	-3082.271564

G-MPO-c



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	8.717222	-0.316350	0.077486
2	6	0	9.492570	0.884142	0.062418
3	6	0	6.659224	1.018739	0.013336
4	6	0	7.443368	2.224567	-0.001576
5	6	0	4.600191	2.355393	-0.048492
6	6	0	9.367128	-1.588957	0.118641
7	6	0	6.529997	-1.440853	0.067742
8	6	0	7.191619	-2.720188	0.109299
9	6	0	4.346098	-2.569611	0.055786
10	6	0	7.304482	-0.245207	0.051870
11	6	0	4.476819	-0.105440	0.003600
12	6	0	5.250513	1.091872	-0.013885
13	6	0	2.423415	1.229786	-0.059560
14	6	0	5.127310	-1.373692	0.039068
15	6	0	2.293670	-1.233259	-0.012133
16	6	0	3.070319	-0.035523	-0.030637
17	6	0	0.241232	0.103403	-0.081671
18	6	0	5.389991	3.563591	-0.062910
19	6	0	2.537093	3.694310	-0.107566
20	6	0	3.336321	4.904098	-0.120211
21	6	0	0.470205	5.043736	-0.162290
22	6	0	3.197823	2.426423	-0.076144
23	6	0	0.365363	2.564892	-0.120465
24	6	0	1.147033	3.762062	-0.131566
25	6	0	-1.704741	3.908909	-0.173011
26	6	0	1.014080	1.299996	-0.094536
27	6	0	-1.809864	1.439187	-0.146160
28	6	0	-1.040851	2.631756	-0.148148
29	6	0	-3.874228	2.775254	-0.192571
30	6	0	5.013948	-3.850840	0.098053
31	6	0	2.162347	-3.701740	0.037627
32	6	0	2.838833	-4.984777	0.083017
33	6	0	-0.022418	-4.845235	0.011386
34	6	0	2.950751	-2.502753	0.022726
35	6	0	0.110576	-2.363720	-0.039370
36	6	0	0.893187	-1.164157	-0.052466
37	6	0	-1.945192	-1.026344	-0.121777
38	6	0	0.776901	-3.634153	0.001755
39	6	0	-2.073776	-3.505522	-0.078900
40	6	0	-1.282625	-2.294421	-0.082418
41	6	0	-4.129472	-2.170191	-0.182548
42	6	0	-1.163523	0.174246	-0.122283
43	6	0	-3.999167	0.314041	-0.201006
44	6	0	-3.224982	1.507821	-0.178038
45	6	0	-6.042896	1.650680	-0.221766

46	6	0	-3.339648	-0.955182	-0.171763
47	6	0	-6.195736	-0.838090	-0.335182
48	6	0	-5.405018	0.392554	-0.246450
49	6	0	2.636479	6.175854	-0.154810
50	1	0	3.235180	7.082725	-0.164012
51	6	0	4.699566	4.822962	-0.099165
52	1	0	5.293605	5.734274	-0.108195
53	6	0	6.765258	3.477665	-0.039924
54	1	0	7.359289	4.388765	-0.049686
55	6	0	8.830339	2.131111	0.022905
56	1	0	9.425634	3.041332	0.012375
57	6	0	10.900872	0.782300	0.088214
58	1	0	11.492993	1.693075	0.077142
59	6	0	11.521256	-0.456826	0.127422
60	1	0	12.605252	-0.513813	0.147000
61	6	0	10.771853	-1.631253	0.142889
62	1	0	11.269193	-2.596666	0.175110
63	6	0	8.575843	-2.766483	0.133890
64	1	0	9.077063	-3.731318	0.166956
65	6	0	6.388232	-3.901294	0.124351
66	1	0	6.888897	-4.866433	0.158553
67	6	0	4.202139	-5.037015	0.112292
68	1	0	4.704067	-6.001621	0.148351
69	6	0	2.019284	-6.183228	0.095763
70	1	0	2.527321	-7.143207	0.134095
71	6	0	1.291092	6.241439	-0.173819
72	1	0	0.783788	7.202243	-0.199876
73	6	0	-0.895242	5.094926	-0.180055
74	1	0	-1.397498	6.059775	-0.203454
75	6	0	-3.086598	3.954335	-0.190875
76	1	0	-3.589846	4.918675	-0.207064
77	6	0	-5.284833	2.808107	-0.202162
78	1	0	-5.786103	3.774480	-0.191685
79	1	0	-1.978332	-5.675945	-0.023522
80	1	0	0.074686	-7.023497	0.070546
81	6	0	-1.383772	-4.764967	-0.028161
82	6	0	0.674861	-6.117630	0.061769
83	6	0	-7.543185	-0.787928	-0.535845
84	1	0	-8.099648	-1.718889	-0.626571
85	6	0	-5.500824	-2.090692	-0.260434
86	1	0	-6.088618	-3.005304	-0.290838
87	6	0	-3.444336	-3.423808	-0.128212
88	1	0	-4.036845	-4.335938	-0.130949
89	6	0	-8.302643	0.496780	-0.665139
90	6	0	-7.544244	1.724637	-0.132428
91	1	0	-8.617128	0.636102	-1.710325
92	1	0	-7.887031	2.603276	-0.689533
93	6	0	-8.103515	1.867242	1.323485
94	6	0	-9.524315	0.491976	0.259916
95	6	0	-10.709637	-0.353769	-0.003462
96	7	0	-9.422967	1.231113	1.292594
97	6	0	-7.263656	1.209422	2.417002
98	1	0	-7.102576	0.149821	2.195689
99	1	0	-6.289998	1.698710	2.508826
100	1	0	-7.788849	1.284819	3.372478
101	6	0	-10.833246	-1.070814	-1.197188
102	6	0	-11.724450	-0.448275	0.956915
103	6	0	-12.837273	-1.244154	0.723786
104	6	0	-11.949987	-1.869135	-1.429282
105	6	0	-12.953135	-1.957670	-0.469951
106	1	0	-11.614342	0.111030	1.880390
107	1	0	-13.617899	-1.314445	1.475137

108	1	0	-10.057309	-1.008699	-1.954926
109	1	0	-12.034276	-2.420551	-2.360611
110	1	0	-13.823484	-2.581572	-0.649578
111	1	0	-8.232458	2.926604	1.574029

0 imaginary frequencies

Zero-point correction=	0.844494 (Hartree/Particle)
Thermal correction to Energy=	0.891972
Thermal correction to Enthalpy=	0.892917
Thermal correction to Gibbs Free Energy=	0.769151
Sum of electronic and zero-point Energies=	-3082.171730
Sum of electronic and thermal Energies=	-3082.124251
Sum of electronic and thermal Enthalpies=	-3082.123307
Sum of electronic and thermal Free Energies=	-3082.247073