Supporting Information for

Viability of Dodecahedrane-Forming Radical Polycyclizations

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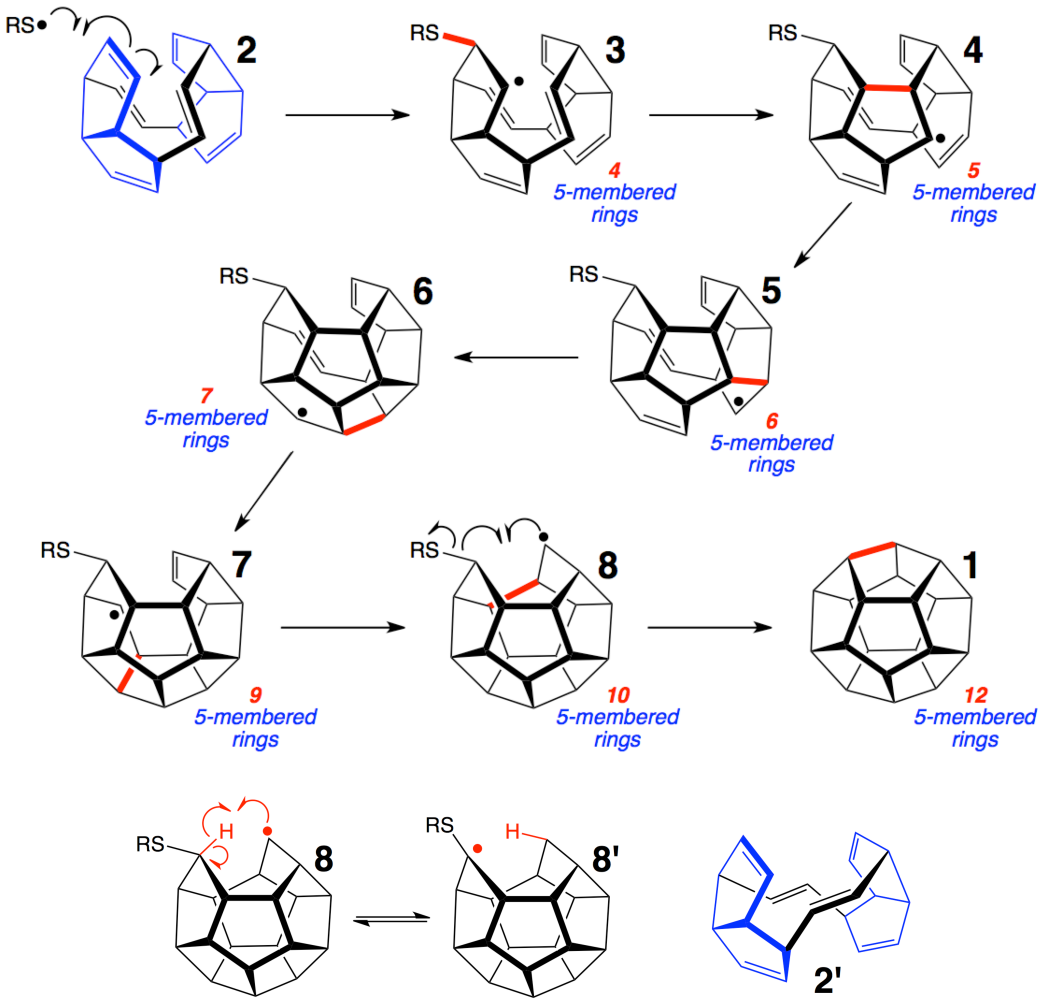

Coordinates and energies:

HS•

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Zero-point correction=                           0.006097 (Hartree/Particle)
 Thermal correction to Energy=                    0.008457
 Thermal correction to Enthalpy=                  0.009402
 Thermal correction to Gibbs Free Energy=        -0.012418
 Sum of electronic and zero-point Energies=           -398.733931
 Sum of electronic and thermal Energies=              -398.731570
 Sum of electronic and thermal Enthalpies=            -398.730626
 Sum of electronic and thermal Free Energies=         -398.752446
-------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type              X           Y           Z
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    1         16             0        0.000000    0.000000    0.079716
    2          1             0        0.000000    0.000000   -1.275458
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2

Zero-point correction= 0.343844 (Hartree/Particle)
Thermal correction to Energy= 0.358552
Thermal correction to Enthalpy= 0.359497
Thermal correction to Gibbs Free Energy= 0.303787
Sum of electronic and zero-point Energies= -773.651359
Sum of electronic and thermal Energies= -773.636651
Sum of electronic and thermal Enthalpies= -773.635707
Sum of electronic and thermal Free Energies= -773.691416

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.778283	0.202297	0.682153
2	6	0	-2.652525	-0.320708	-0.784184
3	6	0	-2.171985	-1.733262	-0.602177
4	6	0	-1.840762	-1.992287	0.665532
5	6	0	-1.881478	-0.755233	1.565143
6	1	0	-3.644148	-0.308251	-1.257092
7	1	0	-2.144471	-2.462694	-1.407555
8	6	0	1.841370	-1.991535	-0.667711
9	6	0	1.881419	-0.753360	-1.565860
10	6	0	2.172392	-1.733799	0.600324
11	1	0	1.474232	-2.946697	-1.036084
12	6	0	2.778305	0.203256	-0.681924
13	1	0	2.406702	-0.973004	-2.507562
14	6	0	2.652661	-0.321367	0.783807
15	1	0	2.145084	-2.464107	1.404913
16	1	0	3.802106	0.023894	-1.036867
17	1	0	3.644251	-0.309218	1.256797
18	6	0	0.423437	-0.450872	-1.882529
19	6	0	-0.289367	0.624172	-1.541408
20	6	0	2.559545	1.688137	-0.517782
21	6	0	2.149287	2.002342	0.715854
22	6	0	-1.807418	0.775075	-1.552706
23	6	0	-2.149420	2.003013	-0.713633
24	6	0	-0.423836	-0.452523	1.883258
25	6	0	0.289237	0.621922	1.540815
26	6	0	1.807156	0.773357	1.553364
27	1	0	-1.473500	-2.947793	1.032876
28	1	0	-2.174373	0.865410	-2.584748
29	1	0	-1.943403	3.012600	-1.062893
30	1	0	1.943146	3.011496	1.066289
31	1	0	2.767683	2.408835	-1.304788
32	1	0	2.173575	0.862347	2.585700
33	1	0	-2.407065	-0.976314	2.506341
34	1	0	-3.802111	0.022535	1.036810
35	6	0	-2.559603	1.687365	0.519693
36	1	0	-2.767687	2.407156	1.307536
37	1	0	-0.091327	-1.307016	-2.323484
38	1	0	0.242070	1.468028	-1.116949
39	1	0	0.090367	-1.307883	2.326474
40	1	0	-0.241918	1.464740	1.114116

