Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information for

Theoretical Studies on the Mechanism by which a Cyclopropane-Containing Farnesyldiphosphate Analog Inactivates Trichodiene Synthase

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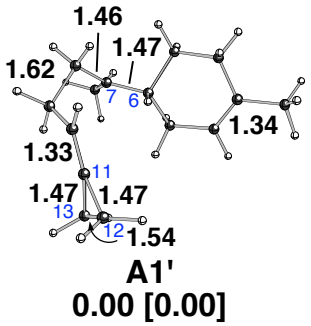
I. Gaussian03 Full Reference

GAUSSIAN03, Revision D.01
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,
V. Bakken, 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., Wallingford CT, 2004.

II. Coordinates and energies

Figure 1a.



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1503162 hartrees (-367181.8234155 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.340540 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367002.5926 kcal/mol (298 Kelvin. 1.0 atm)

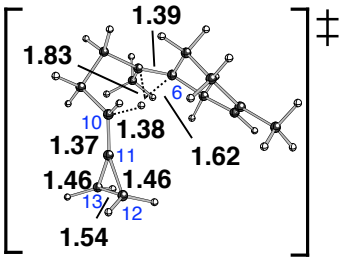
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0150423 hartrees (-367096.93904325 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8080104 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.222529	0.860546	1.076937
2	6	2.958019	0.842030	-0.045721
3	6	2.709621	-0.174790	-1.137908
4	6	1.781383	-1.324901	-0.730751
5	6	0.548713	-0.725827	0.080336
6	6	1.085016	-0.086697	1.372598
7	1	2.317126	0.334326	-2.029830
8	1	2.437055	1.602843	1.842350
9	1	1.446293	-1.876219	-1.613584
10	1	2.303455	-2.026940	-0.071922
11	1	3.665479	-0.618035	-1.449350
12	6	-1.385902	-2.022756	-0.881537
13	6	-2.674395	-1.073272	-0.612882
14	1	-1.740117	-3.055378	-0.900223
15	1	-0.987273	-1.733762	-1.856953
16	6	-2.500221	0.332026	-1.088456
17	1	-3.459009	-1.579622	-1.185925
18	1	-2.965846	-1.109963	0.440312
19	6	-2.634183	1.404268	-0.309172
20	6	-0.443862	-1.794552	0.207170
21	6	-2.705727	2.863915	-0.206855
22	6	-2.926739	1.961292	1.021603
23	1	-2.316394	0.470665	-2.154221
24	1	0.119681	0.045608	-0.578430
25	6	-0.532949	-2.626958	1.424732
26	1	0.423278	-3.159621	1.552298
27	1	-0.623732	-2.001116	2.321771
28	1	-1.340686	-3.358269	1.388247
29	1	1.415465	-0.861457	2.078209
30	1	0.273589	0.457096	1.873249
31	6	4.064822	1.829119	-0.306587
32	1	5.028657	1.317327	-0.418310
33	1	3.889570	2.378310	-1.240458
34	1	4.157072	2.556414	0.503554
35	1	-2.150718	1.955360	1.784990
36	1	-3.937336	1.870776	1.415104
37	1	-1.783110	3.439338	-0.250797

38	1	-3.569246	3.371656	-0.631132



TS (A1'-to-D')
10.35 [7.50]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1288238 hartrees (-367168.3369345 kcal/mol)
Imaginary Frequencies: 1 (-735.7701 1/cm)
Zero-point correction = 0.335537 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366991.0207 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -585.162798 hartrees (-367195.50737298 kcal/mol)

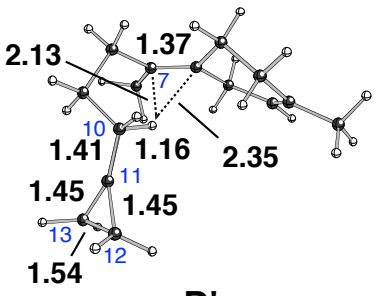
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.9980942 hartrees (-367086.3041105 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7887242 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.347319	-0.176749	1.183000
2	6	2.771994	0.292756	0.001174
3	6	2.067482	-0.081432	-1.282862
4	6	1.127695	-1.290267	-1.133440
5	6	0.300060	-1.277475	0.145664
6	6	1.150032	-1.074246	1.391502
7	1	1.522534	0.794116	-1.667328
8	1	2.886845	0.090680	2.089270
9	1	0.515976	-1.407108	-2.029254
10	1	1.745551	-2.196747	-1.062521
11	1	2.811081	-0.313802	-2.054984
12	6	-1.916563	-1.754934	-0.972143
13	6	-2.551453	-0.324362	-1.084963

14	1	-2.716227	-2.488745	-0.844495
15	1	-1.392732	-1.996983	-1.898110
16	6	-1.475882	0.746505	-0.949260
17	1	-3.054824	-0.225513	-2.051352
18	1	-3.307536	-0.187469	-0.306064
19	6	-1.621842	1.850816	-0.154480
20	6	-1.006987	-1.740201	0.226412
21	6	-1.120794	3.160977	0.240270
22	6	-2.323939	2.507862	0.944797
23	1	-0.796636	0.863312	-1.797390
24	1	-0.638398	0.018900	-0.122123
25	6	-1.683448	-2.074403	1.526418
26	1	-1.837648	-3.162561	1.546838
27	1	-1.115325	-1.809561	2.416348
28	1	-2.681552	-1.627228	1.590861
29	1	1.485582	-2.063692	1.743478
30	1	0.547186	-0.670338	2.212011
31	6	3.964258	1.203373	-0.130778
32	1	4.753869	0.728707	-0.726513
33	1	3.696442	2.132561	-0.650227
34	1	4.384422	1.466461	0.843188
35	1	-2.180547	2.134503	1.957834
36	1	-3.322908	2.897784	0.753500
37	1	-0.178003	3.214808	0.783228
38	1	-1.294738	3.998586	-0.434061



D'
9.56 [8.71]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1324871 hartrees (-367170.63565525 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.337949 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366993.0526 kcal/mol (298 Kelvin. 1.0 atm)

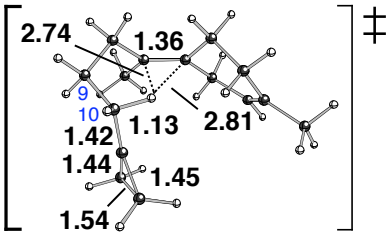
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -584.9985719 hartrees (-367086.60386725 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7894885 hartrees
Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.740987	0.161884	1.122575
2	6	2.865110	0.966694	0.057483
3	6	2.105559	0.681460	-1.219393
4	6	1.577064	-0.765217	-1.292796
5	6	0.930637	-1.216043	-0.005394
6	6	1.830572	-1.042474	1.197566
7	1	1.279272	1.402467	-1.326059
8	1	3.316348	0.370008	2.022400
9	1	0.929035	-0.887625	-2.162178
10	1	2.441342	-1.426168	-1.456526
11	1	2.757084	0.860944	-2.083532
12	6	-1.245599	-2.009213	-1.057164
13	6	-2.424975	-1.011068	-0.917891
14	1	-1.650998	-3.027224	-1.058651
15	1	-0.758928	-1.861977	-2.022985
16	6	-1.844274	0.407184	-0.727371
17	1	-3.072926	-1.034648	-1.799582
18	1	-3.040256	-1.268159	-0.049604
19	6	-2.601848	1.363545	-0.022280
20	6	-0.294124	-1.828194	0.101709
21	6	-2.893830	2.760598	0.227435
22	6	-3.599147	1.629718	0.997980
23	1	-1.360413	0.828125	-1.615982
24	1	-0.943577	0.197219	-0.019659
25	6	-0.783354	-2.382669	1.428550
26	1	-0.072979	-3.111832	1.834001
27	1	-0.908728	-1.610604	2.197337
28	1	-1.742255	-2.894006	1.314861
29	1	2.441773	-1.957460	1.298987
30	1	1.247282	-0.996098	2.123400
31	6	3.757414	2.180112	0.052235
32	1	4.549595	2.080607	-0.700485
33	1	3.192301	3.085353	-0.206118
34	1	4.229863	2.341061	1.024599
35	1	-3.330517	1.470717	2.043240
36	1	-4.638710	1.388564	0.771714
37	1	-2.148853	3.359749	0.753148

38	1	-3.435904	3.313087	-0.541783



TS (D'-to-E1')
16.65 [15.51]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1201734 hartrees (-367162.9088085 kcal/mol)
Imaginary Frequencies: 1 (-362.4992 1/cm)
Zero-point correction = 0.336932 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366985.8632 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -585.157436 hartrees (-367192.14266436 kcal/mol)

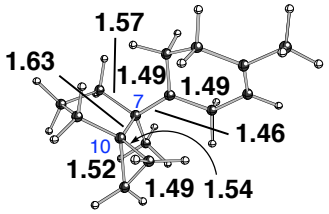
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.9865568 hartrees (-367079.064392 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7820744 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.493650	-0.222941	1.076748
2	6	2.716522	0.442791	-0.069060
3	6	1.959603	0.084389	-1.328070
4	6	1.222010	-1.264116	-1.221220
5	6	0.493145	-1.412645	0.101409
6	6	1.470257	-1.323253	1.259953
7	1	1.252999	0.899489	-1.577458
8	1	3.089988	0.020413	1.954886
9	1	0.578286	-1.406924	-2.091426
10	1	1.977881	-2.060461	-1.269938
11	1	2.652512	0.055799	-2.179155
12	6	-1.803398	-1.688885	-0.927577
13	6	-2.715482	-0.437671	-1.029998

