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New Journal of Chemistry

Supporting Information

Condensation Mechanism of Cage Hexabenzylhexaazaisowurtzitane from Glyoxal and Benzylamine: A Computational Study

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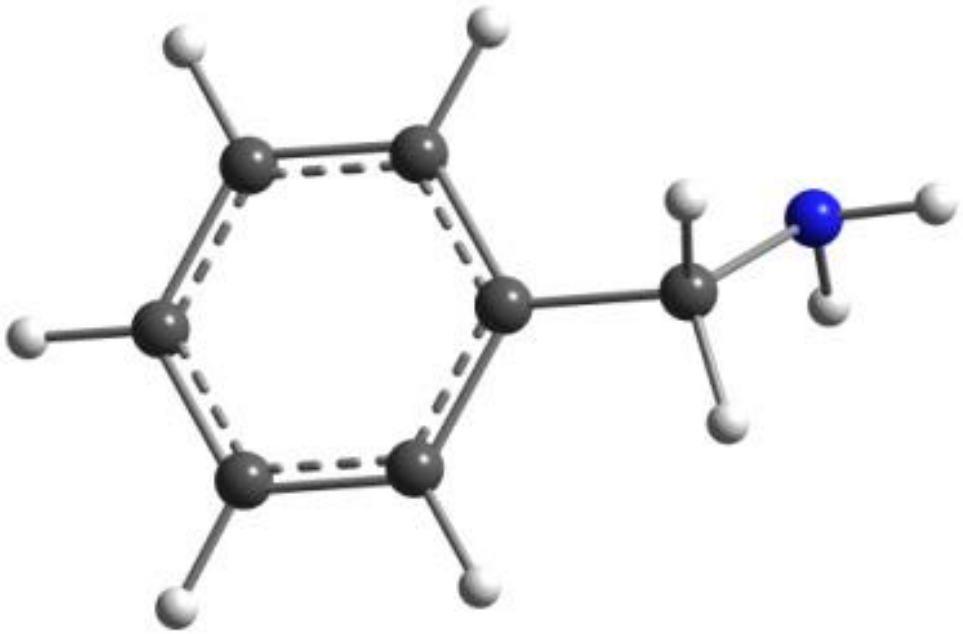
Figure 1

benzylamine:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.774882	1.088809	0.155841
2	6	0	-0.404108	1.269381	-0.044440
3	6	0	0.439667	0.174205	-0.237971
4	6	0	-0.111766	-1.112925	-0.223661
5	6	0	-1.477511	-1.298146	-0.025027
6	6	0	-2.314481	-0.195479	0.165566
7	1	0	-2.417371	1.951081	0.307300
8	1	0	0.013743	2.273253	-0.047836
9	1	0	0.542268	-1.969250	-0.366558
10	1	0	-1.892149	-2.301874	-0.020676
11	1	0	-3.379222	-0.339991	0.321216
12	6	0	1.923459	0.365602	-0.456418
13	7	0	2.697443	-0.363752	0.554717
14	1	0	3.690880	-0.264897	0.364763
15	1	0	2.535332	0.046611	1.471111

16	1	0	2.141588	1.442737	-0.479673
17	1	0	2.200564	-0.040087	-1.435999

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free energy = -326.653967 A.U.

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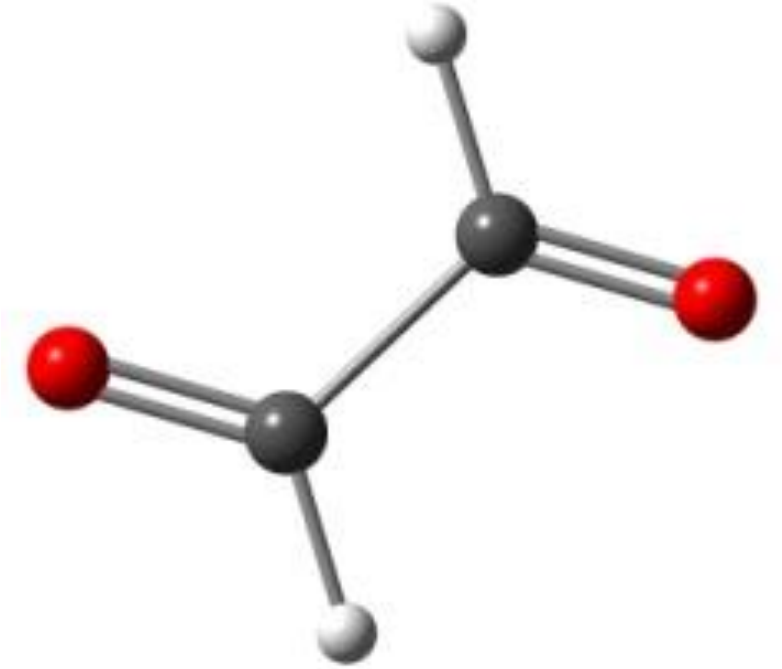

Standard orientation

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1	6	0	0.651591	0.396447	-0.000204
2	8	0	1.714909	-0.172743	0.000242
3	1	0	0.548340	1.495386	-0.000057
4	6	0	-0.651589	-0.396446	-0.000723
5	8	0	-1.714911	0.172741	0.000352
6	1	0	-0.548335	-1.495379	0.000871

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free energy = -227.715472 A.U.

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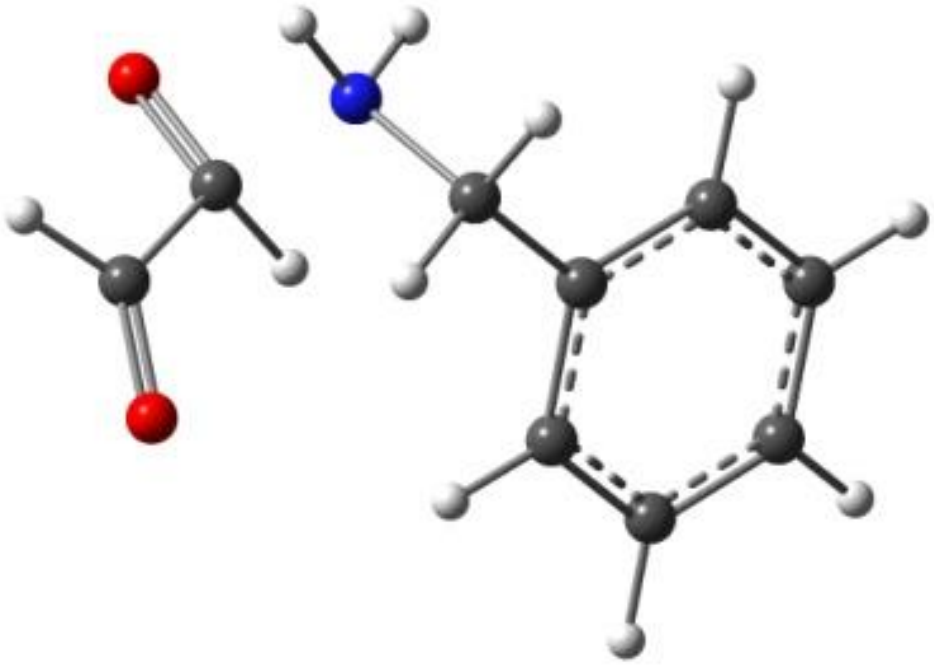

Standard orientation

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1	6	0	3.087734	-0.819691	0.335840
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3	6	0	0.946704	-0.248875	-0.641903
4	6	0	1.150236	1.087937	-0.288314
5	6	0	2.316571	1.468968	0.373549
6	6	0	3.284692	0.515435	0.688626
7	1	0	3.842157	-1.563634	0.571436
8	1	0	1.779734	-2.237680	-0.620227
9	1	0	0.386519	1.824940	-0.525107
10	1	0	2.468666	2.509249	0.643427
11	1	0	4.192186	0.812473	1.204886
12	6	0	-0.318352	-0.673167	-1.343734
13	7	0	-1.311279	-1.230485	-0.376481
14	1	0	-2.088995	-1.679668	-0.867713
15	1	0	-0.888051	-1.963613	0.199969
16	1	0	-0.112428	-1.445846	-2.088041
17	1	0	-0.793921	0.172059	-1.845412
18	6	0	-2.005082	-0.228438	0.760233
19	8	0	-2.756809	-0.928974	1.532840
20	1	0	-1.096598	0.253940	1.171740
21	6	0	-2.762126	0.784452	-0.110319
22	8	0	-2.299515	1.843036	-0.473075

23	1	0	-3.806877	0.491741	-0.341463

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free energy = -554.367125 A.U.

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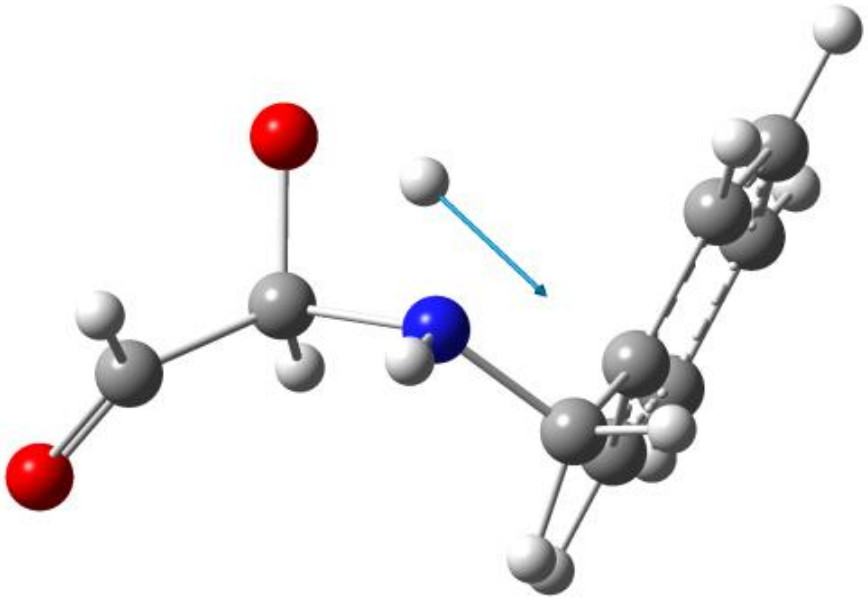

Standard orientation

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3	6	0	-1.035559	-0.088615	0.761237
4	6	0	-1.466384	1.225891	0.574782
5	6	0	-2.603944	1.494899	-0.187917
6	6	0	-3.314930	0.448384	-0.771858
7	1	0	-3.441002	-1.687354	-1.040558
8	1	0	-1.430587	-2.162328	0.322302
9	1	0	-0.912010	2.043487	1.028963
10	1	0	-2.931317	2.520558	-0.325623
11	1	0	-4.198981	0.657116	-1.366114
12	6	0	0.193974	-0.387964	1.583389
13	7	0	1.289022	-0.916722	0.732979
14	1	0	2.048672	-1.291006	1.306703
15	1	0	1.103333	-1.591516	-0.261277
16	1	0	-0.016238	-1.154945	2.332750
17	1	0	0.546568	0.508465	2.100642

18	6	0	1.784671	-0.081898	-0.434201
19	8	0	1.589474	-1.027769	-1.407451
20	1	0	1.181924	0.836188	-0.502104
21	6	0	3.254209	0.274104	-0.280552
22	8	0	3.671735	1.408858	-0.278089
23	1	0	3.938332	-0.596943	-0.230063

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free energy = -554.340829 A.U.

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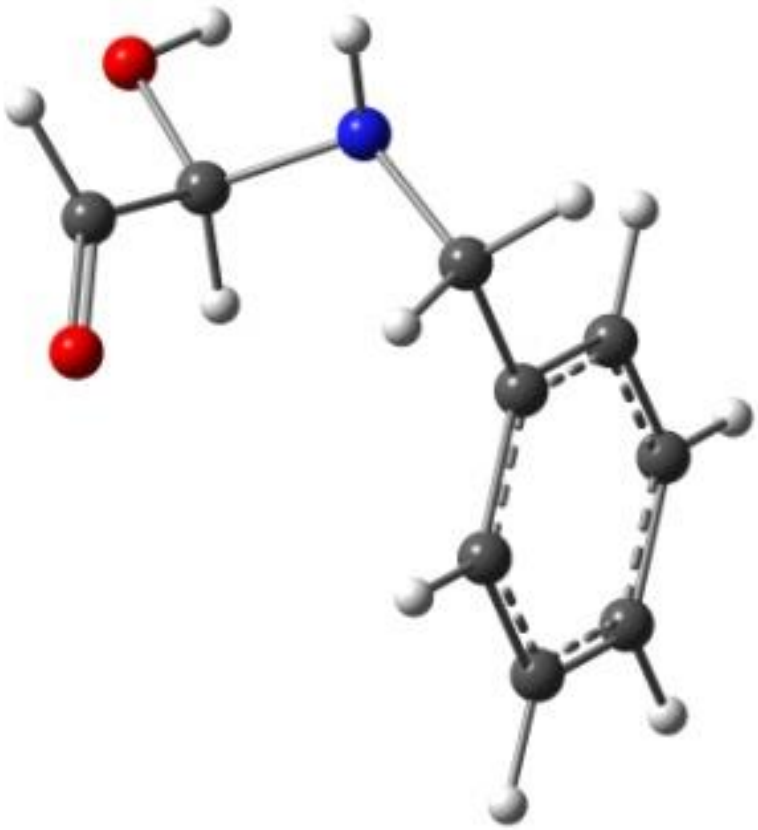

Standard orientation

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1	6	0	-2.827886	-1.124618	-0.269666
2	6	0	-1.623466	-1.147248	0.429448
3	6	0	-0.925730	0.039131	0.681668
4	6	0	-1.450604	1.246047	0.216557
5	6	0	-2.658740	1.273250	-0.483646
6	6	0	-3.349270	0.087932	-0.728087
7	1	0	-3.362127	-2.051200	-0.457015

8	1	0	-1.213816	-2.089370	0.784684
9	1	0	-0.907746	2.170346	0.399518
10	1	0	-3.054239	2.218741	-0.841975
11	1	0	-4.287006	0.105800	-1.274777
12	6	0	0.376166	0.006240	1.452064
13	7	0	1.355454	-0.875431	0.807600
14	1	0	2.131221	-1.080619	1.435137
15	1	0	2.052917	-2.237285	-1.074406
16	1	0	0.202982	-0.400796	2.452913
17	1	0	0.747407	1.034445	1.576812
18	6	0	1.852778	-0.413526	-0.475850
19	8	0	2.587500	-1.431204	-1.100348
20	1	0	0.996259	-0.076266	-1.073675
21	6	0	2.804529	0.748929	-0.265165
22	8	0	2.433708	1.901983	-0.262261
23	1	0	3.849642	0.471167	-0.023479

SCF Done: E(RM062X) = -554.561152884 A.U.

free energy = -554.392997 A.U.

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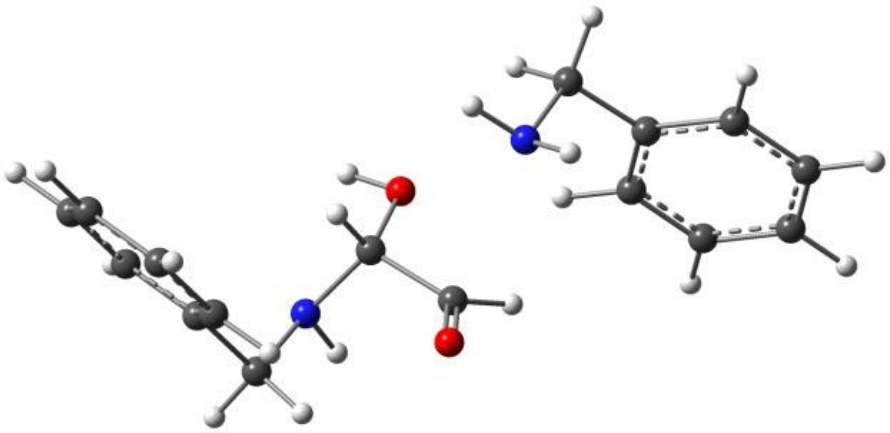

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.201021	0.422027	-1.188605
2	6	0	-4.315523	-0.612255	-0.892690
3	6	0	-3.606962	-0.617833	0.313634
4	6	0	-3.795133	0.431751	1.214748
5	6	0	-4.682464	1.469557	0.923081
6	6	0	-5.386420	1.466703	-0.279669

7	1	0	-5.749899	0.413537	-2.125504
8	1	0	-4.167231	-1.424700	-1.599837
9	1	0	-3.232386	0.438437	2.144922
10	1	0	-4.818279	2.279938	1.632747
11	1	0	-6.076466	2.272653	-0.509945
12	6	0	-2.641518	-1.737611	0.631227
13	7	0	-1.534219	-1.779445	-0.331382
14	1	0	-0.982220	-2.625206	-0.194671
15	1	0	-0.324305	-1.023138	-2.197062
16	1	0	-3.154907	-2.701195	0.552935
17	1	0	-2.295062	-1.627460	1.668019
18	6	0	-0.654396	-0.618365	-0.346560
19	8	0	0.210616	-0.724843	-1.448316
20	1	0	-1.281081	0.282023	-0.387417
21	6	0	0.194803	-0.569595	0.913648
22	8	0	-0.272312	-0.223376	1.980284
23	1	0	1.210250	-0.996967	0.825753
24	6	0	4.592402	-1.409938	-0.133247
25	6	0	3.546301	-0.644152	-0.645390
26	6	0	3.569304	0.751287	-0.542887
27	6	0	4.660526	1.365380	0.077873
28	6	0	5.708882	0.602355	0.594673
29	6	0	5.676235	-0.787776	0.490145
30	1	0	4.564988	-2.492076	-0.221218
31	1	0	2.694588	-1.119383	-1.126824
32	1	0	4.690647	2.450220	0.154669
33	1	0	6.550437	1.093088	1.074299
34	1	0	6.491843	-1.383638	0.888442
35	6	0	2.410317	1.573774	-1.052433
36	7	0	1.371186	1.668533	-0.017004
37	1	0	1.734687	2.163478	0.794927
38	1	0	0.588746	2.218936	-0.364499
39	1	0	1.959276	1.074519	-1.914296
40	1	0	2.779181	2.557206	-1.377769

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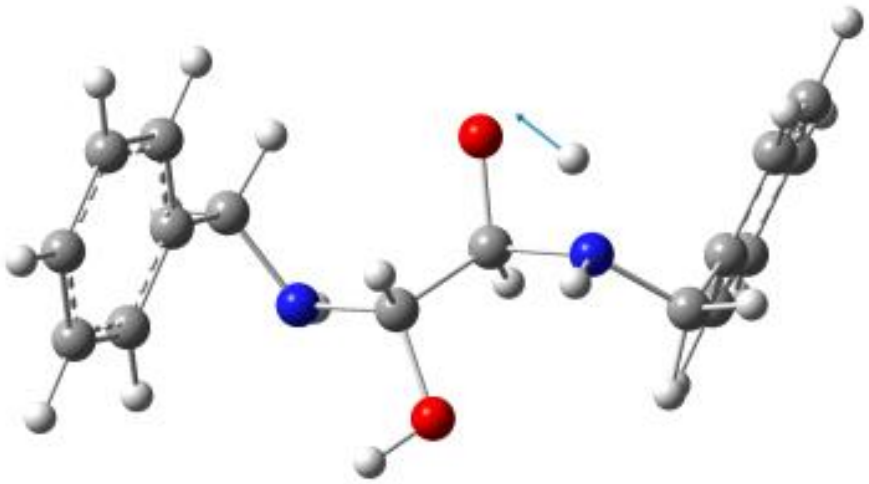

Standard orientation

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1	6	0	-5.196782	1.475551	-0.009008
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3	6	0	-3.636771	-0.249170	-0.690633
4	6	0	-4.076159	-1.047718	0.366848
5	6	0	-5.069669	-0.590581	1.233890
6	6	0	-5.630103	0.671872	1.047416
7	1	0	-5.633844	2.457583	-0.160404
8	1	0	-3.872703	1.640558	-1.698816
9	1	0	-3.639383	-2.032706	0.512769
10	1	0	-5.402754	-1.220009	2.053087
11	1	0	-6.402949	1.029330	1.720642
12	6	0	-2.557398	-0.733814	-1.627701
13	7	0	-1.285016	-0.009695	-1.402583
14	1	0	-0.615110	-0.226037	-2.143049
15	1	0	-1.224249	1.139172	-1.011000
16	1	0	-2.844392	-0.557636	-2.667526
17	1	0	-2.378062	-1.804710	-1.495088
18	6	0	-0.640603	-0.064652	-0.027313
19	8	0	-0.604868	1.290659	0.194078
20	1	0	-1.308866	-0.637604	0.640516
21	6	0	0.715379	-0.760202	-0.077402
22	8	0	0.466487	-2.063751	-0.574335
23	1	0	1.375909	-0.200642	-0.758501
24	6	0	5.184817	1.545728	-0.526962
25	6	0	3.984837	1.524415	0.186634
26	6	0	3.493816	0.331547	0.722424

27	6	0	4.219168	-0.847710	0.520358
28	6	0	5.415862	-0.831312	-0.193560
29	6	0	5.903845	0.367192	-0.718987
30	1	0	5.552187	2.481347	-0.937804
31	1	0	3.422311	2.444518	0.326657
32	1	0	3.833080	-1.779421	0.924108
33	1	0	5.968896	-1.754297	-0.341203
34	1	0	6.834517	0.379724	-1.277802
35	6	0	2.214311	0.323366	1.534709
36	7	0	1.373469	-0.830860	1.206210
37	1	0	1.264622	-2.584662	-0.411489
38	1	0	0.696026	-1.002596	1.945297
39	1	0	1.686805	1.275849	1.394365
40	1	0	2.465859	0.239554	2.597621

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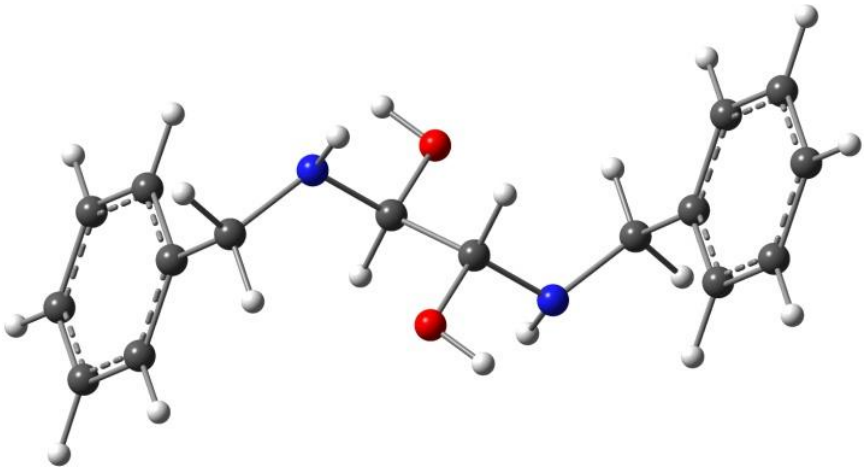

Standard orientation

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3	6	0	3.571623	0.302122	-0.674487
4	6	0	4.220052	1.319042	0.030022
5	6	0	5.375627	1.052442	0.767126
6	6	0	5.891169	-0.241649	0.812406
7	1	0	5.639733	-2.277277	0.149806
8	1	0	3.585721	-1.791187	-1.157450

9	1	0	3.815569	2.328166	0.003759
10	1	0	5.867071	1.854486	1.309622
11	1	0	6.787049	-0.453901	1.387715
12	6	0	2.340828	0.606570	-1.504390
13	7	0	1.299322	-0.406009	-1.320110
14	1	0	0.616764	-0.359317	-2.072026
15	1	0	1.013208	-2.299080	0.043237
16	1	0	2.611963	0.590470	-2.565657
17	1	0	1.987662	1.619849	-1.272458
18	6	0	0.645838	-0.409819	-0.031480
19	8	0	0.281031	-1.732635	0.321440
20	1	0	1.355153	0.002065	0.703756
21	6	0	-0.645866	0.410346	0.031655
22	8	0	-0.281010	1.733198	-0.321123
23	1	0	-1.355140	-0.001448	-0.703674
24	6	0	-5.375723	-1.053116	-0.766680
25	6	0	-4.220121	-1.319396	-0.029506
26	6	0	-3.571576	-0.302139	0.674421
27	6	0	-4.093392	0.995073	0.619083
28	6	0	-5.244716	1.265820	-0.117748
29	6	0	-5.891190	0.240984	-0.812611
30	1	0	-5.867243	-1.855415	-1.308729
31	1	0	-3.815687	-2.328523	-0.002748
32	1	0	-3.585561	1.791412	1.156339
33	1	0	-5.639589	2.276942	-0.151107
34	1	0	-6.787090	0.452998	-1.387976
35	6	0	-2.340772	-0.606313	1.504408
36	7	0	-1.299461	0.406467	1.320219
37	1	0	-1.012988	2.299663	-0.042450
38	1	0	-0.616924	0.359875	2.072162
39	1	0	-1.987393	-1.619522	1.272504
40	1	0	-2.612013	-0.590283	2.565652

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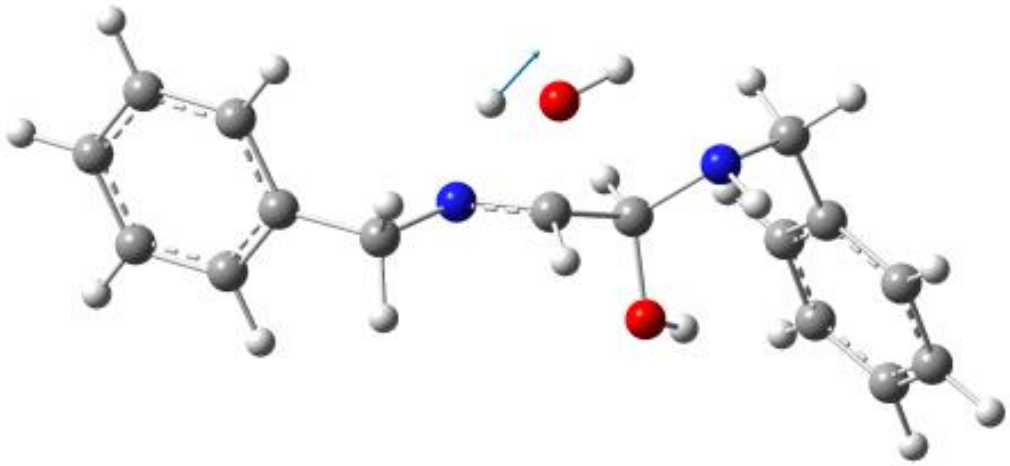


Standard orientation

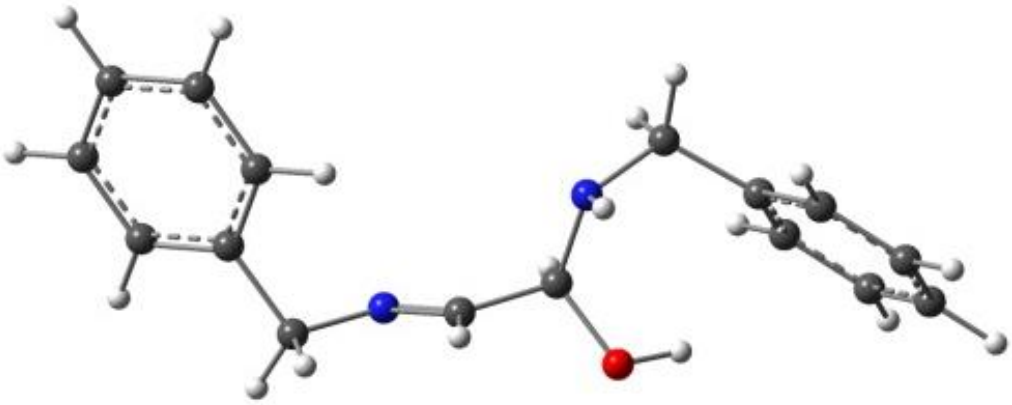
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.274818	2.038069	-0.020577
2	6	0	-4.168603	1.464350	-0.647189
3	6	0	-3.886563	0.103407	-0.496254
4	6	0	-4.733928	-0.673309	0.299336
5	6	0	-5.842245	-0.106181	0.928862
6	6	0	-6.115501	1.252835	0.769620
7	1	0	-5.482698	3.095940	-0.151440
8	1	0	-3.514915	2.077264	-1.263537
9	1	0	-4.523336	-1.733642	0.422869
10	1	0	-6.492849	-0.724298	1.540382
11	1	0	-6.979151	1.696964	1.255050
12	6	0	-2.664408	-0.506727	-1.138339
13	7	0	-1.511416	-0.388649	-0.235698
14	1	0	-2.463242	0.014729	-2.085899
15	1	0	-2.890762	-1.556963	-1.393144
16	6	0	-0.410884	-1.091051	-0.669320
17	1	0	-0.344249	-1.427198	-1.711209
18	6	0	0.932127	-0.596225	-0.125863
19	8	0	1.384012	0.306882	-1.119049
20	1	0	0.730570	-0.071143	0.818543
21	6	0	4.443919	2.113230	0.746417
22	6	0	3.665465	1.044153	1.195784
23	6	0	3.829820	-0.235101	0.654240
24	6	0	4.798717	-0.430354	-0.337319
25	6	0	5.579344	0.632746	-0.785578
26	6	0	5.400721	1.909020	-0.246552
27	1	0	4.303616	3.100920	1.174422

28	1	0	2.921987	1.205223	1.973420
29	1	0	4.938042	-1.422147	-0.762101
30	1	0	6.328325	0.468157	-1.553954
31	1	0	6.008129	2.737886	-0.596011
32	6	0	2.932518	-1.376917	1.088738
33	7	0	1.831380	-1.691178	0.166324
34	1	0	2.109599	0.833807	-0.756097
35	1	0	2.489455	-1.143215	2.062578
36	1	0	3.520508	-2.291182	1.208197
37	1	0	2.187339	-2.089553	-0.701381
38	8	0	-0.716790	-2.451533	0.173291
39	1	0	-1.414416	-1.646872	0.560665
40	1	0	0.076438	-2.660353	0.714287

SCF Done: E(RM062X) = -881.283444886 A.U.

free energy = -880.981242 A.U.

IM3':



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.950327	0.106242	0.840845
2	6	0	5.011859	-0.880299	0.531553
3	6	0	3.874898	-0.568226	-0.215633
4	6	0	3.685774	0.749497	-0.645501
5	6	0	4.618845	1.736602	-0.339031
6	6	0	5.756124	1.415869	0.406080
7	1	0	6.830871	-0.150401	1.421776
8	1	0	5.165667	-1.900632	0.873474
9	1	0	2.799562	1.002329	-1.223679
10	1	0	4.461968	2.754788	-0.681876

11	1	0	6.485319	2.184039	0.644412
12	6	0	2.846499	-1.624229	-0.562349
13	7	0	1.578216	-1.330134	0.101039
14	1	0	3.194771	-2.598609	-0.207786
15	1	0	2.723469	-1.679797	-1.654554
16	6	0	0.599451	-1.009864	-0.633926
17	1	0	0.663484	-0.974724	-1.733190
18	6	0	-0.735491	-0.627505	-0.046223
19	8	0	-1.679501	-1.487163	-0.681921
20	1	0	-0.713387	-0.806008	1.036131
21	6	0	-5.170143	-0.619948	1.148602
22	6	0	-3.912450	-0.043391	1.344232
23	6	0	-3.382322	0.847481	0.405094
24	6	0	-4.141908	1.165852	-0.727268
25	6	0	-5.397490	0.596029	-0.924215
26	6	0	-5.912927	-0.302984	0.012666
27	1	0	-5.566842	-1.313428	1.883553
28	1	0	-3.335968	-0.291601	2.232792
29	1	0	-3.742535	1.863087	-1.460623
30	1	0	-5.975650	0.852480	-1.806540
31	1	0	-6.890245	-0.749465	-0.141088
32	6	0	-1.982793	1.411682	0.569472
33	7	0	-0.950076	0.781834	-0.260418
34	1	0	-2.551407	-1.336958	-0.290396
35	1	0	-1.670435	1.316486	1.614966
36	1	0	-1.984133	2.478202	0.326169
37	1	0	-1.105009	0.968768	-1.248916

SCF Done: E(RM062X) = -804.951196428 A.U.

free energy = -804.667817 A.U.

H_2O:

Standard orientation

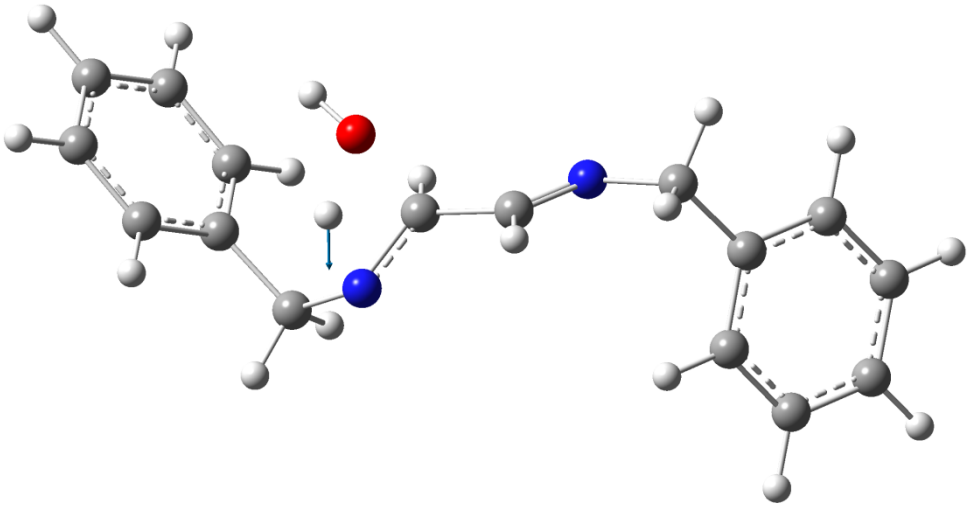
Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	8	0	0.000000	0.000000	0.116946
2	1	0	0.000000	0.766047	-0.467784
3	1	0	0.000000	-0.766047	-0.467784

SCF Done: E(RM062X) = -76.4030304541 A.U.

free energy = -76.38508 A.U.

TS4':



Standard orientation

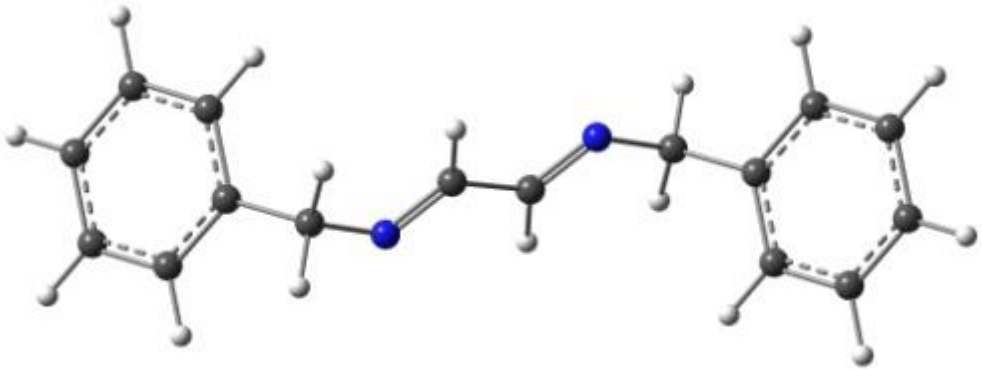
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.833270	-0.267489	1.176671
2	6	0	4.825988	-1.086358	0.662878
3	6	0	3.867612	-0.567665	-0.209409
4	6	0	3.927088	0.785452	-0.558694
5	6	0	4.929872	1.605907	-0.047930
6	6	0	5.886996	1.079406	0.822467
7	1	0	6.573592	-0.682624	1.853633
8	1	0	4.786549	-2.136533	0.940655
9	1	0	3.183091	1.196686	-1.237589
10	1	0	4.967455	2.653846	-0.329294
11	1	0	6.669902	1.717476	1.220390
12	6	0	2.762744	-1.437592	-0.769571
13	7	0	1.480379	-1.069669	-0.173000
14	1	0	2.958564	-2.483129	-0.513520
15	1	0	2.734129	-1.349722	-1.865487
16	6	0	0.596809	-0.595217	-0.946769
17	1	0	0.738277	-0.455692	-2.027380

18	6	0	-0.706239	-0.132532	-0.392551
19	8	0	-1.774923	-1.242128	-1.222880
20	1	0	-0.832203	-0.345501	0.674653
21	6	0	-4.630436	-0.573774	1.772433
22	6	0	-3.527498	0.233107	1.483070
23	6	0	-3.440918	0.915100	0.264900
24	6	0	-4.490269	0.785059	-0.654175
25	6	0	-5.593793	-0.015766	-0.368505
26	6	0	-5.663808	-0.702333	0.845869
27	1	0	-4.682153	-1.097337	2.722187
28	1	0	-2.730897	0.338437	2.216057
29	1	0	-4.434490	1.313960	-1.603304
30	1	0	-6.399145	-0.105218	-1.091125
31	1	0	-6.522011	-1.327950	1.070164
32	6	0	-2.201620	1.706469	-0.107315
33	7	0	-1.261694	0.968105	-0.974630
34	1	0	-2.509666	-1.518478	-0.647115
35	1	0	-1.686976	2.030266	0.806181
36	1	0	-2.495615	2.607878	-0.651987
37	1	0	-1.904611	-0.099047	-1.560875

SCF Done: E(RM062X) = -804.858473584 A.U.

