Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information for

Attack of Radicals and Protons on Ladderane Lipids: Quantum Chemical Calculations and Biological Implications

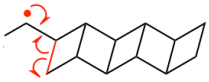
Dustin H. Nouri[a,b] and Dean J. Tantillo*[a]

[‡] *Department of Chemistry, University of California–Davis, 1 Shields Avenue, Davis, CA 95616;* [∫] *Present address: Department of Chemistry, Allan Hancock College, 800 S. College Dr. Santa Maria, CA 93454*

tantillo@chem.ucdavis.edu

Contents

Coordinates and energies

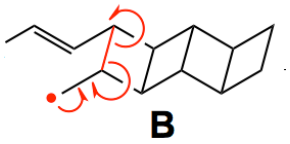


A

Zero-point correction= 0.292169 (Hartree/Particle)
Thermal correction to Energy= 0.304941
Thermal correction to Enthalpy= 0.305885
Thermal correction to Gibbs Free Energy= 0.251312
Sum of electronic and zero-point Energies= -544.438328
Sum of electronic and thermal Energies= -544.425556
Sum of electronic and thermal Enthalpies= -544.424612
Sum of electronic and thermal Free Energies= -544.479185

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.551566	-0.116708	-0.213442
2	6	0	2.307511	1.449481	-0.149297
3	6	0	1.215311	-0.325740	0.571037
4	6	0	0.945821	1.225617	0.542757
5	1	0	0.741882	1.826905	1.435224
6	6	0	-0.000672	-0.568440	-0.339422
7	6	0	-0.246216	0.999586	-0.413858
8	1	0	-0.258374	1.586853	-1.340302
9	6	0	-1.330111	-0.737488	0.422838
10	6	0	-1.585772	0.827270	0.323757
11	1	0	-1.765748	1.485946	1.182366
12	6	0	-2.781814	0.567044	-0.614656
13	1	0	-2.796084	1.119970	-1.560087
14	6	0	-2.535811	-0.989047	-0.503037
15	6	0	-4.137299	0.395678	0.119061
16	1	0	-4.229814	0.947592	1.061562
17	1	0	-5.001865	0.644980	-0.504509
18	6	0	-3.889114	-1.137412	0.241144
19	1	0	-3.816738	-1.533912	1.260505
20	1	0	-4.622060	-1.740999	-0.303705
21	1	0	-2.369889	-1.646774	-1.363054
22	1	0	-1.295172	-1.307003	1.359628
23	1	0	0.152162	-1.218845	-1.209381
24	1	0	1.290345	-0.919284	1.488798
25	1	0	2.490501	-0.490773	-1.245106
26	6	0	3.787861	-0.627349	0.428034
27	1	0	2.286524	1.972768	-1.112754
28	1	0	3.033961	1.949777	0.499490
29	6	0	5.051459	-0.855408	-0.335600
30	1	0	5.615027	0.080022	-0.508866
31	1	0	5.730625	-1.532951	0.195907
32	1	0	4.850972	-1.282880	-1.327198
33	1	0	3.847419	-0.583902	1.515585

mPW1PW91 energy: -544.6318521, S2=0.755246
CCSD(T) energy: -543.0138016, S2=0.765266

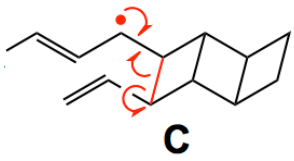


B

Zero-point correction= 0.289965 (Hartree/Particle)
Thermal correction to Energy= 0.303711
Thermal correction to Enthalpy= 0.304655
Thermal correction to Gibbs Free Energy= 0.248590
Sum of electronic and zero-point Energies= -544.442859
Sum of electronic and thermal Energies= -544.429113
Sum of electronic and thermal Enthalpies= -544.428169
Sum of electronic and thermal Free Energies= -544.484233

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.672092	-0.311122	0.192808
2	6	0	-1.814623	2.536986	0.082625
3	6	0	-1.343911	-0.018703	-0.426767
4	6	0	-0.884173	1.527564	-0.464813
5	1	0	-0.604474	1.805407	-1.490616
6	6	0	-0.100378	-0.340073	0.457393
7	6	0	0.341550	1.165741	0.421158
8	1	0	0.478945	1.783945	1.315396
9	6	0	1.160452	-0.740953	-0.334956
10	6	0	1.610154	0.786308	-0.368134
11	1	0	1.816705	1.358370	-1.280947
12	6	0	2.815990	0.443837	0.529150
13	1	0	2.955837	1.061172	1.422943
14	6	0	2.370707	-1.071077	0.561197
15	6	0	4.093933	0.040234	-0.252003
16	1	0	4.195492	0.494094	-1.244581
17	1	0	5.018915	0.230278	0.301739
18	6	0	3.654074	-1.453815	-0.221685
19	1	0	3.480867	-1.926333	-1.195454
20	1	0	4.334996	-2.094698	0.347483
21	1	0	2.165825	-1.630651	1.480142
22	1	0	1.012868	-1.370109	-1.221243
23	1	0	-0.303632	-0.895432	1.379574
24	1	0	-1.295794	-0.482126	-1.419744
25	1	0	-2.830581	0.072422	1.202795
26	6	0	-3.653007	-1.005257	-0.392896
27	1	0	-1.859338	2.739997	1.149097
28	1	0	-2.591222	2.972550	-0.539220
29	6	0	-4.986684	-1.314571	0.224996
30	1	0	-5.809937	-0.905685	-0.376958
31	1	0	-5.155808	-2.398306	0.289558
32	1	0	-5.068625	-0.899031	1.235242
33	1	0	-3.492995	-1.386466	-1.403641

mPW1PW91 energy: -544.6263132, S2=0.755351

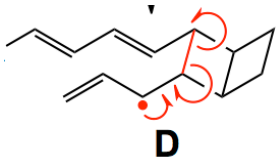


C

Zero-point correction= 0.289884 (Hartree/Particle)
Thermal correction to Energy= 0.304166
Thermal correction to Enthalpy= 0.305111
Thermal correction to Gibbs Free Energy= 0.246753
Sum of electronic and zero-point Energies= -544.475862
Sum of electronic and thermal Energies= -544.461580
Sum of electronic and thermal Enthalpies= -544.460636
Sum of electronic and thermal Free Energies= -544.518993

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.507305	3.585640	0.149685
2	6	0	-1.591070	-0.224437	-0.384251
3	6	0	-0.185795	2.404434	-0.381178
4	1	0	-0.379927	2.235148	-1.441461
5	6	0	-0.274924	-0.139235	0.303541
6	6	0	0.458659	1.278187	0.364329
7	1	0	0.656364	1.598724	1.394681
8	6	0	0.956486	-0.724056	-0.469026
9	6	0	1.699945	0.655893	-0.343025
10	1	0	2.099892	1.217872	-1.194054
11	6	0	2.732969	0.012198	0.609181
12	1	0	2.895208	0.510988	1.570650
13	6	0	2.007369	-1.384802	0.443392
14	6	0	3.981684	-0.563265	-0.107026
15	1	0	4.284490	-0.035143	-1.018574
16	1	0	4.856186	-0.635815	0.547516
17	6	0	3.254649	-1.926306	-0.306103
18	1	0	3.073451	-2.225778	-1.344733
19	1	0	3.743877	-2.761845	0.204507
20	1	0	1.633334	-1.985701	1.279231
21	1	0	0.731749	-1.215857	-1.421605
22	1	0	-0.368211	-0.570108	1.308130
23	1	0	-0.330458	3.806431	1.200600
24	1	0	-0.961239	4.376013	-0.442378
25	1	0	-1.636216	0.086804	-1.428156
26	6	0	-2.759016	-0.686510	0.212001
27	1	0	-2.695781	-0.999474	1.257048
28	6	0	-3.996484	-0.784031	-0.405379
29	1	0	-4.081360	-0.474944	-1.447452
30	6	0	-5.240087	-1.283190	0.259916
31	1	0	-6.032730	-0.519985	0.263568
32	1	0	-5.658761	-2.155937	-0.263156
33	1	0	-5.052353	-1.574514	1.299292

mPW1PW91 energy: -544.6508706, S2=0.789542

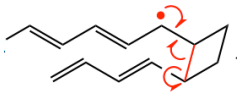


D

Zero-point correction= 0.288580 (Hartree/Particle)
Thermal correction to Energy= 0.303641
Thermal correction to Enthalpy= 0.304585
Thermal correction to Gibbs Free Energy= 0.244158
Sum of electronic and zero-point Energies= -544.492934
Sum of electronic and thermal Energies= -544.477872
Sum of electronic and thermal Enthalpies= -544.476928
Sum of electronic and thermal Free Energies= -544.537355