14	1	-2.464195	-2.557435	-0.819537
15	1	-1.286397	-1.820630	-1.880535
16	6	-1.937262	0.884767	-1.178463
17	1	-3.369941	-0.537613	-1.901261
18	1	-3.368886	-0.373849	-0.154398
19	6	-1.815138	1.759566	-0.063181
20	6	-0.835970	-1.637162	0.243963
21	6	-1.433221	3.067110	0.424853
22	6	-1.945049	1.957013	1.360628
23	1	-2.095836	1.446581	-2.109460
24	1	-0.823975	0.675709	-1.230378
25	6	-1.509362	-1.919239	1.572774
26	1	-1.826694	-2.969426	1.611752
27	1	-0.873233	-1.745625	2.440536
28	1	-2.422477	-1.324383	1.705086
29	1	1.996724	-2.286492	1.368829
30	1	0.960434	-1.170483	2.215243
31	6	3.741664	1.540949	-0.186832
32	1	4.529908	1.266212	-0.899074
33	1	3.292479	2.469117	-0.566058
34	1	4.214727	1.760795	0.773818
35	1	-1.224968	1.459535	2.011848
36	1	-2.957404	1.992559	1.769075
37	1	-0.370971	3.313935	0.458743
38	1	-2.072771	3.909146	0.153301



E1'
-16.86 [-24.13]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1808397 hartrees (-367200.97691175 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.344202 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367016.4016 kcal/mol (298 Kelvin. 1.0 atm)

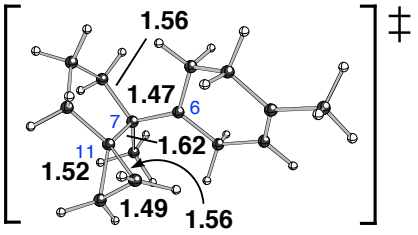
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.057159 hartrees (-367123.3672725 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8573229 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.530180	1.103447	-0.201102
2	6	-2.984085	-0.143039	-0.012799
3	6	-2.053716	-1.323340	-0.174244
4	6	-0.801089	-0.998781	-1.011673
5	6	-0.159062	0.304545	-0.704572
6	6	-1.098269	1.444438	-0.525848
7	1	-1.755251	-1.703707	0.812213
8	1	-3.197642	1.954127	-0.092220
9	1	-0.096468	-1.829039	-1.020865
10	1	-1.120331	-0.859092	-2.063402
11	1	-2.579213	-2.150531	-0.663607
12	6	2.172918	-0.492572	-1.486215
13	6	3.008637	-1.287379	-0.465978
14	1	2.792686	0.071611	-2.187229
15	1	1.560830	-1.167904	-2.088551
16	6	2.071689	-1.439316	0.735707
17	1	3.349795	-2.244759	-0.868150
18	1	3.898844	-0.717685	-0.177377
19	6	1.380163	-0.081743	0.854104
20	6	1.286787	0.505229	-0.665666
21	6	0.437041	0.161690	2.051282
22	6	1.753560	0.857346	1.994120
23	1	2.590698	-1.681627	1.668608
24	1	1.343559	-2.242155	0.566865
25	6	1.794707	1.941574	-0.834782
26	1	1.664021	2.259236	-1.874407
27	1	1.301259	2.675693	-0.196401
28	1	2.863515	1.973787	-0.609466
29	1	-1.031184	1.980298	-1.495627
30	1	-0.691940	2.179768	0.178713
31	6	-4.404198	-0.448594	0.375779
32	1	-4.895982	-1.058414	-0.391848
33	1	-4.437291	-1.027225	1.307486
34	1	-4.990529	0.461907	0.519044
35	1	1.757920	1.926995	1.818778
36	1	2.564339	0.507884	2.628029
37	1	-0.460439	0.760490	1.946578

38	1	0.319382	-0.690702	2.714171



TS (E1'-to-E2')
-14.18 [-21.38]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1763018 hartrees (-367198.1293795 kcal/mol)
Imaginary Frequencies: 1 (-67.2164 1/cm)
Zero-point correction = 0.343934 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367013.1837 kcal/mol (298 Kelvin. 1.0 atm)

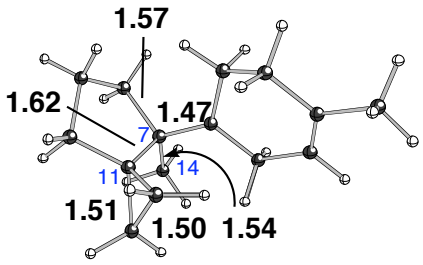
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0525061 hartrees (-367120.44757775 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8521499 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.104517	0.176917	-0.753484
2	6	1.842686	1.748574	-1.246130
3	1	2.887708	1.880400	-0.956909
4	1	1.794671	1.772374	-2.340044
5	1	1.286434	2.607838	-0.869236
6	6	1.344135	0.389786	-0.737353
7	6	2.224880	-0.762885	-1.310724
8	6	1.427682	0.174216	0.862024
9	6	2.428839	-1.841079	-0.230185
10	1	3.186277	-0.317700	-1.580425
11	1	1.801848	-1.163094	-2.237896
12	6	2.174189	-1.150307	1.123615
13	1	1.751068	-2.687304	-0.371108
14	1	3.438394	-2.256557	-0.283726
15	6	-1.052256	1.322227	-0.821643

16	6	-0.744357	-1.160503	-0.820886
17	6	-2.479732	1.044892	-0.421144
18	6	-1.992277	-1.330035	0.070785
19	6	-2.924268	-0.141905	0.014495
20	1	1.622336	-1.796601	1.812186
21	1	-0.040452	-1.978219	-0.691967
22	1	-1.080147	-1.199458	-1.875994
23	1	-2.517624	-2.234290	-0.255198
24	1	-1.686594	-1.521265	1.108540
25	1	-3.150950	1.897994	-0.472295
26	1	-0.653414	2.198010	-0.297825
27	1	-0.994176	1.629932	-1.886779
28	6	-4.336799	-0.366980	0.479436
29	1	-4.924648	0.553234	0.450453
30	1	-4.838467	-1.116954	-0.144003
31	1	-4.351315	-0.750513	1.507387
32	6	0.405707	0.641475	1.939902
33	6	1.689308	1.370947	1.765279
34	1	3.123794	-0.907167	1.613191
35	1	1.658235	2.368854	1.341343
36	1	2.480486	1.223182	2.496012
37	1	-0.514532	1.147060	1.672989
38	1	0.301750	-0.041798	2.777379



E2'
-15.04 [-22.06]

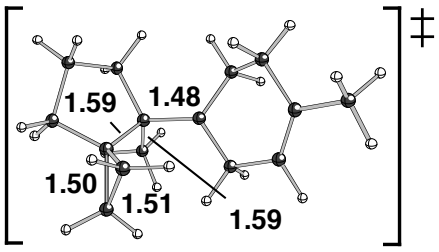
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.177527 hartrees (-367198.8981925 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.343787 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367014.6088 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0534437 hartrees (-367121.03592175 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8540332 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.169545	-0.045590	-0.741475
2	6	-1.776709	-1.462382	-1.574613
3	1	-2.840210	-1.611358	-1.374403
4	1	-1.659876	-1.298498	-2.651338
5	1	-1.264163	-2.389164	-1.313048
6	6	-1.287443	-0.230548	-0.793655
7	6	-2.095505	1.047942	-1.209192
8	6	-1.566317	-0.352137	0.797789
9	6	-2.501887	1.792549	0.073754
10	1	-2.991944	0.701301	-1.731014
11	1	-1.549130	1.670995	-1.923679
12	6	-2.670176	0.671776	1.101886
13	1	-1.730084	2.498242	0.399303
14	1	-3.418047	2.371782	-0.068405
15	6	1.090935	-1.193372	-0.908487
16	6	0.819981	1.275601	-0.611781
17	6	2.526750	-0.987200	-0.500214
18	6	2.075952	1.315481	0.283244
19	6	2.992941	0.132825	0.069563
20	1	-2.622608	1.021079	2.137069
21	1	0.120178	2.073780	-0.374639
22	1	1.153635	1.452294	-1.656153
23	1	2.608876	2.247628	0.067438
24	1	1.780623	1.380277	1.339191
25	1	3.182824	-1.838476	-0.659692
26	1	0.663582	-2.096173	-0.452403
27	1	1.013570	-1.422944	-1.992542
28	6	4.412336	0.282607	0.542002
29	1	4.986735	-0.635091	0.397014
30	1	4.918107	1.095286	0.006712
31	1	4.441624	0.540502	1.608029
32	6	-0.529118	-0.657843	1.897067
33	6	-1.558356	-1.678080	1.510247
34	1	-3.642715	0.182491	0.962881
35	1	-1.221502	-2.570653	0.991461
36	1	-2.396829	-1.855596	2.179620
37	1	0.507293	-0.882310	1.668896
38	1	-0.657509	-0.105174	2.822898



TS (E2'-to-E3')
-7.25 [-13.59]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1652451 hartrees (-367191.19130025 kcal/mol)
Imaginary Frequencies: 1 (-87.5288 1/cm)
Zero-point correction = 0.343920 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367006.6746 kcal/mol (298 Kelvin. 1.0 atm)