2→3 TSS
imaginary: 56.18i cm-1

Zero-point correction= 0.351084 (Hartree/Particle)
Thermal correction to Energy= 0.368456
Thermal correction to Enthalpy= 0.369400
Thermal correction to Gibbs Free Energy= 0.305963
Sum of electronic and zero-point Energies= -1172.392449
Sum of electronic and thermal Energies= -1172.375078
Sum of electronic and thermal Enthalpies= -1172.374134
Sum of electronic and thermal Free Energies= -1172.437571

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.973048	1.089673	-0.897348
2	6	0	-1.962142	1.109638	0.666371
3	6	0	-1.063214	2.269960	0.987020
4	6	0	-0.457574	2.754908	-0.099480
5	6	0	-0.703975	1.919667	-1.356310
6	1	0	-2.978669	1.293298	1.037495
7	1	0	-0.963383	2.684921	1.986318
8	6	0	2.802359	1.116677	1.347913
9	6	0	2.314228	-0.263163	1.793091
10	6	0	3.243840	1.137873	0.087425
11	1	0	2.694925	1.989379	1.987778
12	6	0	3.003966	-1.171353	0.698270
13	1	0	2.721708	-0.517895	2.782750
14	6	0	3.290762	-0.236762	-0.519936
15	1	0	3.580213	2.031393	-0.432222
16	1	0	3.959483	-1.467404	1.151362
17	1	0	4.294687	-0.451226	-0.910700
18	6	0	0.803544	-0.128360	1.916134
19	6	0	-0.138593	-0.735366	1.192393
20	6	0	2.367387	-2.375222	0.047152
21	6	0	2.091198	-2.160865	-1.243804
22	6	0	-1.616397	-0.368726	1.103200
23	6	0	-2.181727	-1.136599	-0.088579
24	6	0	0.627729	1.253618	-1.665236
25	6	0	0.913698	-0.048930	-1.688689
26	6	0	2.290873	-0.704430	-1.654707
27	1	0	0.230083	3.596995	-0.109437
28	1	0	-2.139830	-0.618705	2.032528
29	1	0	1.647893	-2.891546	-1.917037
30	1	0	2.210556	-3.317039	0.566990
31	1	0	2.777894	-0.616318	-2.635855
32	1	0	-0.983286	2.563444	-2.203475
33	1	0	-2.828559	1.672574	-1.266175
34	6	0	-2.190873	-0.361496	-1.216230
35	1	0	0.510621	0.667400	2.604358
36	1	0	0.172407	-1.532509	0.527243
37	1	0	1.444495	1.973718	-1.737601
38	1	0	0.085852	-0.749842	-1.632705
39	1	0	-2.416260	-0.734314	-2.210983
40	1	0	-2.197522	-2.221843	-0.105696
41	16	0	-4.728738	-1.319310	0.253047
42	1	0	-4.935743	-0.009960	-0.015613

3
Zero-point correction= 0.352560 (Hartree/Particle)

Thermal correction to Energy=	0.369635
Thermal correction to Enthalpy=	0.370579
Thermal correction to Gibbs Free Energy=	0.308691
Sum of electronic and zero-point Energies=	-1172.401766
Sum of electronic and thermal Energies=	-1172.384692
Sum of electronic and thermal Enthalpies=	-1172.383748
Sum of electronic and thermal Free Energies=	-1172.445636

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.979566	1.140316	-0.931732
2	6	0	-2.064353	1.153320	0.628170
3	6	0	-1.192301	2.310153	1.021204
4	6	0	-0.523837	2.812781	-0.019077
5	6	0	-0.699506	2.005555	-1.304158
6	1	0	-3.102810	1.320022	0.941633
7	1	0	-1.147351	2.702911	2.033658
8	6	0	2.719232	1.039004	1.440169
9	6	0	2.206027	-0.353144	1.809374
10	6	0	3.203670	1.111342	0.197269
11	1	0	2.605300	1.883002	2.116205
12	6	0	2.897794	-1.218572	0.682127
13	1	0	2.604739	-0.660762	2.787370
14	6	0	3.245915	-0.232098	-0.478910
15	1	0	3.572189	2.022743	-0.266668
16	1	0	3.832300	-1.568120	1.140983
17	1	0	4.260165	-0.447000	-0.841749
18	6	0	0.695197	-0.227800	1.943428
19	6	0	-0.232613	-0.654077	1.084597
20	6	0	2.240793	-2.367558	-0.041610
21	6	0	2.019066	-2.088480	-1.330497
22	6	0	-1.710474	-0.314408	1.076339
23	6	0	-2.375613	-1.138157	-0.063642
24	6	0	0.648899	1.355556	-1.568973
25	6	0	0.924619	0.064076	-1.754977
26	6	0	2.284036	-0.624597	-1.674001
27	1	0	0.164450	3.653582	0.027695
28	1	0	-2.164856	-0.525748	2.050921
29	1	0	1.572430	-2.772572	-2.049097
30	1	0	2.028605	-3.323052	0.431326
31	1	0	2.819454	-0.520801	-2.628500
32	1	0	-0.947860	2.667726	-2.147421
33	1	0	-2.821221	1.719118	-1.343104
34	6	0	-2.156170	-0.302747	-1.279737
35	1	0	0.393218	0.395688	2.789054
36	1	0	0.098185	-1.269522	0.259205
37	1	0	1.476352	2.057636	-1.466048
38	1	0	0.084380	-0.616725	-1.882069
39	1	0	-2.349667	-0.671638	-2.282516
40	1	0	-1.958002	-2.146302	-0.149602
41	16	0	-4.236322	-1.402085	0.167571
42	1	0	-4.143740	-2.289618	1.185420

b3lyp/6-311++g(2d,p)
HF=-1172.9993725

m062x/6-31g(d)

HF=-1172.3978763

wb97xd/6-31g(d)
HF=-1172.5231645

b3lyp/6-31g(d) scrf=(smd,solvent=water)
HF=-1172.7600591

scrf=(smd,solvent=benzene)
HF=-1172.7738429

3→4 TSS
imaginary: 552.48i cm-1
Zero-point correction= 0.352522 (Hartree/Particle)
Thermal correction to Energy= 0.368535
Thermal correction to Enthalpy= 0.369479
Thermal correction to Gibbs Free Energy= 0.310138
Sum of electronic and zero-point Energies= -1172.371151
Sum of electronic and thermal Energies= -1172.355138
Sum of electronic and thermal Enthalpies= -1172.354194
Sum of electronic and thermal Free Energies= -1172.413535