Free energy = -804.582621 A.U.

IM4'



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.967408	-0.691668	-0.742068
2	6	0	-4.801699	-1.238387	-0.205276
3	6	0	-3.915163	-0.441239	0.522349

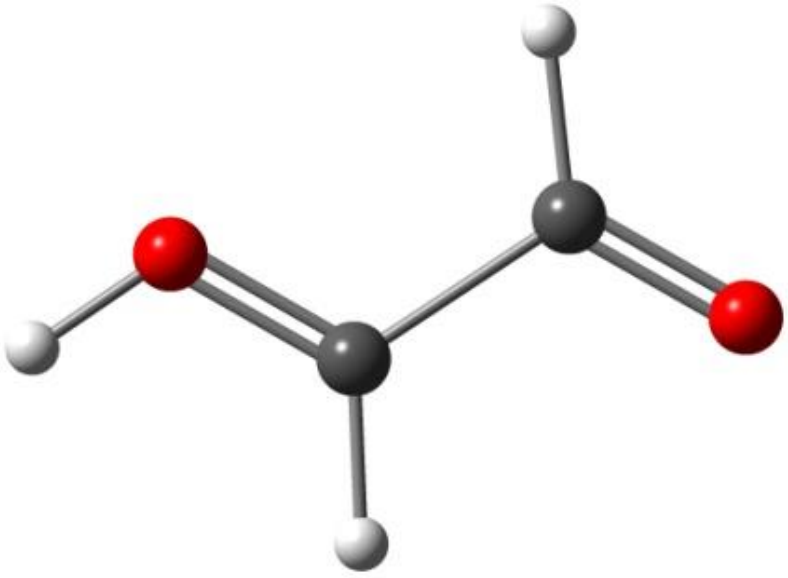
4	6	0	-4.209917	0.912690	0.704668
5	6	0	-5.374615	1.462710	0.171204
6	6	0	-6.256181	0.660055	-0.554047
7	1	0	-6.650073	-1.321163	-1.304657
8	1	0	-4.578605	-2.292384	-0.351185
9	1	0	-3.523665	1.538087	1.271418
10	1	0	-5.595377	2.514618	0.324319
11	1	0	-7.165106	1.085297	-0.968110
12	6	0	-2.627658	-1.013724	1.074456
13	7	0	-1.549374	-0.824918	0.107681
14	1	0	-2.744435	-2.091354	1.228593
15	1	0	-2.391020	-0.547508	2.041498
16	6	0	-0.557337	-0.118258	0.468766
17	1	0	-0.469470	0.341819	1.462199
18	6	0	0.557031	0.118790	-0.468674
19	1	0	0.468841	-0.341092	-1.462170
20	6	0	5.375983	-1.462196	-0.173446
21	6	0	4.211245	-0.912162	-0.706897
22	6	0	3.915215	0.441169	-0.522396
23	6	0	4.800479	1.237734	0.207467
24	6	0	5.966171	0.691018	0.744235
25	6	0	6.256255	-0.660141	0.553980
26	1	0	5.597699	-2.513652	-0.328289
27	1	0	3.526007	-1.537146	-1.275323
28	1	0	4.576336	2.291265	0.355138
29	1	0	6.647852	1.320043	1.308542
30	1	0	7.165213	-1.085322	0.968035
31	6	0	2.627648	1.013568	-1.074418
32	7	0	1.549399	0.824966	-0.107576
33	1	0	2.390959	0.547219	-2.041387
34	1	0	2.744376	2.091187	-1.228757

SCF Done: E(RM062X) = -728.533000377 A.U.

free energy = -728.27676 A.U.

Figure 2

protonized glyoxal:



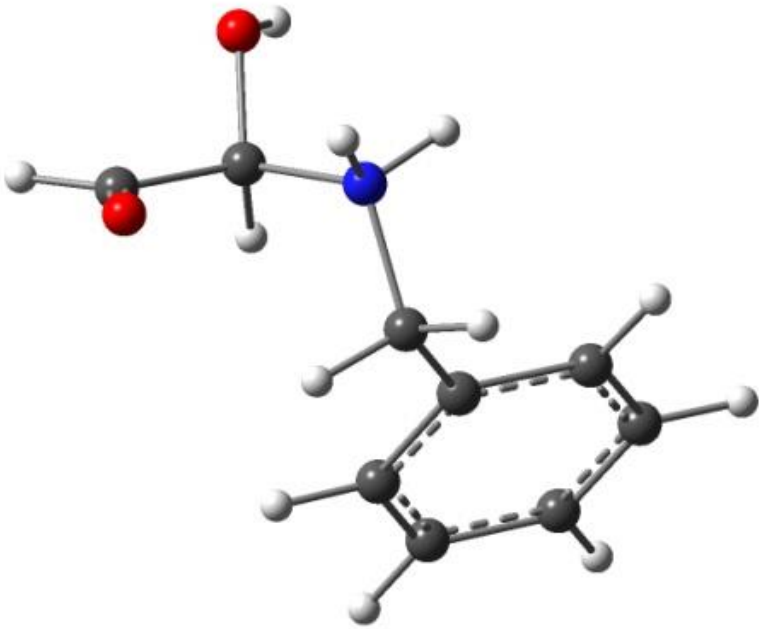
Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.546283	-0.405867	0.000207
2	8	0	-1.618913	0.225153	-0.000176
3	1	0	-0.513704	-1.498276	0.000493
4	6	0	0.734190	0.414014	0.000183
5	8	0	1.768771	-0.192704	-0.000210
6	1	0	0.627036	1.507089	0.000471
7	1	0	-2.439633	-0.317284	-0.000219

SCF Done: E(RM062X) = -228.113458971 A.U.

free energy = -228.073595 A.U.

IM1:



Standard orientation

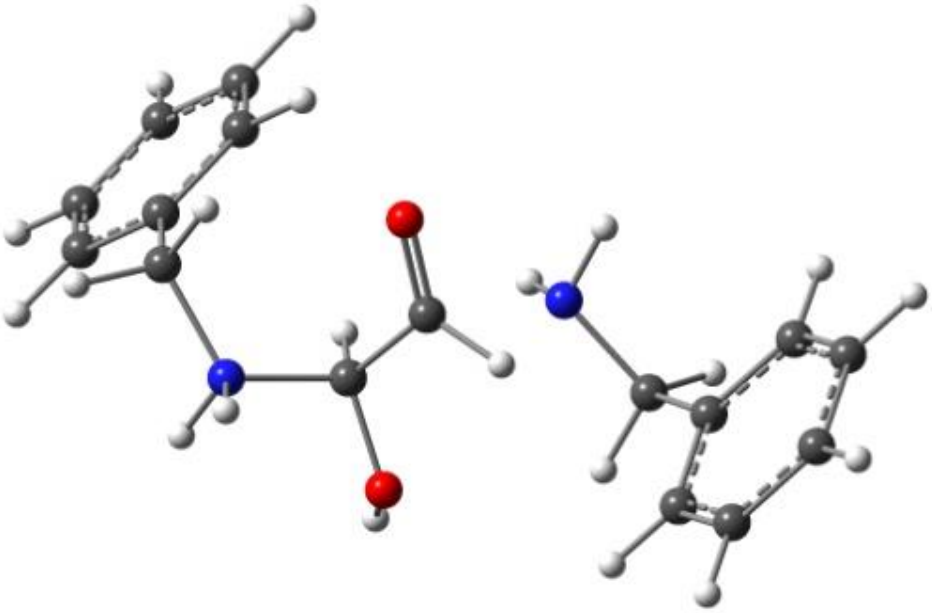
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.112209	-0.935005	0.035542
2	6	0	1.892611	-1.055644	-0.626095
3	6	0	1.005682	0.025101	-0.668351
4	6	0	1.358143	1.232192	-0.058662
5	6	0	2.581143	1.354003	0.599764
6	6	0	3.456089	0.269861	0.649829
7	1	0	3.797082	-1.776093	0.061889
8	1	0	1.637911	-1.988354	-1.124247
9	1	0	0.682014	2.082139	-0.108684
10	1	0	2.850195	2.295232	1.067761
11	1	0	4.409668	0.365848	1.159049
12	6	0	-0.314069	-0.116414	-1.375939
13	7	0	-1.316286	-0.879295	-0.530209
14	1	0	-2.146247	-1.074337	-1.105464
15	1	0	-0.923584	-1.786660	-0.253925
16	1	0	-0.221835	-0.688791	-2.300185
17	1	0	-0.771080	0.847333	-1.602968
18	6	0	-1.779970	-0.172524	0.717435
19	8	0	-2.382218	-1.079563	1.565316
20	1	0	-0.910328	0.327040	1.155933
21	6	0	-2.855564	0.838977	0.309763
22	8	0	-3.226793	0.935722	-0.832367

23	1	0	-3.280377	1.425432	1.137860
24	1	0	-1.774968	-1.366275	2.261136

SCF Done: E(RM062X) = -554.996247229 A.U.

free energy = -554.811951 A.U.

CP1:



Standard orientation

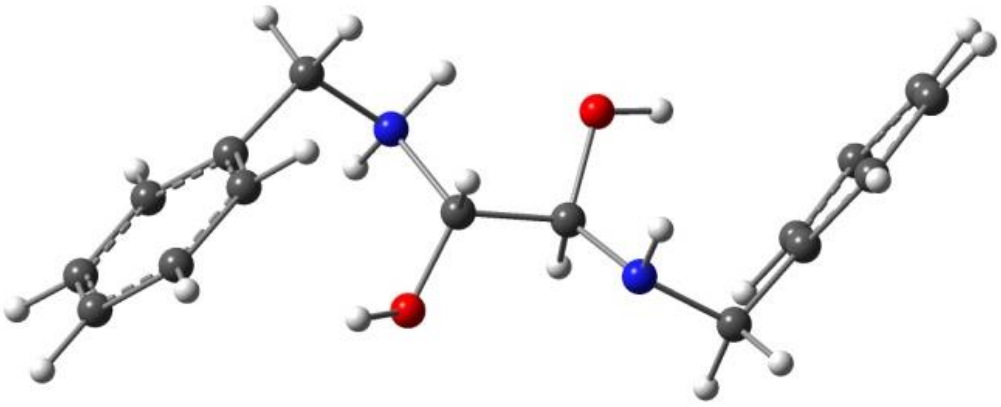
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.076395	0.654998	-0.854283
2	6	0	-4.425034	-0.518708	-0.479422
3	6	0	-3.402814	-0.481310	0.473351
4	6	0	-3.046384	0.737912	1.058790
5	6	0	-3.699839	1.910722	0.684536
6	6	0	-4.712499	1.870088	-0.274001
7	1	0	-5.872348	0.618421	-1.591015
8	1	0	-4.722112	-1.467085	-0.921076
9	1	0	-2.254348	0.763712	1.803337
10	1	0	-3.419917	2.853698	1.143031
11	1	0	-5.223001	2.783126	-0.563375
12	6	0	-2.680568	-1.743847	0.858841
13	7	0	-1.595370	-2.082964	-0.150011
14	1	0	-1.120044	-2.946540	0.138528
15	1	0	-0.104219	-1.020178	-2.335309

16	1	0	-3.345216	-2.608851	0.862489
17	1	0	-2.190059	-1.654317	1.825593
18	6	0	-0.554475	-1.005954	-0.440204
19	8	0	0.201878	-1.424902	-1.512908
20	1	0	-1.114727	-0.088880	-0.621199
21	6	0	0.363233	-0.837708	0.777161
22	8	0	-0.079048	-0.660006	1.887463
23	1	0	1.435256	-0.952499	0.556086
24	6	0	4.660220	-1.121357	-0.333660
25	6	0	3.600265	-0.473003	-0.969311
26	6	0	3.254932	0.835714	-0.620409
27	6	0	3.994417	1.488434	0.371681
28	6	0	5.050332	0.842697	1.013357
29	6	0	5.385159	-0.465540	0.661220
30	1	0	4.918736	-2.137779	-0.614683
31	1	0	3.028206	-0.987978	-1.737132
32	1	0	3.744963	2.513021	0.640289
33	1	0	5.614413	1.361473	1.782353
34	1	0	6.209171	-0.969053	1.157016
35	6	0	2.078607	1.532758	-1.261273
36	7	0	0.917247	1.507141	-0.352349
37	1	0	1.158862	1.976335	0.519202
38	1	0	0.159358	2.053828	-0.758018
39	1	0	1.797842	1.010388	-2.180507
40	1	0	2.366300	2.557393	-1.533883
41	1	0	-2.037827	-2.303585	-1.049888

SCF Done: E(RM062X) = -881.790826441 A.U.

free energy = -881.47059 A.U.

IM2:



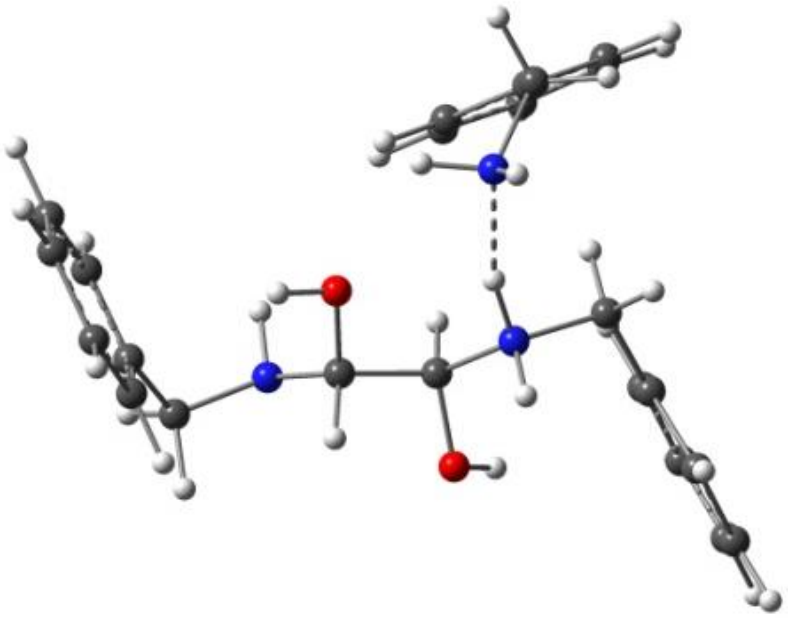
Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.319180	-0.097001	1.207312
2	6	0	-4.322033	0.838516	0.940970
3	6	0	-3.669021	0.851658	-0.297654
4	6	0	-4.042794	-0.083280	-1.268225
5	6	0	-5.040308	-1.025034	-1.003416
6	6	0	-5.677520	-1.034558	0.235871
7	1	0	-5.818512	-0.095861	2.171319
8	1	0	-4.042819	1.564478	1.701683
9	1	0	-3.551321	-0.074496	-2.238780
10	1	0	-5.318625	-1.745925	-1.765906
11	1	0	-6.452959	-1.765073	0.443502
12	6	0	-2.525229	1.814366	-0.552902
13	7	0	-1.253478	1.438813	0.078706
14	1	0	-1.295873	1.547413	1.089938
15	1	0	-2.781327	2.810885	-0.183489
16	1	0	-2.349589	1.900409	-1.630192
17	6	0	-0.749057	0.146640	-0.260895
18	8	0	-1.291862	-0.942485	0.481173
19	1	0	-0.892104	-0.012106	-1.338658
20	6	0	0.756964	0.114699	0.036441
21	8	0	1.425674	0.823323	-0.937468
22	1	0	0.946406	0.481432	1.051370
23	6	0	4.957991	1.212872	0.801312
24	6	0	3.908587	0.387094	1.207563
25	6	0	3.602792	-0.768515	0.481567
26	6	0	4.368701	-1.102443	-0.640078
27	6	0	5.415420	-0.277965	-1.044700
28	6	0	5.707452	0.883241	-0.327446
29	1	0	5.190402	2.107810	1.368818
30	1	0	3.334003	0.638934	2.095714
31	1	0	4.148660	-2.009991	-1.196815
32	1	0	6.004429	-0.542879	-1.916447
33	1	0	6.523404	1.525034	-0.643215
34	6	0	2.431245	-1.627758	0.874115
35	7	0	1.225478	-1.331715	0.015234
36	1	0	2.256393	1.179492	-0.589576
37	1	0	0.429267	-1.912699	0.316185
38	1	0	2.122500	-1.451913	1.906066
39	1	0	2.642967	-2.689845	0.742556
40	1	0	1.424378	-1.572542	-0.962716
41	1	0	-2.218238	-1.074136	0.232419

SCF Done: E(RM062X) = -881.822293373 A.U.

free energy = -881.494609 A.U.

CP2:



Standard orientation

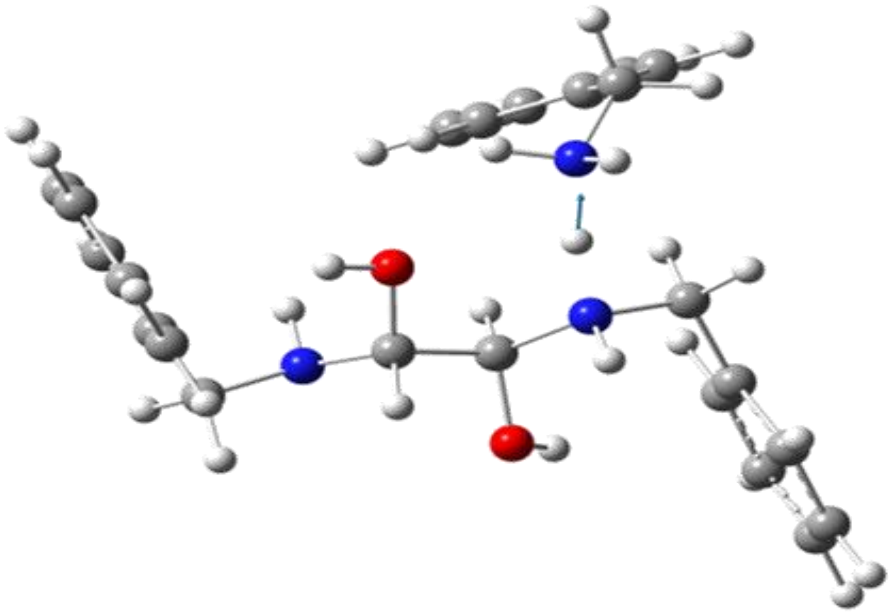
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.671308	0.621004	-0.556521
2	6	0	-4.700674	-0.093577	-1.256432
3	6	0	-4.145471	-1.261859	-0.717011
4	6	0	-4.589907	-1.705065	0.533810
5	6	0	-5.562165	-0.989776	1.239905
6	6	0	-6.102405	0.175480	0.696686
7	1	0	-6.093845	1.523787	-0.986549
8	1	0	-4.368389	0.259435	-2.230444
9	1	0	-4.175719	-2.615929	0.960789
10	1	0	-5.897322	-1.345912	2.208976
11	1	0	-6.858745	0.731383	1.241615
12	6	0	-3.032935	-1.988417	-1.449903
13	7	0	-1.713483	-1.342714	-1.366998
14	1	0	-1.719924	-0.448038	-1.857690
15	1	0	-3.277757	-2.075201	-2.511162
16	1	0	-2.929675	-3.002994	-1.055133
17	6	0	-1.205182	-1.148789	-0.037482
18	8	0	-1.683296	0.011727	0.633503

19	1	0	-1.423245	-2.048365	0.551935
20	6	0	0.321470	-1.015428	-0.132180
21	8	0	0.821152	-2.298870	-0.313373
22	1	0	0.596231	-0.324837	-0.937562
23	6	0	4.650350	-1.921611	-1.191690
24	6	0	3.759063	-0.941103	-0.749673
25	6	0	3.295144	-0.952056	0.570063
26	6	0	3.751087	-1.937228	1.452876
27	6	0	4.640636	-2.915176	1.012301
28	6	0	5.087164	-2.911981	-0.311826
29	1	0	5.002730	-1.907587	-2.217870
30	1	0	3.424054	-0.163891	-1.434545
31	1	0	3.411569	-1.940852	2.486029
32	1	0	4.989106	-3.677620	1.701408
33	1	0	5.779426	-3.674807	-0.653276
34	6	0	2.302938	0.087175	1.019210
35	7	0	0.890595	-0.427777	1.135216
36	1	0	1.663725	-2.271961	-0.797061
37	1	0	0.321217	0.405414	1.499664
38	1	0	2.262882	0.916716	0.310707
39	1	0	2.549165	0.487155	2.005779
40	1	0	0.847466	-1.156704	1.858829
41	1	0	-2.637920	-0.096887	0.789462
42	6	0	0.771045	2.355215	-1.882644
43	6	0	0.240854	2.513571	-0.600086
44	6	0	0.990824	3.133166	0.407781
45	6	0	2.267498	3.612533	0.100066
46	6	0	2.799947	3.456947	-1.181525
47	6	0	2.055977	2.818773	-2.175345
48	1	0	0.184038	1.864191	-2.654026
49	1	0	-0.753859	2.127877	-0.384153
50	1	0	2.862819	4.087400	0.875878
51	1	0	3.799440	3.821023	-1.398479
52	1	0	2.472123	2.685317	-3.168914
53	6	0	0.459220	3.232819	1.820975
54	7	0	-0.188936	1.969550	2.234601
55	1	0	-0.267268	1.955357	3.251207
56	1	0	-1.148107	1.939275	1.890018
57	1	0	-0.226999	4.083615	1.906416
58	1	0	1.293694	3.419670	2.499259

SCF Done: E(RM062X) = -1208.64202921 A.U.

free energy = -1208.17613 A.U.

TS1:



Standard orientation

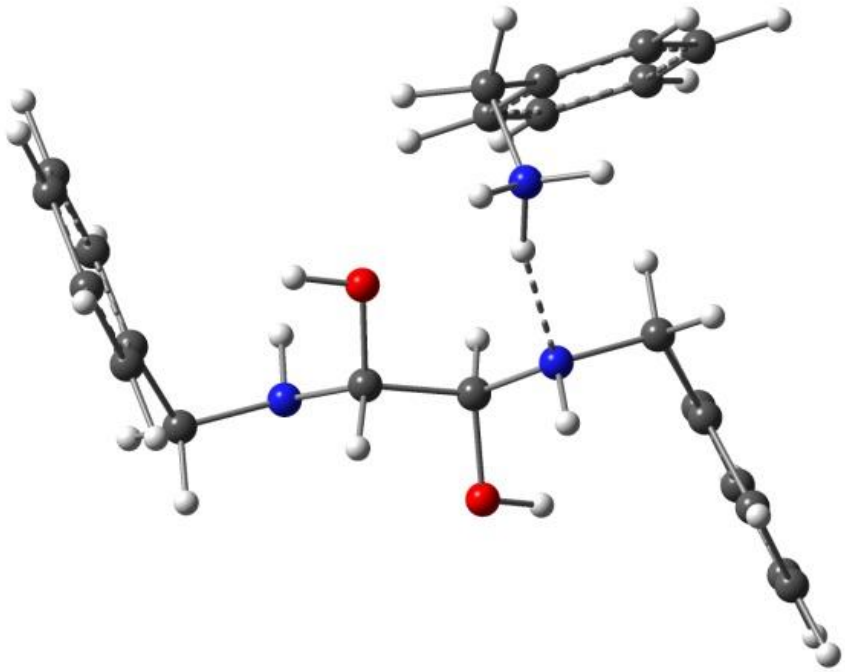
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.664662	0.471482	-0.557789
2	6	0	-4.656974	-0.200631	-1.246783
3	6	0	-4.078292	-1.361114	-0.715589
4	6	0	-4.537888	-1.841188	0.515885
5	6	0	-5.548235	-1.168509	1.211256
6	6	0	-6.111143	-0.010214	0.676536
7	1	0	-6.104996	1.368454	-0.982137
8	1	0	-4.314574	0.178861	-2.207316
9	1	0	-4.105408	-2.746480	0.936905
10	1	0	-5.895017	-1.552809	2.165420
11	1	0	-6.896993	0.512068	1.212856
12	6	0	-2.933181	-2.039673	-1.445807
13	7	0	-1.640906	-1.345465	-1.360806
14	1	0	-1.692440	-0.429014	-1.806169
15	1	0	-3.176162	-2.131840	-2.507456
16	1	0	-2.791487	-3.051695	-1.055964
17	6	0	-1.086841	-1.210398	-0.042452
18	8	0	-1.644169	-0.157933	0.743692
19	1	0	-1.205465	-2.169716	0.477581
20	6	0	0.417972	-0.935955	-0.183435
21	8	0	0.983205	-2.155865	-0.571815
22	1	0	0.584639	-0.142482	-0.922221

23	6	0	4.895342	-1.710292	-1.291705
24	6	0	3.962558	-0.785535	-0.814279
25	6	0	3.433267	-0.914227	0.473656
26	6	0	3.863101	-1.967083	1.289363
27	6	0	4.792101	-2.890402	0.814322
28	6	0	5.307009	-2.765949	-0.479219
29	1	0	5.298601	-1.602338	-2.293408
30	1	0	3.646298	0.039920	-1.448907
31	1	0	3.470306	-2.067863	2.298711
32	1	0	5.117692	-3.705729	1.452406
33	1	0	6.030580	-3.485795	-0.848027
34	6	0	2.405474	0.073785	0.969539
35	7	0	1.010661	-0.452930	1.093805
36	1	0	1.817615	-2.004392	-1.044878
37	1	0	0.406765	0.495207	1.666990
38	1	0	2.353334	0.935340	0.298529
39	1	0	2.677781	0.439429	1.964345
40	1	0	1.003088	-1.237599	1.755555
41	1	0	-2.589144	-0.349435	0.876529
42	6	0	0.245017	2.718728	-1.735540
43	6	0	-0.059280	2.575540	-0.379898
44	6	0	0.821501	3.053387	0.597144
45	6	0	1.999722	3.691172	0.195723
46	6	0	2.301979	3.839938	-1.158038
47	6	0	1.427543	3.347300	-2.128633
48	1	0	-0.441780	2.333727	-2.483622
49	1	0	-0.980269	2.070921	-0.096050
50	1	0	2.695546	4.057693	0.946167
51	1	0	3.224486	4.329699	-1.453727
52	1	0	1.665418	3.452994	-3.182353
53	6	0	0.531626	2.878509	2.071411
54	7	0	-0.094084	1.561218	2.349660
55	1	0	-0.071504	1.376367	3.354897
56	1	0	-1.081313	1.557286	2.087813
57	1	0	-0.117993	3.680528	2.434529
58	1	0	1.464108	2.927290	2.635372

SCF Done: E(RM062X) = -1208.63985717 A.U.

free energy = -1208.17697 A.U.

CP3:



Standard orientation

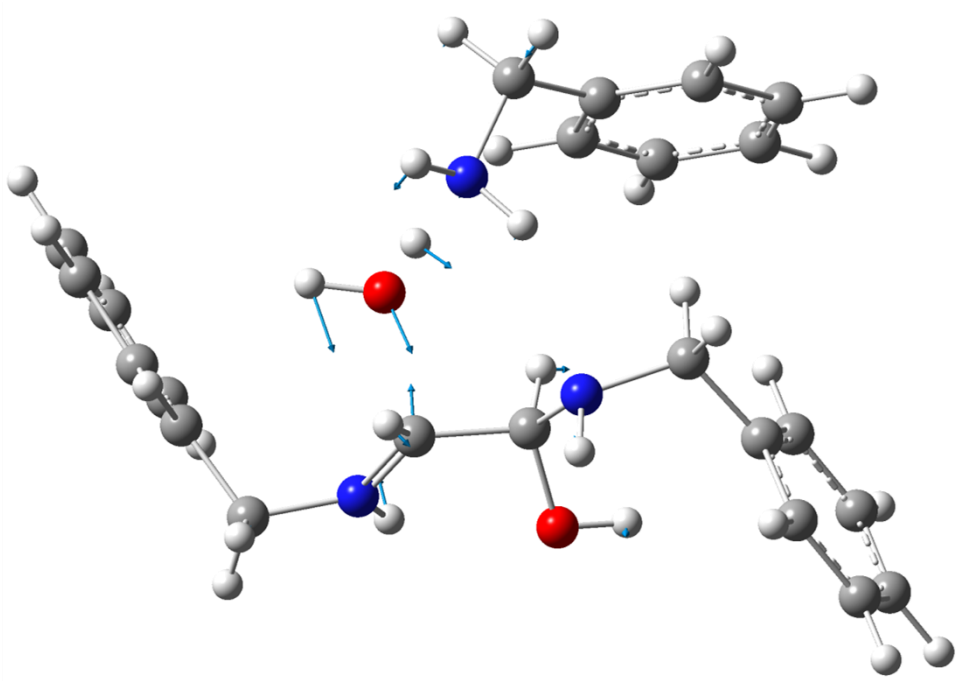
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.492308	0.394736	-0.954035
2	6	0	-4.516768	-0.488989	-1.412135
3	6	0	-4.027319	-1.507526	-0.582613
4	6	0	-4.544451	-1.628991	0.711903
5	6	0	-5.523204	-0.744060	1.175759
6	6	0	-5.995697	0.271063	0.344718
7	1	0	-5.862407	1.178298	-1.607945
8	1	0	-4.127334	-0.386069	-2.422862
9	1	0	-4.177058	-2.417279	1.365306
10	1	0	-5.914540	-0.850538	2.182710
11	1	0	-6.754720	0.959439	0.702672
12	6	0	-2.908504	-2.413840	-1.066833
13	7	0	-1.578617	-1.794631	-1.131478
14	1	0	-1.550633	-1.063386	-1.841524
15	1	0	-3.140000	-2.779179	-2.070843
16	1	0	-2.835823	-3.288048	-0.413273
17	6	0	-1.056059	-1.289750	0.108666
18	8	0	-1.585542	-0.015391	0.497762
19	1	0	-1.261361	-2.033017	0.890956
20	6	0	0.465210	-1.110073	0.000685
21	8	0	0.991307	-2.416339	-0.137069

22	1	0	0.688247	-0.497581	-0.884292
23	6	0	4.800613	-1.641764	-1.263894
24	6	0	3.835318	-0.732726	-0.820085
25	6	0	3.414501	-0.734849	0.514204
26	6	0	3.987261	-1.651989	1.405002
27	6	0	4.950470	-2.558624	0.966392
28	6	0	5.356872	-2.557808	-0.371537
29	1	0	5.115551	-1.631634	-2.302658
30	1	0	3.403418	-0.018052	-1.518449
31	1	0	3.673170	-1.659087	2.446499
32	1	0	5.385201	-3.266141	1.665495
33	1	0	6.105501	-3.265252	-0.713820
34	6	0	2.322704	0.208853	0.974758
35	7	0	0.987367	-0.400843	1.164252
36	1	0	1.914111	-2.352174	-0.432468
37	1	0	0.284160	2.234316	2.811383
38	1	0	2.213396	1.019788	0.247350
39	1	0	2.603135	0.662630	1.930531
40	1	0	1.020703	-1.061864	1.943552
41	1	0	-2.552432	-0.102289	0.559466
42	6	0	1.245242	2.398568	-1.996677
43	6	0	0.188576	2.327194	-1.087793
44	6	0	0.272973	2.986808	0.142009
45	6	0	1.418066	3.729720	0.450091
46	6	0	2.477615	3.795685	-0.454698
47	6	0	2.393701	3.126365	-1.677624
48	1	0	1.174204	1.883044	-2.949574
49	1	0	-0.703448	1.753260	-1.325498
50	1	0	1.485160	4.259908	1.397774
51	1	0	3.363967	4.370876	-0.207587
52	1	0	3.217876	3.177646	-2.382201
53	6	0	-0.839683	2.852504	1.148107
54	7	0	-0.444280	1.854295	2.198622
55	1	0	-1.240922	1.606002	2.793940
56	1	0	-0.073775	0.959087	1.759258
57	1	0	-1.749094	2.473940	0.686019
58	1	0	-1.052424	3.792407	1.658540

SCF Done: E(RM062X) = -1208.65005108 A.U.

free energy = -1208.1824 A.U.

TS2:



Standard orientation

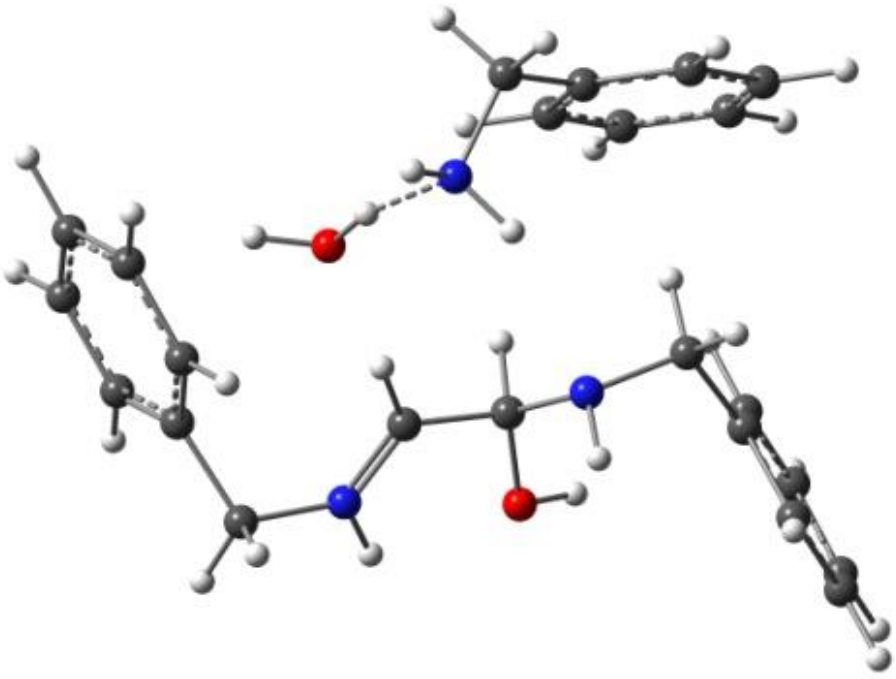
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.396414	-0.191300	1.748720
2	6	0	4.539431	-1.235320	1.405918
3	6	0	4.239129	-1.491509	0.062625
4	6	0	4.817539	-0.698142	-0.932549
5	6	0	5.677720	0.349157	-0.589968
6	6	0	5.964161	0.605719	0.750793
7	1	0	5.622432	0.001754	2.792537
8	1	0	4.097612	-1.851251	2.185473
9	1	0	4.593163	-0.893326	-1.978578
10	1	0	6.120611	0.960682	-1.369590
11	1	0	6.629184	1.420472	1.018564
12	6	0	3.249287	-2.576895	-0.300897
13	7	0	1.874385	-2.198081	0.059299
14	1	0	1.498636	-2.515876	0.950686
15	1	0	3.470415	-3.505811	0.225492
16	1	0	3.271426	-2.779574	-1.373475
17	6	0	1.172873	-1.315678	-0.607573
18	8	0	1.750876	0.477466	-0.113335
19	1	0	1.457966	-1.137907	-1.640994
20	6	0	-0.286719	-1.103344	-0.211408
21	8	0	-0.733122	-2.376377	0.244046
22	1	0	-0.317837	-0.377367	0.609349

23	6	0	-4.509197	-1.885573	1.462828
24	6	0	-3.635318	-0.934007	0.926348
25	6	0	-3.321543	-0.942828	-0.437412
26	6	0	-3.912201	-1.908760	-1.261597
27	6	0	-4.784948	-2.857118	-0.731144
28	6	0	-5.081821	-2.850560	0.635125
29	1	0	-4.740211	-1.869756	2.523422
30	1	0	-3.189743	-0.181490	1.575158
31	1	0	-3.682613	-1.921061	-2.324921
32	1	0	-5.234469	-3.601655	-1.380891
33	1	0	-5.760371	-3.590065	1.048352
34	6	0	-2.310933	0.036128	-1.005600
35	7	0	-0.992521	-0.536200	-1.329742
36	1	0	-1.597296	-2.260472	0.675385
37	1	0	-0.086815	1.639694	-2.161436
38	1	0	-2.148721	0.850023	-0.292167
39	1	0	-2.698647	0.482032	-1.926133
40	1	0	-1.076393	-1.230116	-2.073859
41	1	0	2.724075	0.509317	-0.185801
42	6	0	-1.502329	2.389491	1.947959
43	6	0	-0.507138	2.640982	1.004056
44	6	0	-0.823913	3.248932	-0.218178
45	6	0	-2.150277	3.605607	-0.474692
46	6	0	-3.149698	3.359601	0.471012
47	6	0	-2.827535	2.749020	1.682783
48	1	0	-1.245769	1.916633	2.891399
49	1	0	0.522361	2.360687	1.215467
50	1	0	-2.406404	4.075120	-1.421198
51	1	0	-4.176433	3.640838	0.258409
52	1	0	-3.602311	2.555973	2.418620
53	6	0	0.248094	3.473449	-1.257099
54	7	0	0.707834	2.173603	-1.799424
55	1	0	1.336966	2.334588	-2.587622
56	1	0	1.361925	1.194670	-0.789403
57	1	0	1.114621	3.965303	-0.807770
58	1	0	-0.133736	4.121656	-2.051393

SCF Done: E(RM062X) = -1208.61604932 A.U.

free energy = -1208.15504 A.U.