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.216076	4.122910	0.049609
2	6	0	-1.930864	-0.570225	-0.412474
3	6	0	1.579585	2.863895	-0.394485
4	1	0	2.151555	2.800658	-1.322150
5	6	0	-0.741433	-0.545912	0.214557
6	6	0	1.276891	1.666156	0.245741
7	1	0	0.706798	1.712706	1.173492
8	6	0	0.577113	-0.806453	-0.437539
9	6	0	1.690282	0.325777	-0.242285
10	1	0	2.267224	0.444007	-1.167744
11	6	0	2.444425	-0.620363	0.763331
12	1	0	2.533449	-0.236910	1.783923
13	6	0	1.485412	-1.786521	0.359541
14	6	0	3.644781	-1.379400	0.153923
15	1	0	4.271672	-0.822129	-0.552257
16	1	0	4.295429	-1.812734	0.921025
17	6	0	2.657767	-2.431728	-0.440323
18	1	0	2.532219	-2.381818	-1.527931
19	1	0	2.879027	-3.469749	-0.174380
20	1	0	0.988981	-2.434015	1.087861
21	1	0	0.418847	-1.075915	-1.489319
22	1	0	-0.725058	-0.344104	1.287811
23	1	0	0.644918	4.255132	0.964804
24	1	0	1.485865	5.018579	-0.499874
25	1	0	-1.959343	-0.776661	-1.483850
26	6	0	-3.211238	-0.339883	0.237623
27	6	0	-4.399683	-0.364995	-0.389037
28	6	0	-5.727293	-0.128697	0.266533
29	1	0	-6.248256	0.728421	-0.182760
30	1	0	-6.393103	-0.994704	0.145677
31	1	0	-5.618112	0.066604	1.338805
32	1	0	-4.419923	-0.571217	-1.460678
33	1	0	-3.183117	-0.133522	1.309254

mPW1PW91 energy: -544.6589771, S2=0.791522

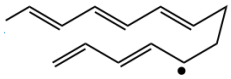


E

Zero-point correction= 0.287881 (Hartree/Particle)
Thermal correction to Energy= 0.303610
Thermal correction to Enthalpy= 0.304554
Thermal correction to Gibbs Free Energy= 0.242469
Sum of electronic and zero-point Energies= -544.524282
Sum of electronic and thermal Energies= -544.508554
Sum of electronic and thermal Enthalpies= -544.507609
Sum of electronic and thermal Free Energies= -544.569694

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.899563	3.634045	-0.172023
2	6	0	2.563614	-0.242606	0.347998
3	6	0	-3.139681	2.643607	0.318933
4	1	0	-2.513042	2.835199	1.190734
5	6	0	1.450669	-0.711845	-0.384392
6	6	0	-3.080751	1.297834	-0.231614
7	1	0	-3.702877	1.103085	-1.107044
8	6	0	0.312136	-1.241957	0.162766
9	6	0	-2.321588	0.306223	0.267709
10	1	0	-1.701300	0.512645	1.141403
11	6	0	-2.258009	-1.078153	-0.278100
12	1	0	-2.892612	-1.153137	-1.169501
13	6	0	-0.851914	-1.742942	-0.622658
14	6	0	-2.541014	-2.292145	0.658492
15	1	0	-2.254257	-2.072971	1.693287
16	1	0	-3.561357	-2.688850	0.661986
17	6	0	-1.445630	-3.090039	-0.087415
18	1	0	-0.776694	-3.717973	0.509233
19	1	0	-1.858428	-3.694745	-0.901685
20	1	0	-0.610280	-1.722252	-1.691182
21	1	0	0.249291	-1.314642	1.250275
22	1	0	1.510930	-0.645847	-1.472712
23	1	0	-4.538347	3.484833	-1.039962
24	1	0	-3.908464	4.623632	0.274681
25	1	0	2.520985	-0.299967	1.436108
26	6	0	3.730636	0.297955	-0.240535
27	6	0	4.818211	0.759427	0.448454
28	6	0	6.050106	1.331804	-0.180518
29	1	0	6.228318	2.365479	0.150132
30	1	0	6.947780	0.760986	0.098550
31	1	0	5.980575	1.335895	-1.273748
32	1	0	4.799898	0.713742	1.538105
33	1	0	3.756560	0.347638	-1.331247

mPW1PW91 energy: -544.6817775, S2=0.813649



F

Zero-point correction= 0.286492 (Hartree/Particle)
Thermal correction to Energy= 0.303002
Thermal correction to Enthalpy= 0.303946
Thermal correction to Gibbs Free Energy= 0.239614
Sum of electronic and zero-point Energies= -544.540909
Sum of electronic and thermal Energies= -544.524399
Sum of electronic and thermal Enthalpies= -544.523455
Sum of electronic and thermal Free Energies= -544.587788

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.831205	0.555173	0.037600
2	1	0	-6.220945	-0.418969	-0.262988
3	6	0	-4.497223	0.719417	0.109126
4	1	0	-4.100849	1.691357	0.408740
5	6	0	-3.525134	-0.312794	-0.186231
6	1	0	-3.919179	-1.286155	-0.483176
7	6	0	-2.183868	-0.145751	-0.118190
8	1	0	-1.789186	0.827597	0.177317
9	6	0	-1.212840	-1.179257	-0.413050
10	1	0	-1.612392	-2.153080	-0.703276
11	6	0	1.131313	-2.086359	-0.652688
12	1	0	0.606692	-3.020561	-0.887463
13	1	0	1.707083	-1.827235	-1.554501
14	6	0	2.117196	-2.355106	0.505117
15	1	0	1.540586	-2.570640	1.416856
16	1	0	2.663130	-3.288746	0.287657
17	6	0	5.685277	2.825765	-0.127988
18	1	0	5.881174	3.667357	-0.784247
19	1	0	6.276831	2.761681	0.781979
20	6	0	-6.848680	1.613268	0.339622
21	1	0	-7.520061	1.302327	1.152453
22	1	0	-6.375021	2.555856	0.634176
23	1	0	-7.488728	1.812793	-0.531384
24	6	0	0.121973	-1.013301	-0.354171
25	1	0	0.515078	-0.040217	-0.058531
26	6	0	3.124636	-1.280231	0.810829
27	1	0	3.677908	-1.415606	1.741420
28	6	0	3.438939	-0.193573	0.040851
29	1	0	2.904310	-0.036922	-0.896251
30	6	0	4.424533	0.765419	0.372871
31	1	0	4.976277	0.632458	1.303805
32	6	0	4.738842	1.887990	-0.428247
33	1	0	4.174732	2.002747	-1.355285

mPW1PW91 energy: -544.6919427, S2=0.817081
CCSD(T) energy: - 543.0857535, 3S2=1.194346

TS A-to-B

Zero-point correction= 0.289939 (Hartree/Particle)
Thermal correction to Energy= 0.302478
Thermal correction to Enthalpy= 0.303422
Thermal correction to Gibbs Free Energy= 0.250227
Sum of electronic and zero-point Energies= -544.417394
Sum of electronic and thermal Energies= -544.404855
Sum of electronic and thermal Enthalpies= -544.403911
Sum of electronic and thermal Free Energies= -544.457106

Imaginary Frequency -671.7196

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.571567	-0.291598	-0.183930
2	6	0	2.229177	1.749593	-0.072032
3	6	0	1.242105	-0.274620	0.580891
4	6	0	0.936880	1.259388	0.541662
5	1	0	0.652405	1.778363	1.466707
6	6	0	0.017861	-0.560470	-0.313119
7	6	0	-0.241171	0.998935	-0.434533
8	1	0	-0.235643	1.560418	-1.376249
9	6	0	-1.311782	-0.718360	0.453040
10	6	0	-1.590191	0.838145	0.286231
11	1	0	-1.794314	1.528331	1.114107
12	6	0	-2.769298	0.519260	-0.656357
13	1	0	-2.775628	1.027353	-1.626624
14	6	0	-2.507233	-1.026616	-0.468078
15	6	0	-4.132651	0.366802	0.066398
16	1	0	-4.247969	0.966429	0.976737
17	1	0	-4.990789	0.569662	-0.582378
18	6	0	-3.865306	-1.154044	0.271822
19	1	0	-3.795953	-1.494103	1.311557
20	1	0	-4.585229	-1.796496	-0.245134
21	1	0	-2.327919	-1.722940	-1.294314
22	1	0	-1.271994	-1.247275	1.413112
23	1	0	0.175422	-1.234918	-1.163217
24	1	0	1.294859	-0.809109	1.536802
25	1	0	2.489223	-0.368392	-1.270299
26	6	0	3.753823	-0.729129	0.378319
27	1	0	2.219840	2.218903	-1.055731
28	1	0	2.983382	2.146122	0.604149
29	6	0	5.039489	-0.887932	-0.375159
30	1	0	5.785637	-0.133982	-0.079548
31	1	0	5.500106	-1.867703	-0.184316
32	1	0	4.886170	-0.793291	-1.456234
33	1	0	3.798779	-0.863501	1.459949

mPW1PW91 energy: -544.6040318, S2=0.79654
CCSD(T) energy: -542.9865044, S2=1.006059