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.910702	1.064042	0.865400
2	6	0	2.086174	1.224152	-0.685158
3	6	0	1.411165	2.542887	-0.978801
4	6	0	0.812485	3.065230	0.096872
5	6	0	0.834224	2.124247	1.292140
6	1	0	3.154498	1.305260	-0.920477
7	1	0	1.449225	3.016475	-1.956689
8	6	0	-3.173774	1.014478	-1.024910
9	6	0	-2.323045	-0.097163	-1.632309
10	6	0	-3.397338	0.814131	0.279286
11	1	0	-3.426066	1.919677	-1.572436
12	6	0	-2.675149	-1.274342	-0.632577
13	1	0	-2.618418	-0.362405	-2.655660
14	6	0	-2.952239	-0.560571	0.722560
15	1	0	-3.894428	1.519202	0.940913
16	1	0	-3.604084	-1.721328	-1.011847
17	1	0	-3.785985	-1.064378	1.229447
18	6	0	-0.875052	0.365286	-1.567229
19	6	0	0.209943	-0.364922	-1.825860
20	6	0	-1.675086	-2.332445	-0.259859
21	6	0	-1.202738	-2.161919	0.978716
22	6	0	1.627730	-0.127398	-1.348347
23	6	0	1.824706	-1.142973	-0.174994
24	6	0	-0.491781	1.410100	1.426487
25	6	0	-0.504023	0.075540	1.833711
26	6	0	-1.698139	-0.883261	1.643208
27	1	0	0.278966	4.012981	0.114474
28	1	0	2.313834	-0.374874	-2.167170
29	1	0	-0.477262	-2.808307	1.466787
30	1	0	-1.401302	-3.154166	-0.916857
31	1	0	-2.071831	-1.104134	2.653616
32	1	0	1.126208	2.639227	2.220369

33	1	0	2.857568	1.293374	1.369124
34	6	0	1.499695	-0.375904	1.086431
35	1	0	-0.730060	1.342873	-1.128974
36	1	0	0.083755	-1.353627	-2.274602
37	1	0	-1.343858	1.828121	0.905694
38	1	0	0.027438	-0.158958	2.757075
39	1	0	1.829937	-0.862585	2.002938
40	1	0	1.231935	-2.048942	-0.302246
41	16	0	3.615604	-1.731320	-0.009895
42	1	0	3.659514	-2.437537	-1.163761

b3lyp/6-311++g(2d,p)
HF=-1172.9669789

m062x/6-31g(d)
HF=-1172.3671378

wb97xd/6-31g(d)
HF=-1172.494497

b3lyp/6-31g(d) scrf=(smd,solvent=water)
HF=-1172.7276122

b3lyp/6-31g(d) scrf=(smd,solvent=benzene)
HF=-1172.7423235

4

Zero-point correction= 0.355529 (Hartree/Particle)
Thermal correction to Energy= 0.371522
Thermal correction to Enthalpy= 0.372466
Thermal correction to Gibbs Free Energy= 0.313256
Sum of electronic and zero-point Energies= -1172.399254
Sum of electronic and thermal Energies= -1172.383261
Sum of electronic and thermal Enthalpies= -1172.382317
Sum of electronic and thermal Free Energies= -1172.441526

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.921071	1.073277	0.782912
2	6	0	2.061678	1.193017	-0.772247
3	6	0	1.384608	2.507783	-1.085808
4	6	0	0.799728	3.053480	-0.015211
5	6	0	0.905599	2.163077	1.216222
6	1	0	3.121927	1.247827	-1.046260
7	1	0	1.383618	2.942185	-2.082432
8	6	0	-3.134979	1.146525	-0.752853
9	6	0	-2.409242	0.050949	-1.529601
10	6	0	-3.176566	0.863249	0.554131
11	1	0	-3.416408	2.096012	-1.201579
12	6	0	-2.727477	-1.181706	-0.591898
13	1	0	-2.794297	-0.111680	-2.544018
14	6	0	-2.749331	-0.559548	0.831880
15	1	0	-3.551122	1.533088	1.323737
16	1	0	-3.734422	-1.523234	-0.867129
17	1	0	-3.525201	-1.058845	1.427569

18	6	0	-0.941149	0.441773	-1.514423
19	6	0	0.104208	-0.304024	-1.873264
20	6	0	-1.781332	-2.338550	-0.439635
21	6	0	-1.102226	-2.277604	0.710990
22	6	0	1.531388	-0.149838	-1.389228
23	6	0	1.647965	-1.143556	-0.190810
24	6	0	-0.344366	1.401387	1.563708
25	6	0	-0.118849	-0.070512	1.728447
26	6	0	-1.387972	-1.027293	1.521711
27	1	0	0.251219	3.992178	-0.010248
28	1	0	2.203147	-0.466172	-2.196222
29	1	0	-0.388235	-3.024611	1.050790
30	1	0	-1.694030	-3.141033	-1.167968
31	1	0	-1.655654	-1.326357	2.542474
32	1	0	1.261711	2.744106	2.085073
33	1	0	2.891467	1.227337	1.260985
34	6	0	1.341557	-0.333252	1.103566
35	1	0	-0.742904	1.365259	-0.989609
36	1	0	-0.066724	-1.248867	-2.394465
37	1	0	-1.214480	1.893593	1.985348
38	1	0	0.086944	-0.214426	2.806001
39	1	0	1.908079	-0.805481	1.912255
40	1	0	1.013226	-2.012726	-0.328429
41	16	0	3.389416	-1.798357	0.029149
42	1	0	3.485618	-2.386260	-1.183783

4→5 TSS

imaginary: 467.33i cm-1

Zero-point correction=	0.356141 (Hartree/Particle)
Thermal correction to Energy=	0.370986
Thermal correction to Enthalpy=	0.371930
Thermal correction to Gibbs Free Energy=	0.315202
Sum of electronic and zero-point Energies=	-1172.382797
Sum of electronic and thermal Energies=	-1172.367952
Sum of electronic and thermal Enthalpies=	-1172.367008
Sum of electronic and thermal Free Energies=	-1172.423736

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.706360	1.142507	0.832641
2	6	0	1.891148	1.332052	-0.708529
3	6	0	1.075586	2.573447	-0.989008
4	6	0	0.335203	2.954766	0.056578
5	6	0	0.517531	2.049400	1.260874
6	1	0	2.947504	1.509260	-0.941695
7	1	0	1.091473	3.080441	-1.951377
8	6	0	-2.804721	1.220239	-0.562223
9	6	0	-2.406927	0.119065	-1.536216
10	6	0	-2.600752	0.848786	0.752684
11	1	0	-3.006915	2.235380	-0.894817
12	6	0	-2.686803	-1.155449	-0.643308
13	1	0	-3.034092	0.112367	-2.438438
14	6	0	-2.563868	-0.665745	0.838872
15	1	0	-3.019592	1.444109	1.558323
16	1	0	-3.726450	-1.438715	-0.854584
17	1	0	-3.428680	-1.028290	1.407811