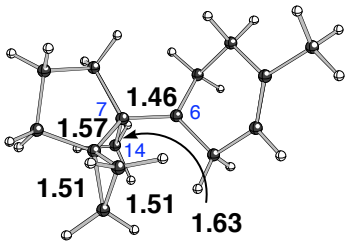
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0400811 hartrees (-367112.65089025 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8393137 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.330045	-0.472888	0.720765
2	6	-1.656942	-0.347155	2.037021
3	1	-2.746953	-0.314641	1.976199
4	1	-1.372123	-1.229396	2.617266
5	1	-1.310323	0.554950	2.541804
6	6	-1.134942	-0.441319	0.534282
7	6	-1.787968	-1.695558	-0.155495
8	6	-1.718473	0.791083	-0.280609
9	6	-2.599678	-1.173100	-1.355135
10	1	-2.449716	-2.185783	0.564919
11	1	-1.067766	-2.451117	-0.466961
12	6	-2.986709	0.244803	-0.934893
13	1	-1.974738	-1.138103	-2.254924
14	1	-3.459033	-1.810819	-1.576691
15	6	1.080363	0.669625	1.298587

16	6	1.201087	-1.622841	0.421824
17	6	2.448750	0.884796	0.664989
18	6	2.230524	-1.171607	-0.679357
19	6	2.967921	0.080496	-0.270956
20	1	-3.309058	0.877079	-1.767108
21	1	0.675211	-2.523613	0.119943
22	1	1.805195	-1.836887	1.314304
23	1	2.921471	-2.012570	-0.802113
24	1	1.734507	-1.039135	-1.650020
25	1	2.968209	1.780979	0.991591
26	1	0.499433	1.591098	1.312467
27	1	1.218899	0.399022	2.364622
28	6	4.274410	0.359380	-0.965357
29	1	4.708658	1.306668	-0.638938
30	1	4.999790	-0.439150	-0.769975
31	1	4.134413	0.403532	-2.052376
32	6	-0.876442	1.768654	-1.075679
33	6	-1.676035	2.238759	0.121257
34	1	-3.809304	0.220085	-0.207989
35	1	-1.144102	2.559040	1.012153
36	1	-2.578622	2.816962	-0.057820
37	1	0.206065	1.758423	-0.988654
38	1	-1.225573	2.034606	-2.069162



E3'
-8.67 [-15.28]

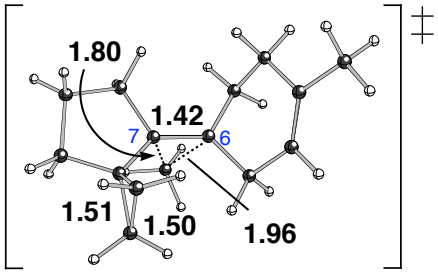
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1683217 hartrees (-367193.12186675 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.344725 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367008.8545 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0435825 hartrees (-367114.84801875 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8432805 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.409513	-0.340705	0.809188
2	6	-1.499841	-0.819036	1.875509
3	1	-1.051221	-1.726960	2.283126
4	1	-1.378463	0.014690	2.567987
5	6	-0.974988	-0.463815	0.374795
6	6	-1.296339	-1.669410	-0.582061
7	6	-1.824209	0.712418	-0.172714
8	6	-2.441662	-1.195056	-1.509966
9	1	-1.587935	-2.549739	-0.001539
10	1	-0.420464	-1.953015	-1.170179
11	6	-3.033924	0.037692	-0.815724
12	1	-2.034382	-0.909711	-2.484959
13	1	-3.177917	-1.983620	-1.683404
14	6	-1.229887	1.920677	-0.868106
15	6	-1.990270	2.083666	0.430022
16	6	1.058772	0.895115	1.308816
17	6	1.330674	-1.502899	0.803721
18	6	2.252341	1.147459	0.369255
19	6	2.387808	-1.233876	-0.328260
20	6	2.867016	0.196286	-0.348589
21	1	-3.551959	0.710706	-1.504016
22	1	0.832871	-2.455755	0.629108
23	1	1.873156	-1.544658	1.754247
24	1	3.222271	-1.926413	-0.170146
25	1	1.955548	-1.493219	-1.302740
26	1	2.572459	2.184605	0.318292
27	1	0.399891	1.758772	1.316776
28	1	1.426949	0.741315	2.333436
29	6	4.057709	0.487397	-1.223562
30	1	4.317670	1.547821	-1.215238
31	1	4.931672	-0.083319	-0.887342
32	1	3.862932	0.188432	-2.260499
33	1	-3.764931	-0.254502	-0.050042
34	1	-2.567920	-0.999070	1.728664
35	1	-0.154343	2.067723	-0.859156
36	1	-1.704305	2.248607	-1.788423
37	1	-1.449988	2.370317	1.326707
38	1	-2.987866	2.511525	0.385392



TS (E3'-to-F')
-7.33 [-14.77]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1654003 hartrees (-367191.28868825 kcal/mol)
Imaginary Frequencies: 1 (-285.4130 1/cm)
Zero-point correction = 0.343936 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367007.1245 kcal/mol (298 Kelvin. 1.0 atm)

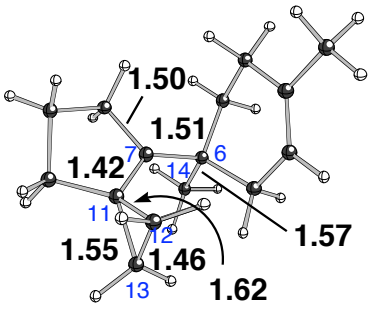
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0419701 hartrees (-367113.83623775 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8423459 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.374234	-0.307003	0.791280
2	6	-1.108979	-0.662887	2.024889
3	1	-0.611272	-1.522178	2.471117
4	1	-1.015901	0.247345	2.610544
5	6	-0.929261	-0.410851	0.248317
6	6	-1.363547	-1.696552	-0.500808
7	6	-1.883088	0.686895	-0.186600
8	6	-2.598468	-1.300112	-1.343802
9	1	-1.600356	-2.499819	0.204002
10	1	-0.546615	-2.062096	-1.127842
11	6	-3.141413	-0.038715	-0.660749
12	1	-2.289017	-1.065400	-2.367039
13	1	-3.330692	-2.108709	-1.400287
14	6	-1.370094	1.875553	-0.995788

15	6	-2.001630	2.094975	0.351233
16	6	1.071119	0.963389	1.206793
17	6	1.330529	-1.473391	0.771653
18	6	2.304605	1.152821	0.330052
19	6	2.347479	-1.229137	-0.374657
20	6	2.890227	0.182384	-0.386212
21	1	-3.746749	0.585198	-1.323481
22	1	0.831978	-2.434074	0.639827
23	1	1.877467	-1.499179	1.720390
24	1	3.166457	-1.948508	-0.257213
25	1	1.889439	-1.456341	-1.347358
26	1	2.704214	2.163710	0.316786
27	1	0.430040	1.838892	1.132227
28	1	1.378489	0.881632	2.259602
29	6	4.104641	0.424716	-1.241853
30	1	4.406202	1.474524	-1.230913
31	1	4.951535	-0.179334	-0.894113
32	1	3.915138	0.133369	-2.282357
33	1	-3.776714	-0.299339	0.197761
34	1	-2.165666	-0.903399	1.895877
35	1	-0.296559	2.008572	-1.088715
36	1	-1.930423	2.142698	-1.886710
37	1	-1.387632	2.435542	1.176962
38	1	-3.011492	2.494382	0.378449



F'

-24.09 [-30.39]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1929463 hartrees (-367208.57380325 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.344777 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367023.7102 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

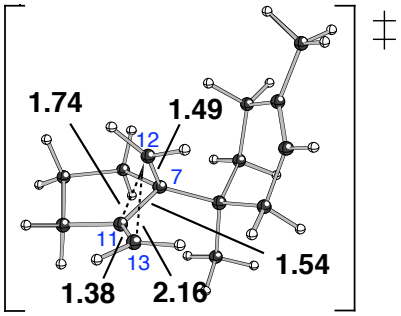
HF = -585.067702 hartrees (-367129.983005 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8676245 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.273996	-0.818645	0.903166
2	6	-0.442136	-1.686034	2.004539
3	1	0.333488	-2.053655	2.682154
4	1	-1.158586	-1.102074	2.588200
5	6	-0.869845	-0.439115	-0.003525
6	6	-1.304248	-1.358433	-1.113380
7	6	-1.813853	0.625069	0.069115
8	6	-2.357690	-0.588436	-1.930539
9	1	-1.758876	-2.236785	-0.621813
10	1	-0.468827	-1.750565	-1.696240
11	6	-2.976761	0.355645	-0.891260
12	1	-1.864200	-0.017751	-2.724452
13	1	-3.086539	-1.250603	-2.401544
14	6	-1.211227	2.131507	0.118906
15	6	-2.007496	1.630101	1.231142
16	6	1.054086	0.333061	1.589068
17	6	1.340392	-1.690106	0.185061
18	6	2.036827	1.016889	0.664557
19	6	2.117671	-0.920978	-0.894400
20	6	2.526319	0.471493	-0.460786
21	1	-3.391701	1.270574	-1.321763
22	1	0.903761	-2.607192	-0.221949
23	1	2.041669	-2.012752	0.962303
24	1	3.016063	-1.493360	-1.158081
25	1	1.546407	-0.851166	-1.832692
26	1	2.390959	1.996968	0.980739
27	1	0.392846	1.067757	2.052602
28	1	1.596148	-0.112961	2.434343
29	6	3.515757	1.182166	-1.345420
30	1	3.728426	2.193283	-0.989344
31	1	4.462658	0.629991	-1.389849
32	1	3.146081	1.251626	-2.376436
33	1	-3.785388	-0.141743	-0.340508
34	1	-0.954602	-2.552853	1.580133
35	1	-0.133686	2.205138	0.197765