TS B-to-C

Zero-point correction= 0.288664 (Hartree/Particle)
Thermal correction to Energy= 0.302050
Thermal correction to Enthalpy= 0.302994
Thermal correction to Gibbs Free Energy= 0.247654
Sum of electronic and zero-point Energies= -544.433364
Sum of electronic and thermal Energies= -544.419979
Sum of electronic and thermal Enthalpies= -544.419034
Sum of electronic and thermal Free Energies= -544.474374

Imaginary frequency -695.1187

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.655389	-0.524659	0.238066
2	6	0	-1.741282	2.580703	0.045007
3	6	0	-1.368451	-0.257236	-0.386147
4	6	0	-0.832534	1.629491	-0.432024
5	1	0	-0.607066	1.700131	-1.498778
6	6	0	-0.081745	-0.395902	0.432723
7	6	0	0.319450	1.110557	0.443864
8	1	0	0.431675	1.662862	1.384103
9	6	0	1.193416	-0.739764	-0.375252
10	6	0	1.616210	0.793266	-0.333002
11	1	0	1.826302	1.409826	-1.215062
12	6	0	2.815356	0.432025	0.566542
13	1	0	2.927068	1.004987	1.493139
14	6	0	2.403088	-1.092553	0.512009
15	6	0	4.112769	0.098334	-0.215128
16	1	0	4.220903	0.611238	-1.177708
17	1	0	5.024796	0.272718	0.364605
18	6	0	3.702008	-1.402844	-0.277737
19	1	0	3.547496	-1.819841	-1.279567
20	1	0	4.389577	-2.063631	0.259711
21	1	0	2.204037	-1.706485	1.396953
22	1	0	1.058070	-1.326963	-1.291298
23	1	0	-0.211958	-0.951447	1.369430
24	1	0	-1.308856	-0.582425	-1.427336
25	1	0	-2.717383	-0.365928	1.317104
26	6	0	-3.768280	-0.909649	-0.415345
27	1	0	-1.856321	2.767959	1.109879
28	1	0	-2.471388	3.041516	-0.614000
29	6	0	-5.105332	-1.147060	0.221459
30	1	0	-5.873085	-0.482680	-0.200206
31	1	0	-5.456417	-2.174313	0.049619
32	1	0	-5.071500	-0.977654	1.303177
33	1	0	-3.711653	-1.068119	-1.493969

mPW1PW91 energy: -544.6114647, S2=0.797202

TS C-to-D

Zero-point correction= 0.287498 (Hartree/Particle)
Thermal correction to Energy= 0.301790
Thermal correction to Enthalpy= 0.302735
Thermal correction to Gibbs Free Energy= 0.244620
Sum of electronic and zero-point Energies= -544.459012
Sum of electronic and thermal Energies= -544.444720
Sum of electronic and thermal Enthalpies= -544.443775
Sum of electronic and thermal Free Energies= -544.501890

Imaginary frequency -714.7710

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.223233	3.224431	0.096535
2	6	0	-1.466011	-0.752291	-0.424481
3	6	0	-0.366777	2.330523	-0.439779
4	1	0	-0.291567	2.274802	-1.527511
5	6	0	-0.246715	-0.533032	0.227717
6	6	0	0.435383	1.390550	0.307902
7	1	0	0.485865	1.584466	1.380697
8	6	0	1.104038	-0.725629	-0.470437
9	6	0	1.655823	0.727966	-0.326431
10	1	0	2.035224	1.263799	-1.205539
11	6	0	2.743470	0.221012	0.658521
12	1	0	2.792641	0.722021	1.630725
13	6	0	2.228030	-1.258256	0.446582
14	6	0	4.086793	-0.158176	-0.013581
15	1	0	4.363620	0.438875	-0.890243
16	1	0	4.929994	-0.145084	0.684483
17	6	0	3.553981	-1.596150	-0.288813
18	1	0	3.435263	-1.866326	-1.344357
19	1	0	4.139841	-2.383402	0.195687
20	1	0	1.930654	-1.927326	1.260489
21	1	0	1.012021	-1.193760	-1.457840
22	1	0	-0.249601	-0.715591	1.304073
23	1	0	-1.342983	3.322831	1.173271
24	1	0	-1.825149	3.881516	-0.523920
25	1	0	-1.467960	-0.806833	-1.514169
26	6	0	-2.728235	-0.808414	0.232191
27	1	0	-2.718732	-0.739938	1.322312
28	6	0	-3.930117	-0.952405	-0.390560
29	1	0	-3.946603	-1.018486	-1.479405
30	6	0	-5.253319	-1.031818	0.306461
31	1	0	-5.930819	-0.230277	-0.022092
32	1	0	-5.768927	-1.978695	0.088978
33	1	0	-5.141445	-0.952455	1.393393

mPW1PW91 energy: -544.6274092, S2=0.838795

TS D-to-E

Zero-point correction= 0.286536 (Hartree/Particle)
Thermal correction to Energy= 0.301486
Thermal correction to Enthalpy= 0.302431
Thermal correction to Gibbs Free Energy= 0.242715
Sum of electronic and zero-point Energies= -544.480261
Sum of electronic and thermal Energies= -544.465311
Sum of electronic and thermal Enthalpies= -544.464367
Sum of electronic and thermal Free Energies= -544.524083

Imaginary frequency -719.9420

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.154159	3.913049	0.033418
2	6	0	-1.753411	-0.827185	-0.399003
3	6	0	0.545911	2.846655	-0.443079
4	1	0	0.685322	2.761644	-1.522360
5	6	0	-0.567744	-0.968793	0.255351
6	6	0	1.131952	1.828438	0.355451
7	1	0	0.989248	1.895975	1.434872
8	6	0	0.726460	-0.984385	-0.373788
9	6	0	1.788197	0.694969	-0.161647
10	1	0	2.119760	0.789848	-1.198275
11	6	0	2.656819	-0.222109	0.712290
12	1	0	2.725199	0.123108	1.749216
13	6	0	1.936763	-1.553290	0.367625
14	6	0	3.957858	-0.739456	0.044477
15	1	0	4.424411	-0.077984	-0.694126
16	1	0	4.718630	-1.024582	0.778226
17	6	0	3.166546	-1.968188	-0.498638
18	1	0	2.971187	-1.940315	-1.576395
19	1	0	3.597539	-2.945022	-0.259773
20	1	0	1.684774	-2.256523	1.168919
21	1	0	0.700471	-1.133420	-1.455149
22	1	0	-0.590098	-1.030786	1.345606
23	1	0	-0.326599	4.047385	1.098586
24	1	0	-0.563399	4.668620	-0.629417
25	1	0	-1.745876	-0.759474	-1.488074
26	6	0	-3.042106	-0.772318	0.248436
27	6	0	-4.221203	-0.650845	-0.395518
28	6	0	-5.563430	-0.591744	0.268106
29	1	0	-6.086860	0.345560	0.031473
30	1	0	-6.217163	-1.406101	-0.075416
31	1	0	-5.477753	-0.664362	1.357713
32	1	0	-4.215601	-0.587008	-1.484913
33	1	0	-3.043898	-0.835349	1.338396

mPW1PW91 energy: -544.6400789, S2=0.846413

TS E-to-F

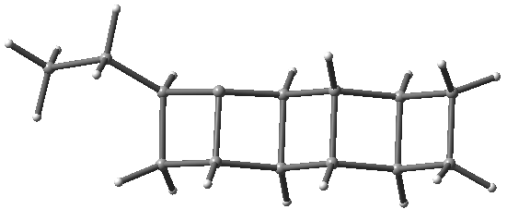
Zero-point correction= 0.285541 (Hartree/Particle)
Thermal correction to Energy= 0.301241
Thermal correction to Enthalpy= 0.302186
Thermal correction to Gibbs Free Energy= 0.240258
Sum of electronic and zero-point Energies= -544.507056
Sum of electronic and thermal Energies= -544.491356
Sum of electronic and thermal Enthalpies= -544.490412
Sum of electronic and thermal Free Energies= -544.552340