18	6	0	-0.958586	0.479378	-1.828265
19	6	0	0.094577	-0.338024	-1.782797
20	6	0	-1.803566	-2.378570	-0.654089
21	6	0	-1.067645	-2.491471	0.458110
22	6	0	1.521471	-0.044617	-1.375779
23	6	0	1.772864	-1.057120	-0.210581
24	6	0	-0.609562	1.104021	1.686325
25	6	0	-0.111764	-0.335800	1.740565
26	6	0	-1.289029	-1.355987	1.434454
27	1	0	-0.337748	3.808490	0.067533
28	1	0	2.207788	-0.254920	-2.206829
29	1	0	-0.384148	-3.311625	0.666307
30	1	0	-1.792592	-3.092970	-1.474356
31	1	0	-1.551987	-1.787442	2.409039
32	1	0	0.783347	2.666167	2.134148
33	1	0	2.619964	1.439977	1.353755
34	6	0	1.354032	-0.342517	1.105008
35	1	0	-0.788454	1.547504	-1.823981
36	1	0	-0.093530	-1.403682	-1.847753
37	1	0	-1.134611	1.424856	2.585477
38	1	0	0.107073	-0.524902	2.801996
39	1	0	1.993070	-0.743550	1.898130
40	1	0	1.258854	-2.002796	-0.374181
41	16	0	3.582631	-1.479283	-0.004619
42	1	0	3.774335	-1.961293	-1.252518

5

Zero-point correction= 0.359066 (Hartree/Particle)
Thermal correction to Energy= 0.373868
Thermal correction to Enthalpy= 0.374812
Thermal correction to Gibbs Free Energy= 0.318345
Sum of electronic and zero-point Energies= -1172.409594
Sum of electronic and thermal Energies= -1172.394792
Sum of electronic and thermal Enthalpies= -1172.393847
Sum of electronic and thermal Free Energies= -1172.450315

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.614976	1.084842	0.903853
2	6	0	1.876195	1.353538	-0.613729
3	6	0	1.037179	2.577120	-0.884253
4	6	0	0.203316	2.860072	0.122346
5	6	0	0.358007	1.918258	1.296214
6	1	0	2.938779	1.554835	-0.791630
7	1	0	1.102335	3.143273	-1.810773
8	6	0	-2.467440	1.361535	-0.420993
9	6	0	-2.371148	0.302131	-1.496574
10	6	0	-2.197390	0.838450	0.953939
11	1	0	-2.556013	2.417736	-0.656033
12	6	0	-2.742454	-1.004153	-0.686059
13	6	0	-2.517634	-0.671811	0.826951
14	1	0	-2.898894	1.335111	1.639011
15	1	0	-3.809681	-1.170170	-0.880419
16	1	0	-3.412809	-0.942361	1.395037
17	6	0	-0.938005	0.561428	-1.941771
18	6	0	0.085815	-0.254738	-1.670588

19	6	0	-1.984463	-2.307077	-0.841327
20	6	0	-1.210072	-2.581726	0.216346
21	6	0	1.536901	0.005315	-1.350274
22	6	0	1.833892	-1.055756	-0.247165
23	6	0	-0.778913	0.905488	1.674664
24	6	0	-0.136305	-0.533505	1.679755
25	6	0	-1.309751	-1.533497	1.303736
26	1	0	-0.494420	3.693743	0.132623
27	1	0	2.191310	-0.135387	-2.221022
28	1	0	-0.581614	-3.464507	0.309333
29	1	0	-2.061130	-2.930866	-1.728979
30	1	0	-1.568310	-2.042897	2.241128
31	1	0	0.568083	2.513027	2.195220
32	1	0	2.481113	1.408239	1.487398
33	6	0	1.339793	-0.430627	1.090783
34	1	0	-0.772966	1.589935	-2.249275
35	1	0	-0.190555	-1.270625	-1.448312
36	1	0	0.068382	-0.756941	2.731538
37	1	0	1.980294	-0.836515	1.880273
38	1	0	-3.087031	0.469144	-2.312982
39	1	0	-1.042648	1.122641	2.715461
40	1	0	1.372680	-2.019158	-0.470162
41	16	0	3.655192	-1.390873	-0.022695
42	1	0	3.895033	-1.796015	-1.289439

5→6 TSS

imaginary: 513.72i cm-1

Zero-point correction= 0.358619 (Hartree/Particle)

Thermal correction to Energy= 0.372485

Thermal correction to Enthalpy= 0.373430

Thermal correction to Gibbs Free Energy= 0.318851

Sum of electronic and zero-point Energies= -1172.391626

Sum of electronic and thermal Energies= -1172.377760

Sum of electronic and thermal Enthalpies= -1172.376815

Sum of electronic and thermal Free Energies= -1172.431393

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.504672	1.117248	0.921221
2	6	0	1.732066	1.449915	-0.588575
3	6	0	0.705917	2.513929	-0.862587
4	6	0	-0.285733	2.571298	0.106770
5	6	0	0.176957	1.806618	1.348346
6	1	0	2.748569	1.822951	-0.762851
7	1	0	0.719885	3.128504	-1.758952
8	6	0	-2.139125	1.431819	-0.263455
9	6	0	-2.219150	0.417130	-1.436806
10	6	0	-2.151670	0.719151	1.079456
11	1	0	-2.787676	2.302263	-0.360055
12	6	0	-2.703145	-0.928801	-0.742525
13	1	0	-2.984338	0.743935	-2.152429
14	6	0	-2.496314	-0.753617	0.789183
15	1	0	-2.902131	1.190641	1.725566
16	1	0	-3.771191	-1.017064	-0.976358
17	1	0	-3.392478	-1.082605	1.324815
18	6	0	-0.844963	0.503344	-2.066748

19	6	0	0.157934	-0.262214	-1.639589
20	6	0	-2.005926	-2.251370	-1.003842
21	6	0	-1.232350	-2.632393	0.022513
22	6	0	1.593361	0.065355	-1.350100
23	6	0	1.965593	-0.976389	-0.257771
24	6	0	-0.788083	0.704815	1.835880
25	6	0	-0.101285	-0.699992	1.659599
26	6	0	-1.289414	-1.663263	1.184856
27	1	0	-0.898045	3.463135	0.218976
28	1	0	2.264760	0.022343	-2.216675
29	1	0	-0.627994	-3.536500	0.037835
30	1	0	-2.101329	-2.794915	-1.940464
31	1	0	-1.546639	-2.234774	2.085783
32	1	0	0.359934	2.526823	2.155283
33	1	0	2.343821	1.491325	1.513385
34	6	0	1.368829	-0.425636	1.075218
35	1	0	-0.669131	1.432740	-2.605248
36	1	0	-0.148614	-1.161584	-1.144320
37	1	0	-0.997970	0.843851	2.902660
38	1	0	0.126472	-1.065088	2.664741
39	1	0	2.030439	-0.773032	1.874988
40	1	0	1.603311	-1.975129	-0.511967
41	16	0	3.801161	-1.131650	0.019358
42	1	0	4.122738	-1.463113	-1.250699