36	1	-1.673342	2.747421	-0.646026
37	1	-1.529780	1.406942	2.176843
38	1	-3.043729	1.948658	1.308163



TS (F'-to-N)
-10.15 [-17.02]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1704882 hartrees (-367194.4813455 kcal/mol)
Imaginary Frequencies: 1 (-243.4134 1/cm)
Zero-point correction = 0.344536 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367008.9229 kcal/mol (298 Kelvin. 1.0 atm)

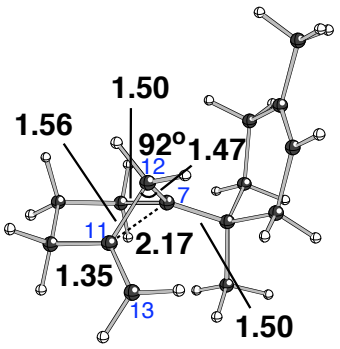
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0461553 hartrees (-367116.46245075 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8480477 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.216072	0.969463	0.630245
2	6	0.558382	2.053616	1.407805
3	1	1.155301	1.616304	2.216078
4	1	1.228200	2.632937	0.765700
5	6	0.825096	0.085263	-0.143492
6	6	1.489462	0.735065	-1.386200
7	6	1.988333	-0.651381	0.540349
8	6	2.800656	-0.027923	-1.654125
9	1	1.701870	1.780906	-1.151799
10	1	0.818576	0.725560	-2.247655

11	6	3.261263	-0.506839	-0.266345
12	6	-1.125760	0.195559	1.619504
13	6	-1.175676	1.632490	-0.396141
14	6	-2.219955	-0.623667	0.971236
15	6	-2.046741	0.630448	-1.167589
16	6	-2.657687	-0.438713	-0.285762
17	1	-0.629652	2.279768	-1.089492
18	1	-1.831804	2.296789	0.178615
19	1	-2.850005	1.176359	-1.678732
20	1	-1.480512	0.149772	-1.981347
21	1	-2.705852	-1.367898	1.600890
22	1	-0.541109	-0.422019	2.312520
23	1	-1.587201	0.943685	2.279318
24	6	-3.775027	-1.249965	-0.886293
25	1	-4.124944	-2.030545	-0.205710
26	1	-4.628873	-0.607662	-1.135400
27	1	-3.460614	-1.726179	-1.823989
28	1	-0.142164	2.759931	1.861765
29	1	2.632764	-0.884342	-2.315253
30	1	3.546939	0.601133	-2.143227
31	1	3.867671	-1.417252	-0.280103
32	1	3.850828	0.270064	0.238531
33	6	1.806194	-1.589885	1.530716
34	6	0.624927	-1.387376	-0.264379
35	1	-0.188050	-1.841309	0.291061
36	1	1.009356	-1.959502	-1.103162
37	1	0.929071	-1.638586	2.160848
38	1	2.605829	-2.294841	1.753377



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1939332 hartrees (-367209.193083 kcal/mol)
Imaginary Frequencies: none

Zero-point correction = 0.344239 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367025.0349 kcal/mol (298 Kelvin. 1.0 atm)

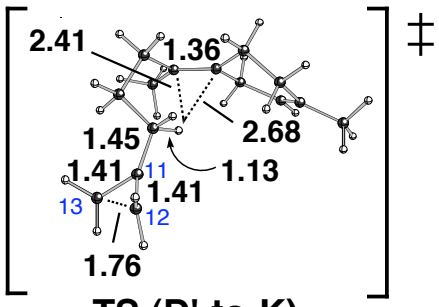
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0638842 hartrees (-367127.5873355 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8616646 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.336287	0.816414	0.784347
2	6	-0.436747	1.788482	1.722838
3	1	-1.143360	2.397612	1.152387
4	1	-0.981248	1.270708	2.515293
5	6	-0.589908	-0.214088	0.202395
6	6	-1.328681	-1.160975	1.092292
7	6	-2.314163	0.210006	-1.043140
8	6	-2.552869	-1.807828	0.413931
9	1	-1.576146	-0.687508	2.046621
10	1	-0.594828	-1.947018	1.341917
11	6	-3.303242	-0.760699	-0.440224
12	6	1.122716	1.617945	-0.275979
13	6	1.405015	0.038305	1.648741
14	6	2.185910	0.807632	-0.979886
15	6	2.287332	-0.908151	0.826787
16	6	2.721674	-0.328957	-0.503641
17	1	0.925391	-0.484189	2.481614
18	1	2.025797	0.825956	2.088768
19	1	3.176899	-1.155351	1.420501
20	1	1.790535	-1.876630	0.656894
21	1	2.550482	1.208979	-1.923642
22	1	0.440863	2.073069	-1.004501
23	1	1.586171	2.472907	0.234618
24	6	3.792381	-1.090283	-1.239818
25	1	4.018038	-0.638843	-2.209096
26	1	4.719708	-1.121393	-0.654359
27	1	3.493781	-2.132936	-1.408280
28	1	0.284650	2.456117	2.200814
29	1	-2.228657	-2.640124	-0.218075
30	1	-3.208524	-2.240225	1.173065
31	1	-3.858651	-1.267129	-1.239033

32	1	-4.035429	-0.214112	0.161714
33	6	-2.578021	1.488906	-1.364924
34	6	-0.878085	-0.359665	-1.227233
35	1	-0.259443	0.232706	-1.892950
36	1	-0.935339	-1.395273	-1.573664
37	1	-1.820860	2.156289	-1.763813
38	1	-3.587424	1.884124	-1.285724



TS (D'-to-K)
12.14 [13.02]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1294552 hartrees (-367168.733138 kcal/mol)
Imaginary Frequencies: 1 (-211.6966 1/cm)
Zero-point correction = 0.339033 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366990.0286 kcal/mol (298 Kelvin. 1.0 atm)

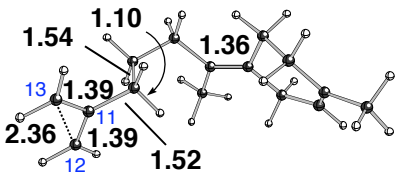
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.9927835 hartrees (-367082.97164625 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7847667 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.986216	0.102648	-1.026963
2	6	-2.949642	1.109158	-0.142110
3	6	-2.067605	1.027195	1.084547
4	6	-1.615171	-0.412699	1.398697
5	6	-1.126280	-1.143596	0.169583
6	6	-2.152115	-1.155669	-0.945535
7	1	-1.194331	1.687031	0.953818

8	1	-3.648138	0.172417	-1.888265
9	1	-0.886042	-0.407298	2.211434
10	1	-2.491462	-0.960979	1.774900
11	1	-2.606384	1.428122	1.952602
12	6	1.119377	-1.832930	1.132453
13	6	2.367017	-1.011352	0.723598
14	1	1.444113	-2.866162	1.306448
15	1	0.745690	-1.461008	2.088689
16	6	1.955927	0.447169	0.441935
17	1	3.124248	-1.041230	1.515245
18	1	2.815832	-1.446226	-0.176679
19	6	2.878155	1.264769	-0.314118
20	6	0.059869	-1.804652	0.053178
21	6	3.531484	2.494709	-0.118059
22	6	4.106817	1.062903	-0.969499
23	1	1.603950	0.982972	1.330979
24	1	1.043445	0.373884	-0.213576
25	6	0.402079	-2.603481	-1.195872
26	1	-0.390186	-3.318017	-1.442646
27	1	0.541888	-1.972372	-2.082796
28	1	1.320530	-3.180976	-1.057668
29	1	-2.818653	-2.024215	-0.799467
30	1	-1.675203	-1.328105	-1.916145
31	6	-3.772409	2.361529	-0.297039
32	1	-4.475312	2.476364	0.537927
33	1	-3.135160	3.256003	-0.294716
34	1	-4.346583	2.357588	-1.227246
35	1	4.365364	1.511219	-1.922672
36	1	4.760130	0.261485	-0.626342
37	1	3.673020	3.237718	-0.895170
38	1	3.721520	2.827580	0.902575



K
1.03 [-7.45]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1478943 hartrees (-367180.30367325 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.339758 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -367002.2525 kcal/mol (298 Kelvin. 1.0 atm)