Imaginary frequency -712.6342

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.786124	4.311082	0.241587
2	6	0	-2.270128	-0.860045	-0.282546
3	6	0	1.857705	3.118998	-0.384486
4	1	0	1.585517	3.061635	-1.439316
5	6	0	-1.105829	-1.069825	0.427718
6	6	0	2.274317	1.886433	0.234852
7	1	0	2.543206	1.929864	1.291411
8	6	0	0.029253	-1.740134	-0.065508
9	6	0	2.359341	0.688464	-0.418457
10	1	0	2.083287	0.663559	-1.474619
11	6	0	2.714910	-0.555240	0.186476
12	1	0	3.137507	-0.477285	1.189793
13	6	0	1.233376	-1.895942	0.643756
14	6	0	3.181753	-1.773653	-0.601988
15	1	0	2.859991	-1.682647	-1.646592
16	1	0	4.268779	-1.933923	-0.604676
17	6	0	2.341037	-2.828911	0.132575
18	1	0	1.973978	-3.652601	-0.490727
19	1	0	2.888865	-3.269382	0.973220
20	1	0	1.168965	-1.735885	1.719801
21	1	0	-0.012781	-2.105194	-1.093497
22	1	0	-1.059931	-0.697413	1.452820
23	1	0	2.046201	4.418581	1.292267
24	1	0	1.465318	5.209513	-0.276318
25	1	0	-2.324525	-1.225376	-1.309002
26	6	0	-3.425555	-0.192684	0.237690
27	6	0	-4.574131	0.018838	-0.450338
28	6	0	-5.783347	0.718302	0.089831
29	1	0	-6.035716	1.605288	-0.509016
30	1	0	-6.669051	0.067265	0.064561
31	1	0	-5.632588	1.042654	1.125145
32	1	0	-4.638663	-0.341649	-1.478173
33	1	0	-3.361314	0.168913	1.265942

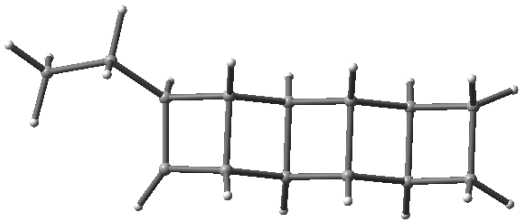
mPW1PW91 energy: -544.6578536, S2=0.89566

Alternative radicals



CCSD(T)=-543.0065801, S2=0.760877

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.545092	-0.273936	0.314831
2	6	0	-1.171236	-0.429289	-0.328419
3	6	0	-0.985628	1.101361	-0.517353
4	6	0	-2.330010	1.282153	0.242787
5	1	0	-2.612150	-0.678137	1.335930
6	1	0	-0.881902	1.620707	-1.475014
7	6	0	0.275673	1.010324	0.369241
8	1	0	0.323226	1.686738	1.231861
9	6	0	0.074454	-0.578163	0.508533
10	1	0	-0.009164	-1.122992	1.456776
11	6	0	-3.728306	-0.800230	-0.507785
12	1	0	-3.662017	-0.399653	-1.529010
13	6	0	-5.090050	-0.451867	0.102315
14	1	0	-5.910947	-0.835375	-0.514281
15	1	0	-5.196431	-0.883387	1.105352
16	1	0	-5.224070	0.632909	0.193917
17	1	0	-3.632459	-1.890335	-0.601987
18	6	0	1.373013	-0.792206	-0.303305
19	6	0	1.569293	0.777631	-0.428868
20	1	0	1.310837	-1.481609	-1.151923
21	1	0	1.664132	1.318214	-1.378240
22	6	0	2.634328	-0.874716	0.580096
23	6	0	2.830942	0.687025	0.452385
24	1	0	2.534990	-1.404335	1.533541
25	1	0	2.888070	1.370425	1.306460
26	6	0	3.948853	-1.094932	-0.213023
27	6	0	4.141184	0.445733	-0.342301
28	1	0	3.837232	-1.647952	-1.152717
29	1	0	4.734240	-1.581927	0.373835
30	1	0	4.145950	0.846975	-1.362288
31	1	0	5.034855	0.816087	0.170053
32	1	0	-3.098499	1.808251	-0.334869
33	1	0	-2.230403	1.772064	1.217800



CCSD(T)=-543.0140672, S2=0.766291

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.539476	-0.211354	-0.292571
2	6	0	1.188851	-0.448545	0.457822
3	6	0	0.992900	1.118823	0.568829
4	6	0	2.291344	1.271325	-0.155828
5	1	0	2.538974	-0.589827	-1.329774
6	1	0	1.230596	-1.116519	1.325164
7	1	0	0.839435	1.668565	1.506812
8	6	0	-0.254555	1.017305	-0.365208
9	1	0	-0.285333	1.695014	-1.225384
10	6	0	-0.046632	-0.550489	-0.456035
11	1	0	0.074064	-1.107540	-1.392926
12	6	0	3.789926	-0.767754	0.415199
13	1	0	3.782359	-0.441465	1.463975
14	6	0	5.098964	-0.333473	-0.250136
15	1	0	5.967967	-0.749502	0.272397
16	1	0	5.144873	-0.669711	-1.293486
17	1	0	5.199402	0.758278	-0.247382
18	1	0	3.723388	-1.865260	0.427803
19	6	0	-1.363049	-0.768497	0.315531
20	6	0	-1.569600	0.803262	0.409228
21	1	0	-1.325216	-1.445276	1.177914
22	1	0	-1.690187	1.363227	1.344612
23	6	0	-2.601174	-0.871875	-0.597453
24	6	0	-2.807710	0.691068	-0.502233
25	1	0	-2.475186	-1.417598	-1.538643
26	1	0	-2.845500	1.358787	-1.369575
27	6	0	-3.935112	-1.084000	0.165025
28	6	0	-4.137608	0.457528	0.262053
29	1	0	-3.846027	-1.620405	1.116788
30	1	0	-4.702869	-1.584593	-0.433615
31	1	0	-4.171465	0.877253	1.274039
32	1	0	-5.019117	0.814164	-0.280337
33	1	0	2.743714	2.132455	-0.643725

Small molecules

NH2OH

CCSD(T)=-131.3502451

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.691485	-0.000924	0.157401
2	1	0	-1.038469	0.812692	-0.355423
3	1	0	-1.039085	-0.808385	-0.364784
4	8	0	0.725451	0.000933	-0.141100
5	1	0	1.114335	-0.005307	0.747200

NH2O•

CCSD(T)=-130.7345566, S2=0.762238

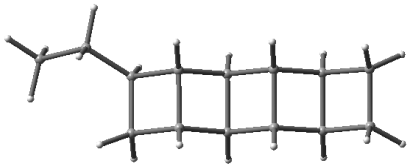
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.028172	0.546984	0.000000
2	1	0	-0.211287	1.029752	0.868651
3	8	0	0.028172	-0.736049	0.000000
4	1	0	-0.211287	1.029752	-0.868651

•NHOH

CCSD(T)=-130.725353, S2=0.761201

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.709034	-0.177978	-0.000026
2	1	0	-1.126700	0.766741	0.000191
3	8	0	0.626987	0.149322	-0.000027
4	1	0	1.074042	-0.715471	0.000206

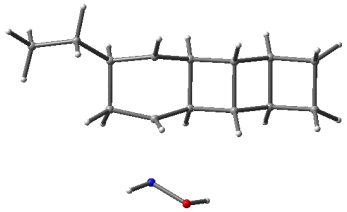
Radical Addition



Zero-point correction= 0.307082 (Hartree/Particle)
Thermal correction to Energy= 0.319392
Thermal correction to Enthalpy= 0.320336
Thermal correction to Gibbs Free Energy= 0.268118
Sum of electronic and zero-point Energies= -545.088704
Sum of electronic and thermal Energies= -545.076394
Sum of electronic and thermal Enthalpies= -545.075450
Sum of electronic and thermal Free Energies= -545.127668

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.500333	-0.221323	-0.265846
2	6	0	1.165394	-0.453841	0.500757
3	6	0	0.953189	1.107069	0.587006
4	6	0	2.308421	1.323018	-0.128041
5	1	0	2.453865	-0.573592	-1.305842
6	1	0	1.218282	-1.115548	1.373393
7	1	0	0.792231	1.653513	1.522411
8	6	0	-0.262665	0.993171	-0.357845
9	1	0	-0.271963	1.650936	-1.235652
10	6	0	-0.067690	-0.582489	-0.411013
11	1	0	0.054600	-1.165026	-1.332545
12	6	0	3.750580	-0.798284	0.398748
13	1	0	3.797251	-0.450765	1.441458
14	6	0	5.048994	-0.426085	-0.325148
15	1	0	5.924386	-0.844308	0.184698
16	1	0	5.048958	-0.804977	-1.354635
17	1	0	5.181329	0.661586	-0.373405
18	1	0	3.656453	-1.892817	0.446480
19	6	0	-1.392282	-0.770437	0.354372
20	6	0	-1.595686	0.804839	0.388244
21	1	0	-1.364753	-1.415795	1.240973
22	1	0	-1.739947	1.396307	1.300793
23	6	0	-2.618340	-0.904937	-0.568974
24	6	0	-2.813212	0.662324	-0.547802
25	1	0	-2.486685	-1.494159	-1.482846
26	1	0	-2.821724	1.291607	-1.444274
27	6	0	-3.964682	-1.070406	0.184246
28	6	0	-4.163472	0.474675	0.191479
29	1	0	-3.889040	-1.550241	1.166880
30	1	0	-4.725763	-1.604225	-0.393856
31	1	0	-4.225788	0.950497	1.177019
32	1	0	-5.027559	0.801581	-0.395917
33	1	0	2.269788	1.900735	-1.058956
34	1	0	3.062790	1.780929	0.522727