6

Zero-point correction= 0.360912 (Hartree/Particle)
Thermal correction to Energy= 0.374777
Thermal correction to Enthalpy= 0.375721
Thermal correction to Gibbs Free Energy= 0.321194
Sum of electronic and zero-point Energies= -1172.416174
Sum of electronic and thermal Energies= -1172.402309
Sum of electronic and thermal Enthalpies= -1172.401364
Sum of electronic and thermal Free Energies= -1172.455892

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.433602	1.150616	0.917234
2	6	0	1.627917	1.507970	-0.590962
3	6	0	0.469682	2.406216	-0.905789
4	6	0	-0.639024	2.331157	0.103264
5	6	0	0.073280	1.737777	1.368461
6	1	0	2.591600	1.999266	-0.770174
7	1	0	0.470270	3.108784	-1.733886
8	6	0	-1.974051	1.472934	-0.134591
9	6	0	-2.119947	0.481105	-1.386601
10	6	0	-2.139664	0.624743	1.167085
11	1	0	-2.803022	2.185418	-0.204312
12	6	0	-2.664168	-0.883473	-0.769417
13	1	0	-2.900645	0.884291	-2.041296
14	6	0	-2.474954	-0.812746	0.768225
15	1	0	-2.915410	1.067144	1.801213
16	1	0	-3.729119	-0.935452	-1.025966
17	1	0	-3.367411	-1.196988	1.272996
18	6	0	-0.798826	0.483174	-2.114131
19	6	0	0.201512	-0.246691	-1.611754

20	6	0	-1.983009	-2.198761	-1.105656
21	6	0	-1.205202	-2.638612	-0.106213
22	6	0	1.628469	0.102972	-1.346191
23	6	0	2.042563	-0.917849	-0.254008
24	6	0	-0.786956	0.589783	1.918641
25	6	0	-0.069148	-0.781980	1.642268
26	6	0	-1.254610	-1.731523	1.107521
27	1	0	-0.994728	3.347800	0.321636
28	1	0	2.298784	0.111822	-2.213460
29	1	0	-0.602427	-3.542984	-0.144622
30	1	0	-2.083934	-2.687083	-2.071363
31	1	0	-1.501511	-2.349438	1.980038
32	1	0	0.219657	2.528251	2.111189
33	1	0	2.256470	1.561999	1.507692
34	6	0	1.389197	-0.402916	1.067972
35	1	0	-0.639006	1.289743	-2.828164
36	1	0	-0.123920	-1.028468	-0.958204
37	1	0	-0.952419	0.696362	2.996364
38	1	0	0.176144	-1.221518	2.612319
39	1	0	2.057864	-0.702071	1.881324
40	1	0	1.733063	-1.932342	-0.518950
41	16	0	3.876955	-0.972469	0.051865
42	1	0	4.238422	-1.268413	-1.216364

6→7 TSS

imaginary: 399.37i cm-1

Zero-point correction=	0.360465 (Hartree/Particle)
Thermal correction to Energy=	0.373563
Thermal correction to Enthalpy=	0.374507
Thermal correction to Gibbs Free Energy=	0.321541
Sum of electronic and zero-point Energies=	-1172.414833
Sum of electronic and thermal Energies=	-1172.401734
Sum of electronic and thermal Enthalpies=	-1172.400790
Sum of electronic and thermal Free Energies=	-1172.453756

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.394812	1.174736	0.907975
2	6	0	1.559427	1.527950	-0.603978
3	6	0	0.318155	2.303043	-0.957409
4	6	0	-0.716054	2.310104	0.134332
5	6	0	0.029396	1.726788	1.383176
6	1	0	2.473890	2.104177	-0.784970
7	1	0	0.340600	3.086709	-1.710757
8	6	0	-2.028693	1.449772	-0.077601
9	6	0	-2.094197	0.496777	-1.359881
10	6	0	-2.163503	0.564162	1.198391
11	1	0	-2.884819	2.130636	-0.138134
12	6	0	-2.622577	-0.897218	-0.790694
13	1	0	-2.866865	0.892376	-2.028738
14	6	0	-2.457242	-0.867678	0.752094
15	1	0	-2.946160	0.962498	1.852740
16	1	0	-3.683828	-0.952120	-1.062168
17	1	0	-3.347202	-1.291241	1.229226
18	6	0	-0.752844	0.567362	-2.060593
19	6	0	0.253208	-0.259617	-1.673865

20	6	0	-1.929457	-2.200957	-1.146317
21	6	0	-1.155636	-2.652265	-0.148629
22	6	0	1.658728	0.127405	-1.349941
23	6	0	2.071506	-0.882178	-0.246013
24	6	0	-0.799383	0.550967	1.932367
25	6	0	-0.055253	-0.801583	1.629804
26	6	0	-1.220717	-1.765893	1.078445
27	1	0	-1.041914	3.339331	0.337519
28	1	0	2.367315	0.160415	-2.187038
29	1	0	-0.545074	-3.550879	-0.198850
30	1	0	-2.018294	-2.672249	-2.121722
31	1	0	-1.455873	-2.401344	1.941620
32	1	0	0.164707	2.511365	2.134260
33	1	0	2.218602	1.604841	1.483693
34	6	0	1.391613	-0.378657	1.064532
35	1	0	-0.644747	1.317684	-2.841640
36	1	0	-0.064149	-1.104961	-1.100236
37	1	0	-0.951274	0.643280	3.013334
38	1	0	0.198120	-1.255357	2.591206
39	1	0	2.061065	-0.651477	1.886736
40	1	0	1.789268	-1.903785	-0.513403
41	16	0	3.903567	-0.897122	0.087328
42	1	0	4.291831	-1.174077	-1.177091

7

Zero-point correction= 0.363880 (Hartree/Particle)
Thermal correction to Energy= 0.376564
Thermal correction to Enthalpy= 0.377508
Thermal correction to Gibbs Free Energy= 0.325225
Sum of electronic and zero-point Energies= -1172.496141
Sum of electronic and thermal Energies= -1172.483457
Sum of electronic and thermal Enthalpies= -1172.482513
Sum of electronic and thermal Free Energies= -1172.534795