CP4:



Standard orientation

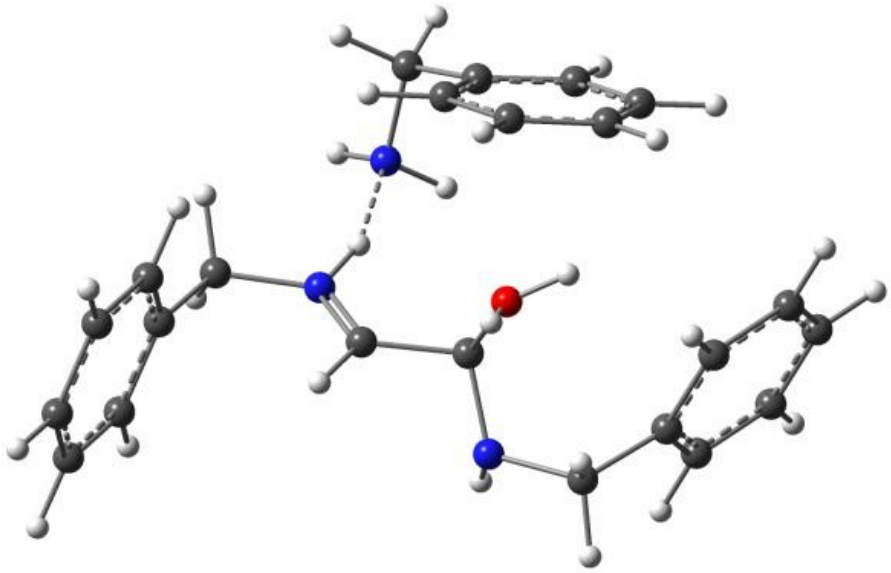
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.339951	-0.213514	1.501437
2	6	0	4.567472	-1.340366	1.222141
3	6	0	4.111411	-1.575025	-0.079359
4	6	0	4.447693	-0.682858	-1.101159
5	6	0	5.213960	0.450612	-0.820888
6	6	0	5.656362	0.688290	0.480801
7	1	0	5.691648	-0.036141	2.512626
8	1	0	4.310212	-2.033076	2.019201
9	1	0	4.113803	-0.870492	-2.118901
10	1	0	5.467307	1.141094	-1.618720
11	1	0	6.252289	1.568058	0.701138
12	6	0	3.205147	-2.747649	-0.353170
13	7	0	1.785714	-2.400454	-0.066165
14	1	0	1.208155	-3.070521	0.453920
15	1	0	3.441328	-3.596350	0.286420
16	1	0	3.253766	-3.070697	-1.394316
17	6	0	1.209071	-1.314544	-0.409728
18	8	0	2.021078	0.756856	1.111854
19	1	0	1.755611	-0.573685	-0.983448
20	6	0	-0.240408	-1.071890	-0.085299

21	8	0	-0.706486	-2.269456	0.510766
22	1	0	-0.257655	-0.235769	0.630026
23	6	0	-4.553417	-1.761761	1.409121
24	6	0	-3.651340	-0.851798	0.847689
25	6	0	-3.266879	-0.965045	-0.492970
26	6	0	-3.815364	-1.991729	-1.270909
27	6	0	-4.715728	-2.899054	-0.715463
28	6	0	-5.082992	-2.788891	0.628824
29	1	0	-4.840356	-1.664940	2.451614
30	1	0	-3.241292	-0.048588	1.458220
31	1	0	-3.533684	-2.082380	-2.317861
32	1	0	-5.133338	-3.691364	-1.328992
33	1	0	-5.783103	-3.496768	1.061001
34	6	0	-2.226740	-0.032937	-1.083327
35	7	0	-0.897035	-0.638599	-1.290900
36	1	0	-1.553744	-2.103134	0.958947
37	1	0	0.449005	1.362145	-1.723249
38	1	0	-2.093403	0.836141	-0.431867
39	1	0	-2.559480	0.336174	-2.057026
40	1	0	-0.957237	-1.413702	-1.951953
41	1	0	2.987137	0.776252	1.212544
42	6	0	-1.867833	2.565251	1.762654
43	6	0	-0.682373	2.702735	1.041045
44	6	0	-0.701362	3.200201	-0.269725
45	6	0	-1.925533	3.560735	-0.838460
46	6	0	-3.115357	3.427084	-0.116518
47	6	0	-3.089137	2.926301	1.184570
48	1	0	-1.840291	2.178248	2.777212
49	1	0	0.263464	2.415720	1.495922
50	1	0	-1.952704	3.941527	-1.856446
51	1	0	-4.059168	3.708224	-0.573585
52	1	0	-4.012454	2.817163	1.745511
53	6	0	0.578901	3.306053	-1.064318
54	7	0	1.154605	1.959245	-1.281714
55	1	0	1.925024	2.033916	-1.947717
56	1	0	1.811504	1.272553	0.288833
57	1	0	1.315967	3.895838	-0.511559
58	1	0	0.378954	3.822807	-2.008947

SCF Done: E(RM062X) = -1208.62427507 A.U.

free energy = -1208.16413 A.U.

CP5:



Standard orientation

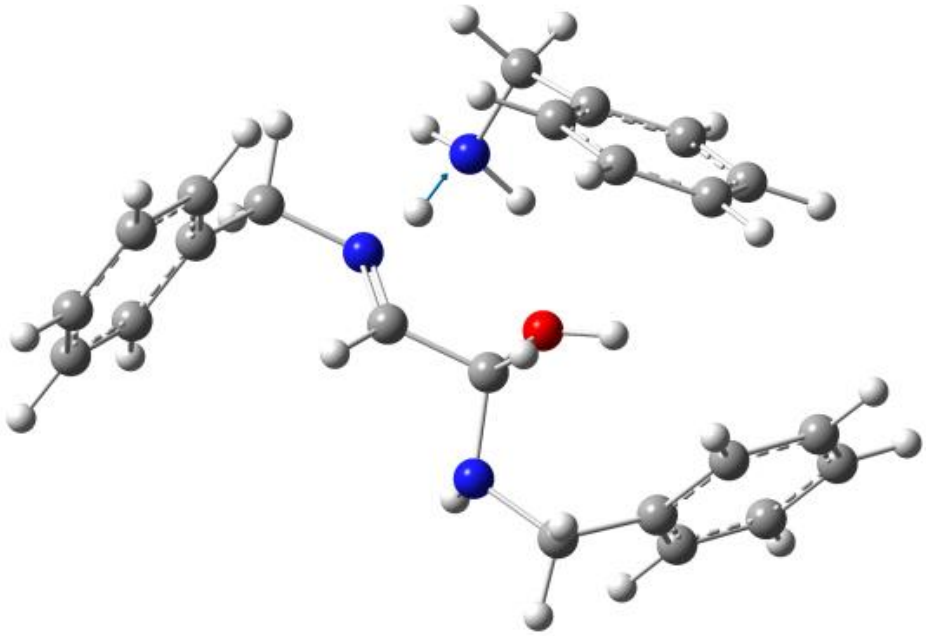
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.313785	-0.413634	1.619728
2	6	0	-4.378662	0.339344	0.911354
3	6	0	-4.058808	0.004602	-0.409166
4	6	0	-4.681561	-1.091142	-1.013459
5	6	0	-5.619976	-1.843669	-0.305943
6	6	0	-5.936086	-1.505559	1.010386
7	1	0	-5.560217	-0.147055	2.642420
8	1	0	-3.894859	1.191082	1.384129
9	1	0	-4.436014	-1.354251	-2.039088
10	1	0	-6.104277	-2.689426	-0.783174
11	1	0	-6.668128	-2.088647	1.560085
12	6	0	-3.030231	0.804936	-1.158447
13	7	0	-1.636409	0.387954	-0.883979
14	1	0	-0.916360	1.054463	-1.338709
15	1	0	-3.077394	1.865718	-0.898007
16	1	0	-3.160010	0.722865	-2.240234
17	6	0	-1.282674	-0.613207	-0.181918
18	1	0	-2.038762	-1.245645	0.279564
19	6	0	0.162281	-0.971516	0.044076
20	8	0	0.950536	-0.100768	-0.738535
21	1	0	0.345324	-0.811372	1.117459
22	6	0	4.623614	-0.918091	0.885207
23	6	0	3.422582	-1.586108	1.145605
24	6	0	2.800387	-2.347336	0.152412

25	6	0	3.405482	-2.440954	-1.107928
26	6	0	4.600237	-1.775672	-1.372262
27	6	0	5.211391	-1.007457	-0.375242
28	1	0	5.096870	-0.332124	1.667815
29	1	0	2.969758	-1.515158	2.132518
30	1	0	2.934825	-3.035282	-1.888278
31	1	0	5.058798	-1.856337	-2.353051
32	1	0	6.142651	-0.489052	-0.581089
33	6	0	1.466557	-3.017902	0.415642
34	7	0	0.307138	-2.379029	-0.230073
35	1	0	1.782353	0.096060	-0.271237
36	1	0	1.272492	-3.041790	1.491789
37	1	0	1.487548	-4.053273	0.067343
38	1	0	0.330973	-2.521509	-1.239081
39	6	0	2.895959	2.163907	0.958381
40	6	0	2.215740	2.808739	-0.076352
41	6	0	0.826937	2.965145	-0.025779
42	6	0	0.129678	2.492082	1.090010
43	6	0	0.804703	1.849016	2.129309
44	6	0	2.188993	1.672897	2.059567
45	1	0	3.973592	2.042079	0.904977
46	1	0	2.767747	3.181773	-0.936257
47	1	0	-0.949271	2.623443	1.147910
48	1	0	0.253180	1.486135	2.991642
49	1	0	2.715982	1.171773	2.866120
50	6	0	0.087867	3.524164	-1.216177
51	7	0	-0.227982	2.409364	-2.140974
52	1	0	-0.744404	2.769095	-2.944782
53	1	0	0.643154	2.027000	-2.512446
54	1	0	0.684366	4.299728	-1.708329
55	1	0	-0.857193	3.972313	-0.900564

SCF Done: E(RM062X) = -1132.21349162 A.U.

free energy = -1131.77537 A.U.

TS3:



Standard orientation

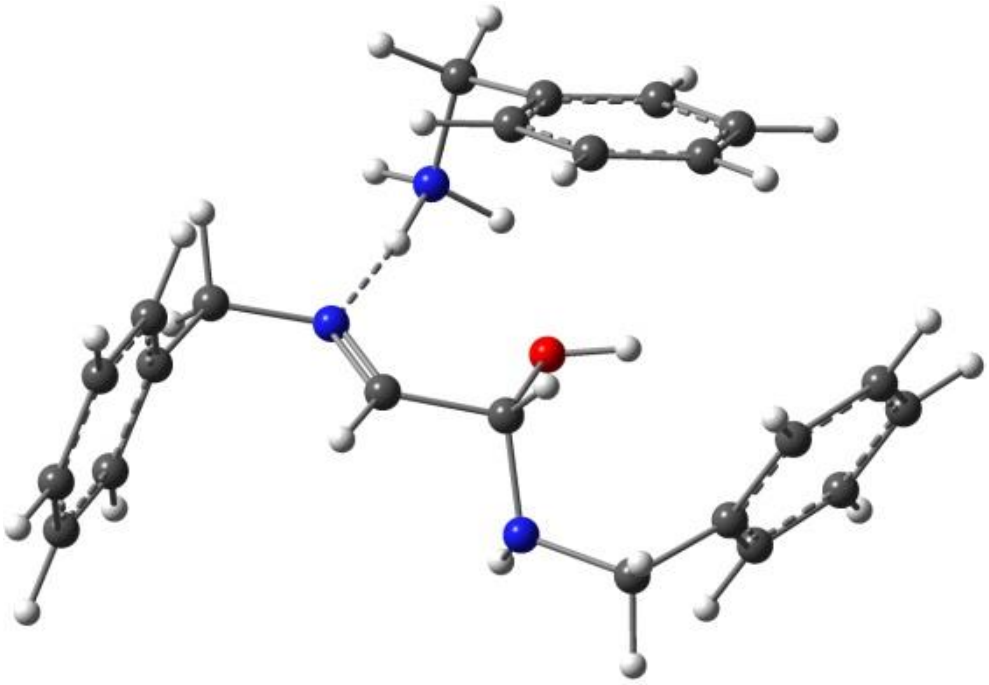
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.362660	-0.294004	1.602753
2	6	0	-4.450439	0.448564	0.853303
3	6	0	-4.067849	0.019152	-0.421769
4	6	0	-4.607203	-1.163077	-0.938665
5	6	0	-5.518912	-1.907945	-0.189921
6	6	0	-5.897331	-1.473950	1.081579
7	1	0	-5.658679	0.049174	2.588911
8	1	0	-4.035445	1.368265	1.259080
9	1	0	-4.313101	-1.501743	-1.929127
10	1	0	-5.934354	-2.823113	-0.599464
11	1	0	-6.608811	-2.051311	1.663463
12	6	0	-3.055596	0.804047	-1.210914
13	7	0	-1.646144	0.430070	-0.959429
14	1	0	-0.878234	1.203080	-1.516203
15	1	0	-3.126575	1.872209	-0.986641
16	1	0	-3.210525	0.686445	-2.286956
17	6	0	-1.298232	-0.547136	-0.224555
18	1	0	-2.046460	-1.167028	0.270501
19	6	0	0.140013	-0.924707	0.019201
20	8	0	0.955640	-0.100222	-0.790108
21	1	0	0.328721	-0.729355	1.085680
22	6	0	4.577667	-0.891698	0.897350

23	6	0	3.366462	-1.535632	1.170096
24	6	0	2.754879	-2.343022	0.206714
25	6	0	3.381541	-2.506627	-1.036250
26	6	0	4.586981	-1.865640	-1.312676
27	6	0	5.187374	-1.051864	-0.345761
28	1	0	5.041338	-0.268571	1.656548
29	1	0	2.896521	-1.408320	2.143226
30	1	0	2.918409	-3.135905	-1.793343
31	1	0	5.061535	-1.999694	-2.279877
32	1	0	6.126726	-0.552261	-0.560983
33	6	0	1.406651	-2.981362	0.479237
34	7	0	0.264822	-2.345651	-0.198596
35	1	0	1.829272	-0.008793	-0.369732
36	1	0	1.203443	-2.964233	1.553962
37	1	0	1.414207	-4.028720	0.168131
38	1	0	0.290490	-2.529343	-1.200750
39	6	0	2.938947	2.231163	0.946369
40	6	0	2.240228	2.795817	-0.120844
41	6	0	0.847318	2.909659	-0.075423
42	6	0	0.162834	2.479190	1.064495
43	6	0	0.858135	1.915278	2.135585
44	6	0	2.246750	1.778848	2.072873
45	1	0	4.019843	2.140899	0.897911
46	1	0	2.780922	3.138091	-1.000482
47	1	0	-0.919923	2.576387	1.115062
48	1	0	0.317643	1.580775	3.015977
49	1	0	2.788095	1.335056	2.903300
50	6	0	0.094093	3.383155	-1.292296
51	7	0	-0.183591	2.214074	-2.170963
52	1	0	-0.662097	2.520177	-3.021298
53	1	0	0.696566	1.785298	-2.465958
54	1	0	0.666618	4.136755	-1.839280
55	1	0	-0.866769	3.818863	-1.010758

SCF Done: E(RM062X) = -1132.21237548 A.U.

free energy = -1131.77822 A.U.

CP6:



Standard orientation

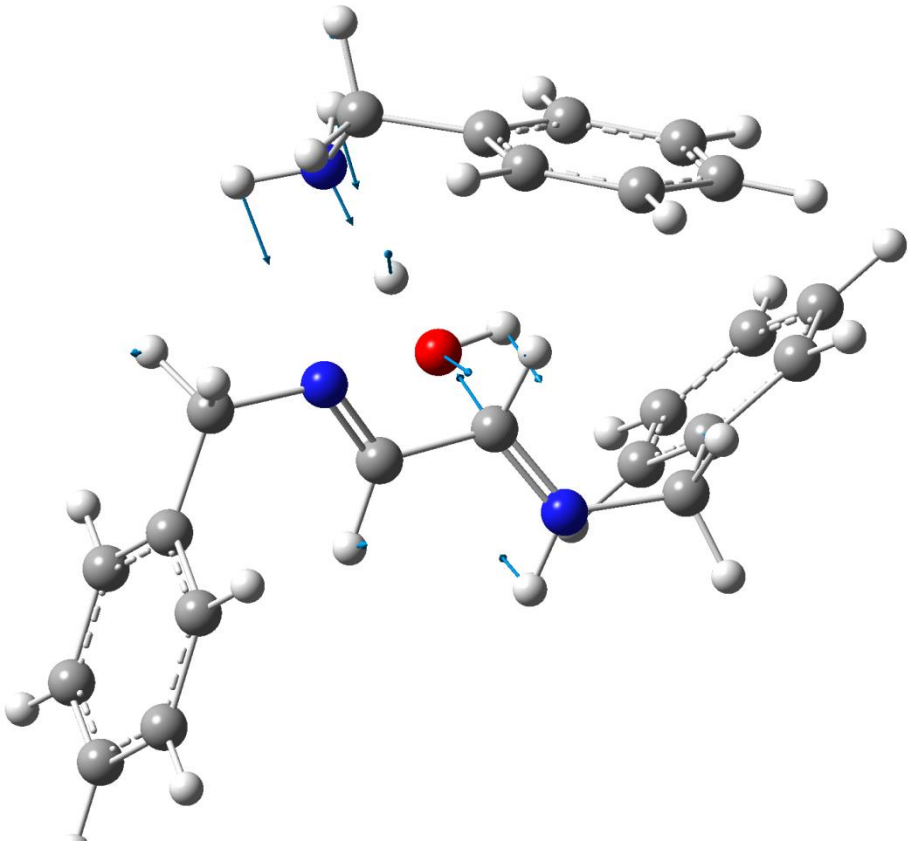
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.409488	-0.206232	1.600208
2	6	0	-4.490687	0.526702	0.847795
3	6	0	-4.103333	0.090325	-0.423460
4	6	0	-4.647212	-1.095052	-0.929906
5	6	0	-5.564812	-1.831867	-0.180312
6	6	0	-5.947719	-1.387897	1.086839
7	1	0	-5.707082	0.145213	2.583252
8	1	0	-4.071892	1.446417	1.250327
9	1	0	-4.349078	-1.443357	-1.916158
10	1	0	-5.981572	-2.748953	-0.584866
11	1	0	-6.663714	-1.958346	1.670216
12	6	0	-3.076335	0.859248	-1.216025
13	7	0	-1.668001	0.475228	-1.014630
14	1	0	-0.487574	1.468525	-1.832967
15	1	0	-3.136049	1.927467	-0.983573
16	1	0	-3.267767	0.761982	-2.289062
17	6	0	-1.356542	-0.480154	-0.241900
18	1	0	-2.096203	-1.067876	0.310388
19	6	0	0.074086	-0.905024	-0.005622
20	8	0	0.924864	-0.123366	-0.834050
21	1	0	0.294565	-0.704891	1.053537
22	6	0	4.487976	-0.977939	0.924987

23	6	0	3.257591	-1.590546	1.182456
24	6	0	2.647649	-2.400921	0.220011
25	6	0	3.296015	-2.598356	-1.007049
26	6	0	4.520984	-1.988189	-1.268570
27	6	0	5.119565	-1.172245	-0.302387
28	1	0	4.948898	-0.352535	1.683815
29	1	0	2.769294	-1.435420	2.142430
30	1	0	2.833115	-3.228715	-1.763418
31	1	0	5.011990	-2.147996	-2.223592
32	1	0	6.074286	-0.697337	-0.505582
33	6	0	1.278560	-3.001262	0.476443
34	7	0	0.160331	-2.333235	-0.207092
35	1	0	1.826918	-0.169061	-0.471434
36	1	0	1.069134	-2.980219	1.550033
37	1	0	1.262183	-4.048385	0.164320
38	1	0	0.174912	-2.528693	-1.207069
39	6	0	3.013676	2.206294	1.099124
40	6	0	2.408105	2.750713	-0.032880
41	6	0	1.017478	2.880875	-0.093861
42	6	0	0.237974	2.486302	0.996406
43	6	0	0.842353	1.942833	2.130434
44	6	0	2.229895	1.792159	2.178614
45	1	0	4.093747	2.106498	1.138753
46	1	0	3.021133	3.068496	-0.873377
47	1	0	-0.843658	2.594057	0.957100
48	1	0	0.231786	1.634717	2.973570
49	1	0	2.700325	1.365246	3.059404
50	6	0	0.366052	3.359172	-1.363412
51	7	0	0.154793	2.192921	-2.285351
52	1	0	-0.250876	2.492678	-3.177871
53	1	0	1.036888	1.710504	-2.484233
54	1	0	0.983247	4.086198	-1.891323
55	1	0	-0.616704	3.792682	-1.178292

SCF Done: E(RM062X) = -1132.21856724 A.U.

free energy = -1131.78108 A.U.

TS4:



Standard orientation

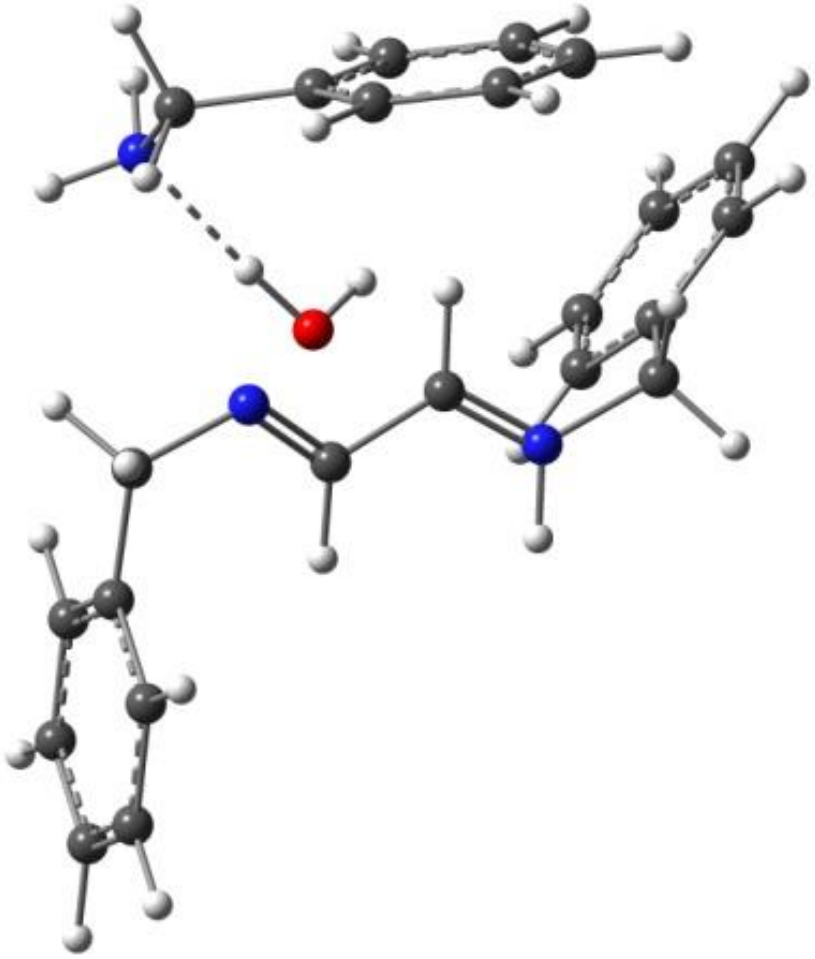
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.694771	-1.056659	-1.367399
2	6	0	4.821217	0.009072	-1.150288
3	6	0	4.247084	0.213855	0.109486
4	6	0	4.558281	-0.668375	1.149308
5	6	0	5.431760	-1.736144	0.936258
6	6	0	6.001460	-1.931634	-0.323188
7	1	0	6.138066	-1.201803	-2.347646
8	1	0	4.583621	0.689441	-1.964848
9	1	0	4.115582	-0.518758	2.131376
10	1	0	5.668937	-2.411806	1.752142
11	1	0	6.684226	-2.759016	-0.489479
12	6	0	3.266484	1.340950	0.321024
13	7	0	1.858105	1.056977	0.025123
14	1	0	-0.338958	0.477574	1.746690
15	1	0	3.532849	2.205827	-0.293737
16	1	0	3.288168	1.685441	1.360556
17	6	0	1.496499	-0.115059	-0.284354
18	1	0	2.160962	-0.984058	-0.359494

19	6	0	0.051944	-0.335203	-0.574532
20	8	0	-0.477561	-0.445455	1.241553
21	1	0	-0.552524	0.547504	-0.773967
22	6	0	-4.979565	-1.772158	0.050128
23	6	0	-3.983428	-1.476474	-0.881123
24	6	0	-2.687118	-1.970657	-0.715308
25	6	0	-2.400578	-2.777438	0.392019
26	6	0	-3.393116	-3.065697	1.329511
27	6	0	-4.684875	-2.562516	1.161547
28	1	0	-5.980517	-1.375308	-0.087679
29	1	0	-4.216195	-0.853043	-1.741194
30	1	0	-1.399394	-3.176918	0.534309
31	1	0	-3.156061	-3.683613	2.189807
32	1	0	-5.455505	-2.784121	1.893016
33	6	0	-1.634020	-1.652459	-1.759156
34	7	0	-0.294683	-1.444035	-1.204058
35	1	0	-1.429914	-0.660060	1.275442
36	1	0	-1.912699	-0.747522	-2.306066
37	1	0	-1.554646	-2.464853	-2.484000
38	1	0	0.332214	-2.242481	-1.158327
39	6	0	-3.281344	1.867582	-0.404292
40	6	0	-2.428756	2.141039	0.666009
41	6	0	-1.195099	2.768072	0.453913
42	6	0	-0.841230	3.137675	-0.847434
43	6	0	-1.692903	2.869332	-1.921452
44	6	0	-2.911849	2.224128	-1.703999
45	1	0	-4.233669	1.378814	-0.222655
46	1	0	-2.732309	1.853931	1.670402
47	1	0	0.120097	3.612859	-1.024598
48	1	0	-1.398082	3.151370	-2.927506
49	1	0	-3.571166	2.005645	-2.538722
50	6	0	-0.242054	3.017755	1.601135
51	7	0	-0.164379	1.837222	2.497130
52	1	0	0.723369	1.852520	2.999933
53	1	0	-0.880467	1.897136	3.221766
54	1	0	-0.544261	3.908573	2.161754
55	1	0	0.754073	3.195297	1.196059

SCF Done: E(RM062X) = -1132.18291672 A.U.

free energy = -1131.75046 A.U.

CP7:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.698470	-1.327622	-1.124804
2	6	0	4.900545	-0.182605	-1.161300
3	6	0	4.130622	0.181199	-0.052087
4	6	0	4.164178	-0.621251	1.094523
5	6	0	4.958037	-1.767435	1.133400
6	6	0	5.727456	-2.121804	0.022570
7	1	0	6.296546	-1.597894	-1.989368
8	1	0	4.877830	0.433255	-2.057059
9	1	0	3.564110	-0.346723	1.959542
10	1	0	4.978455	-2.381288	2.028367
11	1	0	6.348426	-3.011607	0.052174
12	6	0	3.229761	1.389449	-0.104103
13	7	0	1.827226	1.154454	-0.454324
14	1	0	-0.017472	0.372438	1.856725
15	1	0	3.597804	2.127002	-0.824291

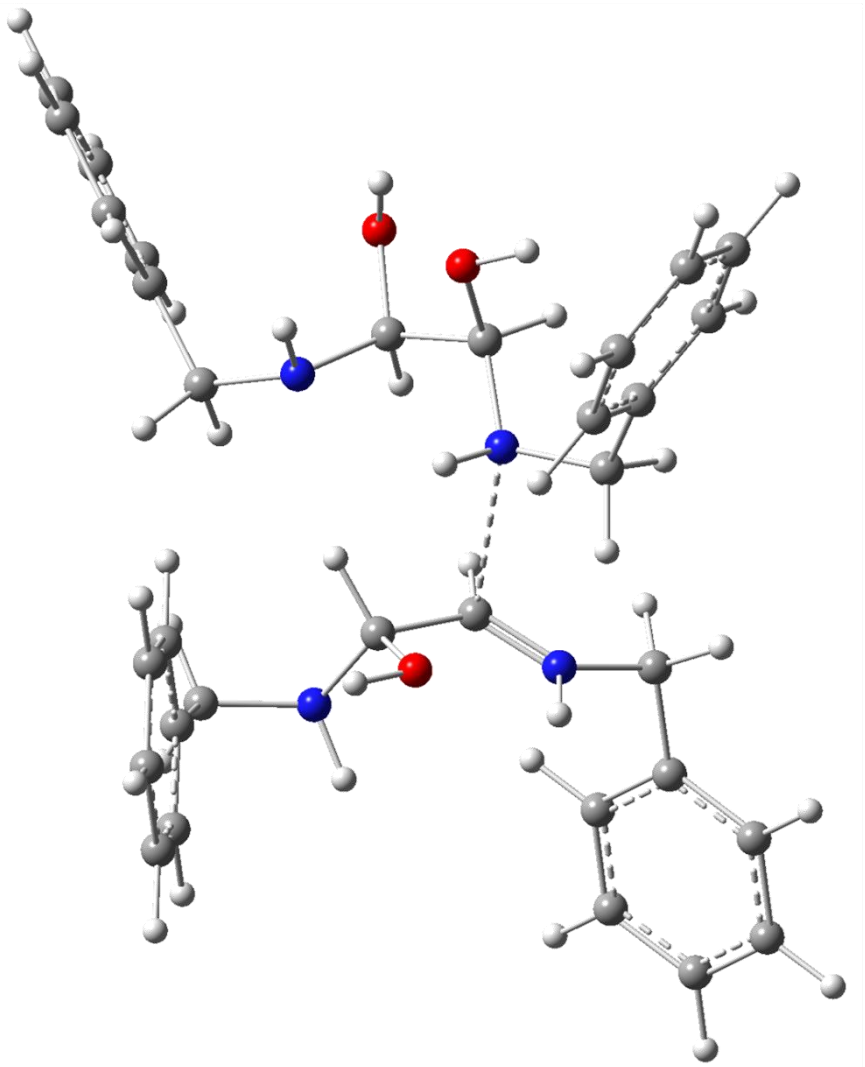
16	1	0	3.204982	1.899174	0.865551
17	6	0	1.433662	-0.018298	-0.734981
18	1	0	2.058247	-0.917283	-0.747674
19	6	0	0.007970	-0.165115	-1.060523
20	8	0	-0.164416	-0.529043	1.458107
21	1	0	-0.655946	0.687791	-0.924473
22	6	0	-4.907300	-2.065351	0.261376
23	6	0	-4.090076	-1.628978	-0.780609
24	6	0	-2.719875	-1.903630	-0.765143
25	6	0	-2.174693	-2.625647	0.299110
26	6	0	-2.992145	-3.055309	1.346460
27	6	0	-4.359020	-2.775732	1.330650
28	1	0	-5.968985	-1.840620	0.242681
29	1	0	-4.519426	-1.064366	-1.605062
30	1	0	-1.111525	-2.848806	0.330122
31	1	0	-2.557161	-3.607977	2.173345
32	1	0	-4.992421	-3.107010	2.147279
33	6	0	-1.880081	-1.431287	-1.934069
34	7	0	-0.464844	-1.244740	-1.574941
35	1	0	-1.061403	-0.787269	1.724439
36	1	0	-2.249854	-0.475048	-2.309163
37	1	0	-1.903903	-2.151325	-2.753532
38	1	0	0.167528	-2.034453	-1.716618
39	6	0	-3.183058	1.703769	-0.064537
40	6	0	-2.200469	2.007327	0.881225
41	6	0	-1.093226	2.789166	0.535556
42	6	0	-0.996555	3.273641	-0.774647
43	6	0	-1.972896	2.971352	-1.724163
44	6	0	-3.069819	2.178618	-1.372768
45	1	0	-4.035643	1.095685	0.222723
46	1	0	-2.303536	1.620190	1.891422
47	1	0	-0.134790	3.872094	-1.059619
48	1	0	-1.873659	3.345302	-2.738550
49	1	0	-3.830842	1.939348	-2.110038
50	6	0	-0.004700	3.117110	1.533996
51	7	0	0.149397	2.063435	2.554329
52	1	0	1.040055	2.196770	3.031733
53	1	0	-0.556352	2.178543	3.281160
54	1	0	-0.207938	4.096362	1.985715
55	1	0	0.939018	3.198621	0.991363

SCF Done: E(RM062X) = -1132.18858418 A.U.

free energy = -1131.75498 A.U.