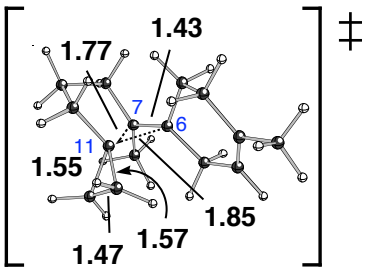
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0023819 hartrees (-367088.99464225 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7879573 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.310213	0.186737	-0.907004
2	6	3.324521	-0.996161	-0.257089
3	6	2.279683	-1.288290	0.793103
4	6	1.669001	-0.003755	1.383327
5	6	1.206175	0.959773	0.316277
6	6	2.265118	1.249831	-0.726769
7	1	1.496594	-1.929331	0.357498
8	1	4.077204	0.398546	-1.649289
9	1	0.880284	-0.258877	2.092896
10	1	2.456327	0.501046	1.964717
11	1	2.724764	-1.878804	1.603838
12	6	-1.097883	1.373346	1.310500
13	6	-2.426176	0.831163	0.725958
14	1	-1.326748	2.339170	1.781719
15	1	-0.776610	0.708834	2.115604
16	6	-2.287042	-0.580488	0.121172
17	1	-3.177580	0.813955	1.524184
18	1	-2.802996	1.523319	-0.037995
19	6	-3.606567	-1.117245	-0.394473
20	6	-0.002925	1.590087	0.288534
21	6	-4.287307	-2.161449	0.222400
22	6	-4.205939	-0.564500	-1.520398
23	1	-1.885461	-1.269739	0.871681
24	1	-1.561864	-0.557936	-0.701020
25	6	-0.338943	2.619979	-0.772361
26	1	0.532623	3.194278	-1.094457
27	1	-0.765683	2.159543	-1.675587
28	1	-1.078219	3.335721	-0.399376
29	1	2.769900	2.199492	-0.467274
30	1	1.806772	1.451529	-1.704489
31	6	4.340240	-2.065230	-0.540489
32	1	4.939388	-2.281168	0.353825

33	1	3.848906	-3.007371	-0.818271
34	1	5.018829	-1.782249	-1.349019
35	1	-5.154668	-0.937290	-1.897094
36	1	-3.743405	0.249707	-2.072095
37	1	-5.240369	-2.516451	-0.159508
38	1	-3.890989	-2.658707	1.103393



TS (E1'-to-H')
-15.00 [-23.92]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1785545 hartrees (-367199.54294875 kcal/mol)
Imaginary Frequencies: 1 (-166.7088 1/cm)
Zero-point correction = 0.344870 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367013.6418 kcal/mol (298 Kelvin. 1.0 atm)

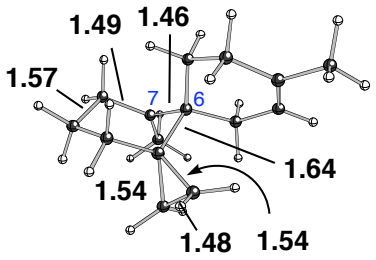
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.05749 hartrees (-367123.574975 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8603345 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.355241	1.126518	-0.203546
2	6	-2.837525	-0.120349	-0.103877
3	6	-1.943830	-1.312713	-0.361481
4	6	-0.680299	-0.955863	-1.156197
5	6	0.018303	0.293153	-0.663149
6	6	-0.925509	1.478159	-0.541423
7	1	-1.674512	-1.788597	0.592586
8	1	-3.013126	1.976359	-0.036511
9	1	-0.014360	-1.813858	-1.230200

10	1	-0.971357	-0.704818	-2.187890
11	1	-2.499034	-2.075255	-0.919977
12	6	2.356084	-0.594045	-1.302741
13	6	2.853379	-1.426299	-0.102650
14	1	3.186508	-0.128752	-1.838809
15	1	1.827410	-1.225353	-2.021410
16	6	1.673905	-1.473386	0.874170
17	1	3.192123	-2.419343	-0.408554
18	1	3.704989	-0.922891	0.368353
19	6	1.029858	-0.087524	0.843464
20	6	1.425431	0.509661	-0.771761
21	6	0.096529	0.283594	2.044997
22	6	1.415917	0.919553	1.951477
23	1	1.991902	-1.698634	1.897041
24	1	0.951789	-2.248369	0.598590
25	6	2.018129	1.899073	-0.868594
26	1	1.420226	2.688081	-0.415378
27	1	3.022065	1.920666	-0.436052
28	1	2.117242	2.135184	-1.935038
29	1	-0.883715	1.987708	-1.518595
30	1	-0.545809	2.223643	0.165461
31	6	-4.267249	-0.415235	0.260724
32	1	-4.775321	-0.944679	-0.554740
33	1	-4.321251	-1.068391	1.140913
34	1	-4.828050	0.496936	0.478158
35	1	1.458570	1.971419	1.692907
36	1	2.228685	0.580992	2.587939
37	1	-0.796042	0.868472	1.866072
38	1	-0.046220	-0.556307	2.718643



H'
-16.92 [-24.83]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1819146 hartrees (-367201.6514115 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.345169 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -367013.6418 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0592419 hartrees (-367124.67429225 kcal/mol)

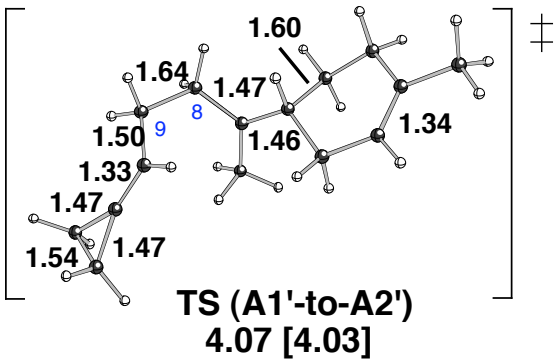
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8613077 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.256534	1.131226	0.268411
2	6	-2.777312	-0.006749	-0.211165
3	6	-1.903090	-0.996279	-0.945961
4	6	-0.601283	-0.371469	-1.459313
5	6	0.136139	0.438331	-0.368017
6	6	-0.805694	1.541834	0.162863
7	1	-1.691458	-1.857282	-0.295141
8	1	-2.900007	1.845744	0.777747
9	1	0.027515	-1.142084	-1.904723
10	1	-0.840823	0.339832	-2.259830
11	1	-2.450973	-1.406908	-1.802783
12	6	2.426955	-0.048854	-1.393280
13	6	2.781929	-1.275430	-0.485568
14	1	3.340129	0.481529	-1.673420
15	1	1.940060	-0.407668	-2.304751
16	6	1.524286	-1.740004	0.254878
17	1	3.220222	-2.062330	-1.104945
18	1	3.545817	-0.961953	0.233935
19	6	0.770566	-0.530504	0.792611
20	6	1.507876	0.856541	-0.642381
21	6	-0.051505	-0.675142	2.085296
22	6	1.255075	0.025926	2.144726
23	1	1.806199	-2.382008	1.095773
24	1	0.883551	-2.347236	-0.391151
25	6	2.079553	2.139800	-0.170482
26	1	1.477482	2.678664	0.557244
27	1	3.108288	2.018544	0.183917
28	1	2.146618	2.771015	-1.073935
29	1	-0.723869	2.406983	-0.511641
30	1	-0.471071	1.911644	1.139053
31	6	-4.229306	-0.369838	-0.053701
32	1	-4.715562	-0.466189	-1.032360

33	1	-4.339134	-1.339503	0.448448
34	1	-4.775140	0.377914	0.526947
35	1	1.241660	1.098412	2.309135
36	1	2.111638	-0.477827	2.582790
37	1	-0.963676	-0.099147	2.176895
38	1	-0.123386	-1.696482	2.449284

Figure 1b.



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.143419 hartrees (-367177.4954225 kcal/mol)
Imaginary Frequencies: 1 (-90.1979 1/cm)
Zero-point correction = 0.340133 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366997.8819 kcal/mol (298 Kelvin. 1.0 atm)

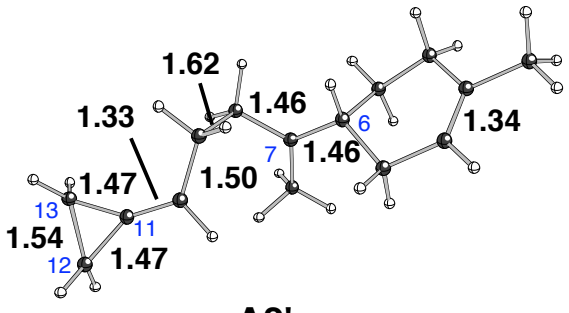
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.008212 hartrees (-367092.65303 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8010827 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.780809	1.500809	0.045319
2	6	3.758294	0.610744	-0.182805
3	6	3.506260	-0.878708	-0.100541
4	6	2.170520	-1.260413	0.550549
5	6	1.034702	-0.304537	-0.040973
6	6	1.352748	1.144687	0.378804

7	1	3.581023	-1.321165	-1.103958
8	1	3.000851	2.563941	-0.019674
9	1	1.944327	-2.313930	0.362373
10	1	2.207872	-1.108244	1.633734
11	1	4.301492	-1.353138	0.490999
12	6	-0.925949	-1.852989	-0.445129
13	6	-2.278509	-1.221460	-1.115817
14	1	-1.268462	-2.707586	0.146140
15	1	-0.279389	-2.203409	-1.251036
16	6	-2.596167	0.226197	-0.892904
17	1	-2.138370	-1.405704	-2.185254
18	1	-3.112121	-1.835648	-0.772480
19	6	-3.722929	0.643998	-0.318834
20	6	-0.216868	-0.905404	0.418764
21	6	-4.607524	1.762590	0.023480
22	6	-5.018411	0.302226	0.289950
23	1	-1.901938	0.968077	-1.291442
24	1	1.104416	-0.402462	-1.131026
25	6	-0.814298	-0.556268	1.711663
26	1	-0.115335	-0.137746	2.436049
27	1	-1.538439	0.246733	1.447287
28	1	-1.408484	-1.364787	2.143088
29	1	1.165533	1.294208	1.449931
30	1	0.670667	1.824122	-0.147216
31	6	5.160470	1.020278	-0.548081
32	1	5.879514	0.672198	0.203754
33	1	5.463009	0.575565	-1.504564
34	1	5.254688	2.105519	-0.633343
35	1	-5.048023	-0.029971	1.325982
36	1	-5.790472	-0.135632	-0.339493
37	1	-4.367792	2.383271	0.884573
38	1	-5.103462	2.295294	-0.785089