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.056675	-1.377837	-1.016829
2	6	0	1.138924	-1.740064	0.489705
3	6	0	-0.302258	-2.074967	0.973459
4	6	0	-1.227561	-2.103430	-0.267804
5	6	0	-0.387317	-1.647378	-1.501579
6	1	0	1.820852	-2.578424	0.655592
7	1	0	-0.323409	-3.028597	1.510157
8	6	0	-2.354725	-1.060843	-0.050221
9	6	0	-2.091135	-0.301323	1.291602
10	6	0	-2.287720	-0.037585	-1.218236
11	1	0	-3.338143	-1.541758	-0.018585
12	6	0	-2.181317	1.232451	0.952426
13	1	0	-2.899340	-0.529626	1.993509
14	6	0	-2.177626	1.365742	-0.601900
15	1	0	-3.163308	-0.132226	-1.868587
16	1	0	-3.131614	1.598223	1.363054
17	1	0	-2.982394	2.034620	-0.923132
18	6	0	-0.771476	-0.917452	1.915712
19	6	0	0.441187	-0.066059	2.093630
20	6	0	-1.063843	2.165465	1.361769

21	6	0	-0.336320	2.585882	0.319097
22	6	0	1.612060	-0.470553	1.254247
23	6	0	2.038919	0.564921	0.163451
24	6	0	-0.979972	-0.307988	-2.009045
25	6	0	0.039243	0.845687	-1.713353
26	6	0	-0.794872	1.978277	-0.984623
27	1	0	-1.639078	-3.104565	-0.431862
28	1	0	2.478967	-0.676410	1.898722
29	1	0	0.485321	3.294731	0.385073
30	1	0	-0.915788	2.490601	2.388035
31	1	0	-0.930796	2.775098	-1.727352
32	1	0	-0.409576	-2.410983	-2.285554
33	1	0	1.788151	-1.955500	-1.589417
34	6	0	1.350539	0.148588	-1.164856
35	1	0	-1.063677	-1.322962	2.896848
36	1	0	0.547429	0.637526	2.913187
37	1	0	-1.184400	-0.352332	-3.083996
38	1	0	0.342037	1.284751	-2.668231
39	1	0	2.082711	0.285916	-1.967254
40	1	0	1.809003	1.583002	0.465729
41	16	0	3.875897	0.511991	-0.169939
42	1	0	4.284265	0.767869	1.093177

b3lyp/6-311++g(2d,p)
HF=-1173.0888444

m062x/6-31g(d)
HF=-1172.5182521

wb97xd/6-31g(d)
HF=-1172.6601356

b3lyp/6-31g(d) scrf=(smd,solvent=water)
HF=-1172.8626853

b3lyp/6-31g(d) scrf=(smd,solvent=benzene)
HF=-1172.8778923

7→8 TSS
imaginary: 401.61i cm-1
Zero-point correction= 0.363957 (Hartree/Particle)
Thermal correction to Energy= 0.375686
Thermal correction to Enthalpy= 0.376630
Thermal correction to Gibbs Free Energy= 0.326393
Sum of electronic and zero-point Energies= -1172.491435
Sum of electronic and thermal Energies= -1172.479706
Sum of electronic and thermal Enthalpies= -1172.478762
Sum of electronic and thermal Free Energies= -1172.529000

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.262264	-2.079632	-0.220928
2	6	0	-0.399570	-1.670725	-1.453965
3	6	0	1.039951	-1.398885	-0.956611
4	6	0	1.081889	-1.659930	0.574797

5	6	0	-0.359738	-2.001542	1.039267
6	1	0	-0.416659	-2.457240	-2.215099
7	1	0	1.770269	-2.028807	-1.472359
8	6	0	1.504989	-0.329157	1.265482
9	6	0	2.044508	0.577244	0.121937
10	6	0	0.283143	0.151344	2.030694
11	1	0	2.313336	-0.495326	1.989609
12	6	0	-0.215080	2.547475	0.247861
13	6	0	-0.842384	2.007896	1.337081
14	1	0	0.476105	0.619843	2.993387
15	1	0	0.589892	3.275456	0.296635
16	1	0	-0.731859	2.417701	2.336897
17	6	0	1.367369	0.107718	-1.191869
18	6	0	0.068779	0.802942	-1.764993
19	6	0	-0.727274	1.967470	-1.041595
20	6	0	-2.117535	1.390335	-0.630899
21	6	0	-0.969983	-0.341590	-2.014912
22	6	0	-2.274390	-0.016437	-1.237487
23	6	0	-0.864782	-0.823695	1.931644
24	6	0	-2.170369	-0.257437	1.273318
25	6	0	-2.102082	1.259255	0.926506
26	1	0	1.783892	-2.462977	0.814168
27	1	0	-1.174719	-0.427406	-3.087249
28	1	0	-2.914119	2.071742	-0.945625
29	1	0	-0.849302	2.764626	-1.786239
30	1	0	-2.973445	1.764738	1.361851
31	1	0	-0.381509	-2.940347	1.601512
32	1	0	-1.669265	-3.087589	-0.351288
33	6	0	-2.395570	-1.030311	-0.063833
34	1	0	-1.121252	-1.186145	2.936451
35	1	0	-3.010799	-0.438714	1.951217
36	1	0	-3.380836	-1.508019	-0.066404
37	1	0	0.371660	1.213369	-2.732650
38	1	0	2.105763	0.193175	-1.996048
39	1	0	-3.146172	-0.078492	-1.896779
40	1	0	1.903204	1.633827	0.328238
41	16	0	3.877887	0.329617	-0.137469
42	1	0	4.271971	0.668696	1.110306

8

Zero-point correction= 0.366900 (Hartree/Particle)
Thermal correction to Energy= 0.378487
Thermal correction to Enthalpy= 0.379431
Thermal correction to Gibbs Free Energy= 0.329614
Sum of electronic and zero-point Energies= -1172.523051
Sum of electronic and thermal Energies= -1172.511464
Sum of electronic and thermal Enthalpies= -1172.510520
Sum of electronic and thermal Free Energies= -1172.560336

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.021757	-1.513684	-0.744707
2	6	0	-1.014501	-1.489061	0.811730
3	6	0	-1.388030	-0.043488	1.252768
4	6	0	-2.051522	0.585322	0.005304
5	6	0	-1.399380	-0.083194	-1.229064