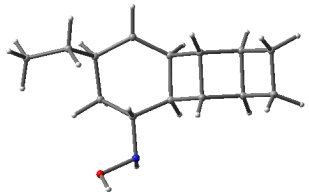
mPW1PW91 energy: - 545.2962531, S2=0.89566



Zero-point correction= 0.334171 (Hartree/Particle)
Thermal correction to Energy= 0.350004
Thermal correction to Enthalpy= 0.350948
Thermal correction to Gibbs Free Energy= 0.289872
Sum of electronic and zero-point Energies= -676.083009
Sum of electronic and thermal Energies= -676.067176
Sum of electronic and thermal Enthalpies= -676.066232
Sum of electronic and thermal Free Energies= -676.127308
1 Imaginary: -1089.1786

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.461948	-0.816016	0.241554
2	6	0	-1.149305	-1.085957	-0.489148
3	6	0	-0.910666	0.883563	-0.291885
4	6	0	-2.309167	0.723686	0.308667
5	1	0	-2.459530	-1.274361	1.244528
6	1	0	-1.182407	-1.626211	-1.438906
7	1	0	-0.763547	1.228910	-1.309492
8	6	0	0.272502	0.399062	0.541785
9	1	0	0.300224	0.861509	1.537246
10	6	0	0.098143	-1.149237	0.355666
11	1	0	0.039451	-1.826326	1.223147
12	6	0	-3.705140	-1.308439	-0.506843
13	1	0	-3.722383	-0.852920	-1.508107
14	6	0	-5.018283	-1.004181	0.221581
15	1	0	-5.881872	-1.365272	-0.348336
16	1	0	-5.043185	-1.485824	1.206774
17	1	0	-5.151958	0.073146	0.377451
18	1	0	-3.616639	-2.392498	-0.665950
19	6	0	1.418471	-1.210379	-0.445809
20	6	0	1.607685	0.348481	-0.232571
21	1	0	1.379841	-1.705575	-1.423353
22	1	0	1.736487	1.076664	-1.040841
23	6	0	2.654867	-1.482112	0.431574
24	6	0	2.834821	0.070787	0.661955
25	1	0	2.537078	-2.211504	1.240158
26	1	0	2.846075	0.545279	1.649402
27	6	0	3.995958	-1.509830	-0.347817
28	6	0	4.180169	0.018222	-0.108230
29	1	0	3.917333	-1.826913	-1.394060
30	1	0	4.766526	-2.121099	0.132549
31	1	0	4.229448	0.645971	-1.005522
32	1	0	5.046427	0.255480	0.517669
33	1	0	-3.057368	1.225784	-0.318099
34	1	0	-2.370333	1.166244	1.310984
35	7	0	-0.750420	2.887476	0.211005
36	1	0	-1.489207	3.237711	-0.414825
37	8	0	0.381524	3.452799	-0.414419
38	1	0	1.091656	3.271183	0.223022

mPW1PW91 energy: -676.2803153, S2=0.823511

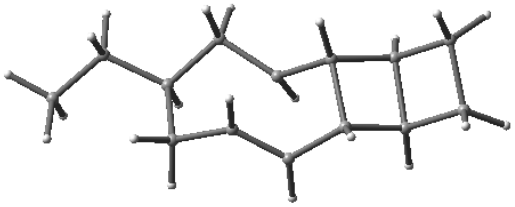


Zero-point correction= 0.338344 (Hartree/Particle)
Thermal correction to Energy= 0.353877
Thermal correction to Enthalpy= 0.354821
Thermal correction to Gibbs Free Energy= 0.294439
Sum of electronic and zero-point Energies= -676.170555
Sum of electronic and thermal Energies= -676.155022
Sum of electronic and thermal Enthalpies= -676.154078
Sum of electronic and thermal Free Energies= -676.214461

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.178768	-1.176587	0.501227
2	6	0	-0.794067	-1.756563	0.433561
3	6	0	-0.961069	1.024641	0.083294
4	6	0	-2.132739	0.341447	0.805403
5	1	0	-2.725880	-1.667239	1.329017
6	1	0	-0.698882	-2.816127	0.195574
7	1	0	-0.998460	0.763311	-0.982474
8	6	0	0.366453	0.543549	0.676287
9	1	0	0.544014	1.071078	1.625134
10	6	0	0.445198	-1.017039	0.790511
11	1	0	0.824300	-1.345346	1.775086
12	6	0	-2.983892	-1.510394	-0.785340
13	1	0	-2.589545	-0.920451	-1.623759
14	6	0	-4.495638	-1.290850	-0.659285
15	1	0	-5.009528	-1.573561	-1.585208
16	1	0	-4.915421	-1.897643	0.152949
17	1	0	-4.744498	-0.243839	-0.454140
18	1	0	-2.798298	-2.561825	-1.042906
19	6	0	1.607056	-1.029818	-0.266114
20	6	0	1.570670	0.548864	-0.291990
21	1	0	1.450104	-1.664030	-1.145069
22	1	0	1.452538	1.150856	-1.199167
23	6	0	3.013620	-0.996653	0.357474
24	6	0	2.959839	0.584384	0.385023
25	1	0	3.180202	-1.620111	1.242790
26	1	0	3.048331	1.187244	1.295299
27	6	0	4.169766	-0.924048	-0.676224
28	6	0	4.146400	0.631835	-0.611087
29	1	0	3.941205	-1.365796	-1.653005
30	1	0	5.106506	-1.363805	-0.319269
31	1	0	3.947928	1.156861	-1.552568
32	1	0	5.056436	1.054718	-0.173452
33	1	0	-3.070993	0.822715	0.515375
34	1	0	-2.013089	0.500259	1.887708
35	7	0	-0.965868	2.495185	0.129763
36	1	0	-1.055637	2.774402	1.110291
37	8	0	-2.209384	2.967046	-0.447935
38	1	0	-1.892162	3.519056	-1.179499

mPW1PW91 energy: -676.375168, S2=0.755363

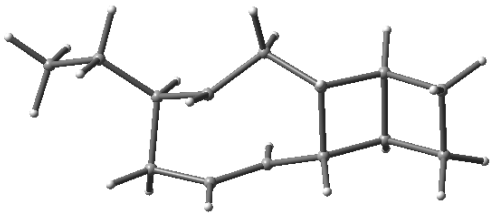
Protonation



Zero-point correction= 0.319477 (Hartree/Particle)
Thermal correction to Energy= 0.332590
Thermal correction to Enthalpy= 0.333534
Thermal correction to Gibbs Free Energy= 0.280038
Sum of electronic and zero-point Energies= -545.453147
Sum of electronic and thermal Energies= -545.440034
Sum of electronic and thermal Enthalpies= -545.439090
Sum of electronic and thermal Free Energies= -545.492586

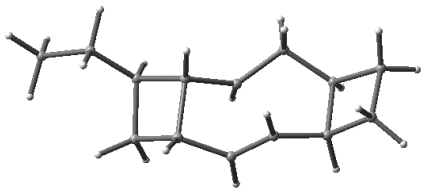
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.503614	-0.291196	-0.311313
2	6	0	1.319980	-1.196986	0.119626
3	6	0	0.697490	1.097763	0.601532
4	6	0	2.135550	1.167753	0.157015
5	1	0	2.529427	-0.281824	-1.409087
6	1	0	1.381178	-1.449012	1.184456
7	1	0	0.535122	0.802229	1.638705
8	6	0	-0.432912	1.501643	-0.095896
9	1	0	-0.336093	2.035639	-1.043195
10	6	0	0.022128	-0.436602	-0.162114
11	1	0	-0.108415	-0.360161	-1.248692
12	6	0	3.860640	-0.793798	0.197436
13	1	0	3.860594	-0.771993	1.296436
14	6	0	5.052251	0.004543	-0.342441
15	1	0	5.992481	-0.403636	0.039911
16	1	0	5.093827	-0.034758	-1.437120
17	1	0	5.009128	1.058839	-0.044822
18	1	0	3.970330	-1.847675	-0.089983
19	6	0	-1.345001	-0.554216	0.537717
20	6	0	-1.760443	0.960567	0.383350
21	1	0	-1.290252	-1.023160	1.524791
22	1	0	-2.162783	1.525139	1.231853
23	6	0	-2.484672	-0.965840	-0.416192
24	6	0	-2.798458	0.555773	-0.705920
25	1	0	-2.243438	-1.694852	-1.194492
26	1	0	-2.689969	1.032440	-1.684504
27	6	0	-3.877128	-1.100017	0.263198
28	6	0	-4.229044	0.362106	-0.147876
29	1	0	-3.839191	-1.290238	1.340599
30	1	0	-4.516140	-1.860720	-0.190295
31	1	0	-4.532237	1.045735	0.651532
32	1	0	-4.983575	0.407018	-0.937085
33	1	0	2.280182	1.895425	-0.646484
34	1	0	2.758203	1.479550	1.000805
35	1	0	1.307649	-2.132942	-0.452062

mPW1PW91 energy: -545.6677753



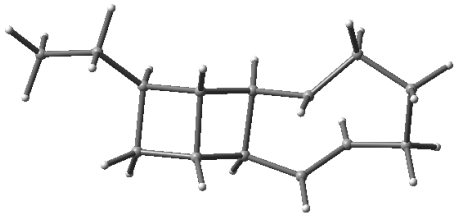
Zero-point correction= 0.319171 (Hartree/Particle)
Thermal correction to Energy= 0.332514
Thermal correction to Enthalpy= 0.333458
Thermal correction to Gibbs Free Energy= 0.279000
Sum of electronic and zero-point Energies= -545.455905
Sum of electronic and thermal Energies= -545.442562
Sum of electronic and thermal Enthalpies= -545.441618
Sum of electronic and thermal Free Energies= -545.496076