Figure 3

CP8



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.915973	-1.703611	-2.729210
2	6	0	4.722250	-1.020604	-2.508010
3	6	0	4.740209	0.270459	-1.968540
4	6	0	5.959696	0.870698	-1.651751
5	6	0	7.156956	0.187559	-1.876893
6	6	0	7.135872	-1.098814	-2.413832
7	1	0	5.896183	-2.704009	-3.149486
8	1	0	3.775171	-1.493333	-2.760142
9	1	0	5.977702	1.873347	-1.233021
10	1	0	8.102256	0.661093	-1.632071
11	1	0	8.066233	-1.629703	-2.588906
12	6	0	3.439870	1.000941	-1.722117

13	7	0	2.680219	0.334454	-0.647792
14	1	0	3.088187	0.339144	0.293328
15	1	0	2.801817	1.012454	-2.606990
16	1	0	3.619423	2.029347	-1.404975
17	6	0	1.557027	-0.273584	-0.782931
18	1	0	1.106110	-0.340072	-1.767516
19	6	0	0.991842	-1.083792	0.353089
20	8	0	1.498721	-0.480460	1.534789
21	1	0	-0.102079	-1.020674	0.302379
22	6	0	-0.649062	-2.396502	4.218410
23	6	0	-0.610150	-2.610672	2.837909
24	6	0	0.447852	-3.319508	2.254899
25	6	0	1.460843	-3.823548	3.080164
26	6	0	1.422265	-3.616245	4.458522
27	6	0	0.368745	-2.898080	5.030132
28	1	0	-1.473734	-1.843375	4.656799
29	1	0	-1.408096	-2.216206	2.210595
30	1	0	2.285735	-4.378035	2.638338
31	1	0	2.212633	-4.013316	5.087751
32	1	0	0.340057	-2.734937	6.102706
33	6	0	0.543726	-3.464733	0.749670
34	7	0	1.385934	-2.443655	0.099643
35	1	0	1.154821	-0.963017	2.307074
36	1	0	-0.451929	-3.404161	0.301535
37	1	0	0.962749	-4.437719	0.484688
38	1	0	2.371440	-2.576705	0.325838
39	6	0	-0.830465	4.772084	2.964518
40	6	0	-0.185789	3.739097	2.286637
41	6	0	0.082932	3.845165	0.916308
42	6	0	-0.291776	5.010563	0.239410
43	6	0	-0.940255	6.048435	0.916326
44	6	0	-1.213349	5.928782	2.278681
45	1	0	-1.034473	4.677972	4.026578
46	1	0	0.108691	2.839359	2.823284
47	1	0	-0.080090	5.108837	-0.823227
48	1	0	-1.228387	6.946211	0.378483
49	1	0	-1.717333	6.732667	2.805664
50	6	0	0.717048	2.684546	0.176085
51	7	0	-0.179115	1.550568	-0.096407
52	1	0	-0.469685	1.114282	0.780593
53	1	0	1.551795	2.292072	0.765632
54	1	0	1.118401	3.029940	-0.782401
55	6	0	-1.365718	1.862475	-0.864858
56	8	0	-2.417773	2.465050	-0.108138

57	1	0	-1.076751	2.513282	-1.697961
58	6	0	-2.000732	0.590741	-1.434275
59	8	0	-3.105739	0.953751	-2.247394
60	1	0	-1.292846	0.100809	-2.107836
61	6	0	-5.567488	-2.182604	-3.298211
62	6	0	-4.299607	-2.133966	-2.715144
63	6	0	-4.139018	-1.717942	-1.391855
64	6	0	-5.273583	-1.365562	-0.651907
65	6	0	-6.541756	-1.407322	-1.230065
66	6	0	-6.692095	-1.815059	-2.558223
67	1	0	-5.676438	-2.503944	-4.329723
68	1	0	-3.425173	-2.408826	-3.300272
69	1	0	-5.167810	-1.053592	0.385497
70	1	0	-7.413014	-1.128156	-0.645230
71	1	0	-7.678778	-1.850641	-3.009757
72	6	0	-2.764337	-1.649669	-0.751692
73	7	0	-2.292823	-0.318784	-0.347661
74	1	0	-3.673768	1.531617	-1.708002
75	1	0	-2.019044	-2.070892	-1.435498
76	1	0	-2.766504	-2.276499	0.146664
77	1	0	-2.948247	0.117675	0.301831
78	1	0	-2.183973	3.384533	0.101764

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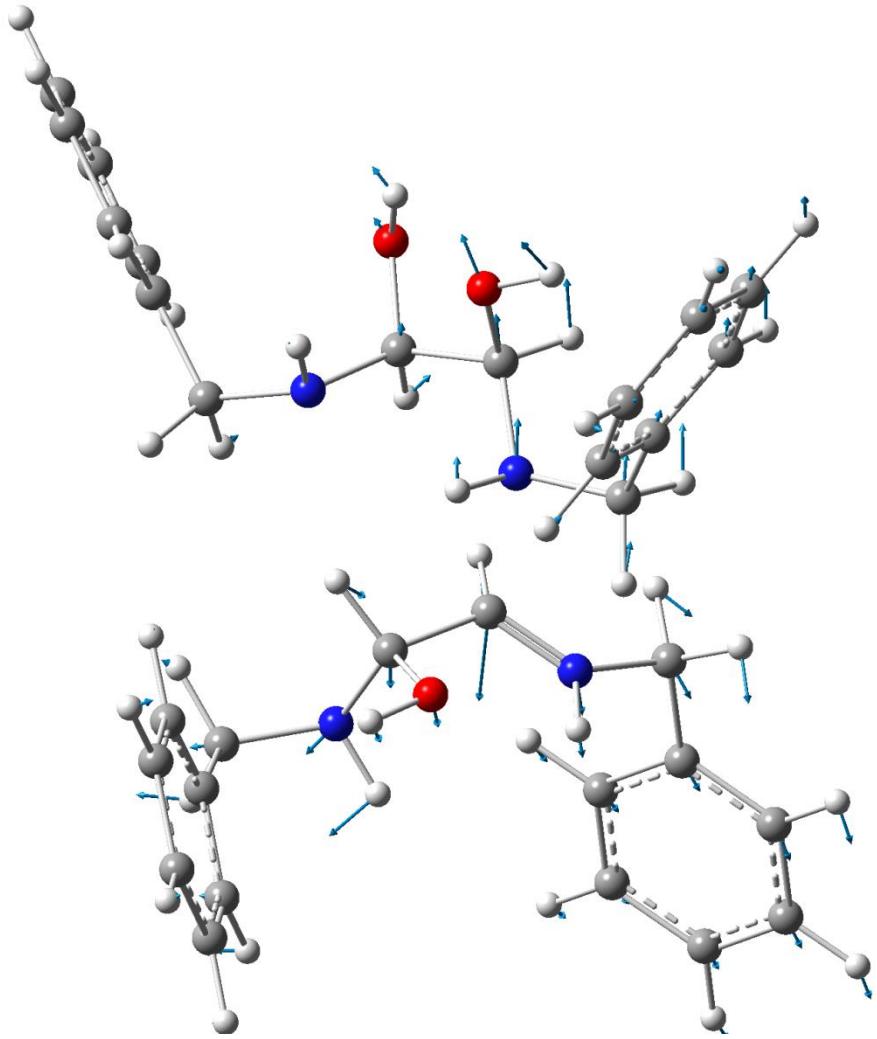
free energy = -1686.20097 A.U.

TS5:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.499564	-1.412395	-3.052974
2	6	0	4.325103	-0.757767	-2.689481
3	6	0	4.369996	0.559038	-2.216541
4	6	0	5.598951	1.211638	-2.109915
5	6	0	6.776963	0.556992	-2.477552
6	6	0	6.728459	-0.754570	-2.947688
7	1	0	5.458015	-2.432800	-3.420399
8	1	0	3.370590	-1.273053	-2.774969
9	1	0	5.638815	2.232799	-1.740220
10	1	0	7.729137	1.070914	-2.392856
11	1	0	7.643266	-1.265107	-3.231690
12	6	0	3.091535	1.262327	-1.817847
13	7	0	2.448994	0.563575	-0.694904
14	1	0	2.947452	0.546534	0.198190

15	1	0	2.370896	1.284805	-2.637783
16	1	0	3.294821	2.289294	-1.509053
17	6	0	1.291899	-0.026141	-0.731646
18	1	0	0.799471	-0.128058	-1.691901
19	6	0	0.936518	-0.975252	0.389217
20	8	0	1.434570	-0.350741	1.568254
21	1	0	-0.152444	-1.087462	0.426744
22	6	0	0.040836	-2.826922	4.393900
23	6	0	-0.068314	-2.961353	3.006543
24	6	0	1.036136	-3.348801	2.238540
25	6	0	2.250461	-3.614693	2.885081
26	6	0	2.362034	-3.483828	4.268299
27	6	0	1.257021	-3.085079	5.025931
28	1	0	-0.823668	-2.524881	4.976647
29	1	0	-1.020995	-2.762175	2.520273
30	1	0	3.113834	-3.923793	2.300081
31	1	0	3.308500	-3.692906	4.757024
32	1	0	1.344001	-2.982453	6.102944
33	6	0	0.948008	-3.411219	0.725964
34	7	0	1.516961	-2.241069	0.034449
35	1	0	1.242309	-0.923314	2.331279
36	1	0	-0.096098	-3.504702	0.414360
37	1	0	1.480166	-4.288507	0.351474
38	1	0	2.531734	-2.208893	0.132551
39	6	0	-1.034819	4.531250	3.184123
40	6	0	-0.355704	3.569109	2.439781
41	6	0	-0.098451	3.774092	1.078917
42	6	0	-0.514791	4.967022	0.479231
43	6	0	-1.197819	5.933528	1.223903
44	6	0	-1.462139	5.715002	2.575532
45	1	0	-1.229677	4.361185	4.238324
46	1	0	-0.021549	2.650094	2.917378
47	1	0	-0.307931	5.144845	-0.573890
48	1	0	-1.519082	6.854220	0.747088
49	1	0	-1.992428	6.464409	3.154406
50	6	0	0.589477	2.692584	0.272157
51	7	0	-0.246345	1.518599	-0.037671
52	1	0	-0.557755	1.074815	0.830163
53	1	0	1.454258	2.324426	0.832060
54	1	0	0.952021	3.100892	-0.676363
55	6	0	-1.428021	1.794428	-0.849077
56	8	0	-2.486409	2.398391	-0.115989
57	1	0	-1.125489	2.426243	-1.691127
58	6	0	-2.045590	0.499337	-1.388754

59	8	0	-3.146619	0.832549	-2.217421
60	1	0	-1.337429	-0.007223	-2.048955
61	6	0	-5.532220	-2.387630	-3.179835
62	6	0	-4.268607	-2.294845	-2.592712
63	6	0	-4.125946	-1.861935	-1.272662
64	6	0	-5.273648	-1.536830	-0.540560
65	6	0	-6.537819	-1.622476	-1.122850
66	6	0	-6.670421	-2.047369	-2.447500
67	1	0	-5.627248	-2.722179	-4.208495
68	1	0	-3.384149	-2.549352	-3.172041
69	1	0	-5.181035	-1.211813	0.494075
70	1	0	-7.419229	-1.363657	-0.543931
71	1	0	-7.653725	-2.117447	-2.902302
72	6	0	-2.757130	-1.735838	-0.629765
73	7	0	-2.329684	-0.375943	-0.276015
74	1	0	-3.735256	1.403088	-1.692685
75	1	0	-1.996762	-2.159351	-1.294990
76	1	0	-2.740790	-2.324611	0.293148
77	1	0	-3.001970	0.065314	0.352465
78	1	0	-2.285507	3.333727	0.054657

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free energy = -1686.19504 A.U.

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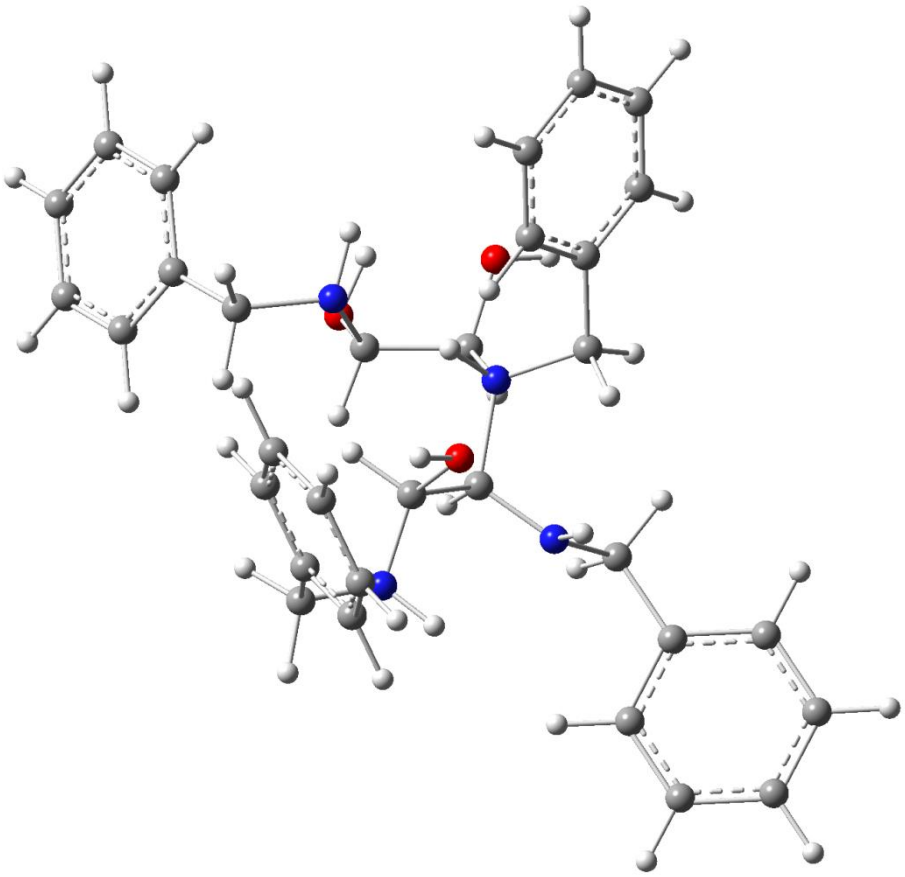

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.303548	-0.304025	-2.483387
2	6	0	-4.938825	-0.483150	-2.268790
3	6	0	-4.476821	-1.566028	-1.510733
4	6	0	-5.399043	-2.461663	-0.967017
5	6	0	-6.769106	-2.284318	-1.180438
6	6	0	-7.223146	-1.206266	-1.938467
7	1	0	-6.652211	0.536645	-3.075392
8	1	0	-4.220885	0.218891	-2.686497
9	1	0	-5.048943	-3.301559	-0.372133
10	1	0	-7.477912	-2.986173	-0.752186
11	1	0	-8.286736	-1.066026	-2.104639
12	6	0	-2.992575	-1.751461	-1.289690
13	7	0	-2.421224	-0.558362	-0.666824
14	1	0	-2.869594	-0.265637	0.197293
15	1	0	-2.486839	-1.884719	-2.252454
16	1	0	-2.824744	-2.662714	-0.701376
17	6	0	-1.047177	-0.312258	-0.740839

18	1	0	-0.702488	-0.502420	-1.758517
19	6	0	-0.720716	1.126718	-0.334878
20	8	0	-1.098100	1.173048	1.047551
21	1	0	0.361247	1.296674	-0.424248
22	6	0	0.211088	4.750244	2.208251
23	6	0	0.253961	4.193189	0.926462
24	6	0	-0.907752	4.095175	0.151571
25	6	0	-2.113660	4.579178	0.675494
26	6	0	-2.159443	5.138420	1.951297
27	6	0	-0.996650	5.221370	2.723017
28	1	0	1.119359	4.816118	2.799049
29	1	0	1.199623	3.829911	0.528052
30	1	0	-3.021765	4.515747	0.080007
31	1	0	-3.099870	5.510965	2.345271
32	1	0	-1.033546	5.654482	3.717565
33	6	0	-0.879298	3.415523	-1.204230
34	7	0	-1.379647	2.033029	-1.219941
35	1	0	-0.870106	2.047180	1.409862
36	1	0	0.146055	3.400506	-1.586238
37	1	0	-1.483465	3.978882	-1.918933
38	1	0	-2.389180	1.984541	-1.092534
39	6	0	1.289956	-1.212335	4.311626
40	6	0	0.512218	-1.054248	3.164997
41	6	0	0.013292	-2.175023	2.493173
42	6	0	0.275497	-3.451058	2.994670
43	6	0	1.041534	-3.609002	4.149362
44	6	0	1.557520	-2.490374	4.805011
45	1	0	1.677826	-0.337880	4.824441
46	1	0	0.281413	-0.053962	2.800872
47	1	0	-0.117259	-4.326893	2.483930
48	1	0	1.239482	-4.604914	4.532763
49	1	0	2.159640	-2.613083	5.699768
50	6	0	-0.837239	-1.995067	1.257214
51	7	0	-0.114998	-1.226113	0.184062
52	1	0	0.525774	-0.572351	0.668411
53	1	0	-1.722408	-1.411058	1.507726
54	1	0	-1.158641	-2.952103	0.843459
55	6	0	0.818582	-2.053645	-0.672731
56	8	0	1.494454	-2.986882	0.105764
57	1	0	0.225523	-2.519763	-1.463635
58	6	0	1.896230	-1.110978	-1.251458
59	8	0	2.783375	-1.885826	-2.021537
60	1	0	1.449217	-0.397472	-1.949133
61	6	0	5.804197	0.497753	-3.361288

62	6	0	4.647148	0.811824	-2.645461
63	6	0	4.541904	0.496648	-1.288883
64	6	0	5.619877	-0.129142	-0.652294
65	6	0	6.775725	-0.449371	-1.363570
66	6	0	6.869875	-0.137534	-2.722536
67	1	0	5.871745	0.746646	-4.415985
68	1	0	3.816162	1.299143	-3.150281
69	1	0	5.557991	-0.367878	0.407726
70	1	0	7.604411	-0.936508	-0.858806
71	1	0	7.769736	-0.384385	-3.277284
72	6	0	3.276739	0.804631	-0.514345
73	7	0	2.458233	-0.364676	-0.148600
74	1	0	3.142974	-2.585309	-1.448002
75	1	0	2.644351	1.483469	-1.096394
76	1	0	3.524482	1.315502	0.419986
77	1	0	2.976791	-0.987172	0.474028
78	1	0	1.096359	-3.867545	0.022679

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free energy = -1686.20325 A.U.

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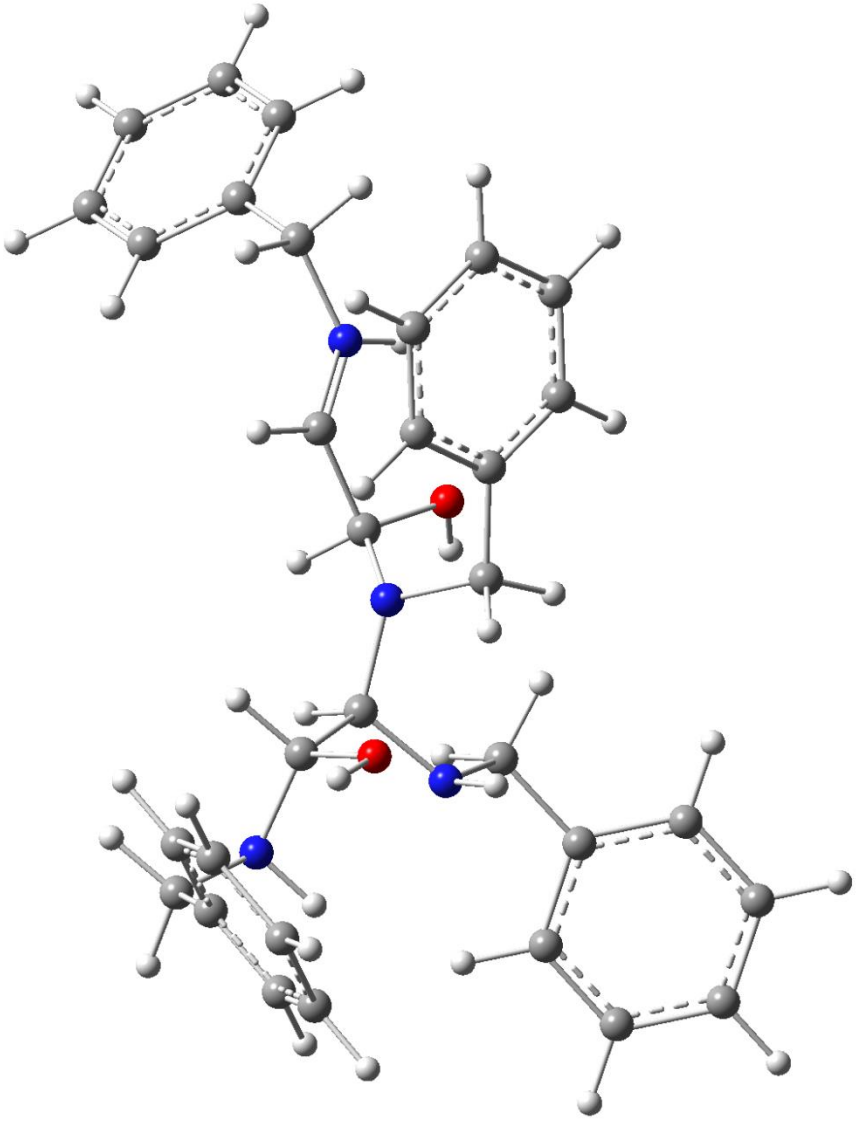


Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.656388	4.726851	-0.947312
2	6	0	3.655834	3.778280	-1.147000
3	6	0	2.575154	3.686015	-0.260678
4	6	0	2.517662	4.554140	0.831273
5	6	0	3.520501	5.506997	1.036052
6	6	0	4.590245	5.595666	0.146784
7	1	0	5.486927	4.793016	-1.643594
8	1	0	3.706277	3.100217	-1.995471
9	1	0	1.684937	4.487663	1.527431
10	1	0	3.464748	6.175860	1.889388
11	1	0	5.368896	6.335957	0.302232

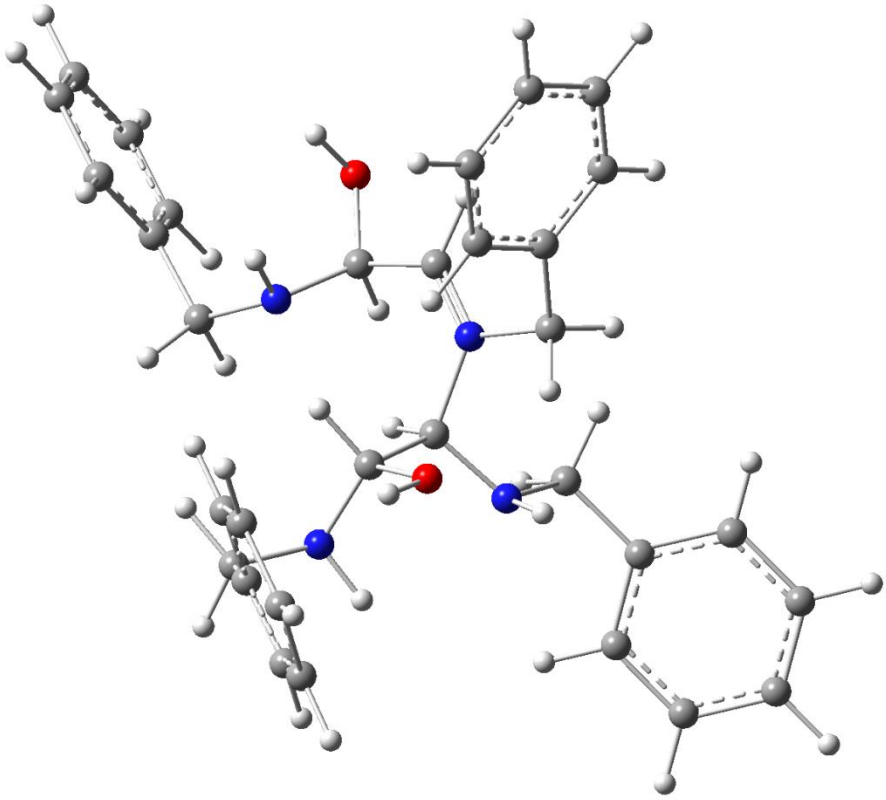
12	6	0	1.497753	2.651363	-0.490575
13	7	0	2.056477	1.301680	-0.424158
14	1	0	2.477888	1.124905	0.487515
15	1	0	1.076854	2.780115	-1.495580
16	1	0	0.683829	2.815394	0.231603
17	6	0	1.141619	0.238980	-0.778310
18	1	0	0.783131	0.432946	-1.793756
19	6	0	1.930528	-1.074603	-0.858172
20	8	0	2.472968	-1.292847	0.450227
21	1	0	1.234417	-1.884890	-1.106802
22	6	0	4.428658	-4.864386	0.277732
23	6	0	3.756684	-4.189659	-0.746950
24	6	0	4.278510	-3.010567	-1.289492
25	6	0	5.497605	-2.524137	-0.797693
26	6	0	6.171182	-3.193477	0.222153
27	6	0	5.635174	-4.364922	0.766449
28	1	0	4.008515	-5.776168	0.690863
29	1	0	2.814771	-4.582284	-1.123718
30	1	0	5.918202	-1.610372	-1.212110
31	1	0	7.113393	-2.803795	0.594972
32	1	0	6.158008	-4.884377	1.563228
33	6	0	3.515151	-2.237749	-2.352128
34	7	0	2.902997	-0.978478	-1.915631
35	1	0	2.930344	-2.149787	0.459236
36	1	0	2.719571	-2.871506	-2.756600
37	1	0	4.186393	-1.996211	-3.180945
38	1	0	3.599839	-0.276883	-1.669386
39	6	0	-2.431765	-2.154800	2.893433
40	6	0	-1.296765	-1.631860	2.272585
41	6	0	-1.048588	-0.253053	2.288124
42	6	0	-1.938146	0.592899	2.954121
43	6	0	-3.075633	0.074404	3.575226
44	6	0	-3.327305	-1.299390	3.539765
45	1	0	-2.618637	-3.223946	2.872307
46	1	0	-0.602327	-2.290428	1.754260
47	1	0	-1.754831	1.664152	2.958635
48	1	0	-3.768287	0.740663	4.080251
49	1	0	-4.216808	-1.702182	4.014566
50	6	0	0.122367	0.303493	1.515975
51	7	0	-0.061435	0.072608	0.072757
52	1	0	1.039482	-0.209901	1.807408
53	1	0	0.231660	1.371254	1.745075
54	6	0	-1.307201	0.545664	-0.455869
55	8	0	-1.749578	1.814794	-0.006757

56	1	0	-1.239764	0.520909	-1.552525
57	6	0	-2.430182	-0.423038	-0.154785
58	1	0	-2.266786	-1.482251	-0.336776
59	6	0	-6.502831	-0.595293	-3.029455
60	6	0	-5.583578	-0.922194	-2.035515
61	6	0	-5.804522	-0.521732	-0.713603
62	6	0	-6.949659	0.210493	-0.393995
63	6	0	-7.872000	0.537467	-1.389811
64	6	0	-7.649321	0.135816	-2.706490
65	1	0	-6.329054	-0.912681	-4.052609
66	1	0	-4.693561	-1.493774	-2.288234
67	1	0	-7.124560	0.523209	0.632045
68	1	0	-8.761757	1.104172	-1.135345
69	1	0	-8.367358	0.388049	-3.480411
70	6	0	-4.792731	-0.866239	0.354830
71	7	0	-3.591554	-0.019880	0.197460
72	1	0	-4.463407	-1.905227	0.292805
73	1	0	-5.186818	-0.679578	1.354201
74	1	0	-3.691748	0.992350	0.343179
75	1	0	-1.419623	2.509755	-0.598103

SCF Done: E(RM062X) = -1610.39929113 A.U.

free energy = -1609.80226 A.U.

IM8-S1:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.362644	-3.240334	-2.316890
2	6	0	-4.047223	-2.828773	-2.112642
3	6	0	-3.432157	-3.012570	-0.868049
4	6	0	-4.155043	-3.606133	0.168886
5	6	0	-5.473898	-4.020794	-0.032879
6	6	0	-6.079098	-3.838897	-1.276032
7	1	0	-5.829593	-3.098429	-3.286643
8	1	0	-3.489031	-2.362238	-2.920767
9	1	0	-3.684837	-3.749636	1.138770
10	1	0	-6.024698	-4.485290	0.779095
11	1	0	-7.102909	-4.162541	-1.436119
12	6	0	-2.015008	-2.544529	-0.646581
13	7	0	-1.963739	-1.077587	-0.649794
14	1	0	-2.695952	-0.648990	-0.086655
15	1	0	-1.366297	-2.895047	-1.456475
16	1	0	-1.631807	-2.976830	0.289002
17	6	0	-0.687796	-0.501487	-0.445645
18	1	0	0.020834	-0.910668	-1.162325
19	6	0	-0.708952	1.020506	-0.638773

20	8	0	-1.713415	1.506140	0.253817
21	1	0	0.272708	1.420348	-0.362556
22	6	0	-1.247918	5.490251	-0.032159
23	6	0	-0.580729	4.494161	-0.752106
24	6	0	-1.240007	3.776512	-1.756643
25	6	0	-2.577928	4.082533	-2.039274
26	6	0	-3.245544	5.076497	-1.325773
27	6	0	-2.582048	5.780591	-0.316435
28	1	0	-0.724652	6.036688	0.746288
29	1	0	0.460771	4.272794	-0.528234
30	1	0	-3.099533	3.535270	-2.821408
31	1	0	-4.281861	5.304094	-1.555275
32	1	0	-3.102030	6.554085	0.239711
33	6	0	-0.545549	2.637592	-2.479899
34	7	0	-0.925870	1.290336	-2.031110
35	1	0	-1.725029	2.478112	0.213744
36	1	0	0.538033	2.732177	-2.360844
37	1	0	-0.759810	2.688191	-3.550156
38	1	0	-1.888035	1.065139	-2.280976
39	6	0	0.623517	1.641642	4.546297
40	6	0	-0.005917	1.137727	3.411390
41	6	0	-0.366368	-0.214170	3.350008
42	6	0	-0.098006	-1.053697	4.432589
43	6	0	0.528341	-0.545903	5.573436
44	6	0	0.890741	0.798910	5.629800
45	1	0	0.899353	2.690332	4.591457
46	1	0	-0.227032	1.788801	2.567553
47	1	0	-0.379431	-2.102618	4.388360
48	1	0	0.732720	-1.201441	6.413751
49	1	0	1.376808	1.193515	6.516419
50	6	0	-1.044905	-0.737883	2.112178
51	7	0	-0.108495	-0.817707	0.940744
52	1	0	-1.849469	-0.070172	1.812528
53	1	0	-1.448637	-1.742013	2.264016
54	6	0	1.101781	-1.199496	1.107259
55	1	0	1.427067	-1.420111	2.124155
56	6	0	2.122870	-1.399146	-0.002910
57	8	0	3.227435	-2.099898	0.534891
58	1	0	1.692042	-2.089021	-0.738780
59	6	0	6.402321	-2.192192	-1.948758
60	6	0	5.065641	-1.835940	-2.132798
61	6	0	4.603706	-0.576884	-1.740173
62	6	0	5.505824	0.328531	-1.169254
63	6	0	6.842050	-0.024733	-0.978148

64	6	0	7.292724	-1.288322	-1.366458
65	1	0	6.747517	-3.174450	-2.256434
66	1	0	4.371093	-2.547893	-2.572173
67	1	0	5.164663	1.318675	-0.873392
68	1	0	7.532022	0.686179	-0.534062
69	1	0	8.332489	-1.564068	-1.220258
70	6	0	3.144218	-0.196835	-1.897466
71	7	0	2.364624	-0.141974	-0.648342
72	1	0	3.862025	-1.466900	0.910790
73	1	0	2.639750	-0.903744	-2.562973
74	1	0	3.061846	0.793227	-2.353567
75	1	0	2.739125	0.552644	-0.002308

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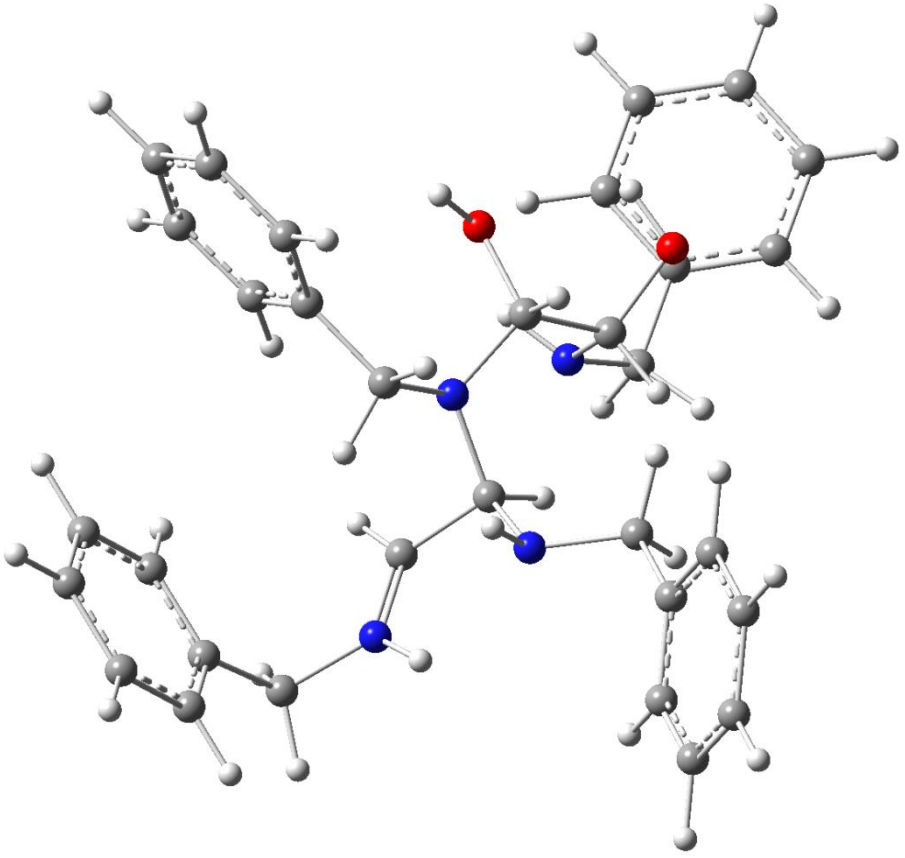
free energy = -1609.79913 A.U.

IM8-S2:



Standard orientation

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

1	6	0	3.236753	5.542914	0.036836
2	6	0	2.325962	4.545213	-0.303044
3	6	0	1.464223	4.012122	0.664018
4	6	0	1.533079	4.487979	1.974703
5	6	0	2.445261	5.489467	2.318734
6	6	0	3.297660	6.018308	1.350676
7	1	0	3.898080	5.953681	-0.719911
8	1	0	2.275948	4.174434	-1.324061
9	1	0	0.869365	4.077400	2.731459
10	1	0	2.488915	5.853015	3.340662
11	1	0	4.006042	6.797359	1.615031
12	6	0	0.478133	2.932592	0.284662
13	7	0	1.195024	1.742890	-0.205253
14	1	0	1.819276	1.409806	0.531195
15	1	0	-0.163974	3.284958	-0.529223
16	1	0	-0.162607	2.707334	1.147584
17	6	0	0.354937	0.661626	-0.691426
18	1	0	-0.513566	1.079585	-1.211919
19	6	0	1.099915	-0.099157	-1.760797
20	1	0	0.646537	-0.991538	-2.187875
21	6	0	4.304256	-3.377598	-0.752610
22	6	0	3.548530	-2.617839	-1.643797
23	6	0	4.037350	-1.394306	-2.115098
24	6	0	5.288694	-0.939045	-1.694878
25	6	0	6.047721	-1.702841	-0.806519
26	6	0	5.555090	-2.918953	-0.332215
27	1	0	3.919792	-4.326124	-0.390945
28	1	0	2.580550	-2.985855	-1.978090
29	1	0	5.671001	0.010818	-2.059209
30	1	0	7.020699	-1.346512	-0.484224
31	1	0	6.145519	-3.511024	0.359655
32	6	0	3.166353	-0.535854	-3.004914
33	7	0	2.265856	0.256281	-2.137221
34	1	0	2.540379	-1.133475	-3.667679
35	1	0	3.747331	0.169596	-3.597243
36	1	0	2.620134	1.116447	-1.688807
37	6	0	0.161359	-4.651466	0.903796
38	6	0	0.315336	-3.318117	0.534386
39	6	0	0.736368	-2.366773	1.471470
40	6	0	0.994852	-2.770594	2.782770
41	6	0	0.840006	-4.109269	3.156622
42	6	0	0.425497	-5.051701	2.218042
43	1	0	-0.171386	-5.380148	0.170934
44	1	0	0.079721	-3.002685	-0.478533

45	1	0	1.315687	-2.037893	3.519314
46	1	0	1.039991	-4.409436	4.180479
47	1	0	0.301487	-6.090841	2.506352
48	6	0	0.962311	-0.924769	1.061690
49	7	0	-0.118619	-0.360947	0.236816
50	1	0	1.892159	-0.897763	0.476725
51	1	0	1.140551	-0.315954	1.961727
52	6	0	-1.325808	-0.072235	1.012357
53	8	0	-2.010045	-1.276226	1.325690
54	1	0	-1.075927	0.452102	1.947459
55	6	0	-2.383281	0.757404	0.264214
56	8	0	-3.488624	0.936041	1.133299
57	1	0	-2.029691	1.776002	0.081915
58	6	0	-7.446655	0.974690	-0.633963
59	6	0	-6.165169	1.304954	-1.079448
60	6	0	-5.183608	0.321653	-1.230772
61	6	0	-5.513481	-1.006572	-0.936547
62	6	0	-6.790772	-1.341689	-0.486089
63	6	0	-7.763036	-0.350575	-0.332135
64	1	0	-8.194865	1.752703	-0.515819
65	1	0	-5.922768	2.341745	-1.300599
66	1	0	-4.773023	-1.794569	-1.058416
67	1	0	-7.028295	-2.376576	-0.258566
68	1	0	-8.757067	-0.609950	0.018745
69	6	0	-3.798379	0.680940	-1.743880
70	7	0	-2.663690	0.127771	-1.001954
71	1	0	-3.786560	0.048818	1.402597
72	1	0	-3.687728	1.769509	-1.761547
73	1	0	-3.708330	0.336170	-2.779061
74	1	0	-2.742799	-0.881419	-0.886438
75	1	0	-1.557960	-1.743255	2.046636

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free energy = -1609.79808 A.U.