A2'
-0.31 [-0.11]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1508119 hartrees (-367182.13446725 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.340544 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367003.1122 kcal/mol (298 Kelvin. 1.0 atm)

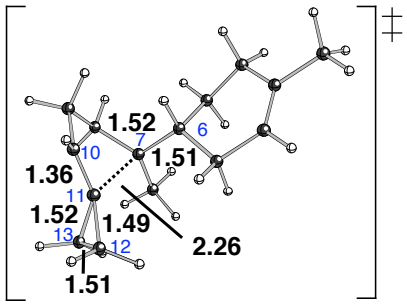
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0152269 hartrees (-367097.05487975 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8077035 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.080102	-1.368108	0.265366
2	6	-3.952953	-0.449148	-0.174728
3	6	-3.552898	0.999041	-0.351066
4	6	-2.207006	1.365128	0.286788
5	6	-1.157167	0.222995	-0.055856
6	6	-1.637773	-1.091089	0.610282
7	1	-3.549985	1.250318	-1.421258
8	1	-3.401787	-2.401268	0.376480
9	1	-1.865576	2.337614	-0.080929
10	1	-2.299336	1.429036	1.375637
11	1	-4.316184	1.647563	0.100566
12	6	1.101077	1.189335	-0.653643
13	6	1.943424	-0.082170	-1.205894
14	1	1.824453	1.907724	-0.263439
15	1	0.583678	1.594316	-1.528645
16	6	2.828885	-0.755064	-0.205662
17	1	1.232759	-0.783888	-1.652223
18	1	2.539595	0.353988	-2.011837
19	6	4.133990	-0.502591	-0.102843
20	6	0.151393	0.736314	0.356720
21	6	5.422837	-0.829875	0.512170
22	6	5.307418	0.237398	-0.591970
23	1	2.392620	-1.526479	0.429025
24	1	-1.171715	0.101825	-1.145409
25	6	0.565294	0.804694	1.768303
26	1	-0.151691	0.402571	2.481351
27	1	1.530687	0.274621	1.856599
28	1	0.811230	1.844791	2.025537

29	1	-1.506590	-1.045952	1.698987
30	1	-1.009553	-1.919130	0.259675
31	6	-5.373610	-0.788827	-0.539560
32	1	-6.082652	-0.242561	0.094665
33	1	-5.592031	-0.502881	-1.576277
34	1	-5.573484	-1.857764	-0.432994
35	1	5.435417	1.278746	-0.302920
36	1	5.699872	-0.002944	-1.578224
37	1	5.623318	-0.489202	1.526042
38	1	5.890109	-1.779240	0.259155



TS (A2'-to-C')
12.31 [9.61]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1319081 hartrees (-367170.27233275 kcal/mol)
Imaginary Frequencies: 1 (-268.5814 1/cm)
Zero-point correction = 0.341743 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -584.7964178 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -585.1670489 hartrees (-367198.174855239 kcal/mol)

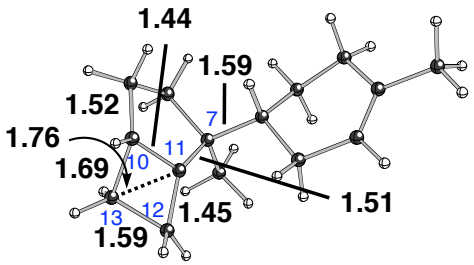
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0009371 hartrees (-367088.08803025 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.7964178 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.448395	-0.295888	0.087003
2	6	-1.191827	-0.579846	2.035882

3	1	-2.195562	-0.900205	2.314146
4	1	-0.487747	-1.258855	2.540635
5	1	-0.986142	0.417118	2.433448
6	6	-0.921786	-0.704204	0.571493
7	6	-1.630751	-1.837187	-0.152577
8	6	-2.360339	0.703908	-0.446418
9	6	-1.842120	-1.431925	-1.615008
10	1	-2.584221	-2.041951	0.340653
11	1	-1.024578	-2.748729	-0.065854
12	6	-2.131785	0.033765	-1.608095
13	1	-0.946991	-1.617592	-2.220916
14	1	-2.646446	-1.992200	-2.112797
15	6	0.879110	1.152862	0.393738
16	6	1.523675	-1.263639	0.687232
17	6	2.327431	1.387579	0.033805
18	6	2.861616	-1.043121	-0.030604
19	6	3.230518	0.417852	-0.177270
20	1	0.490073	-0.427925	-0.999127
21	1	1.216914	-2.311167	0.593599
22	1	1.642720	-1.048271	1.754740
23	1	3.647281	-1.563516	0.532928
24	1	2.848828	-1.520656	-1.021814
25	1	2.629432	2.428294	-0.063849
26	1	0.248349	1.845983	-0.175340
27	1	0.717528	1.389941	1.454872
28	6	4.654106	0.706084	-0.574312
29	1	4.832065	1.777340	-0.697108
30	1	5.356005	0.326105	0.178488
31	1	4.906459	0.208004	-1.519240
32	6	-2.810791	2.091913	-0.152415
33	6	-3.447825	0.940379	0.584997
34	1	-2.004892	0.593119	-2.536638
35	1	-3.225815	0.833026	1.640055
36	1	-4.439024	0.603105	0.293834
37	1	-2.145613	2.722872	0.432691
38	1	-3.374387	2.614969	-0.922119



C'
-16.04 [-24.76]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1805479 hartrees (-367200.79380725 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.345210 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367015.4942 kcal/mol (298 Kelvin. 1.0 atm)

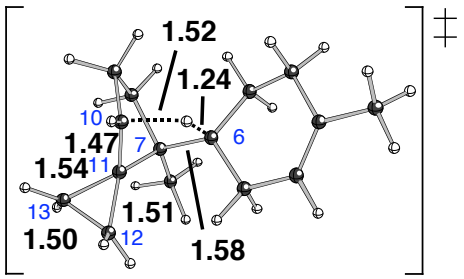
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0591656 hartrees (-367124.626414 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.860944 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.455111	-0.217291	0.016766
2	6	-1.147307	-0.374541	2.063651
3	1	-2.192351	-0.383816	2.392063
4	1	-0.672059	-1.258073	2.494522
5	1	-0.660210	0.505117	2.492662
6	6	-1.039625	-0.418107	0.533349
7	6	-1.661607	-1.712947	-0.084485
8	6	-1.787236	0.675227	-0.186892
9	6	-2.247905	-1.313101	-1.460470
10	1	-2.455942	-2.081655	0.573374
11	1	-0.925806	-2.514689	-0.166792
12	6	-2.511800	0.172558	-1.321586
13	1	-1.530719	-1.460401	-2.275511
14	1	-3.147620	-1.874469	-1.727351
15	6	0.983680	1.227412	0.144552
16	6	1.438054	-1.177711	0.713850
17	6	2.459672	1.323626	-0.165070

18	6	2.804251	-1.134780	0.013996
19	6	3.291963	0.274590	-0.247327
20	1	0.450384	-0.470574	-1.052669
21	1	1.060181	-2.205706	0.723565
22	1	1.564031	-0.870667	1.758542
23	1	3.538843	-1.665824	0.632812
24	1	2.767406	-1.689699	-0.935818
25	1	2.845234	2.326627	-0.336860
26	1	0.442507	1.895481	-0.542113
27	1	0.791045	1.619635	1.154996
28	6	4.748599	0.422846	-0.598990
29	1	5.011713	1.461804	-0.813561
30	1	5.387416	0.069089	0.219986
31	1	5.002672	-0.181818	-1.479102
32	6	-2.474099	1.832233	0.354359
33	6	-3.546245	0.749361	-0.112405
34	1	-2.721080	0.785378	-2.195164
35	1	-3.887363	0.030643	0.624825
36	1	-4.342782	1.228184	-0.676019
37	1	-2.355465	2.034310	1.414899
38	1	-2.563075	2.724866	-0.261075



TS (C'-to-E1')
4.08 [-4.75]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1435432 hartrees (-367177.573358 kcal/mol)
Imaginary Frequencies: 1 (-434.4638 1/cm)
Zero-point correction = 0.340262 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -366994.8548 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -585.1761043 hartrees (-367203.857209293 kcal/mol)