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.364784	-0.079426	0.238547
2	6	0	-1.079429	-0.376870	-0.543620
3	6	0	-0.929912	1.542776	-0.569884
4	6	0	-2.365683	1.454606	-0.057342
5	1	0	-2.186167	-0.254685	1.306719
6	1	0	-0.729071	1.889008	-1.582909
7	6	0	0.138729	1.177203	0.227069
8	1	0	-0.068213	0.989973	1.282282
9	6	0	0.037579	-1.322371	-0.143540
10	1	0	0.009869	-1.496936	0.937805
11	6	0	-3.596409	-0.875771	-0.206598
12	1	0	-3.765284	-0.709068	-1.279606
13	6	0	-4.855840	-0.503869	0.585361
14	1	0	-5.709923	-1.095090	0.242903
15	1	0	-4.724445	-0.696478	1.656058
16	1	0	-5.115292	0.553603	0.460698
17	1	0	-3.388346	-1.947025	-0.085606
18	6	0	1.416815	-0.765296	-0.569716
19	6	0	1.481521	0.808738	-0.263056
20	1	0	1.629139	-1.002813	-1.617319
21	1	0	1.783763	1.415635	-1.122865
22	6	0	2.586911	-1.000995	0.415349
23	6	0	2.594725	0.526613	0.790173
24	1	0	2.446342	-1.798777	1.148900
25	1	0	2.402902	0.905435	1.797931
26	6	0	4.007247	-0.845515	-0.196215
27	6	0	4.037531	0.651858	0.238078
28	1	0	4.067335	-1.031978	-1.273483
29	1	0	4.762770	-1.463196	0.294750
30	1	0	4.181971	1.393256	-0.554465
31	1	0	4.766938	0.853815	1.026262
32	1	0	-2.566923	2.092720	0.807454
33	1	0	-3.069896	1.719276	-0.850093
34	1	0	-1.238475	-0.379475	-1.626887
35	1	0	-0.143003	-2.287282	-0.636164



Zero-point correction= 0.319277 (Hartree/Particle)
Thermal correction to Energy= 0.332560
Thermal correction to Enthalpy= 0.333504
Thermal correction to Gibbs Free Energy= 0.279239
Sum of electronic and zero-point Energies= -545.455261
Sum of electronic and thermal Energies= -545.441978
Sum of electronic and thermal Enthalpies= -545.441033
Sum of electronic and thermal Free Energies= -545.495298

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.419278	-0.326117	-0.257668
2	6	0	1.056664	-0.245950	0.496834
3	6	0	1.090634	1.317937	0.396375
4	6	0	2.320550	1.209447	-0.550608
5	1	0	2.396205	-0.960347	-1.152585
6	1	0	1.241686	1.912796	1.300957
7	6	0	-0.270932	1.530778	-0.252249
8	1	0	-0.355191	1.996404	-1.235143
9	6	0	-0.182026	-0.446549	-0.377375
10	6	0	3.594888	-0.745052	0.629962
11	1	0	3.618609	-0.111382	1.528365
12	6	0	4.944137	-0.671707	-0.092052
13	1	0	5.756255	-0.972326	0.576793
14	1	0	4.965181	-1.337121	-0.962756
15	1	0	5.164276	0.343848	-0.441058
16	1	0	3.419004	-1.770504	0.981715
17	6	0	-1.332857	-1.412879	-0.162798
18	6	0	-1.400236	1.042264	0.372767
19	1	0	-1.420887	-1.667963	0.898620
20	1	0	-1.289809	0.746413	1.417761
21	6	0	-2.644476	-0.791718	-0.698777
22	6	0	-2.707197	0.738775	-0.264687
23	1	0	-2.726033	-0.933277	-1.780108
24	1	0	-2.931967	1.416385	-1.092795
25	6	0	-3.946344	-1.063945	0.103212
26	6	0	-3.919312	0.391775	0.651941
27	1	0	-3.875710	-1.857031	0.852973
28	1	0	-4.806440	-1.276024	-0.535639
29	1	0	-3.694280	0.466323	1.720584
30	1	0	-4.812978	0.986478	0.453508
31	1	0	2.108518	1.469167	-1.593011
32	1	0	3.185231	1.794763	-0.229461
33	1	0	0.982473	-0.737255	1.471334
34	1	0	0.032544	-0.333157	-1.444748
35	1	0	-1.093311	-2.338545	-0.704570



Zero-point correction= 0.319328 (Hartree/Particle)
Thermal correction to Energy= 0.332526
Thermal correction to Enthalpy= 0.333471
Thermal correction to Gibbs Free Energy= 0.279741
Sum of electronic and zero-point Energies= -545.453997
Sum of electronic and thermal Energies= -545.440798
Sum of electronic and thermal Enthalpies= -545.439854
Sum of electronic and thermal Free Energies= -545.493584

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.446395	-0.179635	0.262076
2	6	0	-1.064154	-0.412658	-0.427592
3	6	0	-0.972405	1.136099	-0.716878
4	6	0	-2.409637	1.319487	-0.183350
5	1	0	-2.384589	-0.297436	1.352175
6	1	0	-0.726616	1.566940	-1.692197
7	6	0	0.127447	1.253097	0.384463
8	1	0	-0.129839	1.886237	1.241346
9	6	0	0.149248	-0.320082	0.516567
10	6	0	-3.607426	-1.020699	-0.267687
11	1	0	-3.655818	-0.918454	-1.361374
12	6	0	-4.955652	-0.633661	0.348701
13	1	0	-5.762634	-1.249021	-0.061014
14	1	0	-4.949653	-0.772080	1.436212
15	1	0	-5.204637	0.414727	0.146402
16	1	0	-3.397894	-2.080425	-0.066607
17	6	0	1.502631	-0.545824	-0.187395
18	6	0	1.544631	1.459876	-0.085233
19	1	0	1.771577	1.982781	-1.016935
20	6	0	2.547699	-1.638747	0.070042
21	6	0	2.532100	0.732035	0.572205
22	1	0	2.527613	-1.917987	1.128605
23	1	0	2.320612	0.476827	1.611715
24	6	0	3.923506	-1.057491	-0.335208
25	6	0	3.939785	0.448644	0.100988
26	1	0	4.049434	-1.122787	-1.420248
27	1	0	4.738543	-1.628373	0.115108
28	1	0	4.227561	1.100840	-0.728682
29	1	0	4.642563	0.628494	0.918466
30	1	0	-2.553207	2.082953	0.588055
31	1	0	-3.114198	1.520035	-0.996525
32	1	0	-1.038582	-1.177676	-1.209656
33	1	0	0.088840	-0.798275	1.499081
34	1	0	1.394119	-0.415853	-1.271984
35	1	0	2.288539	-2.524110	-0.522141

IRC plots (note that these IRCs are shown in the ladderane formation direction):