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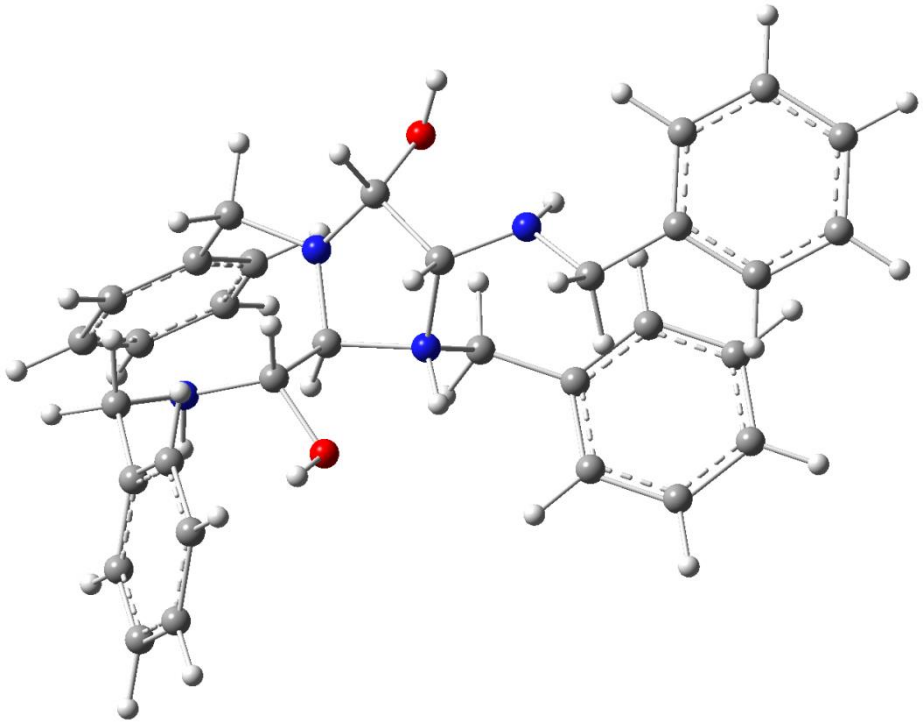


Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.092145	0.814794	3.490231
2	6	0	1.961771	0.298303	2.857880
3	6	0	2.084857	-0.743286	1.931747
4	6	0	3.345613	-1.288094	1.675129
5	6	0	4.476092	-0.777414	2.312225
6	6	0	4.352138	0.281247	3.212967
7	1	0	2.987956	1.626735	4.202626
8	1	0	0.982058	0.708853	3.095862
9	1	0	3.449955	-2.114267	0.975148
10	1	0	5.452882	-1.199221	2.097307
11	1	0	5.233548	0.685767	3.700480
12	6	0	0.859831	-1.270902	1.229367
13	7	0	0.209824	-0.219648	0.360837
14	1	0	0.100459	-1.569300	1.955792
15	1	0	1.082276	-2.127261	0.591138
16	6	0	-1.198352	-0.578908	-0.005712
17	1	0	-1.690334	-1.041322	0.857098
18	6	0	-1.991723	0.689354	-0.389270
19	8	0	-1.567162	1.683302	0.547680
20	1	0	-1.743455	1.005887	-1.410654
21	6	0	-3.515562	4.992047	-0.626151

22	6	0	-3.589350	3.708329	-1.176180
23	6	0	-4.282214	2.688001	-0.514709
24	6	0	-4.915097	2.977730	0.700971
25	6	0	-4.846226	4.256534	1.250702
26	6	0	-4.141339	5.266782	0.589570
27	1	0	-2.972890	5.773603	-1.148633
28	1	0	-3.101887	3.501039	-2.126589
29	1	0	-5.461406	2.194165	1.221566
30	1	0	-5.341322	4.467222	2.193563
31	1	0	-4.084819	6.262148	1.018628
32	6	0	-4.289322	1.271716	-1.058611
33	7	0	-3.380171	0.345015	-0.370345
34	1	0	-1.977499	2.536814	0.323229
35	1	0	-4.016650	1.277186	-2.118275
36	1	0	-5.292468	0.844415	-0.983378
37	1	0	-3.689101	0.160375	0.583725
38	6	0	-4.933893	-3.701171	0.412886
39	6	0	-4.239468	-2.923428	-0.517372
40	6	0	-2.856631	-3.053590	-0.655427
41	6	0	-2.170534	-3.964746	0.155841
42	6	0	-2.859556	-4.738332	1.088443
43	6	0	-4.245368	-4.608546	1.218100
44	1	0	-6.009568	-3.592199	0.513008
45	1	0	-4.771864	-2.201987	-1.132159
46	1	0	-1.091600	-4.060080	0.051940
47	1	0	-2.318785	-5.443684	1.712182
48	1	0	-4.783315	-5.209677	1.944694
49	6	0	-2.094541	-2.231433	-1.672308
50	7	0	-0.969521	-1.544482	-1.047006
51	1	0	-2.773413	-1.536930	-2.181446
52	1	0	-1.659066	-2.897789	-2.423490
53	6	0	0.168184	-1.193090	-1.848257
54	8	0	0.999257	-2.335198	-1.954189
55	1	0	-0.089980	-0.832780	-2.852239
56	6	0	0.859211	-0.050232	-1.067135
57	1	0	0.483506	0.922770	-1.391837
58	6	0	6.319817	0.093753	-2.309893
59	6	0	4.948990	0.201017	-2.062948
60	6	0	4.483315	0.930672	-0.965222
61	6	0	5.409209	1.555273	-0.122795
62	6	0	6.777004	1.456987	-0.372672
63	6	0	7.237453	0.721060	-1.467139
64	1	0	6.668441	-0.480038	-3.163227
65	1	0	4.239767	-0.283940	-2.727547

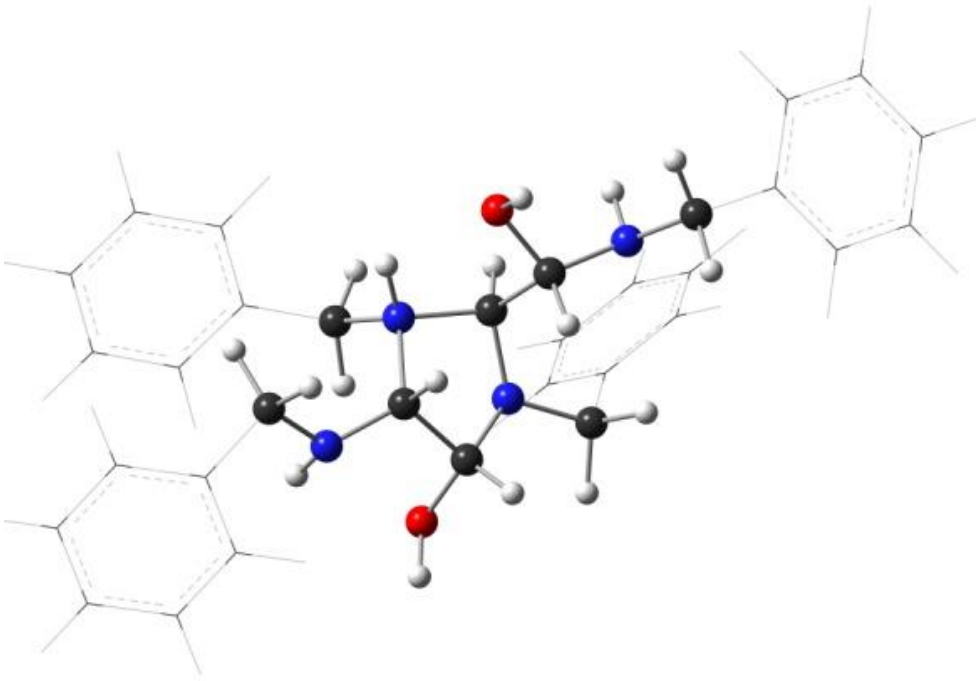
66	1	0	5.057157	2.114843	0.740944
67	1	0	7.483501	1.944488	0.292216
68	1	0	8.302549	0.635659	-1.658869
69	6	0	3.005483	1.080213	-0.678340
70	7	0	2.250753	-0.075107	-1.160767
71	1	0	2.615904	1.962524	-1.199451
72	1	0	2.873490	1.254165	0.398810
73	1	0	1.498563	-2.287865	-2.785135
74	1	0	2.662318	-0.977858	-0.936260
75	1	0	0.190496	0.688421	0.846763

SCF Done: E(RM062X) = -1610.42188874 A.U.

free energy = -1609.8242 A.U.

Figure 4

IM9:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.824690	1.273633	3.427107
2	6	0	-2.607791	1.175340	2.746679
3	6	0	-2.512309	1.613751	1.417053
4	6	0	-3.631545	2.179102	0.786696
5	6	0	-4.842002	2.284883	1.476645

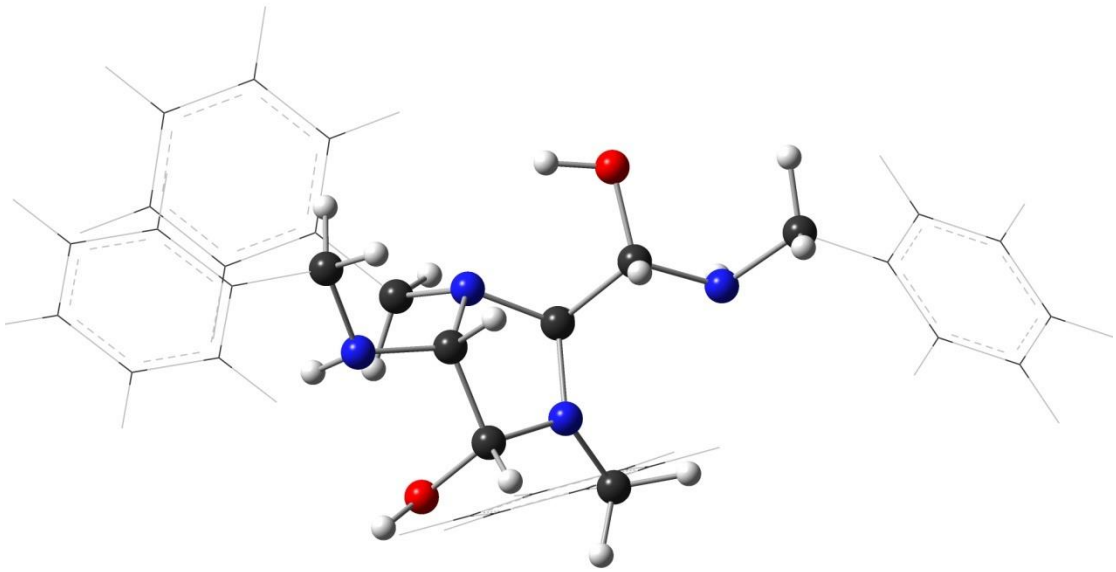
6	6	0	-4.942571	1.826368	2.794214
7	1	0	-3.898576	0.924393	4.458695
8	1	0	-1.739218	0.767542	3.265647
9	1	0	-3.561971	2.549857	-0.237510
10	1	0	-5.709792	2.728686	0.985076
11	1	0	-5.890131	1.905617	3.329633
12	6	0	-1.205949	1.553856	0.680037
13	7	0	-0.689825	0.132196	0.595395
14	1	0	-0.437363	2.128203	1.211940
15	1	0	-1.273481	1.925973	-0.348828
16	6	0	0.753583	0.086246	0.192809
17	1	0	1.295442	0.894114	0.696116
18	6	0	1.382350	-1.265250	0.609785
19	8	0	0.783345	-1.605438	1.866511
20	1	0	1.144170	-2.039767	-0.129174
21	6	0	7.134781	-1.387321	1.771769
22	6	0	5.775106	-1.696412	1.866904
23	6	0	5.041849	-1.996789	0.709343
24	6	0	5.676794	-1.981204	-0.541335
25	6	0	7.036599	-1.671031	-0.630543
26	6	0	7.767307	-1.374348	0.524504
27	1	0	7.702823	-1.156136	2.673218
28	1	0	5.288674	-1.703952	2.842224
29	1	0	5.110496	-2.209859	-1.444334
30	1	0	7.528044	-1.660497	-1.603727
31	1	0	8.827750	-1.133978	0.452884
32	6	0	3.576910	-2.332102	0.810266
33	7	0	2.798439	-1.093812	0.620830
34	1	0	0.891561	-2.552662	2.047105
35	1	0	3.356725	-2.818207	1.779467
36	1	0	3.281625	-3.034665	0.014396
37	1	0	3.064159	-0.387990	1.307237
38	6	0	4.813498	2.445499	-0.715495
39	6	0	4.009967	1.375068	-1.118789
40	6	0	2.707128	1.611421	-1.579329
41	6	0	2.212260	2.923803	-1.625989
42	6	0	3.017597	3.989605	-1.217340
43	6	0	4.319750	3.752693	-0.763987
44	1	0	5.827441	2.259337	-0.361514
45	1	0	4.396330	0.354528	-1.066573
46	1	0	1.197497	3.109174	-1.977905
47	1	0	2.630821	5.008015	-1.253688
48	1	0	4.947693	4.585771	-0.449465
49	6	0	1.852807	0.461273	-2.051579

50	7	0	0.650773	0.341042	-1.218784
51	1	0	2.426538	-0.481515	-2.065654
52	1	0	1.492919	0.660933	-3.072606
53	6	0	-0.509027	-0.296893	-1.776789
54	8	0	-1.198096	0.651342	-2.570089
55	1	0	-0.276008	-1.180454	-2.385326
56	6	0	-1.343276	-0.741934	-0.551767
57	1	0	-1.077649	-1.758309	-0.252552
58	6	0	-6.451310	-2.325718	-2.116522
59	6	0	-5.179515	-2.200681	-1.551927
60	6	0	-4.993849	-1.410074	-0.407270
61	6	0	-6.089165	-0.750419	0.168190
62	6	0	-7.360353	-0.882487	-0.398233
63	6	0	-7.543348	-1.667997	-1.540456
64	1	0	-6.592402	-2.938535	-3.007115
65	1	0	-4.329887	-2.714729	-2.001503
66	1	0	-5.955438	-0.134716	1.058767
67	1	0	-8.210610	-0.370269	0.052862
68	1	0	-8.535140	-1.768345	-1.980966
69	6	0	-3.628876	-1.287154	0.215169
70	7	0	-2.717064	-0.648976	-0.748598
71	1	0	-3.222244	-2.284179	0.441312
72	1	0	-3.678131	-0.728891	1.170511
73	1	0	-1.669089	0.187371	-3.280535
74	1	0	-3.028806	0.236882	-1.137308
75	1	0	-0.779297	-0.357486	1.496996

ONIOM: extrapolated energy = -686.371990949413 A.U.

free energy = -685.802195 A.U.

IM10:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.544919	-0.532822	3.453008
2	6	0	-2.396391	-0.332494	2.682738
3	6	0	-2.358987	0.696560	1.729289
4	6	0	-3.477449	1.526951	1.560616
5	6	0	-4.620660	1.327018	2.339426
6	6	0	-4.657617	0.297919	3.285813
7	1	0	-3.570944	-1.336081	4.189673
8	1	0	-1.528406	-0.976167	2.820819
9	1	0	-3.458796	2.334398	0.829134
10	1	0	-5.486351	1.976525	2.207682
11	1	0	-5.549800	0.144600	3.891602
12	6	0	-1.101305	0.972745	0.942504
13	7	0	-0.522658	-0.254076	0.336605
14	1	0	-0.348487	1.355779	1.650584
15	1	0	-1.259789	1.764227	0.187821
16	6	0	0.897945	-0.084743	0.011052
17	1	0	1.340766	0.698249	0.645733
18	6	0	1.649061	-1.393497	0.309102
19	8	0	1.309511	-1.831496	1.625299
20	1	0	1.349932	-2.157808	-0.422651
21	6	0	7.428646	-1.479134	1.261450
22	6	0	6.068018	-1.772291	1.386976
23	6	0	5.312728	-2.100291	0.251045
24	6	0	5.928324	-2.127684	-1.008839

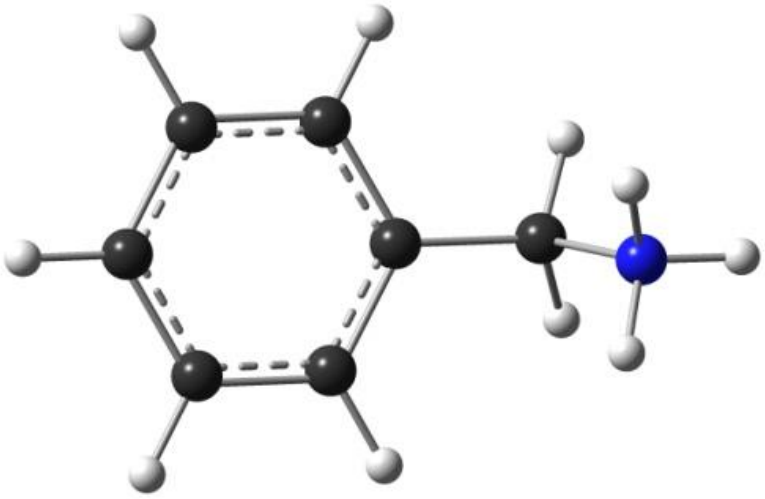
25	6	0	7.289271	-1.832965	-1.129105
26	6	0	8.041453	-1.509255	0.004594
27	1	0	8.013072	-1.226785	2.146389
28	1	0	5.597114	-1.746711	2.369354
29	1	0	5.345655	-2.376680	-1.895358
30	1	0	7.764675	-1.855891	-2.109833
31	1	0	9.102465	-1.281419	-0.090890
32	6	0	3.846324	-2.422151	0.387177
33	7	0	3.062698	-1.189211	0.178560
34	1	0	0.349594	-1.663571	1.698684
35	1	0	3.636383	-2.883185	1.370148
36	1	0	3.534689	-3.145933	-0.384145
37	1	0	3.352950	-0.479362	0.852549
38	6	0	3.447098	3.895528	0.375149
39	6	0	3.310929	2.719699	-0.368418
40	6	0	2.120629	2.458821	-1.063621
41	6	0	1.069239	3.382864	-1.001988
42	6	0	1.206626	4.556299	-0.256592
43	6	0	2.395840	4.815804	0.432700
44	1	0	4.374928	4.094090	0.911092
45	1	0	4.134905	2.007272	-0.406567
46	1	0	0.136202	3.176235	-1.536203
47	1	0	0.385463	5.271174	-0.212741
48	1	0	2.502790	5.731750	1.012111
49	6	0	1.997795	1.185453	-1.882185
50	7	0	0.969717	0.274105	-1.405059
51	1	0	2.963175	0.652875	-1.886735
52	1	0	1.758174	1.440180	-2.926669
53	6	0	-0.322648	0.218714	-2.005265
54	8	0	-0.905236	1.519846	-2.162483
55	1	0	-0.294400	-0.262772	-2.991300
56	6	0	-1.105886	-0.634474	-0.993320
57	1	0	-0.833136	-1.682464	-1.163910
58	6	0	-6.524907	-1.361880	-2.526673
59	6	0	-5.172748	-1.478156	-2.195477
60	6	0	-4.767411	-1.405066	-0.853669
61	6	0	-5.727540	-1.215862	0.150570
62	6	0	-7.079889	-1.104613	-0.185103
63	6	0	-7.481135	-1.176963	-1.522493
64	1	0	-6.835047	-1.417135	-3.570044
65	1	0	-4.428541	-1.621655	-2.978499
66	1	0	-5.421501	-1.151179	1.196018
67	1	0	-7.822726	-0.960168	0.599272
68	1	0	-8.535346	-1.089642	-1.781944

69	6	0	-3.312721	-1.557083	-0.488095
70	7	0	-2.520193	-0.521131	-1.171180
71	1	0	-2.944466	-2.536047	-0.835325
72	1	0	-3.176324	-1.533740	0.611807
73	1	0	-1.610914	1.448407	-2.825843
74	1	0	-2.845388	0.416321	-0.941010

ONIOM: extrapolated energy = -685.930318408357 A.U.

free energy = -685.375648 A.U.

protonized benzylamine:



Standard orientation

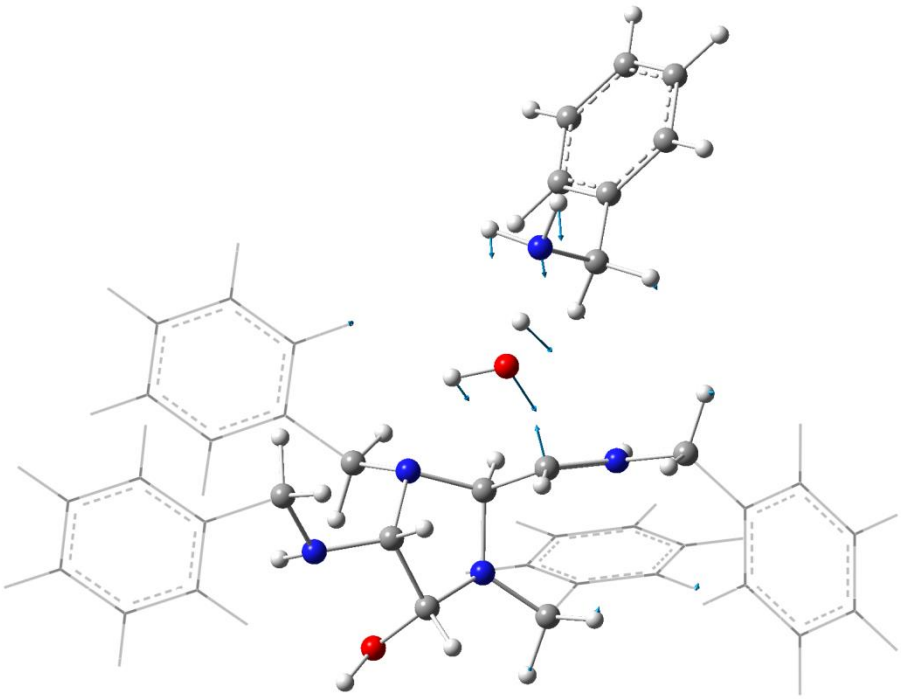
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.705481	-1.176519	0.129606
2	6	0	0.340897	-1.234617	-0.154296
3	6	0	-0.388755	-0.055834	-0.334570
4	6	0	0.255250	1.181581	-0.226937
5	6	0	1.618189	1.239116	0.059361
6	6	0	2.343932	0.059550	0.236963
7	1	0	2.267960	-2.094969	0.262094
8	1	0	-0.153956	-2.197977	-0.245161
9	1	0	-0.305101	2.102142	-0.373206
10	1	0	2.113522	2.201419	0.137308
11	1	0	3.406467	0.103710	0.453739

12	6	0	-1.864680	-0.112313	-0.620411
13	7	0	-2.645766	0.072981	0.658541
14	1	0	-3.658681	0.038810	0.495541
15	1	0	-2.417361	-0.655179	1.344501
16	1	0	-2.170377	-1.074003	-1.029187
17	1	0	-2.187472	0.682916	-1.291298
18	1	0	-2.436522	0.976486	1.097589

SCF Done: E(RM062X) = -327.228262417 A.U.

free energy = -327.080322 A.U.

TS6:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.576564	3.568700	-0.272986
2	6	0	2.622371	2.568021	-0.071117
3	6	0	2.783698	1.642934	0.971803
4	6	0	3.900101	1.735126	1.816362
5	6	0	4.846045	2.744500	1.615753
6	6	0	4.688130	3.660668	0.570860
7	1	0	3.450722	4.282368	-1.087824
8	1	0	1.751282	2.507634	-0.722621
9	1	0	4.032645	1.028885	2.635984

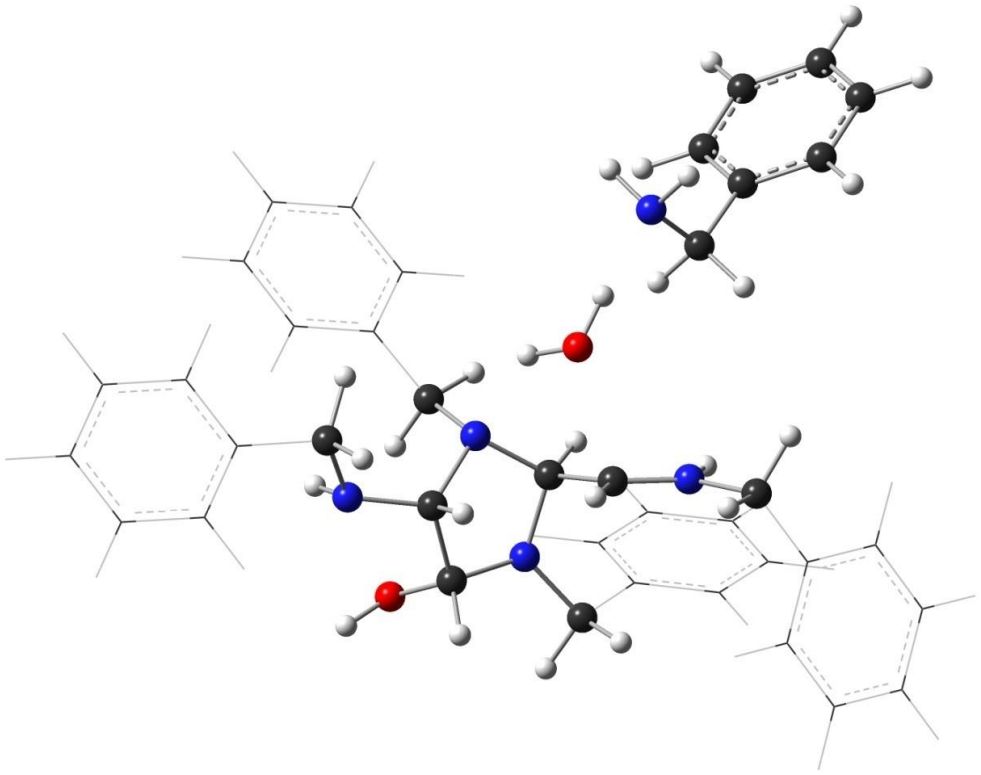
10	1	0	5.710321	2.816245	2.277046
11	1	0	5.428231	4.445292	0.415782
12	6	0	1.731030	0.598724	1.240421
13	7	0	1.337848	-0.130007	-0.000246
14	1	0	0.828796	1.112841	1.608012
15	1	0	2.040214	-0.104858	2.032683
16	6	0	0.018266	-0.725215	0.160915
17	1	0	-0.642047	-0.072835	0.746828
18	6	0	-0.664650	-0.979053	-1.183433
19	8	0	-0.173717	0.726291	-2.093782
20	1	0	-0.121828	-1.498109	-1.966693
21	6	0	-5.868746	-3.338297	-1.028840
22	6	0	-5.000006	-2.346916	-1.493944
23	6	0	-3.688545	-2.683382	-1.859458
24	6	0	-3.252343	-4.013641	-1.763299
25	6	0	-4.125724	-4.999454	-1.297155
26	6	0	-5.432812	-4.663225	-0.928194
27	1	0	-6.889089	-3.076505	-0.744529
28	1	0	-5.346013	-1.315010	-1.571304
29	1	0	-2.236168	-4.283256	-2.054512
30	1	0	-3.787231	-6.034007	-1.221902
31	1	0	-6.112296	-5.435282	-0.564077
32	6	0	-2.748474	-1.617864	-2.346013
33	7	0	-1.965126	-1.127127	-1.191290
34	1	0	0.663291	0.885138	-1.603091
35	1	0	-3.279267	-0.764227	-2.787959
36	1	0	-2.034770	-2.000896	-3.084225
37	1	0	-2.494284	-0.780909	-0.390513
38	6	0	-4.254133	-1.840238	2.425987
39	6	0	-3.239744	-2.454225	1.685961
40	6	0	-1.895408	-2.216567	2.006664
41	6	0	-1.575403	-1.368998	3.077600
42	6	0	-2.593006	-0.754999	3.812157
43	6	0	-3.933413	-0.988130	3.487299
44	1	0	-5.298488	-2.028119	2.173724
45	1	0	-3.504017	-3.127921	0.868389
46	1	0	-0.530498	-1.189767	3.334998
47	1	0	-2.340792	-0.095263	4.643050
48	1	0	-4.725922	-0.509086	4.062086
49	6	0	-0.809151	-2.911488	1.218083
50	7	0	0.255463	-1.983529	0.850676
51	1	0	-1.237723	-3.416161	0.329739
52	1	0	-0.349404	-3.689186	1.847232
53	6	0	1.584637	-2.455184	0.605395

54	8	0	2.259006	-2.593163	1.852210
55	1	0	1.608107	-3.419711	0.081038
56	6	0	2.185981	-1.343844	-0.284438
57	1	0	1.992718	-1.610208	-1.329285
58	6	0	7.795482	-1.836349	-1.029595
59	6	0	6.408316	-1.748190	-1.169502
60	6	0	5.759723	-0.516518	-0.989487
61	6	0	6.511485	0.622908	-0.669694
62	6	0	7.899696	0.530548	-0.534060
63	6	0	8.543734	-0.697438	-0.713256
64	1	0	8.295529	-2.794835	-1.168560
65	1	0	5.826597	-2.636259	-1.414965
66	1	0	6.015839	1.584284	-0.525070
67	1	0	8.480401	1.419528	-0.287698
68	1	0	9.625667	-0.767408	-0.607146
69	6	0	4.266392	-0.413149	-1.162669
70	7	0	3.597346	-1.228716	-0.133936
71	1	0	3.974351	-0.818340	-2.144570
72	1	0	3.935815	0.644434	-1.139401
73	1	0	3.051831	-3.134402	1.703955
74	1	0	3.852301	-0.944369	0.810100
75	1	0	-1.181800	3.522306	-1.071143
76	6	0	-5.456778	5.496639	-1.137266
77	6	0	-4.772528	4.310648	-1.409118
78	6	0	-3.784360	3.843312	-0.536160
79	6	0	-3.493315	4.581886	0.616564
80	6	0	-4.173917	5.768279	0.891215
81	6	0	-5.157773	6.228287	0.013486
82	1	0	-6.223953	5.847379	-1.820660
83	1	0	-5.011647	3.741873	-2.304798
84	1	0	-2.732655	4.223657	1.306845
85	1	0	-3.940927	6.330049	1.790472
86	1	0	-5.691369	7.149034	0.227649
87	6	0	-3.000250	2.589834	-0.854590
88	7	0	-1.745584	2.849750	-1.593750
89	1	0	-0.796642	1.518802	-1.895985
90	1	0	-1.964600	3.308932	-2.479129
91	1	0	-3.604347	1.908920	-1.459214
92	1	0	-2.735855	2.069793	0.070136

ONIOM: extrapolated energy = -1013.144484473952 A.U.

Free energy = -1012.44059 A.U.

CP9:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.504258	3.375929	-0.391032
2	6	0	2.557119	2.382647	-0.130462
3	6	0	2.708496	1.540561	0.982100
4	6	0	3.810745	1.704801	1.833832
5	6	0	4.750735	2.706096	1.573065
6	6	0	4.600820	3.541470	0.461461
7	1	0	3.385831	4.025739	-1.258776
8	1	0	1.699593	2.256595	-0.795437
9	1	0	3.937143	1.060432	2.704049
10	1	0	5.604308	2.834599	2.239845
11	1	0	5.336103	4.320284	0.260434
12	6	0	1.661842	0.508362	1.312512
13	7	0	1.237280	-0.251125	0.101341
14	1	0	0.771130	1.035983	1.688354
15	1	0	1.990814	-0.173101	2.115858
16	6	0	-0.085636	-0.818658	0.286863
17	1	0	-0.731190	-0.160089	0.880191
18	6	0	-0.762473	-1.081393	-1.044624
19	8	0	0.221240	0.926758	-2.300927

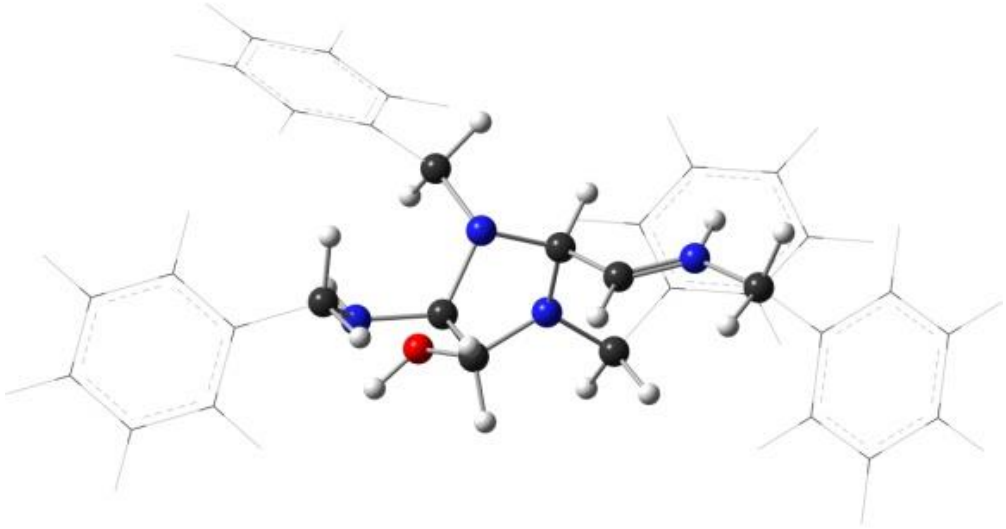
20	1	0	-0.205721	-1.481313	-1.885634
21	6	0	-6.037143	-2.999353	-1.159849
22	6	0	-5.110906	-2.031912	-1.559439
23	6	0	-3.822080	-2.421459	-1.952699
24	6	0	-3.466979	-3.779451	-1.954548
25	6	0	-4.398322	-4.740486	-1.554449
26	6	0	-5.681984	-4.351973	-1.155005
27	1	0	-7.039943	-2.697037	-0.852831
28	1	0	-5.396693	-0.978596	-1.566058
29	1	0	-2.469280	-4.089642	-2.270503
30	1	0	-4.123916	-5.796889	-1.554969
31	1	0	-6.407063	-5.105591	-0.842214
32	6	0	-2.820702	-1.385830	-2.368631
33	7	0	-2.039124	-1.010525	-1.159082
34	1	0	0.842408	0.871699	-1.545629
35	1	0	-3.289289	-0.468996	-2.743599
36	1	0	-2.107553	-1.755530	-3.111091
37	1	0	-2.576605	-0.659490	-0.360418
38	6	0	-4.442452	-1.808148	2.238188
39	6	0	-3.397923	-2.454814	1.571872
40	6	0	-2.076159	-2.286568	2.009301
41	6	0	-1.809903	-1.479242	3.124800
42	6	0	-2.857480	-0.833130	3.786386
43	6	0	-4.174333	-0.993988	3.343155
44	1	0	-5.469274	-1.941196	1.894342
45	1	0	-3.623516	-3.104902	0.724424
46	1	0	-0.783785	-1.356156	3.474285
47	1	0	-2.647084	-0.204661	4.652721
48	1	0	-4.990294	-0.489023	3.860539
49	6	0	-0.957724	-3.008767	1.294633
50	7	0	0.130025	-2.091215	0.962323
51	1	0	-1.343013	-3.529226	0.395636
52	1	0	-0.537103	-3.776693	1.960892
53	6	0	1.458297	-2.573429	0.725326
54	8	0	2.129367	-2.691201	1.974217
55	1	0	1.473346	-3.545529	0.216191
56	6	0	2.067408	-1.478879	-0.179678
57	1	0	1.863177	-1.753042	-1.220550
58	6	0	7.662537	-2.092832	-1.004559
59	6	0	6.277246	-1.978470	-1.144112
60	6	0	5.648708	-0.741359	-0.933068
61	6	0	6.417739	0.376721	-0.580909
62	6	0	7.803994	0.258057	-0.445385
63	6	0	8.428377	-0.974997	-0.656676

64	1	0	8.147280	-3.055298	-1.168318
65	1	0	5.681848	-2.850382	-1.413591
66	1	0	5.937313	1.341857	-0.411847
67	1	0	8.398630	1.130445	-0.174129
68	1	0	9.508887	-1.065341	-0.550963
69	6	0	4.157391	-0.611753	-1.103955
70	7	0	3.480226	-1.378745	-0.042955
71	1	0	3.849518	-1.043247	-2.069389
72	1	0	3.849750	0.452837	-1.114497
73	1	0	2.927622	-3.226861	1.834219
74	1	0	3.750382	-1.070243	0.889031
75	1	0	-0.621470	4.032247	-1.389785
76	6	0	-5.086049	5.480546	-0.868029
77	6	0	-4.292799	4.401650	-1.260794
78	6	0	-3.172736	4.028283	-0.509584
79	6	0	-2.860865	4.753660	0.645993
80	6	0	-3.651232	5.833562	1.042530
81	6	0	-4.765803	6.199800	0.285066
82	1	0	-5.954279	5.757356	-1.458107
83	1	0	-4.548266	3.841562	-2.157522
84	1	0	-1.995709	4.470017	1.241547
85	1	0	-3.399940	6.386467	1.942454
86	1	0	-5.382435	7.038298	0.593369
87	6	0	-2.281860	2.897446	-0.975236
88	7	0	-1.181137	3.321700	-1.861908
89	1	0	-0.239991	1.804306	-2.220556
90	1	0	-1.569402	3.779359	-2.686943
91	1	0	-2.874477	2.157858	-1.521121
92	1	0	-1.836544	2.388834	-0.114422

ONIOM: extrapolated energy = -1013.147295343788 A.U.

Free energy = -1012.44684 A.U.