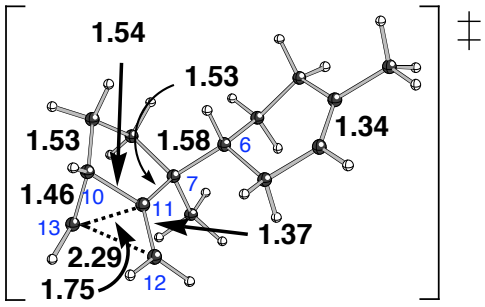
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0223408 hartrees (-367101.518852 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8212501 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.234144	0.145912	0.360244
2	6	1.670152	-0.068912	2.150330
3	1	2.741858	0.082165	2.313992
4	1	1.143124	0.560078	2.874778
5	1	1.436204	-1.112049	2.381339
6	6	1.293656	0.307693	0.724638
7	6	1.738683	1.737079	0.299890
8	6	1.886992	-0.504005	-0.451964
9	6	1.473638	1.739875	-1.231439
10	1	2.805850	1.852189	0.508463
11	1	1.219171	2.537882	0.827560
12	6	1.253012	0.281277	-1.518919
13	1	0.644112	2.371432	-1.563232
14	1	2.348565	2.056452	-1.817787
15	6	-0.849693	-1.233267	0.581950
16	6	-1.220219	1.247168	0.712399
17	6	-2.293577	-1.335274	0.154453
18	6	-2.547424	1.127638	-0.058687
19	6	-3.073878	-0.288179	-0.150264
20	1	-0.117003	0.189103	-0.869218
21	1	-0.798490	2.244923	0.577356
22	1	-1.416483	1.136222	1.790471
23	1	-3.293297	1.767973	0.427031
24	1	-2.433455	1.539757	-1.073320
25	1	-2.697118	-2.343458	0.095692
26	1	-0.257296	-2.013746	0.097235
27	1	-0.759599	-1.435663	1.662468
28	6	-4.499365	-0.441254	-0.608643
29	1	-4.787583	-1.491882	-0.692857
30	1	-5.189139	0.048820	0.089581
31	1	-4.651596	0.033832	-1.586260
32	6	2.240906	-1.968083	-0.523359
33	6	3.343015	-0.959295	-0.630110
34	1	1.027708	-0.093310	-2.519833
35	1	3.991358	-0.798749	0.226898
36	1	3.820123	-0.804995	-1.593117
37	1	2.168812	-2.538072	0.397953

38	1	1.963645	-2.519146	-1.418304



TS (C'-to-J)
-9.52 [-15.40]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1692899 hartrees (-367193.72941225 kcal/mol)
Imaginary Frequencies: 1 (-147.8454 1/cm)
Zero-point correction = 0.344350 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367008.6399 kcal/mol (298 Kelvin. 1.0 atm)

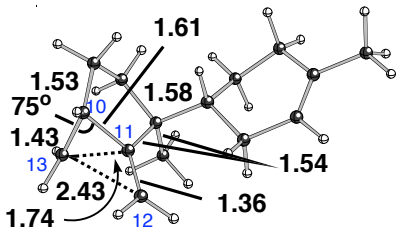
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.0433931 hartrees (-367114.72917025 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8441597 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.423200	-0.181361	0.049706
2	6	-1.163771	-0.269212	2.099314
3	1	-2.207830	-0.266610	2.431262
4	1	-0.684004	-1.141110	2.549233
5	1	-0.675387	0.618553	2.511145
6	6	-1.064760	-0.341420	0.565681
7	6	-1.684698	-1.659371	0.003832
8	6	-1.896029	0.735356	-0.140680
9	6	-2.240664	-1.329387	-1.396294
10	1	-2.487588	-2.005411	0.664885
11	1	-0.954793	-2.469179	-0.034101
12	6	-2.704779	0.125214	-1.305202

13	1	-1.463403	-1.392804	-2.162781
14	1	-3.055030	-1.992719	-1.699367
15	6	1.014499	1.235873	0.190757
16	6	1.391194	-1.175770	0.723817
17	6	2.483164	1.282165	-0.169256
18	6	2.744481	-1.185767	-0.001415
19	6	3.275181	0.204508	-0.276768
20	1	0.410073	-0.415903	-1.024467
21	1	0.981365	-2.190844	0.746106
22	1	1.549636	-0.873893	1.766202
23	1	3.474393	-1.741808	0.600680
24	1	2.666313	-1.739177	-0.949755
25	1	2.898113	2.271551	-0.351543
26	1	0.487130	1.945493	-0.464809
27	1	0.880354	1.610982	1.217655
28	6	4.725620	0.302961	-0.669268
29	1	5.019285	1.332631	-0.889107
30	1	5.374250	-0.076032	0.130509
31	1	4.932838	-0.308027	-1.557210
32	6	-2.020539	2.058915	0.196231
33	6	-3.629377	0.488819	-0.232933
34	1	-2.784215	0.715498	-2.215742
35	1	-3.873620	-0.196477	0.572256
36	1	-4.284675	1.346173	-0.337765
37	1	-1.559264	2.453781	1.098219
38	1	-2.560274	2.766200	-0.426642



J
-9.61 [-14.95]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -585.1695311 hartrees (-367193.88076525 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.344443 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367009.1325 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -585.0427731 hartrees (-367114.34012025 kcal/mol)

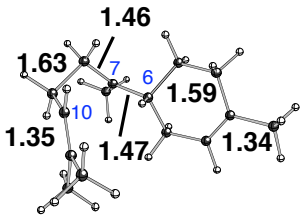
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -584.8430213 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.413527	-0.165451	0.066480
2	6	-1.177889	-0.317407	2.110760
3	1	-2.222394	-0.341141	2.439627
4	1	-0.683654	-1.194644	2.534057
5	1	-0.707126	0.567363	2.548833
6	6	-1.076417	-0.335106	0.573993
7	6	-1.675108	-1.643393	-0.031355
8	6	-1.944826	0.758685	-0.068371
9	6	-2.203989	-1.282749	-1.432287
10	1	-2.486021	-2.017171	0.603929
11	1	-0.936823	-2.444683	-0.078737
12	6	-2.756894	0.133469	-1.309590
13	1	-1.405272	-1.284508	-2.178247
14	1	-2.981512	-1.968839	-1.782060
15	6	1.023510	1.241503	0.225746
16	6	1.377509	-1.176564	0.722860
17	6	2.488211	1.276451	-0.148615
18	6	2.724036	-1.195222	-0.014597
19	6	3.267666	0.191580	-0.279541
20	1	0.401865	-0.379723	-1.011800
21	1	0.958820	-2.187964	0.741027
22	1	1.548774	-0.886054	1.766488
23	1	3.453649	-1.765986	0.573886
24	1	2.630287	-1.736991	-0.968311
25	1	2.912051	2.263649	-0.322119
26	1	0.502837	1.966804	-0.419000
27	1	0.901751	1.605643	1.258483
28	6	4.714699	0.280230	-0.685589
29	1	5.017377	1.309602	-0.894196
30	1	5.367490	-0.117459	0.101584
31	1	4.905497	-0.320537	-1.584160
32	6	-1.921440	2.101984	0.169546
33	6	-3.646908	0.435633	-0.229219
34	1	-2.803918	0.769780	-2.189900
35	1	-3.883699	-0.295817	0.537271
36	1	-4.285891	1.310724	-0.256177

37	1	-1.287728	2.530794	0.940261
38	1	-2.550482	2.795298	-0.382073

Figure 2a.



A1
0.00 [0.00]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4146838 hartrees (-367975.2140845 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.363052 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367782.467 kcal/mol (298 Kelvin. 1.0 atm)

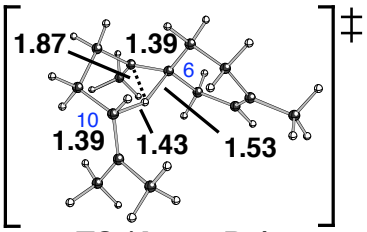
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2752278 hartrees (-367887.7054445 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0586615 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.294619	0.628322	1.173158
2	6	2.970260	0.787724	0.024316
3	6	2.654425	-0.041777	-1.201406
4	6	1.731369	-1.236013	-0.934600
5	6	0.553025	-0.774265	0.026528
6	6	1.162984	-0.350617	1.373226
7	1	2.224982	0.605317	-1.979775
8	1	2.557130	1.237877	2.034815
9	1	1.342710	-1.636130	-1.874960
10	1	2.278121	-2.038710	-0.427973
11	1	3.588099	-0.433500	-1.627816
12	6	-1.440478	-1.893679	-1.027790

13	6	-2.691605	-0.946632	-0.579133
14	1	-1.834117	-2.901840	-1.170038
15	1	-1.073306	-1.484886	-1.971858
16	6	-2.495801	0.494196	-0.897898
17	1	-3.507760	-1.359740	-1.181503
18	1	-2.942733	-1.134235	0.466492
19	6	-2.515625	1.541814	-0.041576
20	6	-0.453615	-1.839979	0.040170
21	6	-2.405946	2.951743	-0.562453
22	1	-3.296945	3.530870	-0.290204
23	1	-1.550849	3.468415	-0.108855
24	1	-2.296328	2.985445	-1.648967
25	6	-2.683878	1.431526	1.451372
26	1	-3.631504	1.892539	1.756952
27	1	-2.681426	0.406221	1.826935
28	1	-1.893014	1.990441	1.965940
29	1	-2.387700	0.714523	-1.959935
30	1	0.094914	0.094333	-0.476140
31	6	-0.511324	-2.837352	1.130001
32	1	0.430764	-3.409785	1.121626
33	1	-0.532640	-2.351991	2.113636
34	1	-1.343412	-3.535122	1.031417
35	1	1.521224	-1.229945	1.926503
36	1	0.385929	0.108236	1.998002
37	6	4.073449	1.800258	-0.134457
38	1	5.024923	1.309212	-0.373245
39	1	3.858248	2.489022	-0.961283
40	1	4.213545	2.391820	0.773496



TS (A1-to-D1)
8.05 [4.96]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3972994 hartrees (-367964.3053735 kcal/mol)
Imaginary Frequencies: 1 (-923.0860 1/cm)
Zero-point correction = 0.358495 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367773.2245 kcal/mol (298 Kelvin. 1.0 atm)