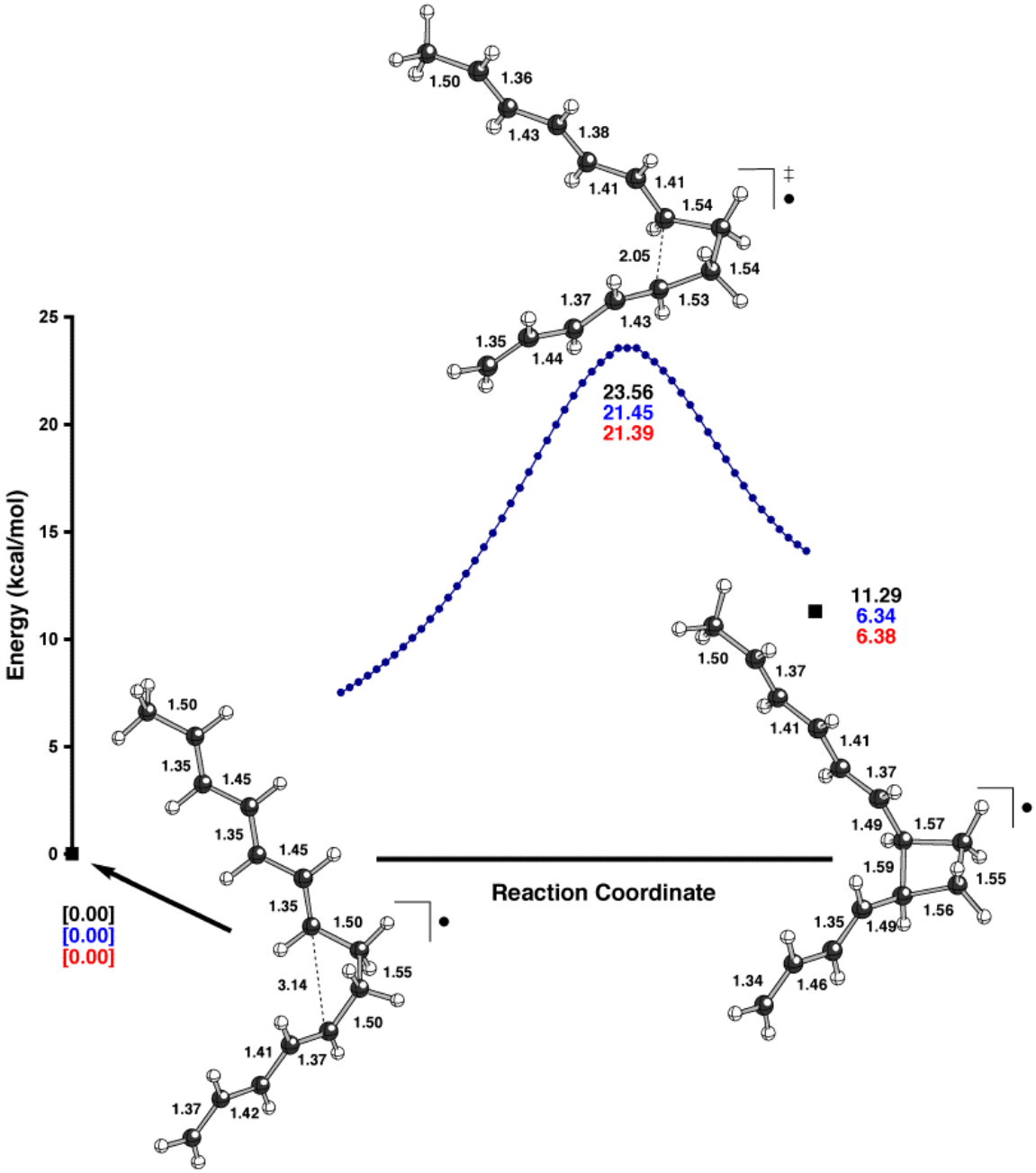


Figure S1. Select distances are shown in Å. Energies are color coded as follows: Black is UB3LYP/6-31G(d), Blue is UmPW1PW91/6-31G(d), and Red is a UmPW1PW91/6-31G(d) single point calculation on the UB3LYP/6-31G(d) optimized structure.

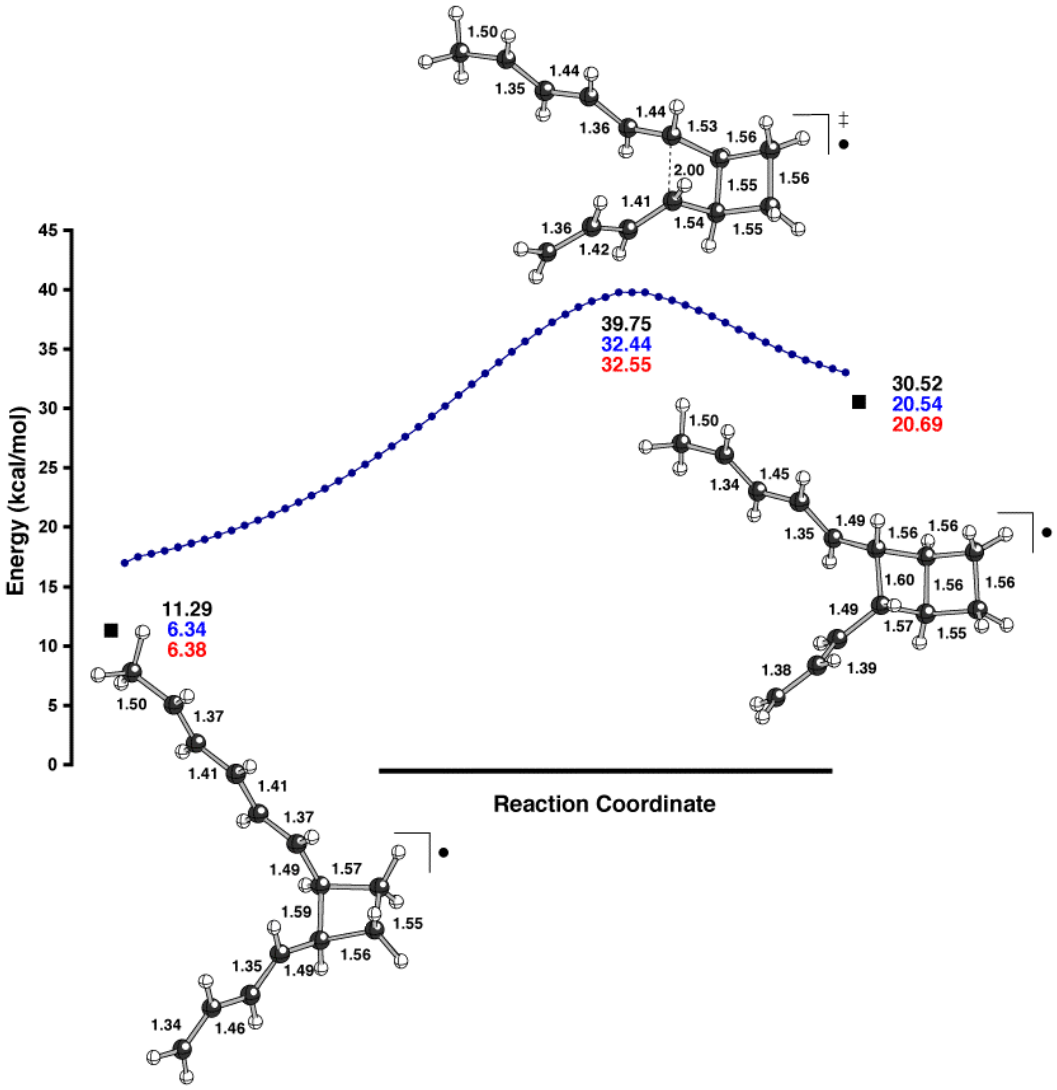


Figure S2. Select distances are shown in Å. Energies are color coded as follows: Black is UB3LYP/6-31G(d), Blue is UmPW1PW91/6-31G(d), and Red is a UmPW1PW91/6-31G(d) single point calculation on the UB3LYP/6-31G(d) optimized structure.