IM11:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.884740	2.143729	2.831681
2	6	0	-2.702593	1.825501	2.158281
3	6	0	-2.615273	2.005488	0.769376
4	6	0	-3.715128	2.516646	0.063820
5	6	0	-4.890825	2.844901	0.745128
6	6	0	-4.979638	2.655623	2.127756
7	1	0	-3.951189	1.997315	3.910099
8	1	0	-1.846408	1.435212	2.709102
9	1	0	-3.657219	2.668099	-1.014220
10	1	0	-5.740898	3.249944	0.194978
11	1	0	-5.898717	2.908366	2.655499
12	6	0	-1.328139	1.732941	0.034733
13	7	0	-0.704583	0.445318	0.447553
14	1	0	-0.616379	2.531729	0.295389
15	1	0	-1.464552	1.776392	-1.060439
16	6	0	0.713100	0.442054	0.157943
17	1	0	1.161050	1.435830	0.279500
18	6	0	1.411036	-0.508665	1.105434
19	1	0	0.952798	-1.453652	1.387940
20	6	0	6.976271	-0.961352	1.136300
21	6	0	5.808352	-0.675069	1.848586
22	6	0	4.667258	-1.470008	1.664153
23	6	0	4.702467	-2.556211	0.775830
24	6	0	5.873680	-2.836799	0.068299
25	6	0	7.009726	-2.039275	0.245779

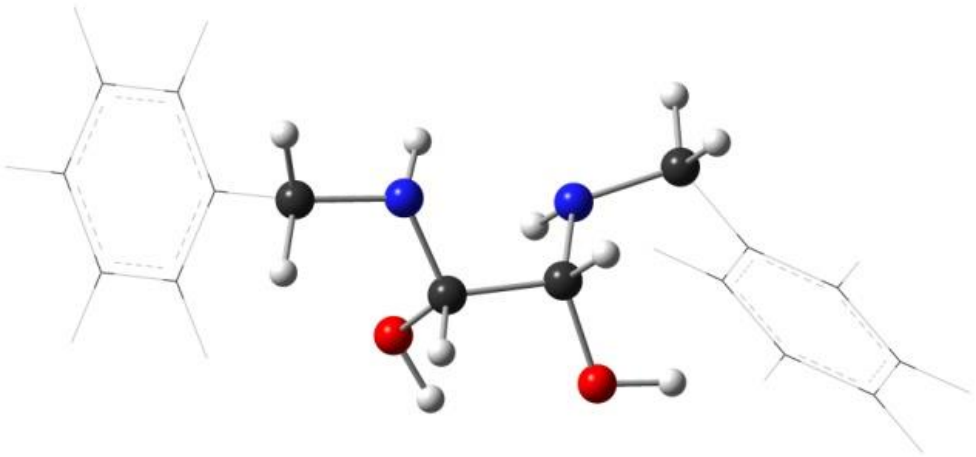
26	1	0	7.863886	-0.342198	1.277682
27	1	0	5.791017	0.164657	2.545922
28	1	0	3.820882	-3.184618	0.636854
29	1	0	5.902079	-3.680882	-0.622906
30	1	0	7.923220	-2.260367	-0.309354
31	6	0	3.407969	-1.161408	2.417203
32	7	0	2.586779	-0.266112	1.553247
33	1	0	3.593604	-0.614725	3.347736
34	1	0	2.806464	-2.049985	2.628353
35	1	0	3.025462	0.620440	1.281666
36	6	0	5.251167	1.734065	-0.976583
37	6	0	4.372289	0.660972	-1.147833
38	6	0	3.077475	0.886262	-1.636892
39	6	0	2.674119	2.188833	-1.964968
40	6	0	3.555796	3.258611	-1.789619
41	6	0	4.844160	3.033808	-1.293508
42	1	0	6.257258	1.554291	-0.594490
43	1	0	4.708817	-0.351005	-0.914633
44	1	0	1.670814	2.365054	-2.355385
45	1	0	3.238160	4.271147	-2.041938
46	1	0	5.530190	3.869928	-1.156778
47	6	0	2.143974	-0.284975	-1.835749
48	7	0	0.844839	-0.028889	-1.215576
49	1	0	2.602102	-1.216930	-1.450304
50	1	0	1.966231	-0.429943	-2.911823
51	6	0	-0.311678	-0.780402	-1.600507
52	8	0	-0.928985	-0.131602	-2.705733
53	1	0	-0.071224	-1.814598	-1.878853
54	6	0	-1.186078	-0.753908	-0.324779
55	1	0	-0.920938	-1.633587	0.271305
56	6	0	-6.403027	-3.238123	-0.772211
57	6	0	-5.132111	-2.907147	-0.294139
58	6	0	-4.812622	-1.569934	-0.014581
59	6	0	-5.772877	-0.569257	-0.222734
60	6	0	-7.041975	-0.904853	-0.702002
61	6	0	-7.359856	-2.238772	-0.976579
62	1	0	-6.648183	-4.278642	-0.985907
63	1	0	-4.390261	-3.690197	-0.139565
64	1	0	-5.531765	0.472789	-0.009338
65	1	0	-7.785781	-0.123984	-0.861272
66	1	0	-8.350340	-2.498750	-1.348274
67	6	0	-3.446399	-1.212581	0.512574
68	7	0	-2.575238	-0.856139	-0.621050
69	1	0	-2.987871	-2.077269	1.016587

70	1	0	-3.517374	-0.402361	1.264490
71	1	0	-1.584612	-0.743643	-3.079608
72	1	0	-2.916304	-0.044461	-1.132526

ONIOM: extrapolated energy = -609.929849544766 A.U.

Free energy = -609.387167 A.U.

IM3:



Standard orientation

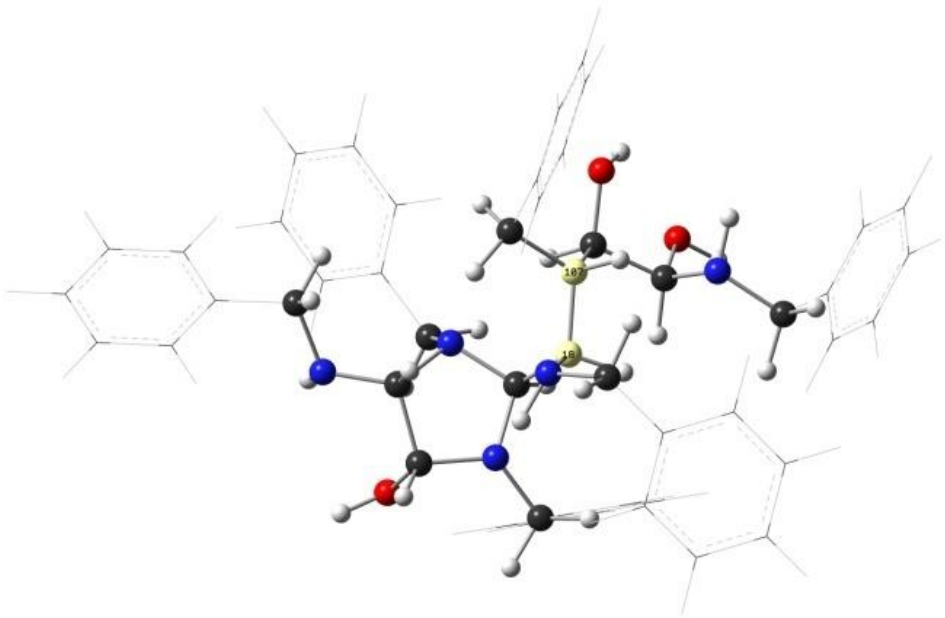
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.533477	2.035590	-0.150725
2	6	0	3.439328	1.504573	0.537235
3	6	0	3.396874	0.135644	0.839475
4	6	0	4.461525	-0.693204	0.459108
5	6	0	5.555927	-0.157014	-0.226276
6	6	0	5.592771	1.206255	-0.534500
7	1	0	4.562367	3.099970	-0.386275
8	1	0	2.622314	2.158755	0.841468
9	1	0	4.443979	-1.756556	0.699884
10	1	0	6.382500	-0.804813	-0.519995
11	1	0	6.445638	1.622456	-1.070159
12	6	0	2.211470	-0.441650	1.587918
13	7	0	0.939642	-0.381850	0.865560
14	1	0	0.702722	0.570084	0.589173
15	1	0	2.087812	0.100668	2.538028
16	1	0	2.393075	-1.496181	1.849842
17	6	0	0.798682	-1.254585	-0.269897
18	8	0	1.564213	-0.876514	-1.422484

19	1	0	1.067391	-2.270035	0.040022
20	6	0	-0.650476	-1.238380	-0.761553
21	8	0	-0.959513	0.080260	-1.235621
22	1	0	-0.743112	-1.944788	-1.596236
23	6	0	-4.544576	1.548738	-1.029625
24	6	0	-3.815745	0.358563	-1.099621
25	6	0	-3.716641	-0.473391	0.024259
26	6	0	-4.345445	-0.099518	1.220777
27	6	0	-5.072184	1.092728	1.288242
28	6	0	-5.175761	1.916761	0.163205
29	1	0	-4.620435	2.191523	-1.906168
30	1	0	-3.300916	0.084419	-2.021439
31	1	0	-4.269521	-0.736990	2.101392
32	1	0	-5.559124	1.379237	2.220046
33	1	0	-5.744846	2.843949	0.216062
34	6	0	-2.946643	-1.774414	-0.045901
35	7	0	-1.524614	-1.652289	0.286650
36	1	0	-0.285229	0.303235	-1.901232
37	1	0	-3.018579	-2.211584	-1.054587
38	1	0	-3.392273	-2.508130	0.645619
39	1	0	-1.362519	-1.080201	1.113274
40	1	0	2.510471	-0.936182	-1.212074

ONIOM: extrapolated energy = -419.378767555472 A.U.

free energy = -419.081387 A.U.

IM12:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.558322	1.417069	-3.284393
2	6	0	-2.675784	0.793523	-2.397851
3	6	0	-2.791778	-0.578889	-2.135690
4	6	0	-3.801768	-1.320905	-2.768994
5	6	0	-4.677126	-0.694954	-3.660069
6	6	0	-4.557029	0.674242	-3.921061
7	1	0	-3.464508	2.485662	-3.481443
8	1	0	-1.901029	1.385108	-1.900023
9	1	0	-3.904699	-2.388878	-2.574815
10	1	0	-5.456891	-1.276876	-4.153064
11	1	0	-5.240136	1.159665	-4.617564
12	6	0	-1.803222	-1.301066	-1.254342
13	7	0	-1.473113	-0.546865	-0.011240
14	1	0	-0.868274	-1.411439	-1.828722
15	1	0	-2.139398	-2.327364	-1.025125
16	6	0	-0.180884	-0.950789	0.534292
17	1	0	0.427060	-1.413873	-0.255447
18	6	0	0.661156	0.235964	1.107184
19	1	0	1.724915	-0.048492	1.091389
20	6	0	4.798598	-0.222849	3.293888
21	6	0	3.728208	0.642028	3.045473
22	6	0	2.449515	0.331285	3.526315
23	6	0	2.251092	-0.841538	4.270065
24	6	0	3.322114	-1.705528	4.511531
25	6	0	4.596596	-1.398806	4.022339
26	1	0	5.793801	0.022553	2.920923
27	1	0	3.894730	1.562559	2.484514
28	1	0	1.264816	-1.080247	4.668924
29	1	0	3.164553	-2.619178	5.086138
30	1	0	5.431124	-2.074051	4.212581
31	6	0	1.287677	1.261450	3.249882
32	7	0	0.246371	0.647766	2.411470
33	1	0	1.636103	2.187747	2.763787
34	1	0	0.812042	1.568800	4.191433
35	1	0	-0.160206	-0.165703	2.873207
36	6	0	2.729635	-4.261598	-0.953703
37	6	0	2.299609	-3.572936	0.184235
38	6	0	0.976236	-3.707887	0.629405
39	6	0	0.088764	-4.531490	-0.076180
40	6	0	0.521076	-5.217614	-1.213676

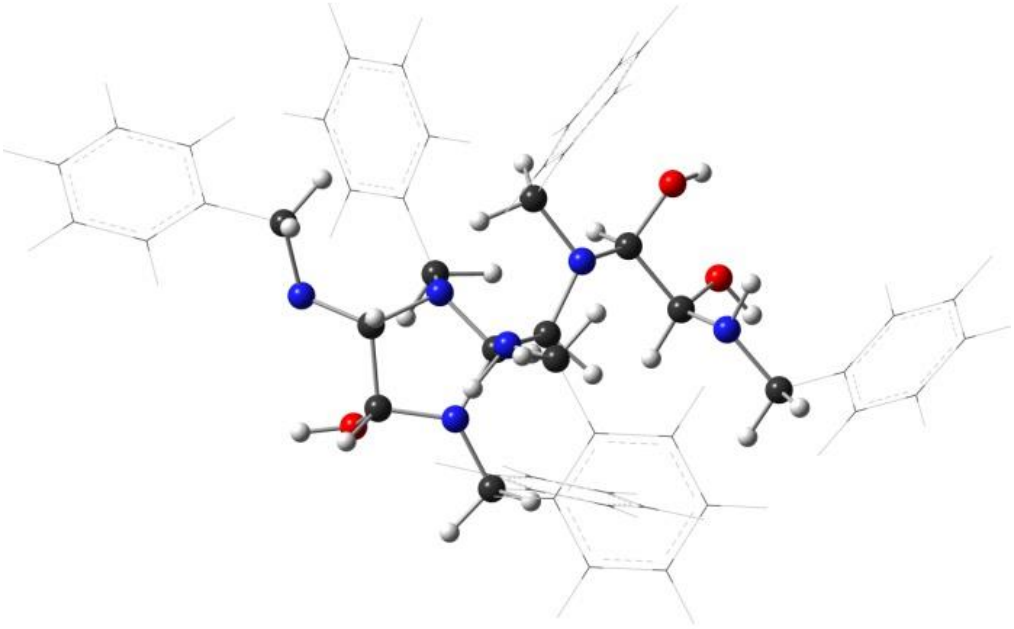
41	6	0	1.842228	-5.085040	-1.653840
42	1	0	3.759804	-4.156916	-1.294492
43	1	0	3.000339	-2.935659	0.724102
44	1	0	-0.948125	-4.625503	0.263083
45	1	0	-0.172772	-5.857865	-1.758543
46	1	0	2.179059	-5.622122	-2.540098
47	6	0	0.522490	-2.969431	1.872736
48	7	0	-0.446094	-1.913150	1.599531
49	1	0	1.395605	-2.527035	2.387617
50	1	0	0.059961	-3.670195	2.582472
51	6	0	-1.855944	-2.105122	1.768213
52	8	0	-2.316025	-3.280918	1.104696
53	1	0	-2.122675	-2.169748	2.829420
54	6	0	-2.415610	-0.821149	1.130236
55	1	0	-2.277311	-0.007390	1.852577
56	6	0	-8.095578	-0.382367	1.441933
57	6	0	-6.715865	-0.198895	1.561956
58	6	0	-5.953333	0.158420	0.439081
59	6	0	-6.583083	0.328007	-0.801848
60	6	0	-7.964297	0.145967	-0.916592
61	6	0	-8.722406	-0.208850	0.203369
62	1	0	-8.684784	-0.659334	2.316096
63	1	0	-6.228984	-0.334794	2.527287
64	1	0	-5.997401	0.601490	-1.681068
65	1	0	-8.450197	0.280733	-1.883008
66	1	0	-9.798803	-0.349546	0.112170
67	6	0	-4.468184	0.377390	0.571654
68	7	0	-3.809555	-0.911453	0.846174
69	1	0	-4.261043	1.041463	1.426271
70	1	0	-4.058488	0.876061	-0.329682
71	1	0	-3.140960	-3.566538	1.529305
72	1	0	-4.004638	-1.603124	0.124669
73	6	0	6.757291	1.284162	-3.352865
74	6	0	5.985572	1.526817	-2.213408
75	6	0	5.448765	0.453288	-1.487855
76	6	0	5.702237	-0.861943	-1.901552
77	6	0	6.477266	-1.100013	-3.040544
78	6	0	7.002708	-0.028594	-3.769357
79	1	0	7.170780	2.120972	-3.917185
80	1	0	5.807407	2.552773	-1.890244
81	1	0	5.303142	-1.704232	-1.335040
82	1	0	6.672078	-2.124753	-3.359635
83	1	0	7.604590	-0.215675	-4.658917
84	6	0	4.606511	0.713588	-0.257903

85	7	0	3.299199	1.323939	-0.550273
86	1	0	3.409891	2.232015	-1.002604
87	1	0	5.142674	1.388930	0.423025
88	1	0	4.417814	-0.219611	0.296297
89	6	0	2.387508	0.519530	-1.318927
90	8	0	2.619795	0.477927	-2.720194
91	1	0	2.391287	-0.497624	-0.913219
92	6	0	0.984091	1.143660	-1.244897
93	8	0	0.982887	2.378714	-1.900801
94	1	0	0.224145	0.471694	-1.650386
95	6	0	0.232663	5.941334	-0.164725
96	6	0	-0.062884	4.609046	-0.464068
97	6	0	-0.351650	3.705390	0.569222
98	6	0	-0.349899	4.145959	1.902398
99	6	0	-0.052656	5.478694	2.196367
100	6	0	0.239238	6.377096	1.164242
101	1	0	0.456832	6.642219	-0.969801
102	1	0	-0.062850	4.269014	-1.503776
103	1	0	-0.587217	3.450872	2.710453
104	1	0	-0.050286	5.819170	3.232666
105	1	0	0.469762	7.417970	1.396100
106	6	0	-0.693214	2.278198	0.261201
107	7	0	0.608566	1.460874	0.171280
108	1	0	1.350046	2.235028	-2.792939
109	1	0	-1.209448	2.156569	-0.700391
110	1	0	-1.284581	1.818194	1.055160
111	1	0	1.397753	2.051357	0.487323
112	1	0	3.432733	-0.021529	-2.907212

ONIOM: extrapolated energy = -1029.341549227254 A.U.

Free energy = -1028.48531 A.U.

IM13:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.783714	1.680454	-3.210022
2	6	0	-2.868115	1.013286	-2.393139
3	6	0	-2.974546	-0.371232	-2.197306
4	6	0	-4.002586	-1.083108	-2.834935
5	6	0	-4.909889	-0.413415	-3.660666
6	6	0	-4.804294	0.968530	-3.848738
7	1	0	-3.699352	2.757875	-3.353559
8	1	0	-2.062275	1.570664	-1.897669
9	1	0	-4.095109	-2.160092	-2.696456
10	1	0	-5.702915	-0.971549	-4.159047
11	1	0	-5.513649	1.488088	-4.491518
12	6	0	-1.943886	-1.122955	-1.389488
13	7	0	-1.641473	-0.493481	-0.080519
14	1	0	-1.007839	-1.107916	-1.972935
15	1	0	-2.220788	-2.188688	-1.279126
16	6	0	-0.323009	-0.893312	0.417561
17	1	0	0.249619	-1.330653	-0.414326
18	6	0	0.549233	0.258444	0.992821
19	1	0	1.567317	-0.154246	1.110462
20	6	0	4.491631	-0.130348	3.648929
21	6	0	3.469109	0.700613	3.180479
22	6	0	2.147780	0.494217	3.597812

23	6	0	1.858516	-0.551084	4.488423
24	6	0	2.881182	-1.383239	4.950103
25	6	0	4.199912	-1.173739	4.532359
26	1	0	5.518707	0.036722	3.325038
27	1	0	3.701439	1.505256	2.481903
28	1	0	0.835794	-0.714507	4.826977
29	1	0	2.651396	-2.195275	5.639665
30	1	0	4.996692	-1.821296	4.895590
31	6	0	1.032872	1.396571	3.097663
32	7	0	0.040829	0.696646	2.281703
33	1	0	1.442081	2.223397	2.495266
34	1	0	0.514830	1.846784	3.960817
35	1	0	-0.293593	-0.134467	2.768143
36	6	0	2.983751	-4.071371	-0.876171
37	6	0	2.429621	-3.473403	0.259488
38	6	0	1.048597	-3.550853	0.492046
39	6	0	0.230111	-4.229455	-0.421085
40	6	0	0.786331	-4.823275	-1.556323
41	6	0	2.164041	-4.745399	-1.786588
42	1	0	4.058078	-4.013671	-1.050514
43	1	0	3.077586	-2.956963	0.967389
44	1	0	-0.849295	-4.284085	-0.242392
45	1	0	0.145395	-5.348981	-2.263990
46	1	0	2.596857	-5.209320	-2.672077
47	6	0	0.461136	-2.902613	1.732745
48	7	0	-0.563825	-1.914464	1.447838
49	1	0	1.269280	-2.425813	2.320271
50	1	0	0.017450	-3.675877	2.379300
51	6	0	-1.954743	-2.185954	1.581454
52	8	0	-2.359524	-3.335033	0.823837
53	1	0	-2.233378	-2.347965	2.631017
54	6	0	-2.563854	-0.886385	1.029366
55	1	0	-2.457856	-0.119289	1.805790
56	6	0	-8.244327	-0.602670	1.542210
57	6	0	-6.866452	-0.385524	1.619764
58	6	0	-6.150551	0.010261	0.479143
59	6	0	-6.826581	0.185997	-0.736317
60	6	0	-8.205630	-0.030569	-0.809035
61	6	0	-8.916670	-0.424932	0.328387
62	1	0	-8.796533	-0.909496	2.430359
63	1	0	-6.345084	-0.524759	2.566306
64	1	0	-6.277952	0.492340	-1.628436
65	1	0	-8.726734	0.108446	-1.756213
66	1	0	-9.991296	-0.592635	0.270143

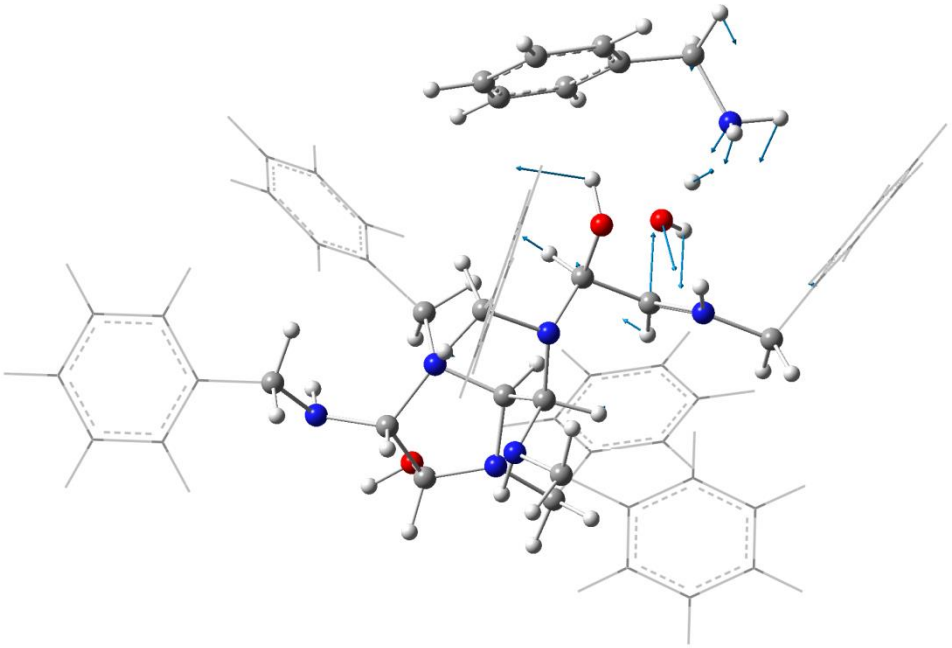
67	6	0	-4.666671	0.263907	0.566382
68	7	0	-3.959955	-1.016879	0.737493
69	1	0	-4.443343	0.881894	1.451059
70	1	0	-4.308360	0.829844	-0.317097
71	1	0	-3.225145	-3.620932	1.159413
72	1	0	-4.115619	-1.637091	-0.055630
73	6	0	7.086617	1.230892	-2.891249
74	6	0	6.230662	1.246795	-1.786898
75	6	0	5.706445	0.046039	-1.286482
76	6	0	6.056448	-1.169271	-1.891115
77	6	0	6.916069	-1.181056	-2.993826
78	6	0	7.429680	0.017766	-3.497651
79	1	0	7.489365	2.166839	-3.279703
80	1	0	5.975848	2.195577	-1.314870
81	1	0	5.666725	-2.110149	-1.502118
82	1	0	7.185681	-2.128838	-3.460916
83	1	0	8.097052	0.007382	-4.358960
84	6	0	4.780531	0.060150	-0.084889
85	7	0	3.541253	0.809623	-0.263555
86	1	0	3.695141	1.784087	-0.515797
87	1	0	5.318676	0.492034	0.773397
88	1	0	4.505101	-0.968166	0.204657
89	6	0	2.551893	0.236016	-1.122429
90	8	0	2.915006	0.142682	-2.512951
91	1	0	2.323272	-0.775130	-0.763962
92	6	0	1.300035	1.133506	-1.175675
93	8	0	1.690419	2.379525	-1.740966
94	1	0	0.584999	0.653695	-1.872387
95	6	0	0.551547	5.936237	-0.446638
96	6	0	0.288861	4.592767	-0.726435
97	6	0	-0.160189	3.734101	0.287076
98	6	0	-0.337565	4.235997	1.585772
99	6	0	-0.073084	5.579712	1.863349
100	6	0	0.369236	6.433478	0.847805
101	1	0	0.898833	6.597814	-1.239166
102	1	0	0.452261	4.198332	-1.731513
103	1	0	-0.680333	3.572516	2.380021
104	1	0	-0.212670	5.962618	2.873556
105	1	0	0.571489	7.480875	1.064061
106	6	0	-0.494466	2.289063	-0.009240
107	7	0	0.691087	1.414877	0.099805
108	1	0	2.055536	2.176157	-2.619829
109	1	0	-0.943191	2.194669	-1.022724
110	1	0	-1.247264	1.925705	0.702057

111	1	0	3.678298	-0.451235	-2.601225

ONIOM: extrapolated energy = -1028.893895875458 A.U.

Free energy = -1028.05261 A.U.

TS7:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.644909	3.299930	-0.705838
2	6	0	-2.868268	2.139575	-0.657463
3	6	0	-3.087790	1.103882	-1.576511
4	6	0	-4.089292	1.244283	-2.550408
5	6	0	-4.857782	2.410265	-2.601018
6	6	0	-4.638135	3.440111	-1.680081
7	1	0	-3.473972	4.099096	0.015824
8	1	0	-2.087344	2.032705	0.105308
9	1	0	-4.269450	0.450066	-3.274625
10	1	0	-5.631925	2.516362	-3.361626
11	1	0	-5.238607	4.348074	-1.722180
12	6	0	-2.205325	-0.121090	-1.595550
13	7	0	-2.012460	-0.735534	-0.257306
14	1	0	-1.210870	0.205794	-1.945064
15	1	0	-2.563373	-0.859604	-2.337249
16	6	0	-0.798582	-1.552930	-0.209923

17	1	0	-0.177485	-1.310536	-1.087962
18	6	0	0.102205	-1.333107	1.037042
19	1	0	1.055241	-1.853885	0.814230
20	6	0	3.940182	-3.551874	2.765992
21	6	0	2.906969	-2.656850	3.060262
22	6	0	1.571567	-3.077028	2.992208
23	6	0	1.279319	-4.400271	2.629166
24	6	0	2.313685	-5.288715	2.325108
25	6	0	3.645813	-4.866619	2.393184
26	1	0	4.978533	-3.226066	2.834803
27	1	0	3.144624	-1.633818	3.352185
28	1	0	0.245426	-4.743526	2.592330
29	1	0	2.082018	-6.315313	2.039841
30	1	0	4.451484	-5.562252	2.160555
31	6	0	0.449801	-2.106780	3.323106
32	7	0	-0.495528	-1.901749	2.225710
33	1	0	0.864009	-1.124957	3.602837
34	1	0	-0.113135	-2.482619	4.192148
35	1	0	-0.931731	-2.782127	1.954118
36	6	0	2.474463	-3.219576	-3.263556
37	6	0	1.799405	-3.581499	-2.094366
38	6	0	0.397447	-3.560103	-2.056945
39	6	0	-0.320332	-3.173589	-3.196817
40	6	0	0.357502	-2.808074	-4.362057
41	6	0	1.755862	-2.829314	-4.397757
42	1	0	3.564077	-3.246950	-3.292224
43	1	0	2.367558	-3.897468	-1.219386
44	1	0	-1.415424	-3.156161	-3.166086
45	1	0	-0.204791	-2.507855	-5.246553
46	1	0	2.283364	-2.546048	-5.308122
47	6	0	-0.319784	-3.964261	-0.781747
48	7	0	-1.232409	-2.953049	-0.274976
49	1	0	0.425215	-4.203719	0.001252
50	1	0	-0.895830	-4.885597	-0.958193
51	6	0	-2.643834	-3.036253	-0.444836
52	8	0	-3.014721	-3.162859	-1.823321
53	1	0	-3.063750	-3.883914	0.110649
54	6	0	-3.091813	-1.693083	0.151846
55	1	0	-3.029034	-1.781134	1.242983
56	6	0	-8.737541	-1.086988	0.122007
57	6	0	-7.383932	-1.241553	0.430844
58	6	0	-6.502009	-0.158271	0.293278
59	6	0	-6.988542	1.078667	-0.152981
60	6	0	-8.344560	1.229915	-0.456849

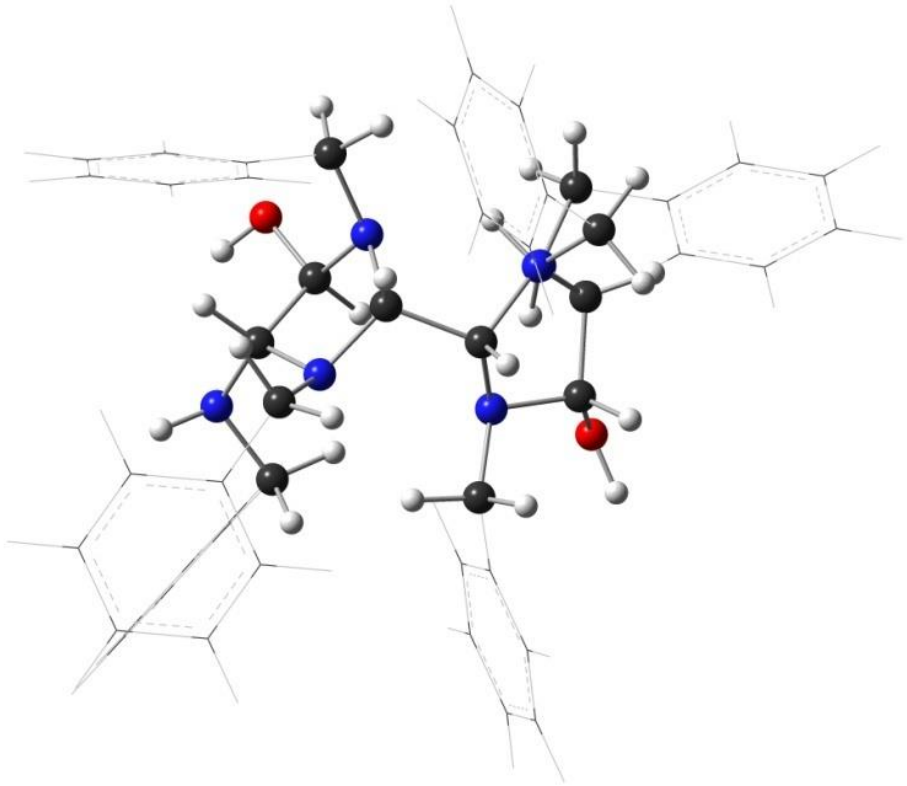
61	6	0	-9.220744	0.148895	-0.320864
62	1	0	-9.418638	-1.931179	0.228019
63	1	0	-7.008459	-2.204702	0.775164
64	1	0	-6.309890	1.925363	-0.267723
65	1	0	-8.718336	2.194105	-0.801227
66	1	0	-10.276966	0.268446	-0.558467
67	6	0	-5.044790	-0.313755	0.647191
68	7	0	-4.444334	-1.370955	-0.183650
69	1	0	-4.951035	-0.628897	1.699188
70	1	0	-4.508102	0.652001	0.552661
71	1	0	-3.920760	-3.510676	-1.859125
72	1	0	-4.543494	-1.170688	-1.177399
73	6	0	7.379482	1.298243	-0.518749
74	6	0	6.400379	0.534444	0.122354
75	6	0	5.564789	-0.304685	-0.629593
76	6	0	5.716498	-0.378963	-2.021467
77	6	0	6.699944	0.384875	-2.656430
78	6	0	7.530957	1.224393	-1.907329
79	1	0	8.030507	1.949382	0.067312
80	1	0	6.295297	0.590890	1.207219
81	1	0	5.080214	-1.037540	-2.614048
82	1	0	6.820657	0.322724	-3.739434
83	1	0	8.299898	1.817450	-2.405128
84	6	0	4.512825	-1.131685	0.061922
85	7	0	3.355420	-0.286382	0.397136
86	1	0	3.490574	0.463949	1.075444
87	1	0	4.891955	-1.565713	0.995423
88	1	0	4.150733	-1.951740	-0.570939
89	6	0	2.275481	-0.180584	-0.344660
90	8	0	2.602647	0.919524	-1.875720
91	1	0	2.036298	-1.024335	-0.988268
92	6	0	1.166222	0.720968	0.209322
93	8	0	1.786854	1.881858	0.722844
94	1	0	0.508770	1.006553	-0.626924
95	6	0	0.811115	3.489005	4.283189
96	6	0	0.472988	2.838760	3.093331
97	6	0	-0.199163	1.609068	3.125678
98	6	0	-0.530455	1.038370	4.364846
99	6	0	-0.189671	1.689461	5.553179
100	6	0	0.480933	2.916308	5.515330
101	1	0	1.332002	4.445407	4.249477
102	1	0	0.743175	3.283141	2.134160
103	1	0	-1.057375	0.084105	4.399422
104	1	0	-0.448824	1.240548	6.511656

105	1	0	0.743397	3.424030	6.442113
106	6	0	-0.620533	0.916629	1.850468
107	7	0	0.459205	0.071844	1.288490
108	1	0	1.686755	2.601330	0.074113
109	1	0	-0.946990	1.663041	1.093421
110	1	0	-1.484123	0.266417	2.038669
111	1	0	2.885840	0.388219	-2.641601
112	1	0	3.348876	1.654890	-1.690518
113	6	0	1.114735	5.345628	0.413577
114	6	0	2.349625	5.135702	-0.203583
115	6	0	2.439664	4.381185	-1.379143
116	6	0	1.269894	3.846002	-1.935605
117	6	0	0.033324	4.056925	-1.321387
118	6	0	-0.044761	4.802741	-0.142415
119	1	0	1.059816	5.931704	1.325399
120	1	0	3.251731	5.558656	0.232012
121	1	0	1.328557	3.255198	-2.846116
122	1	0	-0.867361	3.638440	-1.763032
123	1	0	-1.005336	4.964978	0.336414
124	6	0	3.787609	4.087398	-1.992361
125	7	0	4.321498	2.818469	-1.431229
126	1	0	5.232474	2.618309	-1.851497
127	1	0	4.494450	2.932362	-0.429938
128	1	0	4.479665	4.914191	-1.811232
129	1	0	3.692415	3.949631	-3.070943

ONIOM: extrapolated energy = -1356.116259174763 A.U.

Free energy = -1355.12469 A.U.