6	1	0	-1.734064	-2.209320	1.209719
7	1	0	-2.124842	-0.079398	2.060556
8	6	0	0.054046	2.455774	-0.036759
9	6	0	0.627447	1.861477	1.206060
10	6	0	0.614243	1.821606	-1.265354
11	1	0	-0.593810	3.326894	-0.047882
12	6	0	2.040674	1.373314	0.750920
13	1	0	0.711024	2.627178	1.987185
14	6	0	2.032203	1.348051	-0.809862
15	1	0	0.688813	2.561104	-2.072082
16	1	0	2.812024	2.055861	1.120814
17	1	0	2.799321	2.017912	-1.210467
18	6	0	-0.098173	0.615728	1.873380
19	6	0	0.970443	-0.517872	1.994772
20	6	0	2.260279	-0.072171	1.252686
21	6	0	2.436913	-0.989543	0.006557
22	6	0	0.426282	-1.790790	1.289617
23	6	0	1.303882	-2.051860	0.029873
24	6	0	-0.118190	0.555135	-1.884886
25	6	0	0.949150	-0.582283	-1.980270
26	6	0	2.246899	-0.113174	-1.266857
27	1	0	0.449384	-2.651182	1.966004
28	1	0	3.424210	-1.462511	0.008977
29	1	0	3.131919	-0.137641	1.911819
30	1	0	3.111283	-0.200420	-1.932931
31	1	0	-2.145183	-0.142860	-2.028875
32	1	0	-1.744749	-2.246953	-1.112748
33	6	0	0.413208	-1.831547	-1.228296
34	1	0	-0.415749	0.851030	-2.895169
35	1	0	1.149786	-0.819527	-3.030213
36	1	0	0.428511	-2.713539	-1.876378
37	1	0	1.182686	-0.720176	3.049791
38	1	0	-0.384618	0.944340	2.876983
39	1	0	1.712277	-3.067463	0.044314
40	16	0	-3.870881	0.152806	-0.079378
41	1	0	-4.228521	0.723681	1.092239
42	1	0	-2.000304	1.671651	-0.017278

8→1 TSS

imaginary: 724.35i cm-1

Zero-point correction= 0.365314 (Hartree/Particle)
Thermal correction to Energy= 0.376713
Thermal correction to Enthalpy= 0.377657
Thermal correction to Gibbs Free Energy= 0.327906
Sum of electronic and zero-point Energies= -1172.494799
Sum of electronic and thermal Energies= -1172.483400
Sum of electronic and thermal Enthalpies= -1172.482456
Sum of electronic and thermal Free Energies= -1172.532208

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.299182	-2.032093	0.125727
2	6	0	-0.413641	-1.861705	-1.143381
3	6	0	1.011241	-1.459798	-0.682036
4	6	0	1.005978	-1.362614	0.873734
5	6	0	-0.422929	-1.703622	1.369920

6	1	0	-0.390536	-2.785504	-1.729919
7	1	0	1.760630	-2.182936	-1.012221
8	6	0	1.325478	0.111116	1.269546
9	6	0	1.784696	0.765156	-0.036669
10	6	0	0.040816	0.707529	1.938747
11	1	0	2.131231	0.144605	2.004316
12	6	0	0.130046	2.203465	-0.137132
13	6	0	-0.610810	1.879048	1.133051
14	1	0	0.307763	1.071164	2.936073
15	1	0	0.687244	3.136542	-0.194718
16	1	0	-0.667582	2.765059	1.776656
17	6	0	1.333971	-0.046324	-1.255545
18	6	0	0.056010	0.458628	-2.006305
19	6	0	-0.602188	1.720759	-1.361567
20	6	0	-2.025093	1.313752	-0.869365
21	6	0	-0.996704	-0.689430	-1.980128
22	6	0	-2.270796	-0.167929	-1.257889
23	6	0	-1.012187	-0.435492	2.049177
24	6	0	-2.279978	-0.008754	1.256756
25	6	0	-2.030652	1.412155	0.686488
26	1	0	1.754318	-2.035471	1.297459
27	1	0	-1.232196	-1.015940	-2.998095
28	1	0	-2.782391	1.973432	-1.303844
29	1	0	-0.653139	2.518124	-2.112465
30	1	0	-2.791134	2.121070	1.027921
31	1	0	-0.405927	-2.546388	2.068213
32	1	0	-1.698913	-3.049167	0.188331
33	6	0	-2.446223	-0.984933	0.055520
34	1	0	-1.256543	-0.631229	3.098167
35	1	0	-3.166397	-0.023981	1.898854
36	1	0	-3.426132	-1.471979	0.082733
37	1	0	0.332954	0.692513	-3.038979
38	1	0	2.148204	-0.095721	-1.981595
39	1	0	-3.152049	-0.265287	-1.899768
40	1	0	2.285864	1.718550	-0.102193
41	16	0	4.012081	0.021106	-0.075879
42	1	0	4.354315	0.711356	1.037233

8→8′ TSS

imaginary: 1447.90i cm-1

Zero-point correction= 0.362549 (Hartree/Particle)
Thermal correction to Energy= 0.373538
Thermal correction to Enthalpy= 0.374482
Thermal correction to Gibbs Free Energy= 0.325791
Sum of electronic and zero-point Energies= -1172.512993
Sum of electronic and thermal Energies= -1172.502004
Sum of electronic and thermal Enthalpies= -1172.501060
Sum of electronic and thermal Free Energies= -1172.549751

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.675443	-1.845337	0.022778
2	6	0	-0.752685	-1.805716	-1.230775
3	6	0	0.715785	-1.762406	-0.738649
4	6	0	0.704497	-1.737079	0.816455
5	6	0	-0.771212	-1.763849	1.287925

6	1	0	-0.930752	-2.673440	-1.873848
7	1	0	1.290653	-2.617403	-1.106938
8	6	0	1.342963	-0.387003	1.266548
9	6	0	2.021175	0.192319	0.016180
10	6	0	0.199569	0.485360	1.909020
11	1	0	2.095866	-0.562505	2.040229
12	6	0	0.545015	2.247291	-0.029678
13	6	0	-0.230759	1.835674	1.214123
14	1	0	0.534303	0.743833	2.918255
15	1	0	0.940081	3.263981	-0.044216
16	1	0	-0.160422	2.624960	1.970386
17	6	0	1.359865	-0.427968	-1.223314
18	6	0	0.227121	0.422543	-1.913133
19	6	0	-0.212458	1.794400	-1.270658
20	6	0	-1.698258	1.631134	-0.814586
21	6	0	-1.039035	-0.481970	-1.993753
22	6	0	-2.210655	0.243916	-1.275767
23	6	0	-1.068791	-0.415464	2.001530
24	6	0	-2.229491	0.285983	1.242368
25	6	0	-1.709697	1.656946	0.742588
26	1	0	1.273452	-2.579546	1.220666
27	1	0	-1.292551	-0.685515	-3.039268
28	1	0	-2.311869	2.442249	-1.219283
29	1	0	-0.129741	2.558517	-2.050895
30	1	0	-2.328560	2.481069	1.111439
31	1	0	-0.958969	-2.609715	1.956899
32	1	0	-2.278016	-2.759313	0.033572
33	6	0	-2.576151	-0.578722	-0.005354
34	1	0	-1.337454	-0.583699	3.049578
35	1	0	-3.104054	0.403858	1.890215
36	1	0	-3.637119	-0.848945	-0.008628
37	1	0	0.578474	0.646671	-2.924562
38	1	0	2.120707	-0.626261	-1.985616
39	1	0	-3.075548	0.339790	-1.940016
40	1	0	1.628341	1.418002	-0.009654
41	16	0	3.833104	0.086455	-0.076752
42	1	0	4.105382	0.699822	1.096629