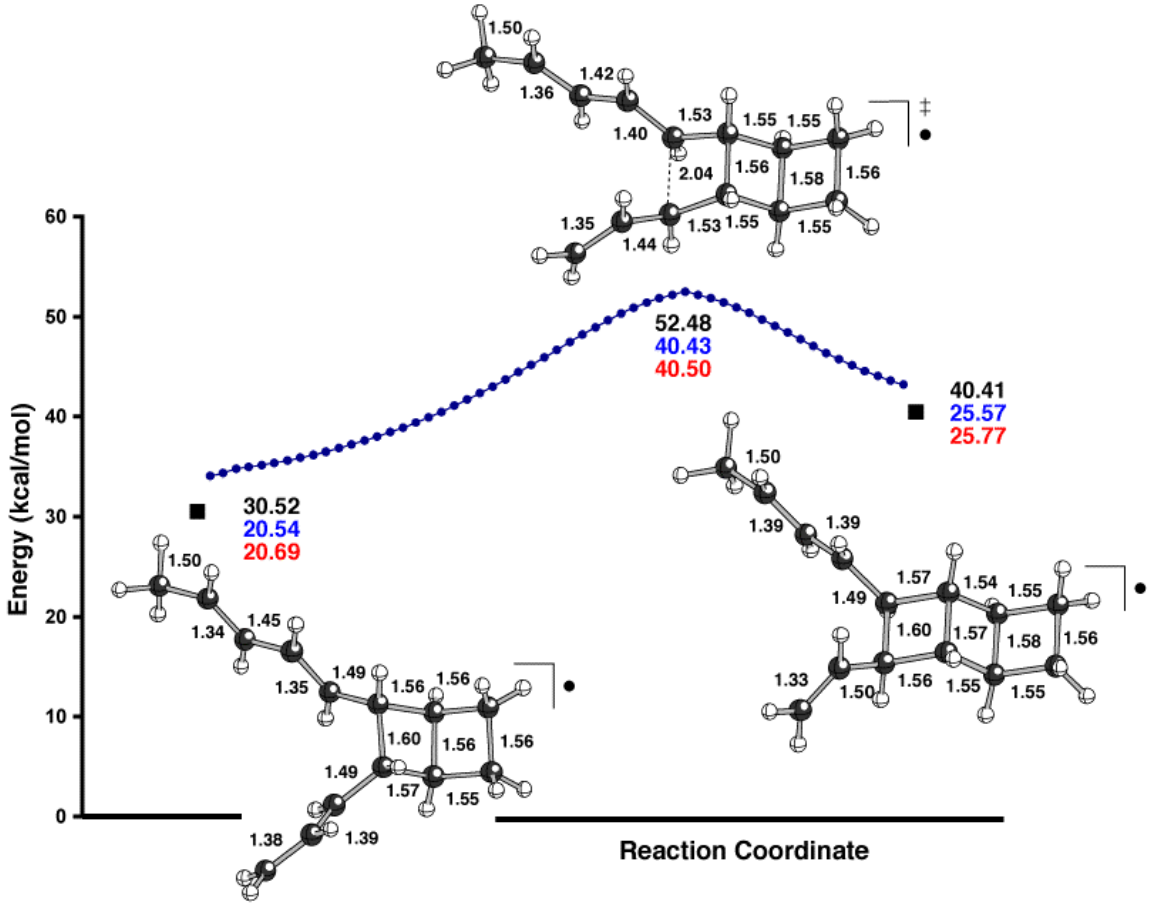


Figure S3. Select distances are shown in Å. Energies are color coded as follows: Black is UB3LYP/6-31G(d), Blue is UmPW1PW91/6-31G(d), and Red is a UmPW1PW91/6-31G(d) single point calculation on the UB3LYP/6-31G(d) optimized structure.

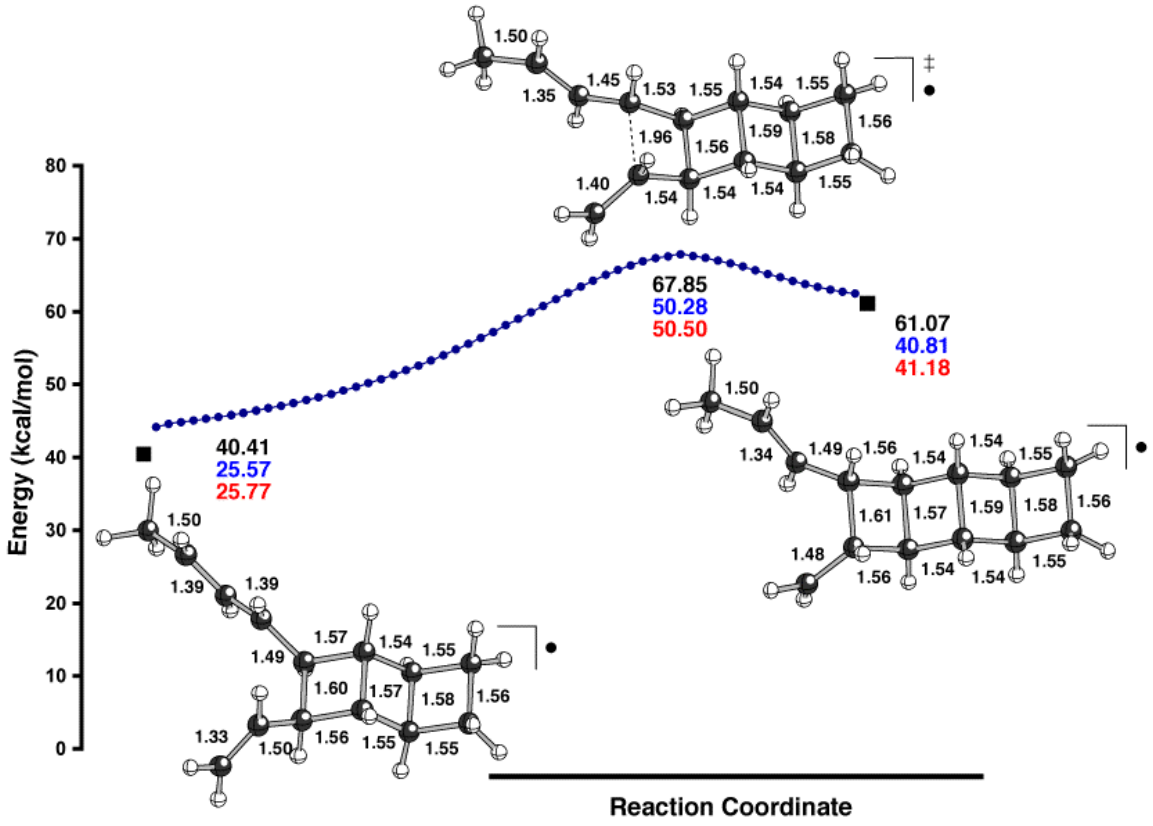


Figure S4. Select distances are shown in Å. Energies are color coded as follows: Black is UB3LYP/6-31G(d), Blue is UmPW1PW91/6-31G(d), and Red is a UmPW1PW91/6-31G(d) single point calculation on the UB3LYP/6-31G(d) optimized structure.

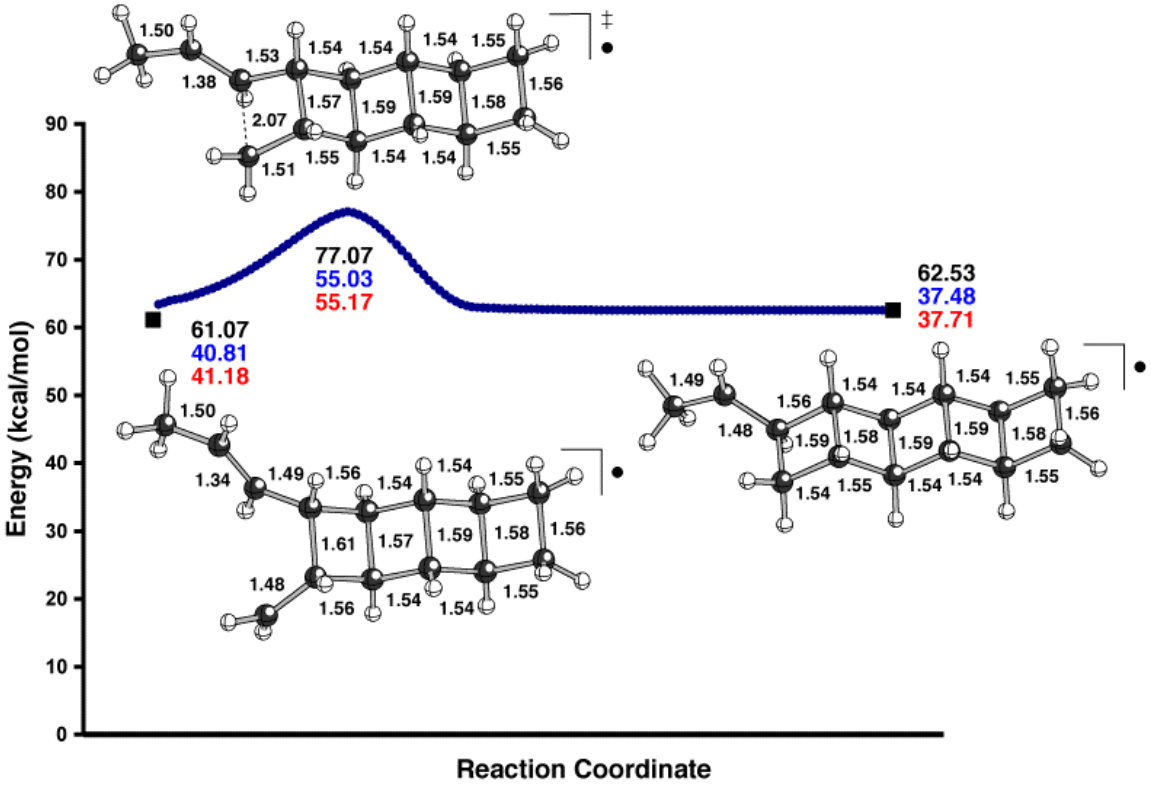


Figure S5. Select distances are shown in Å. Energies are color coded as follows: Black is UB3LYP/6-31G(d), Blue is UmPW1PW91/6-31G(d), and Red is a UmPW1PW91/6-31G(d) single point calculation on the UB3LYP/6-31G(d) optimized structure.

Full Gaussian Citations

Gaussian 03, Revision B.04,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven,
K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi,
V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega,
G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota,
R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao,
H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross,
C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev,
A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala,
K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg,
V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain,
O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari,
J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford,
J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz,
I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham,
C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill,
B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople,
Gaussian, Inc., Pittsburgh PA, 2003.

Gaussian 09, Revision B.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.