IM14:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.808281	-0.814070	2.313483
2	6	0	-3.595646	-0.136912	2.160978
3	6	0	-3.511460	0.970901	1.304256
4	6	0	-4.650996	1.399182	0.607271
5	6	0	-5.862150	0.719332	0.764567
6	6	0	-5.942948	-0.387707	1.615417
7	1	0	-4.869471	-1.675892	2.978816
8	1	0	-2.709074	-0.472777	2.702746
9	1	0	-4.598753	2.263162	-0.055099
10	1	0	-6.746588	1.054446	0.221693
11	1	0	-6.888612	-0.915694	1.735951
12	6	0	-2.206449	1.712607	1.154051
13	7	0	-1.254517	0.951331	0.326406
14	1	0	-1.753127	1.861353	2.147367
15	1	0	-2.377587	2.722177	0.720313
16	6	0	0.096997	1.529615	0.317704
17	1	0	0.108451	2.526447	0.784583
18	6	0	1.107190	0.650041	1.134430
19	1	0	1.120874	0.998083	2.179473

20	6	0	1.409479	4.746078	2.765922
21	6	0	1.953944	3.465218	2.643426
22	6	0	2.768556	3.153052	1.544004
23	6	0	3.057575	4.137974	0.586978
24	6	0	2.511716	5.418098	0.716459
25	6	0	1.684737	5.722459	1.802476
26	1	0	0.773623	4.986237	3.620445
27	1	0	1.752111	2.720824	3.416174
28	1	0	3.715457	3.913481	-0.255604
29	1	0	2.737144	6.182702	-0.029778
30	1	0	1.260776	6.723619	1.902869
31	6	0	3.380415	1.789087	1.412088
32	7	0	2.492371	0.893573	0.572209
33	1	0	3.510145	1.292831	2.381150
34	1	0	4.348952	1.828417	0.900018
35	1	0	2.299634	1.305023	-0.368446
36	6	0	-2.258864	5.338875	-0.481373
37	6	0	-1.061879	4.615998	-0.494464
38	6	0	-0.744646	3.804394	-1.592501
39	6	0	-1.621582	3.742175	-2.686090
40	6	0	-2.814309	4.468850	-2.671157
41	6	0	-3.136851	5.265265	-1.566924
42	1	0	-2.504638	5.964934	0.377049
43	1	0	-0.375750	4.699289	0.349476
44	1	0	-1.369326	3.114473	-3.544726
45	1	0	-3.493922	4.416597	-3.522263
46	1	0	-4.068972	5.830038	-1.554970
47	6	0	0.558396	3.033904	-1.625618
48	7	0	0.536857	1.661307	-1.074091
49	1	0	1.324519	3.583864	-1.053254
50	1	0	0.931703	2.954661	-2.654082
51	6	0	-0.292565	0.676594	-1.779944
52	8	0	-0.355101	0.961047	-3.149895
53	1	0	0.153844	-0.311818	-1.608448
54	6	0	-1.649573	0.780200	-1.081871
55	6	0	-3.357469	-4.515069	-2.894738
56	6	0	-2.567444	-3.511310	-2.326851
57	6	0	-3.101877	-2.670652	-1.339702
58	6	0	-4.432861	-2.840974	-0.928708
59	6	0	-5.219098	-3.844203	-1.500982
60	6	0	-4.683425	-4.683298	-2.483757
61	1	0	-2.938222	-5.167351	-3.660748
62	1	0	-1.536466	-3.383014	-2.654383
63	1	0	-4.854990	-2.191626	-0.160600

64	1	0	-6.252756	-3.973260	-1.179983
65	1	0	-5.297564	-5.465587	-2.927666
66	6	0	-2.253517	-1.590990	-0.716023
67	7	0	-2.514417	-0.324795	-1.419854
68	1	0	-1.180043	-1.831891	-0.805323
69	1	0	-2.466064	-1.511405	0.367555
70	1	0	-1.089148	0.428992	-3.504596
71	1	0	-3.490987	-0.058088	-1.316826
72	6	0	6.346445	-3.639294	-1.452683
73	6	0	5.258446	-2.842536	-1.818322
74	6	0	5.285548	-1.462148	-1.571232
75	6	0	6.410235	-0.884997	-0.966123
76	6	0	7.497757	-1.685840	-0.604192
77	6	0	7.466779	-3.062840	-0.844458
78	1	0	6.322492	-4.712578	-1.643989
79	1	0	4.391268	-3.296944	-2.297683
80	1	0	6.444784	0.188926	-0.781529
81	1	0	8.371961	-1.233981	-0.134576
82	1	0	8.314917	-3.685973	-0.561048
83	6	0	4.102554	-0.601163	-1.955084
84	7	0	2.937173	-0.808889	-1.085039
85	1	0	2.553010	-1.746519	-1.175964
86	1	0	3.783781	-0.819840	-2.983661
87	1	0	4.367578	0.466782	-1.932631
88	6	0	3.106234	-0.481910	0.292283
89	1	0	4.154051	-0.436736	0.610405
90	6	0	2.263732	-1.369536	1.205757
91	8	0	2.349917	-2.687501	0.753034
92	1	0	2.626952	-1.297972	2.244044
93	6	0	-0.672840	-4.735753	3.463494
94	6	0	-0.405442	-3.365694	3.405371
95	6	0	-0.227778	-2.733578	2.163491
96	6	0	-0.319562	-3.490465	0.987382
97	6	0	-0.584141	-4.860901	1.049276
98	6	0	-0.762964	-5.486400	2.286775
99	1	0	-0.810919	-5.220142	4.430515
100	1	0	-0.338984	-2.791604	4.329834
101	1	0	-0.170385	-3.001067	0.018622
102	1	0	-0.652559	-5.442055	0.129478
103	1	0	-0.971310	-6.554775	2.334717
104	6	0	0.002504	-1.242924	2.146395
105	7	0	0.920589	-0.794388	1.071925
106	1	0	2.224437	-3.303779	1.492183
107	1	0	0.407347	-0.908025	3.125938

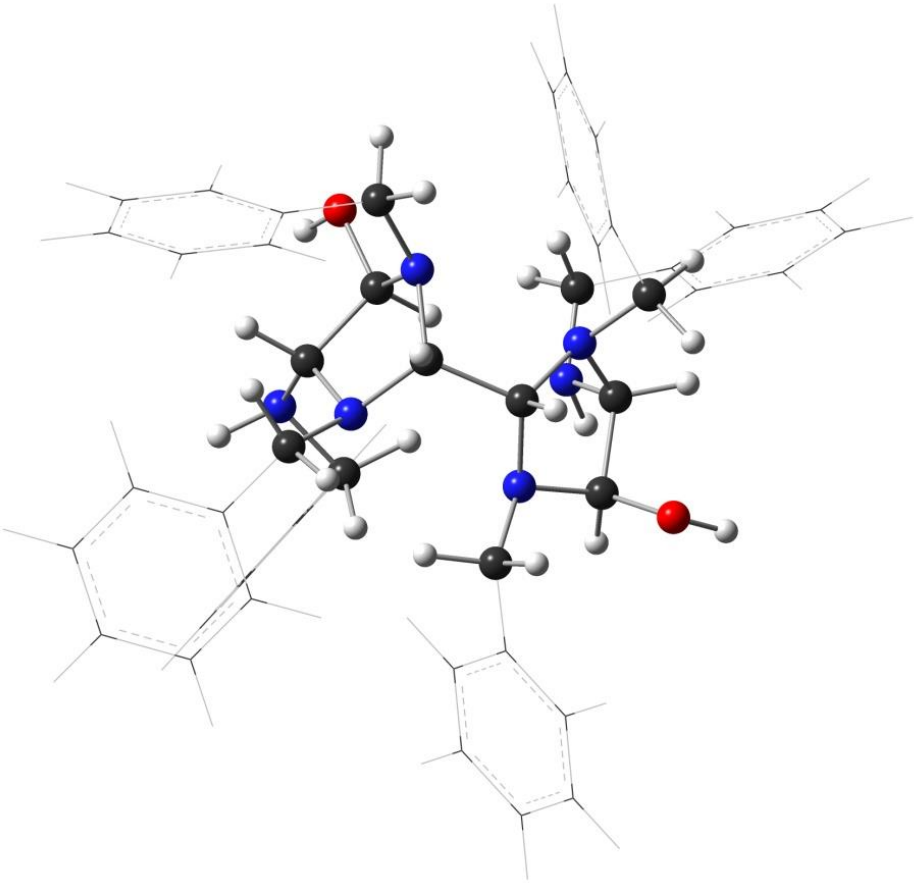
108	1	0	-0.959344	-0.731390	1.990618
109	1	0	-2.154897	1.686683	-1.455804

ONIOM: extrapolated energy = -952.926454813244 A.U.

Free energy = -952.093521 A.U.

Figure 5

IM15:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.226132	-0.114656	1.042694
2	6	0	-3.943693	0.367761	1.314282
3	6	0	-3.478007	1.528290	0.679265
4	6	0	-4.309793	2.205859	-0.224926
5	6	0	-5.593598	1.721542	-0.491465
6	6	0	-6.053112	0.560791	0.138918
7	1	0	-5.583060	-1.018159	1.537016
8	1	0	-3.292294	-0.158939	2.016114
9	1	0	-3.959028	3.110907	-0.720847

10	1	0	-6.237455	2.250411	-1.194254
11	1	0	-7.053124	0.184481	-0.072271
12	6	0	-2.090440	2.050738	0.972038
13	7	0	-1.075314	1.193244	0.352155
14	1	0	-1.925749	2.069655	2.062157
15	1	0	-2.000169	3.104100	0.619902
16	6	0	0.324020	1.507966	0.748355
17	1	0	0.322073	2.341130	1.461151
18	6	0	1.066803	0.292272	1.456462
19	1	0	1.387810	0.669216	2.448237
20	6	0	3.679992	3.983277	2.159680
21	6	0	3.407161	2.614996	2.247555
22	6	0	3.745432	1.760692	1.187197
23	6	0	4.352473	2.290298	0.037672
24	6	0	4.625532	3.658199	-0.044136
25	6	0	4.293466	4.506844	1.017431
26	1	0	3.416977	4.642225	2.986840
27	1	0	2.936869	2.216448	3.145498
28	1	0	4.600566	1.635702	-0.796728
29	1	0	5.098402	4.064506	-0.937955
30	1	0	4.511403	5.571679	0.953752
31	6	0	3.534942	0.270257	1.313752
32	7	0	2.260917	-0.187307	0.744976
33	1	0	3.623683	-0.033137	2.379836
34	1	0	4.341364	-0.255019	0.764567
35	6	0	-1.554742	5.835453	0.210936
36	6	0	-0.443219	4.994163	0.325399
37	6	0	-0.005719	4.253495	-0.781642
38	6	0	-0.675123	4.380669	-2.007765
39	6	0	-1.785990	5.219847	-2.118477
40	6	0	-2.229705	5.946857	-1.008297
41	1	0	-1.893737	6.406307	1.075302
42	1	0	0.080403	4.919260	1.278151
43	1	0	-0.323398	3.810544	-2.871806
44	1	0	-2.306048	5.311201	-3.071839
45	1	0	-3.096283	6.600848	-1.095139
46	6	0	1.220912	3.363919	-0.669808
47	7	0	1.031800	1.930678	-0.455705
48	1	0	1.848498	3.713353	0.168995
49	1	0	1.832637	3.475840	-1.577678
50	6	0	0.367700	1.149505	-1.486253
51	8	0	0.635805	1.650907	-2.774608
52	1	0	0.724598	0.113910	-1.390237
53	6	0	-1.117262	1.205756	-1.112288

54	6	0	-2.652054	-3.824850	-3.771447
55	6	0	-1.911148	-2.922732	-3.002610
56	6	0	-2.545881	-2.146006	-2.022321
57	6	0	-3.928846	-2.278474	-1.821677
58	6	0	-4.665632	-3.180152	-2.593656
59	6	0	-4.029462	-3.955549	-3.568880
60	1	0	-2.154422	-4.426892	-4.531427
61	1	0	-0.838911	-2.822590	-3.166385
62	1	0	-4.429964	-1.676736	-1.062586
63	1	0	-5.739310	-3.279710	-2.435214
64	1	0	-4.605230	-4.658481	-4.168784
65	6	0	-1.749834	-1.175663	-1.183767
66	7	0	-1.883131	0.167624	-1.779761
67	1	0	-0.682807	-1.450558	-1.157916
68	1	0	-2.095868	-1.191857	-0.126807
69	1	0	0.028438	1.184013	-3.373949
70	1	0	-2.866205	0.434427	-1.804573
71	6	0	5.226029	-4.488592	-2.233063
72	6	0	4.046194	-3.742218	-2.296443
73	6	0	3.978998	-2.479089	-1.690717
74	6	0	5.101080	-1.973562	-1.020128
75	6	0	6.280249	-2.721088	-0.958964
76	6	0	6.345134	-3.979226	-1.565998
77	1	0	5.274028	-5.469703	-2.705605
78	1	0	3.178736	-4.144187	-2.819372
79	1	0	5.052255	-0.992080	-0.535913
80	1	0	7.150426	-2.322147	-0.437765
81	1	0	7.264703	-4.561182	-1.519600
82	6	0	2.692780	-1.673890	-1.756487
83	7	0	1.730640	-2.022492	-0.713221
84	1	0	1.538362	-3.023747	-0.732718
85	1	0	2.208252	-1.823424	-2.735885
86	1	0	2.903585	-0.595933	-1.662842
87	6	0	2.169699	-1.641482	0.625844
88	1	0	3.143503	-2.091806	0.881417
89	6	0	1.136903	-2.019033	1.683650
90	6	0	-1.993155	-3.945191	4.483094
91	6	0	-1.319842	-2.745498	4.233497
92	6	0	-1.431525	-2.123825	2.980962
93	6	0	-2.226091	-2.713769	1.987164
94	6	0	-2.894009	-3.913624	2.237304
95	6	0	-2.779329	-4.532222	3.487097
96	1	0	-1.903855	-4.423450	5.458383
97	1	0	-0.706998	-2.297384	5.014684

98	1	0	-2.313400	-2.221570	1.009043
99	1	0	-3.506692	-4.367848	1.458940
100	1	0	-3.301555	-5.467430	3.683337
101	6	0	-0.735406	-0.806491	2.724135
102	7	0	0.238128	-0.905045	1.631617
103	1	0	-0.243712	-0.448664	3.652828
104	1	0	-1.487194	-0.054727	2.430962
105	1	0	-1.522810	2.163758	-1.480991
106	8	0	1.771641	-2.088732	2.968627
107	1	0	2.255349	-2.927706	3.028335
108	1	0	0.605000	-2.958548	1.480068

ONIOM: extrapolated energy = -952.472076552539 A.U.

Free energy = -951.655572 A.U.

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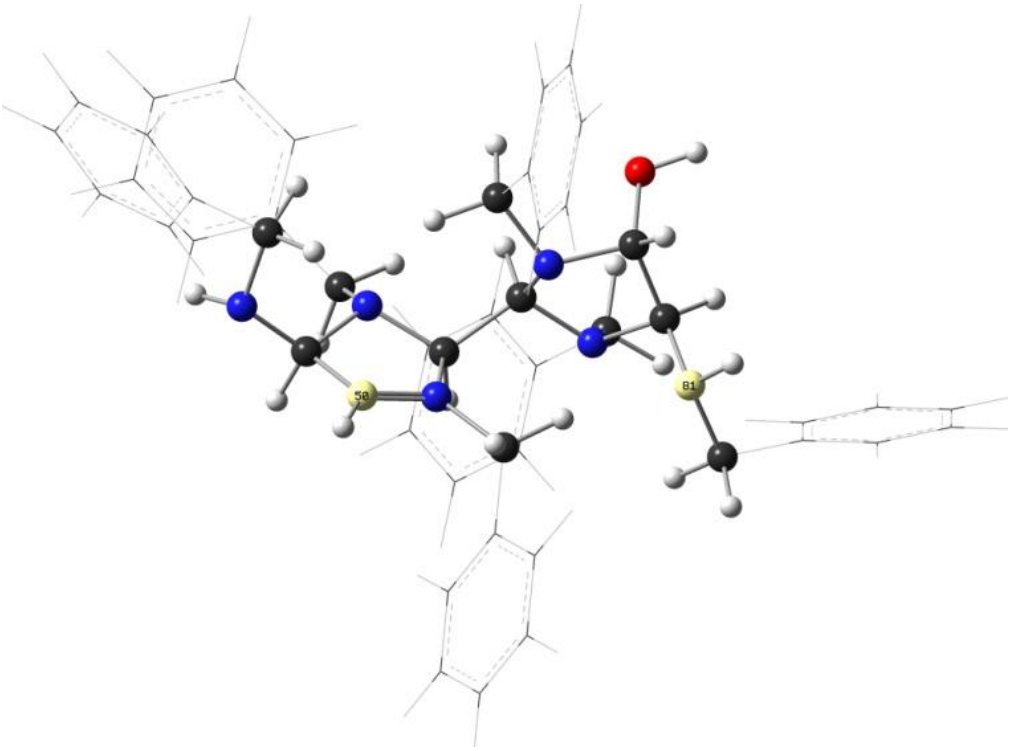


Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.586266	-1.255004	-3.107291
2	6	0	-3.319749	-1.223002	-2.517970
3	6	0	-2.954218	-2.207493	-1.587234
4	6	0	-3.863530	-3.220170	-1.249272
5	6	0	-5.129327	-3.246708	-1.841838

6	6	0	-5.492374	-2.266399	-2.770786
7	1	0	-4.867248	-0.490907	-3.833033
8	1	0	-2.614494	-0.434474	-2.781853
9	1	0	-3.587232	-3.992941	-0.531321
10	1	0	-5.834368	-4.036274	-1.579138
11	1	0	-6.479212	-2.291121	-3.233161
12	6	0	-1.573214	-2.198052	-0.985679
13	7	0	-1.406743	-1.054997	-0.068728
14	1	0	-0.830249	-2.095958	-1.792909
15	1	0	-1.350531	-3.147821	-0.459491
16	6	0	-0.011864	-0.792065	0.271346
17	1	0	0.566683	-1.718980	0.440399
18	6	0	0.724418	0.063390	-0.780576
19	1	0	0.317580	-0.254723	-1.760690
20	6	0	0.879911	-4.434625	-2.292069
21	6	0	1.347438	-3.133008	-2.498898
22	6	0	2.125598	-2.503730	-1.516766
23	6	0	2.447847	-3.193072	-0.338313
24	6	0	1.973934	-4.490733	-0.133449
25	6	0	1.186796	-5.112772	-1.108684
26	1	0	0.274959	-4.921190	-3.058527
27	1	0	1.111031	-2.616913	-3.430452
28	1	0	3.072220	-2.710905	0.416866
29	1	0	2.222058	-5.021328	0.786603
30	1	0	0.818335	-6.126077	-0.948447
31	6	0	2.656698	-1.111677	-1.756165
32	7	0	2.177954	-0.145462	-0.746642
33	1	0	2.394802	-0.763313	-2.775638
34	1	0	3.761480	-1.136665	-1.688678
35	6	0	1.760845	-1.822007	5.294152
36	6	0	1.184434	-0.816012	4.514270
37	6	0	1.619737	-0.620685	3.194651
38	6	0	2.637946	-1.426780	2.667395
39	6	0	3.210105	-2.431746	3.451148
40	6	0	2.770947	-2.631939	4.763885
41	1	0	1.422557	-1.973929	6.320335
42	1	0	0.404061	-0.184683	4.941001
43	1	0	2.992954	-1.260336	1.639566
44	1	0	4.002642	-3.058791	3.040204
45	1	0	3.218005	-3.417061	5.375443
46	6	0	1.011033	0.462746	2.349959
47	7	0	-0.138218	-0.140912	1.604817
48	1	0	1.709645	0.884587	1.618538
49	1	0	0.587079	1.275228	2.953096

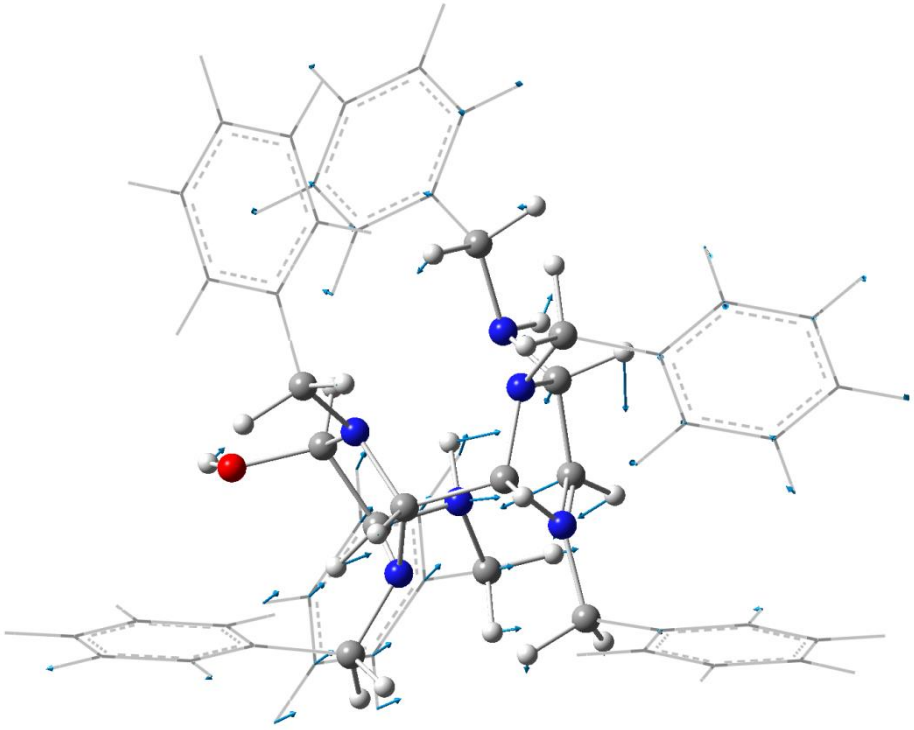
50	6	0	-1.300832	-0.335167	2.097720
51	1	0	-1.580129	0.019208	3.086005
52	6	0	-2.152181	-1.180924	1.196824
53	6	0	-7.166940	1.567128	2.154927
54	6	0	-5.802399	1.328688	1.969845
55	6	0	-5.350338	0.715043	0.791970
56	6	0	-6.273572	0.338912	-0.194609
57	6	0	-7.636991	0.580088	-0.005020
58	6	0	-8.085784	1.194225	1.168579
59	1	0	-7.514988	2.044594	3.071071
60	1	0	-5.090878	1.618193	2.742755
61	1	0	-5.930562	-0.141552	-1.112081
62	1	0	-8.351680	0.288534	-0.774883
63	1	0	-9.149166	1.381828	1.314304
64	6	0	-3.879266	0.463138	0.585432
65	7	0	-3.537003	-0.823735	1.216857
66	1	0	-3.284588	1.250005	1.080131
67	1	0	-3.618394	0.480590	-0.489064
68	1	0	-4.112766	-1.585349	0.865356
69	6	0	7.749456	2.078328	-0.808064
70	6	0	6.643272	1.956498	0.037152
71	6	0	5.756642	0.880420	-0.115579
72	6	0	5.988412	-0.069221	-1.119320
73	6	0	7.096050	0.053826	-1.962781
74	6	0	7.978358	1.127594	-1.808539
75	1	0	8.436432	2.916106	-0.685932
76	1	0	6.472987	2.699308	0.816532
77	1	0	5.297765	-0.909961	-1.248609
78	1	0	7.271564	-0.689004	-2.741201
79	1	0	8.842539	1.223290	-2.465149
80	6	0	4.555245	0.756394	0.802152
81	7	0	3.418844	1.582982	0.391200
82	1	0	3.704497	2.559550	0.327565
83	1	0	4.834522	1.049135	1.826596
84	1	0	4.203077	-0.289134	0.853396
85	6	0	2.823538	1.175346	-0.873279
86	1	0	3.563010	1.140027	-1.689392
87	6	0	1.671623	2.101611	-1.262031
88	6	0	-1.408565	5.760779	-1.323255
89	6	0	-1.287475	4.400404	-1.621197
90	6	0	-0.859897	3.500950	-0.633501
91	6	0	-0.554370	3.973944	0.651644
92	6	0	-0.673131	5.335030	0.943070
93	6	0	-1.101690	6.230414	-0.042542

94	1	0	-1.742507	6.456568	-2.093263
95	1	0	-1.527585	4.043807	-2.622742
96	1	0	-0.219025	3.277432	1.419622
97	1	0	-0.433114	5.699102	1.942209
98	1	0	-1.195924	7.291239	0.187199
99	6	0	-0.769990	2.029003	-0.951911
100	7	0	0.553465	1.498040	-0.578346
101	1	0	-0.977647	1.834653	-2.020809
102	1	0	-1.525398	1.480419	-0.374146
103	1	0	-2.077608	-2.206285	1.605977
104	8	0	1.450419	2.039087	-2.669491
105	1	0	2.108521	2.592554	-3.118486
106	1	0	1.804917	3.140160	-0.936862

ONIOM: extrapolated energy = -876.505160350794 A.U.

Free energy = -875.703513 A.U.

TS8:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.278892	3.327359	0.997814
2	6	0	-3.986980	3.238924	0.471878
3	6	0	-3.688093	2.278890	-0.506393

4	6	0	-4.695897	1.418943	-0.962829
5	6	0	-5.988663	1.515303	-0.439505
6	6	0	-6.282032	2.465838	0.543050
7	1	0	-5.504774	4.073225	1.760234
8	1	0	-3.219330	3.930389	0.819593
9	1	0	-4.482576	0.675235	-1.730616
10	1	0	-6.769310	0.842814	-0.798446
11	1	0	-7.290193	2.537436	0.950394
12	6	0	-2.290985	2.208223	-1.095260
13	7	0	-1.404450	1.212784	-0.490018
14	1	0	-1.799371	3.189161	-1.008181
15	1	0	-2.343252	1.989176	-2.172308
16	6	0	-1.668176	-0.183370	-0.770518
17	1	0	-2.494239	-0.300968	-1.478141
18	6	0	-0.369189	-0.969181	-1.291667
19	1	0	-0.605266	-1.386897	-2.279273
20	6	0	3.473924	-4.313983	-2.612807
21	6	0	2.499626	-4.091637	-1.635239
22	6	0	1.248117	-3.570893	-1.995489
23	6	0	0.980932	-3.276462	-3.340210
24	6	0	1.959401	-3.495899	-4.314080
25	6	0	3.205968	-4.016649	-3.952927
26	1	0	4.444903	-4.719469	-2.329055
27	1	0	2.718136	-4.322967	-0.593243
28	1	0	0.008471	-2.881944	-3.633687
29	1	0	1.747782	-3.264494	-5.357830
30	1	0	3.966060	-4.191286	-4.713378
31	6	0	0.170387	-3.390831	-0.945509
32	7	0	0.013489	-2.044236	-0.384161
33	1	0	0.347799	-4.070882	-0.097299
34	1	0	-0.804274	-3.687104	-1.367558
35	6	0	-6.439462	-1.419283	1.397575
36	6	0	-5.056986	-1.504551	1.584027
37	6	0	-4.227371	-1.858337	0.510039
38	6	0	-4.785297	-2.112797	-0.751115
39	6	0	-6.168568	-2.025405	-0.931506
40	6	0	-6.997087	-1.683447	0.142256
41	1	0	-7.084215	-1.148440	2.234380
42	1	0	-4.629767	-1.301781	2.566666
43	1	0	-4.148176	-2.388626	-1.591567
44	1	0	-6.601554	-2.227281	-1.911918
45	1	0	-8.076614	-1.622678	0.000943
46	6	0	-2.745041	-2.017396	0.724784
47	7	0	-2.058365	-0.728148	0.546916

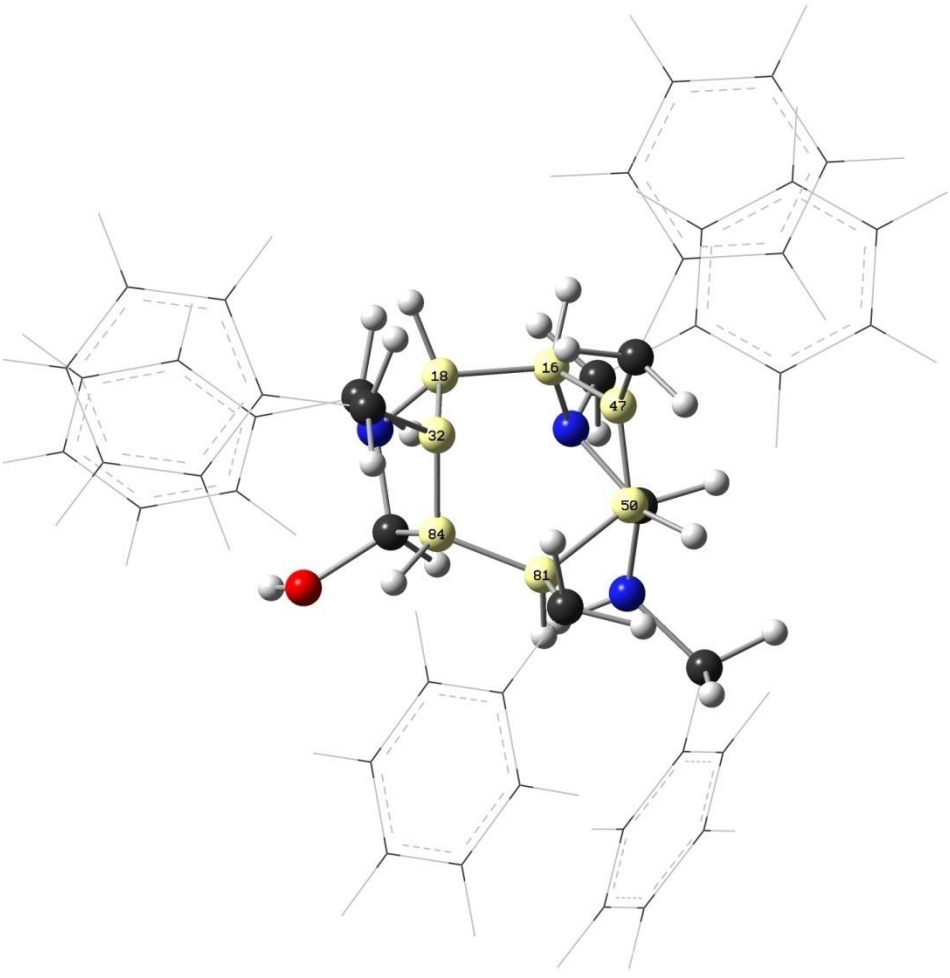
48	1	0	-2.307339	-2.734329	0.020394
49	1	0	-2.525340	-2.374044	1.739791
50	6	0	-1.441083	-0.047026	1.475490
51	1	0	-1.637337	-0.243487	2.524825
52	6	0	-1.132410	1.343889	0.937750
53	6	0	4.255198	3.137138	1.523623
54	6	0	3.023864	2.694228	1.037891
55	6	0	1.899397	3.532695	1.091673
56	6	0	2.021580	4.820784	1.631867
57	6	0	3.258021	5.263016	2.112679
58	6	0	4.374635	4.423389	2.061792
59	1	0	5.124909	2.481930	1.481888
60	1	0	2.922663	1.689793	0.607519
61	1	0	1.156951	5.481949	1.678378
62	1	0	3.349557	6.266104	2.529181
63	1	0	5.335949	4.769794	2.438804
64	6	0	0.572947	3.050884	0.561929
65	7	0	0.208434	1.810651	1.271419
66	1	0	0.653962	2.802198	-0.509325
67	1	0	-0.201780	3.836480	0.672864
68	1	0	0.214564	2.002360	2.275291
69	6	0	3.833881	-1.859314	4.451750
70	6	0	2.580503	-1.453711	3.986698
71	6	0	1.770346	-2.351811	3.275407
72	6	0	2.218922	-3.659749	3.046199
73	6	0	3.473443	-4.061875	3.515247
74	6	0	4.283440	-3.162937	4.215319
75	1	0	4.461919	-1.158083	5.002120
76	1	0	2.234192	-0.438984	4.183268
77	1	0	1.591826	-4.371407	2.509236
78	1	0	3.818730	-5.080340	3.334498
79	1	0	5.261818	-3.477121	4.578453
80	6	0	0.416893	-1.907181	2.767685
81	7	0	0.527101	-0.918471	1.677416
82	1	0	1.091781	-0.112781	1.952161
83	1	0	-0.159241	-1.460146	3.592779
84	1	0	-0.164383	-2.759842	2.382340
85	6	0	1.085520	-1.509908	0.437440
86	1	0	1.789078	-2.310026	0.699722
87	6	0	1.805559	-0.483523	-0.466194
88	6	0	4.087511	2.807313	-2.453192
89	6	0	3.292456	1.659672	-2.405629
90	6	0	1.910227	1.750146	-2.625294
91	6	0	1.332340	3.001331	-2.890482

92	6	0	2.131837	4.146968	-2.938764
93	6	0	3.510210	4.052531	-2.723408
94	1	0	5.160958	2.731576	-2.281632
95	1	0	3.742381	0.686011	-2.199236
96	1	0	0.258418	3.082102	-3.058691
97	1	0	1.678580	5.116077	-3.146247
98	1	0	4.131841	4.945597	-2.764457
99	6	0	1.052748	0.507104	-2.665487
100	7	0	0.765129	-0.061335	-1.349367
101	1	0	1.528050	-0.248322	-3.322759
102	1	0	0.075818	0.751637	-3.115449
103	1	0	-1.898114	2.003275	1.391996
104	8	0	2.849166	-1.121061	-1.197362
105	1	0	3.627467	-1.204667	-0.623594
106	1	0	2.223457	0.369359	0.099509

ONIOM: extrapolated energy = -876.486472777099 A.U.

Free energy = -875.679321 A.U.

IM17:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.929974	0.454173	1.523849
2	6	0	4.578178	0.699960	1.779379
3	6	0	3.670266	-0.366836	1.854526
4	6	0	4.130948	-1.680556	1.691248
5	6	0	5.483330	-1.922536	1.432626
6	6	0	6.384303	-0.856596	1.346790
7	1	0	6.631326	1.286718	1.464228
8	1	0	4.233462	1.724394	1.925421
9	1	0	3.439429	-2.520012	1.766548
10	1	0	5.834256	-2.945844	1.294791
11	1	0	7.438148	-1.046894	1.145576
12	6	0	2.203603	-0.094110	2.136702
13	7	0	1.370311	0.032552	0.936379
14	1	0	2.093803	0.843430	2.703782
15	1	0	1.787878	-0.895532	2.764900
16	6	0	1.191125	-1.177052	0.118304
17	1	0	1.828193	-1.998817	0.470610
18	6	0	-0.327516	-1.668632	0.091744
19	1	0	-0.368056	-2.750380	0.251194
20	6	0	-5.203355	-2.346215	-0.006793
21	6	0	-4.130567	-1.907022	-0.788678
22	6	0	-2.999948	-2.719707	-0.947175
23	6	0	-2.951730	-3.973833	-0.319828
24	6	0	-4.024844	-4.407253	0.463587
25	6	0	-5.152789	-3.595155	0.620074
26	1	0	-6.080939	-1.711588	0.114680
27	1	0	-4.169538	-0.922084	-1.253381
28	1	0	-2.079278	-4.615720	-0.440438
29	1	0	-3.982530	-5.380921	0.951461
30	1	0	-5.989437	-3.934565	1.229823
31	6	0	-1.845451	-2.278231	-1.818638
32	7	0	-0.905768	-1.327256	-1.205816
33	1	0	-2.219690	-1.814232	-2.744246
34	1	0	-1.252491	-3.150898	-2.134694
35	6	0	5.325803	-3.092374	-1.785909
36	6	0	4.284616	-2.204151	-2.068371
37	6	0	2.952726	-2.636265	-1.985637
38	6	0	2.670580	-3.959802	-1.618593
39	6	0	3.716008	-4.844650	-1.338795

40	6	0	5.043536	-4.413042	-1.421402
41	1	0	6.360314	-2.754171	-1.848831
42	1	0	4.507889	-1.174806	-2.348240
43	1	0	1.638670	-4.304886	-1.553353
44	1	0	3.494575	-5.873908	-1.055594
45	1	0	5.856965	-5.104405	-1.202464
46	6	0	1.826587	-1.684967	-2.311344
47	7	0	1.633432	-0.751638	-1.203554
48	1	0	0.896876	-2.230792	-2.540814
49	1	0	2.084664	-1.087912	-3.200039
50	6	0	1.332517	0.599306	-1.333342
51	1	0	1.867988	1.082942	-2.149781
52	6	0	1.757820	1.131414	0.053439
53	6	0	1.685623	6.562361	2.211381
54	6	0	2.141822	5.403835	1.576234
55	6	0	1.388313	4.826398	0.543661
56	6	0	0.174516	5.413226	0.155477
57	6	0	-0.277577	6.570937	0.794861
58	6	0	0.476505	7.147488	1.822106
59	1	0	2.274367	7.009828	3.012626
60	1	0	3.083535	4.950227	1.885625
61	1	0	-0.419052	4.971762	-0.644571
62	1	0	-1.220973	7.025288	0.490769
63	1	0	0.122574	8.050991	2.318177
64	6	0	1.881718	3.581563	-0.146468
65	7	0	1.322842	2.407402	0.543234
66	1	0	2.979708	3.507987	-0.085699
67	1	0	1.626690	3.613496	-1.225059
68	1	0	0.329904	2.476461	0.743833
69	6	0	-2.975955	3.704471	-3.724649
70	6	0	-1.783492	3.066041	-3.374400
71	6	0	-1.653870	1.679577	-3.550029
72	6	0	-2.712792	0.944213	-4.103294
73	6	0	-3.901559	1.589445	-4.455409
74	6	0	-4.036914	2.967787	-4.261809
75	1	0	-3.076843	4.781873	-3.582145
76	1	0	-0.957096	3.655881	-2.975697
77	1	0	-2.614358	-0.129144	-4.271724
78	1	0	-4.724890	1.014722	-4.883200
79	1	0	-4.967607	3.468767	-4.533171
80	6	0	-0.370908	0.990081	-3.179368
81	7	0	-0.207729	0.949616	-1.670367
82	1	0	0.492404	1.527273	-3.589576
83	1	0	-0.331522	-0.054575	-3.514101

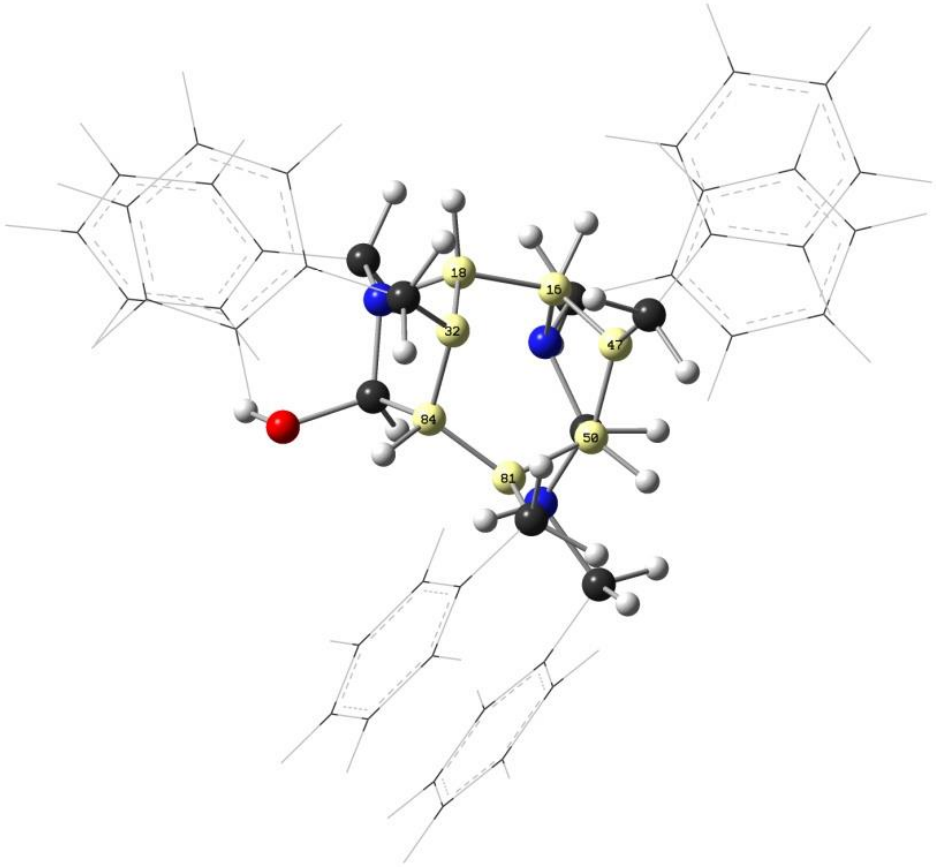
84	6	0	-1.297891	0.039552	-1.070449
85	1	0	-2.207580	0.271968	-1.630414
86	6	0	-1.582573	0.281136	0.431334
87	6	0	-4.244118	-2.226291	3.999272
88	6	0	-3.055902	-2.198849	3.264160
89	6	0	-2.272986	-1.035956	3.235694
90	6	0	-2.689027	0.097584	3.950092
91	6	0	-3.876998	0.064927	4.685922
92	6	0	-4.656539	-1.095733	4.711970
93	1	0	-4.850855	-3.131935	4.015221
94	1	0	-2.743055	-3.079915	2.702906
95	1	0	-2.086330	1.005891	3.941081
96	1	0	-4.195643	0.947887	5.240422
97	1	0	-5.582619	-1.119042	5.285241
98	6	0	-0.971651	-1.002624	2.465310
99	7	0	-1.217093	-0.978830	1.024521
100	1	0	-0.390754	-1.909404	2.698540
101	1	0	-0.365892	-0.131097	2.774552
102	1	0	2.855495	1.201011	-0.046975
103	8	0	-2.961262	0.590781	0.522528
104	1	0	-3.189166	0.734982	1.456210
105	1	0	-1.007749	1.108910	0.866727
106	1	0	-0.367802	1.899388	-1.307902

ONIOM: extrapolated energy = -876.493315999749 A.U.