8′

Zero-point correction= 0.367429 (Hartree/Particle)
Thermal correction to Energy= 0.379263
Thermal correction to Enthalpy= 0.380207
Thermal correction to Gibbs Free Energy= 0.329204
Sum of electronic and zero-point Energies= -1172.532223
Sum of electronic and thermal Energies= -1172.520390
Sum of electronic and thermal Enthalpies= -1172.519445
Sum of electronic and thermal Free Energies= -1172.570448

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.850678	-1.718767	0.007409
2	6	0	-0.932610	-1.761966	-1.249859
3	6	0	0.528715	-1.892732	-0.765551
4	6	0	0.524783	-1.883451	0.793521
5	6	0	-0.938655	-1.746940	1.269372
6	1	0	-1.210360	-2.592093	-1.907343

7	1	0	1.006799	-2.801493	-1.143589
8	6	0	1.325565	-0.618789	1.249820
9	6	0	2.064182	-0.218257	0.008240
10	6	0	0.280575	0.390983	1.881787
11	1	0	2.035253	-0.882180	2.043205
12	6	0	0.725949	2.293213	-0.011273
13	6	0	-0.036763	1.788561	1.233510
14	1	0	0.648467	0.601643	2.890933
15	1	0	0.627183	3.388364	-0.017213
16	1	0	0.086438	2.528133	2.032835
17	6	0	1.330620	-0.633362	-1.231484
18	6	0	0.289175	0.369246	-1.881439
19	6	0	-0.032078	1.774251	-1.252725
20	6	0	-1.521093	1.751761	-0.792115
21	6	0	-1.067068	-0.401242	-1.987013
22	6	0	-2.165475	0.427862	-1.265904
23	6	0	-1.076540	-0.377810	1.989943
24	6	0	-2.171223	0.442945	1.253842
25	6	0	-1.524217	1.760879	0.767138
26	1	0	1.001581	-2.787185	1.185054
27	1	0	-1.328784	-0.557718	-3.038744
28	1	0	-2.057657	2.623293	-1.181467
29	1	0	0.095529	2.504160	-2.059916
30	1	0	-2.061666	2.637107	1.144531
31	1	0	-1.219234	-2.569327	1.935374
32	1	0	-2.544287	-2.565850	0.010934
33	6	0	-2.612817	-0.365356	-0.002299
34	1	0	-1.343083	-0.521902	3.042250
35	1	0	-3.024070	0.634682	1.912969
36	1	0	-3.696634	-0.520508	-0.003685
37	1	0	0.663681	0.567511	-2.890282
38	1	0	2.042503	-0.903552	-2.021265
39	1	0	-3.015402	0.611431	-1.931092
40	16	0	3.791560	0.113965	-0.081314
41	1	0	3.991310	0.413075	1.220516
42	1	0	1.795406	2.082796	-0.012491

2′

Zero-point correction= 0.343455 (Hartree/Particle)
Thermal correction to Energy= 0.358219
Thermal correction to Enthalpy= 0.359163
Thermal correction to Gibbs Free Energy= 0.302277
Sum of electronic and zero-point Energies= -773.594361
Sum of electronic and thermal Energies= -773.579596
Sum of electronic and thermal Enthalpies= -773.578652
Sum of electronic and thermal Free Energies= -773.635539

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.871770	0.249885	0.618724
2	6	0	2.784777	-0.297847	-0.798952
3	6	0	2.559186	0.987006	-1.567652
4	6	0	2.346927	2.019447	-0.733404
5	6	0	1.926595	1.524216	0.680484
6	1	0	3.764351	-0.706529	-1.084946
7	1	0	2.702916	1.076198	-2.641658

8	6	0	-2.366427	-2.026029	-0.781665
9	6	0	-1.891081	-1.607221	0.602362
10	6	0	-2.755291	-0.967878	-1.497361
11	1	0	-2.224960	-3.036432	-1.156598
12	6	0	-2.784193	-0.298440	0.799149
13	1	0	-2.151884	-2.337479	1.380487
14	6	0	-2.872161	0.249318	-0.618403
15	1	0	-3.032564	-0.978710	-2.548366
16	1	0	-3.763499	-0.707317	1.085845
17	1	0	-3.856070	0.711368	-0.778397
18	6	0	-0.375874	-1.518565	0.557078
19	6	0	0.376750	-1.518369	-0.557473
20	6	0	-2.558779	0.986573	1.567792
21	6	0	-2.347596	2.019122	0.733389
22	6	0	1.891946	-1.606878	-0.602489
23	6	0	2.367037	-2.025678	0.781620
24	6	0	0.394020	1.625577	0.547345
25	6	0	-0.395008	1.625514	-0.547708
26	6	0	-1.927645	1.524027	-0.680543
27	1	0	2.218342	3.052841	-1.046871
28	1	0	2.153015	-2.337134	-1.380549
29	1	0	-2.219576	3.052596	1.046841
30	1	0	-2.701946	1.075740	2.641869
31	1	0	-2.246572	2.178714	-1.498468
32	1	0	2.245169	2.179156	1.498373
33	1	0	3.855296	0.712597	0.779162
34	6	0	2.755131	-0.967378	1.497544
35	1	0	0.116002	-1.511896	1.525886
36	1	0	-0.114978	-1.511337	-1.526341
37	1	0	-0.106491	1.621939	1.513620
38	1	0	0.105315	1.621622	-1.514077
39	1	0	3.031893	-0.978210	2.548681
40	1	0	2.225747	-3.036134	1.156481

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comparison of methods

3 → 3to4TS (all electronic energies, kcal/mol)

b3lyp/6-31g(d)
19.2

b3lyp/6-311++g(2d,p)
20.3

m062x/6-31g(d)
19.3

wb97xd/6-31g(d)
18.0

b3lyp/6-31g(d) scrf=(smd,solvent=water)
20.4

b3lyp/6-31g(d) scrf=(smd,solvent=benzene)
19.8

3 → 7 (all electronic energies, kcal/mol)

b3lyp/6-31g(d)
-66.3

b3lyp/6-311++g(2d,p)
-56.1

m062x/6-31g(d)
-75.5

wb97xd/6-31g(d)
-86.0

b3lyp/6-31g(d) scrf=(smd,solvent=water)
-64.4

b3lyp/6-31g(d) scrf=(smd,solvent=benzene)
-65.3

preliminary results on other addition modes

Since there are three nonequivalent alkene carbons in **2**, reactions involving HS• addition to the other two possible positions (**9** and **10** shown below) were also calculated and produced similar energy surfaces with activation barriers of 29.4 kcal/mol and 10.1 kcal/mol for **9** and **10**, respectively (B3LYP/6-31G(d)). While the barrier for the pathway involving **10** is high, we expect the initial addition of RS• to be reversible, allowing either of the pathways involving **3** or **9** to occur readily.