Free energy = -875.683123 A.U.

Figure 6

IM18:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.642127	1.890736	1.806574
2	6	0	4.272700	1.728170	2.034299
3	6	0	3.701379	0.447483	2.013185
4	6	0	4.517860	-0.669116	1.784493
5	6	0	5.887387	-0.503460	1.559010
6	6	0	6.451565	0.776052	1.566230
7	1	0	6.079631	2.888975	1.819650
8	1	0	3.651116	2.601431	2.233490
9	1	0	4.089211	-1.671247	1.783645
10	1	0	6.516524	-1.374963	1.377816
11	1	0	7.518706	0.903573	1.389343
12	6	0	2.211512	0.270002	2.267294
13	7	0	1.375060	0.280246	1.075153
14	1	0	1.846555	1.077467	2.925043
15	1	0	2.043612	-0.673795	2.810834
16	6	0	1.566325	-0.811896	0.105528
17	1	0	2.402483	-1.460565	0.405080

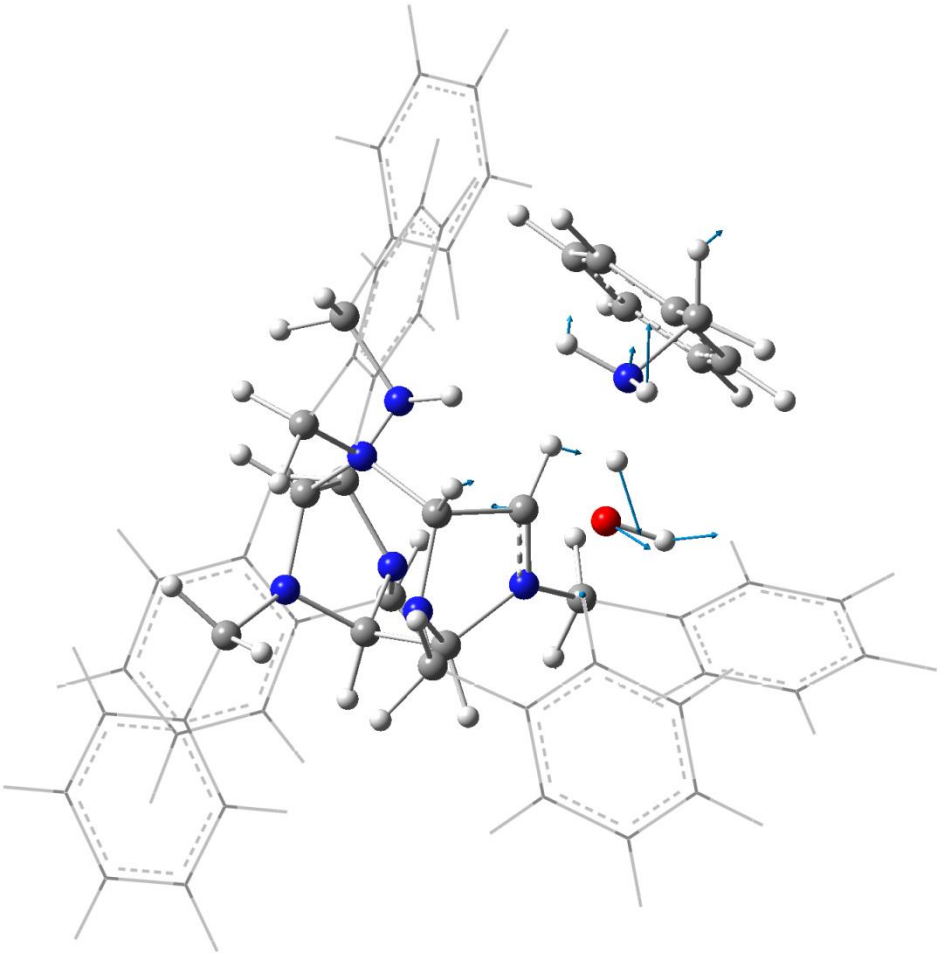
18	6	0	0.253094	-1.711274	-0.047863
19	1	0	0.524850	-2.772929	-0.011064
20	6	0	-4.436295	-3.431832	-0.481275
21	6	0	-3.434913	-2.681138	-1.103326
22	6	0	-2.154218	-3.224568	-1.277925
23	6	0	-1.882734	-4.519835	-0.813481
24	6	0	-2.884785	-5.265078	-0.184905
25	6	0	-4.164482	-4.725433	-0.023448
26	1	0	-5.430823	-3.007081	-0.351104
27	1	0	-3.642789	-1.660652	-1.426447
28	1	0	-0.889862	-4.949620	-0.938878
29	1	0	-2.668066	-6.269627	0.176278
30	1	0	-4.946309	-5.309128	0.459474
31	6	0	-1.081164	-2.453365	-2.023300
32	7	0	-0.386486	-1.387138	-1.309683
33	1	0	-1.518960	-1.998887	-2.928535
34	1	0	-0.307922	-3.154327	-2.386228
35	6	0	6.021554	-1.508582	-2.201184
36	6	0	4.806744	-0.836127	-2.361605
37	6	0	3.596623	-1.512669	-2.150618
38	6	0	3.612587	-2.864263	-1.775490
39	6	0	4.829572	-3.532381	-1.615896
40	6	0	6.035448	-2.856536	-1.828803
41	1	0	6.960305	-0.980115	-2.366548
42	1	0	4.801405	0.215042	-2.647249
43	1	0	2.676006	-3.395784	-1.609794
44	1	0	4.838223	-4.582840	-1.325475
45	1	0	6.983104	-3.378829	-1.705118
46	6	0	2.277533	-0.795164	-2.340842
47	7	0	1.910485	-0.099268	-1.116193
48	1	0	1.498396	-1.499784	-2.681952
49	1	0	2.383868	-0.026665	-3.126215
50	6	0	1.111661	1.107006	-1.113112
51	1	0	1.554105	1.833124	-1.799997
52	6	0	1.380167	1.548468	0.340902
53	6	0	-1.001377	6.605407	2.388720
54	6	0	-0.012162	5.706184	1.978735
55	6	0	-0.242861	4.861486	0.883901
56	6	0	-1.470905	4.920961	0.207174
57	6	0	-2.456841	5.818885	0.621476
58	6	0	-2.223617	6.663633	1.712289
59	1	0	-0.818143	7.261740	3.239703
60	1	0	0.936491	5.663580	2.513011
61	1	0	-1.658160	4.261467	-0.649507

62	1	0	-3.409673	5.861678	0.093404
63	1	0	-2.992986	7.364564	2.033763
64	6	0	0.820721	3.896315	0.424667
65	7	0	0.492810	2.542630	0.914350
66	1	0	1.807524	4.177046	0.829364
67	1	0	0.904937	3.933094	-0.681981
68	1	0	-0.451991	2.323338	0.597881
69	6	0	-3.833507	3.122356	-2.925670
70	6	0	-2.535095	2.730566	-2.591788
71	6	0	-1.937205	1.641981	-3.243571
72	6	0	-2.650659	0.950242	-4.233945
73	6	0	-3.948520	1.347976	-4.567765
74	6	0	-4.542393	2.432728	-3.915016
75	1	0	-4.294317	3.967913	-2.414776
76	1	0	-1.982232	3.270023	-1.812860
77	1	0	-2.197650	0.102660	-4.747392
78	1	0	-4.498842	0.808750	-5.338930
79	1	0	-5.554372	2.739688	-4.175789
80	6	0	-0.520945	1.230648	-2.913543
81	7	0	-0.334116	1.050354	-1.457522
82	1	0	0.160593	2.027331	-3.254731
83	1	0	-0.240349	0.309030	-3.465153
84	6	0	-1.096770	-0.139082	-1.028379
85	1	0	-2.040767	-0.118969	-1.581221
86	6	0	-1.477949	-0.228782	0.474056
87	6	0	-3.345489	-3.798081	3.674964
88	6	0	-2.215756	-3.361806	2.977641
89	6	0	-1.792418	-2.029403	3.086695
90	6	0	-2.511192	-1.139096	3.898733
91	6	0	-3.639826	-1.579913	4.595689
92	6	0	-4.059142	-2.909279	4.485677
93	1	0	-3.671188	-4.834399	3.585580
94	1	0	-1.669310	-4.055982	2.338984
95	1	0	-2.189998	-0.102039	3.994553
96	1	0	-4.193988	-0.884287	5.225886
97	1	0	-4.938881	-3.251216	5.028922
98	6	0	-0.554374	-1.549711	2.357704
99	7	0	-0.803547	-1.423652	0.927462
100	1	0	0.255237	-2.285199	2.505396
101	1	0	-0.209802	-0.590119	2.787604
102	1	0	2.393140	1.986406	0.340904
103	8	0	-2.899576	-0.324952	0.533638
104	1	0	-3.156397	-0.427904	1.464987
105	1	0	-1.168854	0.639962	1.064950

ONIOM: extrapolated energy = -876.054263366222 A.U.

Free energy = -875.260406 A.U.

TS9:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.404786	3.536299	-1.332514
2	6	0	-4.127745	3.058771	-1.640829
3	6	0	-3.915095	1.684969	-1.825943
4	6	0	-4.994627	0.797292	-1.716772
5	6	0	-6.269854	1.277796	-1.405689
6	6	0	-6.477291	2.647141	-1.212051
7	1	0	-5.564249	4.604903	-1.188090
8	1	0	-3.299845	3.760608	-1.742747
9	1	0	-4.845101	-0.270992	-1.872529
10	1	0	-7.103344	0.581257	-1.310456

11	1	0	-7.471906	3.020119	-0.970784
12	6	0	-2.527624	1.167353	-2.168242
13	7	0	-1.731265	0.734595	-1.026300
14	1	0	-1.947894	1.952255	-2.681165
15	1	0	-2.610474	0.328148	-2.878327
16	6	0	-2.210842	-0.402262	-0.239809
17	1	0	-3.145538	-0.811512	-0.641970
18	6	0	-1.107455	-1.564663	-0.200102
19	1	0	-1.496959	-2.498745	-0.615295
20	6	0	2.091939	-5.434269	0.211534
21	6	0	1.518866	-4.404035	0.963723
22	6	0	0.144483	-4.146059	0.871176
23	6	0	-0.652733	-4.936377	0.028878
24	6	0	-0.077164	-5.966077	-0.720666
25	6	0	1.295943	-6.217145	-0.630124
26	1	0	3.161706	-5.629180	0.285632
27	1	0	2.145885	-3.795551	1.617328
28	1	0	-1.726753	-4.759611	-0.037170
29	1	0	-0.700906	-6.577102	-1.373079
30	1	0	1.742588	-7.024172	-1.210441
31	6	0	-0.499039	-3.076267	1.728832
32	7	0	-0.617528	-1.739023	1.143742
33	1	0	0.053637	-2.959722	2.673669
34	1	0	-1.514126	-3.404921	2.013547
35	6	0	-6.852485	-0.343266	1.570507
36	6	0	-5.546583	0.012552	1.919700
37	6	0	-4.501844	-0.909955	1.764213
38	6	0	-4.774073	-2.188414	1.255188
39	6	0	-6.081329	-2.539717	0.907558
40	6	0	-7.122236	-1.618950	1.064859
41	1	0	-7.661904	0.376520	1.692060
42	1	0	-5.341416	1.009136	2.308909
43	1	0	-3.969117	-2.912117	1.131765
44	1	0	-6.289176	-3.534650	0.513840
45	1	0	-8.140737	-1.894849	0.794500
46	6	0	-3.091377	-0.537269	2.163522
47	7	0	-2.433217	0.172166	1.073822
48	1	0	-2.534172	-1.429890	2.494091
49	1	0	-3.118374	0.159106	3.019372
50	6	0	-1.346597	1.091643	1.296763
51	1	0	-1.643938	1.823462	2.051783
52	6	0	-1.366044	1.796487	-0.088463
53	6	0	1.833527	5.837743	-2.321354
54	6	0	0.973905	4.896619	-1.747770

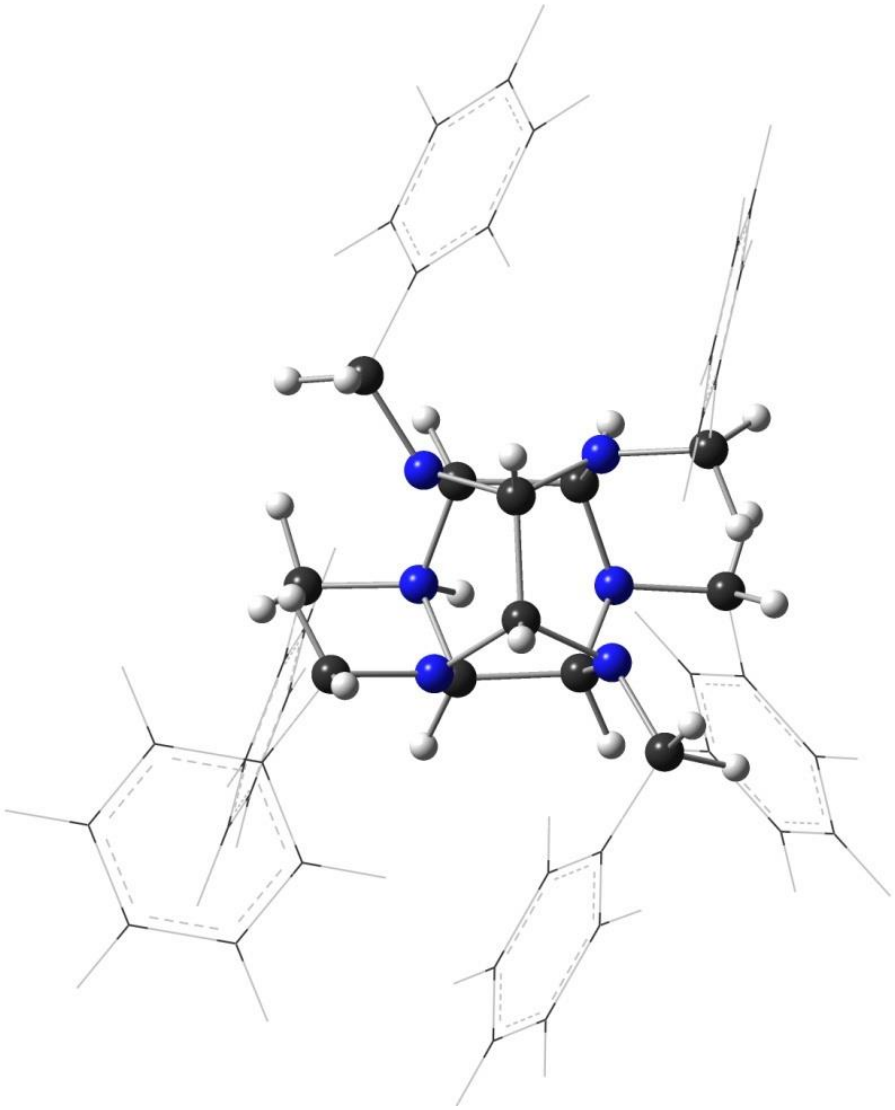
55	6	0	0.946583	4.724761	-0.356277
56	6	0	1.778095	5.513575	0.455716
57	6	0	2.631394	6.456429	-0.122813
58	6	0	2.663372	6.619132	-1.511740
59	1	0	1.854128	5.963671	-3.403999
60	1	0	0.323609	4.293001	-2.381633
61	1	0	1.760323	5.395685	1.538983
62	1	0	3.274364	7.066848	0.511513
63	1	0	3.331281	7.353164	-1.960236
64	6	0	0.000490	3.748642	0.297033
65	7	0	-0.206548	2.542389	-0.524478
66	1	0	-0.980644	4.243917	0.407710
67	1	0	0.342270	3.492142	1.320242
68	1	0	0.622153	1.949481	-0.469624
69	6	0	3.658543	1.773029	3.863308
70	6	0	2.338299	1.745509	3.406403
71	6	0	1.517386	0.645309	3.695147
72	6	0	2.030803	-0.427427	4.439187
73	6	0	3.354231	-0.398344	4.887960
74	6	0	4.169892	0.700754	4.601496
75	1	0	4.289771	2.637009	3.650811
76	1	0	1.942894	2.580915	2.827823
77	1	0	1.400294	-1.284184	4.679475
78	1	0	3.748819	-1.233896	5.467479
79	1	0	5.199541	0.724921	4.958328
80	6	0	0.075844	0.633547	3.241213
81	7	0	-0.020330	0.579321	1.761505
82	1	0	-0.407387	1.560640	3.584363
83	1	0	-0.475836	-0.209481	3.704893
84	6	0	0.435928	-0.742720	1.298322
85	1	0	1.182843	-1.101022	2.009921
86	6	0	1.043159	-0.706674	-0.101621
87	6	0	2.137006	-4.052581	-3.362334
88	6	0	1.256717	-3.209382	-2.678186
89	6	0	1.098270	-1.879432	-3.088462
90	6	0	1.809384	-1.406671	-4.202415
91	6	0	2.684687	-2.254739	-4.885568
92	6	0	2.853638	-3.578041	-4.464797
93	1	0	2.260185	-5.085755	-3.033070
94	1	0	0.694749	-3.596552	-1.824608
95	1	0	1.676901	-0.379486	-4.544798
96	1	0	3.236687	-1.882747	-5.749685
97	1	0	3.539134	-4.237251	-4.997127
98	6	0	0.132261	-0.944348	-2.398893

99	7	0	0.103333	-1.124974	-0.944719
100	1	0	-0.883176	-1.139780	-2.770215
101	1	0	0.360712	0.110436	-2.616658
102	1	0	-2.189416	2.525807	-0.013818
103	1	0	1.745971	0.064890	-0.417524
104	8	0	2.276922	-1.999721	0.120162
105	1	0	2.562449	-2.319373	-0.757679
106	1	0	3.156399	-1.738602	0.713623
107	6	0	3.418106	2.402575	-0.517762
108	6	0	4.148883	1.513323	0.269008
109	6	0	4.608568	0.304475	-0.263115
110	6	0	4.336791	0.005088	-1.602014
111	6	0	3.609624	0.895925	-2.394436
112	6	0	3.140884	2.093924	-1.851465
113	1	0	3.076926	3.341533	-0.090205
114	1	0	4.370968	1.769460	1.303220
115	1	0	4.697891	-0.927252	-2.029267
116	1	0	3.410463	0.655220	-3.434378
117	1	0	2.570479	2.786395	-2.463995
118	6	0	5.316081	-0.686154	0.630147
119	7	0	4.313071	-1.324845	1.523646
120	1	0	4.736844	-2.100384	2.036092
121	1	0	4.007454	-0.654044	2.234029
122	1	0	6.099826	-0.197564	1.214822
123	1	0	5.773687	-1.476448	0.033929

ONIOM: extrapolated energy =-1203.277144511885 A.U.

Free energy = -1202.33204 A.U.

IM19:



Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.762712	3.768041	1.583837
2	6	0	-3.603339	3.606225	0.820948
3	6	0	-3.575281	2.676515	-0.230014
4	6	0	-4.718380	1.918494	-0.515249
5	6	0	-5.878876	2.088689	0.246320
6	6	0	-5.903126	3.010704	1.296740
7	1	0	-4.778998	4.489541	2.400703
8	1	0	-2.726941	4.215164	1.042337
9	1	0	-4.704975	1.184853	-1.322008
10	1	0	-6.766686	1.497848	0.018463
11	1	0	-6.808523	3.141318	1.888684
12	6	0	-2.324938	2.532302	-1.071955

13	7	0	-1.420933	1.440311	-0.683756
14	1	0	-1.740653	3.465970	-1.044172
15	1	0	-2.585216	2.369154	-2.127900
16	6	0	-1.833115	0.061588	-0.962234
17	1	0	-2.597311	0.037244	-1.744494
18	6	0	-0.554558	-0.777636	-1.418729
19	1	0	-0.716274	-1.209505	-2.409694
20	6	0	4.042927	-3.156121	-1.586335
21	6	0	2.814576	-3.134537	-0.919317
22	6	0	1.621035	-3.024774	-1.647218
23	6	0	1.667597	-2.934052	-3.045743
24	6	0	2.897746	-2.959295	-3.709364
25	6	0	4.086863	-3.072922	-2.981802
26	1	0	4.968337	-3.243696	-1.016699
27	1	0	2.792310	-3.216423	0.167186
28	1	0	0.746113	-2.849706	-3.621249
29	1	0	2.929144	-2.893021	-4.797100
30	1	0	5.044718	-3.096648	-3.500510
31	6	0	0.284083	-3.075633	-0.934103
32	7	0	-0.248785	-1.804164	-0.438406
33	1	0	0.348872	-3.754621	-0.068547
34	1	0	-0.482722	-3.506069	-1.597572
35	6	0	-6.740299	-1.300926	-0.613038
36	6	0	-5.578428	-1.243060	0.162574
37	6	0	-4.351298	-1.650189	-0.379416
38	6	0	-4.296902	-2.114575	-1.702563
39	6	0	-5.459495	-2.165352	-2.475724
40	6	0	-6.683069	-1.759828	-1.932413
41	1	0	-7.693735	-0.989334	-0.186101
42	1	0	-5.628981	-0.878044	1.188182
43	1	0	-3.349446	-2.443472	-2.128434
44	1	0	-5.412676	-2.524559	-3.503803
45	1	0	-7.589345	-1.803490	-2.535331
46	6	0	-3.099685	-1.633257	0.468090
47	7	0	-2.389577	-0.364861	0.313446
48	1	0	-2.459465	-2.497734	0.219188
49	1	0	-3.369403	-1.718490	1.534221
50	6	0	-1.480790	0.099869	1.340619
51	1	0	-2.031493	0.313836	2.260700
52	6	0	-0.960879	1.419113	0.676847
53	6	0	4.924754	2.683790	1.128060
54	6	0	3.717391	2.576566	0.431516
55	6	0	2.504362	2.812573	1.091884
56	6	0	2.507840	3.166807	2.451370

57	6	0	3.716779	3.269686	3.142983
58	6	0	4.926650	3.027198	2.483175
59	1	0	5.867373	2.499818	0.610235
60	1	0	3.730338	2.316016	-0.629050
61	1	0	1.571015	3.368208	2.973580
62	1	0	3.716794	3.542079	4.199508
63	1	0	5.869868	3.108683	3.025291
64	6	0	1.197465	2.707742	0.357341
65	7	0	0.551262	1.389467	0.715519
66	1	0	1.311919	2.743344	-0.730717
67	1	0	0.507129	3.503670	0.662501
68	6	0	2.359682	-1.665317	4.978900
69	6	0	1.241931	-1.292514	4.228340
70	6	0	0.591645	-2.237287	3.419806
71	6	0	1.066144	-3.555898	3.371769
72	6	0	2.182361	-3.924694	4.128539
73	6	0	2.831302	-2.981532	4.931238
74	1	0	2.864148	-0.928774	5.604499
75	1	0	0.874802	-0.266794	4.265958
76	1	0	0.567188	-4.298863	2.749772
77	1	0	2.546917	-4.951532	4.091165
78	1	0	3.701892	-3.270927	5.518913
79	6	0	-0.632089	-1.846888	2.626558
80	7	0	-0.319630	-0.716415	1.734289
81	1	0	-1.425319	-1.520938	3.317921
82	1	0	-1.027826	-2.706682	2.055230
83	6	0	0.508604	-1.108187	0.602453
84	1	0	1.320082	-1.741216	0.973182
85	6	0	1.101750	0.166402	-0.098465
86	6	0	4.720800	0.720491	-2.725393
87	6	0	3.384381	0.365214	-2.523218
88	6	0	2.369592	1.315954	-2.695757
89	6	0	2.702887	2.623255	-3.085567
90	6	0	4.040053	2.972670	-3.291709
91	6	0	5.051576	2.023633	-3.109464
92	1	0	5.505652	-0.024041	-2.587761
93	1	0	3.128334	-0.658697	-2.238041
94	1	0	1.922634	3.369722	-3.237829
95	1	0	4.294159	3.988655	-3.595817
96	1	0	6.093836	2.298949	-3.269040
97	6	0	0.912091	0.950740	-2.542232
98	7	0	0.666890	0.033933	-1.429497
99	1	0	0.592974	0.415755	-3.452367
100	1	0	0.279611	1.853047	-2.468158

101	1	0	-1.271051	2.302957	1.238106
102	1	0	2.187457	0.271973	-0.003599
103	1	0	0.783173	1.148845	1.692025

ONIOM: extrapolated energy = -800.100974601493 A.U.

Free energy = -799.314614 A.U.

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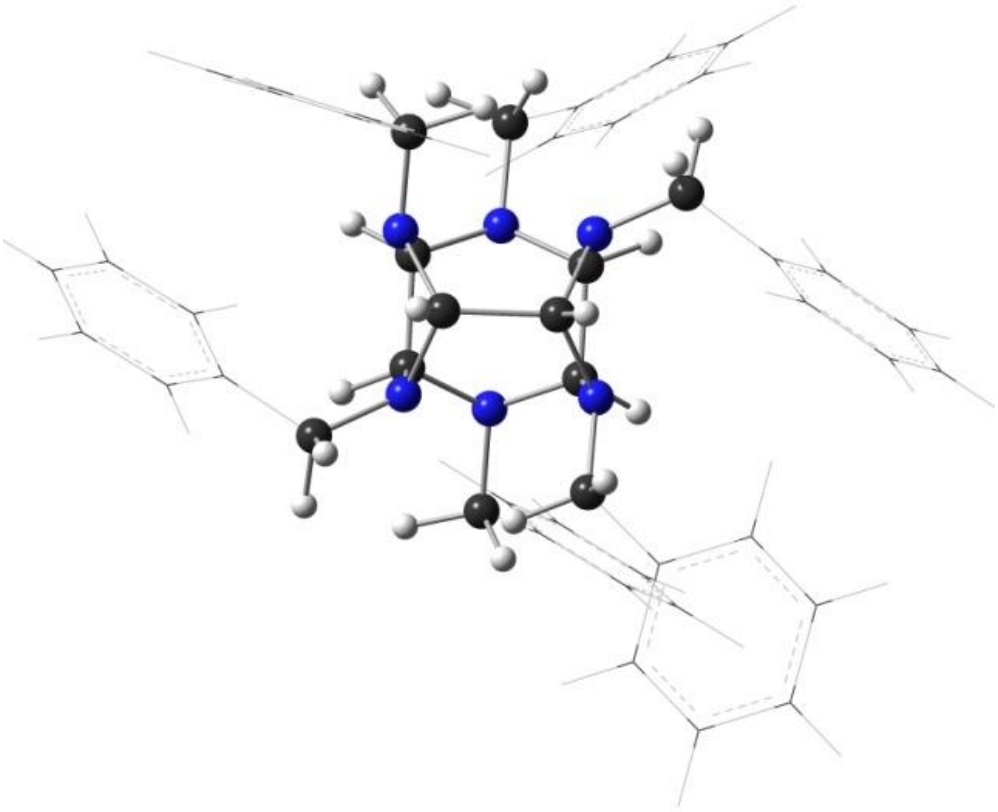

Standard orientation

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.792329	-2.286768	-3.224680
2	6	0	-3.617318	-2.549970	-2.515536
3	6	0	-3.594787	-2.430309	-1.117821
4	6	0	-4.759658	-2.050347	-0.437875
5	6	0	-5.935329	-1.794713	-1.150293
6	6	0	-5.954686	-1.911889	-2.543392
7	1	0	-4.802932	-2.378103	-4.310415
8	1	0	-2.720467	-2.853709	-3.054537
9	1	0	-4.748191	-1.937452	0.645814
10	1	0	-6.838570	-1.500676	-0.615771

11	1	0	-6.871495	-1.712733	-3.095851
12	6	0	-2.329043	-2.760648	-0.346443
13	7	0	-1.389323	-1.671807	-0.114453
14	1	0	-1.776886	-3.556715	-0.877178
15	1	0	-2.589878	-3.184417	0.638209
16	6	0	-1.794390	-0.598533	0.782571
17	1	0	-2.545981	-0.951183	1.498711
18	6	0	-0.509848	-0.055174	1.571065
19	1	0	-0.677267	-0.143822	2.650934
20	6	0	4.074393	1.919901	2.760968
21	6	0	2.836089	2.204075	2.178380
22	6	0	1.650207	1.825198	2.824537
23	6	0	1.716241	1.156238	4.055246
24	6	0	2.956558	0.874083	4.635057
25	6	0	4.137434	1.258304	3.991779
26	1	0	4.992832	2.217106	2.255369
27	1	0	2.796310	2.724176	1.221727
28	1	0	0.801363	0.853751	4.562921
29	1	0	3.002368	0.355844	5.592498
30	1	0	5.102695	1.042049	4.446607
31	6	0	0.302271	2.198519	2.232011
32	7	0	-0.242591	1.327405	1.198853
33	1	0	0.365572	3.212978	1.800123
34	1	0	-0.453186	2.263679	3.034315
35	6	0	-6.688507	0.662217	1.337205
36	6	0	-5.570178	0.990923	0.564685
37	6	0	-4.313723	1.129584	1.170239
38	6	0	-4.186906	0.935148	2.554802
39	6	0	-5.305534	0.601875	3.322065
40	6	0	-6.558880	0.466590	2.715308
41	1	0	-7.664228	0.559784	0.862650
42	1	0	-5.676325	1.132222	-0.510334
43	1	0	-3.213781	1.048173	3.032441
44	1	0	-5.202001	0.450118	4.396191
45	1	0	-7.430938	0.211103	3.315201
46	6	0	-3.105946	1.538923	0.353544
47	7	0	-2.384525	0.371137	-0.134493
48	1	0	-2.464655	2.207411	0.957205
49	1	0	-3.436986	2.110832	-0.531845
50	6	0	-1.462731	0.475905	-1.262309
51	1	0	-2.031453	0.693965	-2.173209
52	6	0	-0.855625	-0.976771	-1.301004
53	6	0	5.025040	-1.798197	-2.286105
54	6	0	3.806210	-2.074165	-1.659275

55	6	0	2.600093	-1.832512	-2.330548
56	6	0	2.625469	-1.307123	-3.632345
57	6	0	3.845294	-1.030982	-4.254295
58	6	0	5.047950	-1.277221	-3.583160
59	1	0	5.960010	-1.989429	-1.759908
60	1	0	3.798881	-2.476128	-0.644488
61	1	0	1.690260	-1.112014	-4.155649
62	1	0	3.859891	-0.624112	-5.265102
63	1	0	5.998283	-1.063478	-4.069692
64	6	0	1.274575	-2.149964	-1.673773
65	7	0	0.588103	-0.909410	-1.303201
66	1	0	1.415201	-2.839281	-0.820434
67	1	0	0.633671	-2.681667	-2.397709
68	6	0	1.976831	4.230755	-3.618522
69	6	0	0.910256	3.459231	-3.150451
70	6	0	0.399952	3.672684	-1.861003
71	6	0	0.966226	4.664196	-1.046560
72	6	0	2.031982	5.435154	-1.520159
73	6	0	2.539489	5.220155	-2.805119
74	1	0	2.370881	4.061308	-4.620507
75	1	0	0.474865	2.686527	-3.783158
76	1	0	0.578206	4.839148	-0.043830
77	1	0	2.468584	6.205099	-0.884131
78	1	0	3.370527	5.820917	-3.171678
79	6	0	-0.766005	2.850511	-1.357068
80	7	0	-0.369394	1.447990	-1.212043
81	1	0	-1.588558	2.898856	-2.091729
82	1	0	-1.153870	3.273792	-0.409913
83	6	0	0.499056	1.225136	-0.071766
84	1	0	1.299341	1.973335	-0.092891
85	6	0	1.101680	-0.226050	-0.119133
86	6	0	4.744473	-2.010974	2.020865
87	6	0	3.412949	-1.590634	1.972468
88	6	0	2.395098	-2.504054	1.666098
89	6	0	2.724616	-3.847023	1.417943
90	6	0	4.057046	-4.264325	1.471747
91	6	0	5.070325	-3.347752	1.770841
92	1	0	5.529963	-1.293456	2.257001
93	1	0	3.157292	-0.546295	2.174655
94	1	0	1.943643	-4.569935	1.185372
95	1	0	4.306192	-5.307653	1.279581
96	1	0	6.108023	-3.674311	1.810223
97	6	0	0.938088	-2.097137	1.651890
98	7	0	0.735382	-0.724603	1.207754

99	1	0	0.566064	-2.143238	2.693952
100	1	0	0.334250	-2.821128	1.075627
101	1	0	-1.182122	-1.492958	-2.208888
102	1	0	2.194221	-0.205690	-0.211485

ONIOM: extrapolated energy = -799.649968202027 A.U.

Free ennergy = -798.878821 A.U.