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -586.4302411 hartrees (-367990.840592661 kcal/mol)

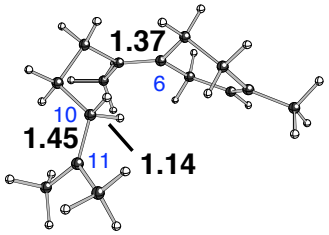
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2627619 hartrees (-367879.88309225 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0443193 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.284004	-0.468784	1.199884
2	6	2.775645	0.058111	0.069191
3	6	2.071747	-0.139263	-1.253902
4	6	1.015805	-1.255174	-1.225047
5	6	0.163730	-1.275921	0.045398
6	6	1.010124	-1.272245	1.313786
7	1	1.624236	0.813735	-1.573978
8	1	2.826043	-0.327644	2.132831
9	1	0.411959	-1.226958	-2.133349
10	1	1.537531	-2.222271	-1.231340
11	1	2.809905	-0.379618	-2.029032
12	6	-2.056433	-1.492060	-1.113638
13	6	-2.564899	-0.002356	-1.026034
14	1	-2.921267	-2.159069	-1.082894
15	1	-1.551118	-1.644031	-2.068500
16	6	-1.407791	0.960734	-0.832390
17	1	-3.087529	0.239274	-1.956869
18	1	-3.295813	0.082131	-0.218448
19	6	-1.363483	2.014780	0.070547
20	6	-1.159534	-1.710467	0.066541
21	6	-0.323464	3.081184	-0.064515
22	1	-0.813180	4.062692	-0.115910
23	1	0.315584	3.108794	0.826956
24	1	0.299979	2.957245	-0.951301
25	6	-2.293756	2.151552	1.234199
26	1	-3.043165	2.920064	0.995598
27	1	-2.831543	1.235170	1.479495
28	1	-1.761133	2.508186	2.121479
29	1	-0.774584	1.086266	-1.712765
30	1	-0.577065	0.057093	-0.106576
31	6	-1.848189	-2.188808	1.311495
32	1	-1.957186	-3.280083	1.223282

33	1	-1.303911	-1.993880	2.234416
34	1	-2.864228	-1.790079	1.397334
35	1	1.253419	-2.314560	1.576120
36	1	0.430536	-0.891769	2.162627
37	6	4.049242	0.861743	0.035613
38	1	4.806172	0.367427	-0.586042
39	1	3.881605	1.853006	-0.405291
40	1	4.468258	1.000727	1.035388



D1
3.92 [3.09]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4067226 hartrees (-367970.2184315 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.361338 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367779.3364 kcal/mol (298 Kelvin. 1.0 atm)

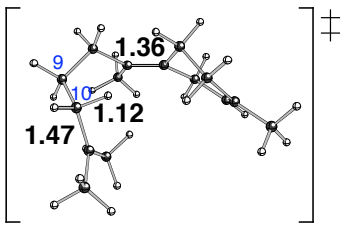
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2685837 hartrees (-367883.53627175 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0514714 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.936450	-0.041459	-1.041774
2	6	-2.958568	0.966144	-0.157805
3	6	-2.075372	0.932395	1.070325
4	6	-1.555130	-0.482126	1.393502
5	6	-1.025293	-1.196944	0.172418
6	6	-2.032826	-1.250019	-0.956646
7	1	-1.234116	1.632177	0.937361
8	1	-3.597730	-0.010427	-1.905665

9	1	-0.832570	-0.438894	2.210760
10	1	-2.406446	-1.071168	1.766002
11	1	-2.633162	1.310770	1.936188
12	6	1.211337	-1.845902	1.189854
13	6	2.430029	-0.964231	0.818783
14	1	1.571493	-2.869077	1.351383
15	1	0.800165	-1.507475	2.142805
16	6	1.940687	0.468857	0.531397
17	1	3.162432	-0.947726	1.633366
18	1	2.929949	-1.383656	-0.059234
19	6	2.764903	1.392518	-0.215361
20	6	0.180027	-1.835731	0.083594
21	6	2.653287	2.847491	0.015167
22	1	3.641347	3.229837	0.320698
23	1	2.439442	3.363669	-0.931268
24	1	1.915861	3.118228	0.770918
25	6	3.720750	0.923328	-1.242914
26	1	4.642307	0.613323	-0.720625
27	1	3.363918	0.031500	-1.766379
28	1	3.995158	1.706057	-1.952553
29	1	1.514632	0.948095	1.419130
30	1	1.033592	0.315816	-0.142179
31	6	0.557771	-2.644944	-1.147234
32	1	-0.128445	-3.489071	-1.285124
33	1	0.524472	-2.061942	-2.074390
34	1	1.562804	-3.065687	-1.056205
35	1	-2.649675	-2.156911	-0.824426
36	1	-1.535948	-1.392682	-1.922229
37	6	-3.848504	2.171191	-0.314863
38	1	-4.558996	2.246363	0.518082
39	1	-3.261749	3.099492	-0.310295
40	1	-4.418621	2.135985	-1.246772



TS (D1-to-D2)
8.54 [7.34]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3994222 hartrees (-367965.6374305 kcal/mol)

Imaginary Frequencies: 1 (-54.9328 1/cm)
Zero-point correction = 0.361407 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367772.7331 kcal/mol (298 Kelvin. 1.0 atm)

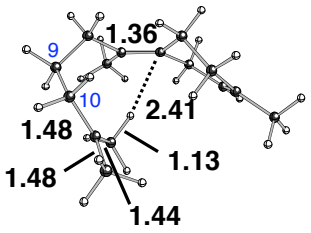
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2618917 hartrees (-367879.33704175 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0479467 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.709598	-1.324523	-0.182286
2	6	-1.012421	-2.508406	1.251862
3	1	-2.043366	-2.255568	1.528380
4	1	-1.012065	-3.588626	1.054509
5	1	-0.384103	-2.342717	2.127705
6	6	-0.564751	-1.761779	0.009981
7	6	-1.657274	-1.677941	-1.044754
8	6	-2.091507	1.635661	0.371233
9	6	-2.760785	-0.629037	-0.772235
10	1	-2.156044	-2.654268	-1.100257
11	1	-1.246671	-1.493809	-2.040582
12	6	-2.282526	0.849272	-0.851916
13	1	-3.547136	-0.747384	-1.524091
14	1	-3.243092	-0.817628	0.192584
15	6	-2.257890	3.097068	0.324600
16	1	-3.264499	3.289718	0.744616
17	1	-1.559891	3.619844	0.985092
18	1	-2.248846	3.508515	-0.686744
19	6	-1.662308	0.988822	1.606974
20	1	-1.433165	1.677952	2.418755
21	1	-2.403731	0.244942	1.931776
22	1	-0.786029	0.355141	1.346486
23	6	1.809075	-1.468280	0.853423
24	6	1.250257	-0.728477	-1.466498
25	6	2.751289	-0.283751	0.891285
26	6	1.901828	0.651250	-1.245741
27	6	2.798742	0.692383	-0.027445
28	1	0.503683	-0.665567	-2.261318
29	1	2.031808	-1.408789	-1.834042
30	1	2.481963	0.920494	-2.137894

31	1	1.131358	1.437580	-1.160292
32	1	3.432611	-0.249882	1.739722
33	1	1.406045	-1.630537	1.856887
34	1	2.385985	-2.381834	0.629238
35	6	3.743625	1.861806	0.072193
36	1	4.325324	1.835875	0.997260
37	1	4.445285	1.872674	-0.771468
38	1	3.200889	2.816150	0.038404
39	1	-1.229473	0.857458	-1.226932
40	1	-2.836552	1.435856	-1.591851



D2
8.18 [6.83]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3998298 hartrees (-367965.8931995 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.361237 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367773.8532 kcal/mol (298 Kelvin. 1.0 atm)

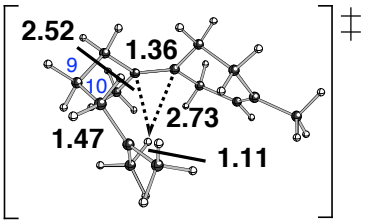
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.262534 hartrees (-367879.740085 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0475994 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.590618	-1.345602	0.293722
2	6	1.086309	-2.581597	-1.150153
3	1	2.040910	-2.256756	-1.582441
4	1	1.241954	-3.618568	-0.824176
5	1	0.349718	-2.601915	-1.953127
6	6	0.691048	-1.725048	0.035589

7	6	1.861390	-1.466096	0.979766
8	6	1.852430	1.716207	-0.456474
9	6	2.952700	-0.467869	0.516777
10	1	2.369794	-2.428215	1.126031
11	1	1.518667	-1.161882	1.972254
12	6	2.596090	1.028756	0.619287
13	1	3.822157	-0.617299	1.164882
14	1	3.304506	-0.703121	-0.494149
15	6	1.667448	3.177165	-0.359345
16	1	2.320762	3.632382	-1.124592
17	1	0.650550	3.466033	-0.649757
18	1	1.932747	3.594042	0.613353
19	6	1.275938	0.990286	-1.564104
20	1	0.774958	1.604588	-2.311243
21	1	1.990407	0.291614	-2.017536
22	1	0.553849	0.269491	-1.080768
23	6	-1.767662	-1.690894	-0.597660
24	6	-1.044404	-0.586602	1.523929
25	6	-2.779943	-0.571591	-0.710029
26	6	-1.780201	0.718887	1.159148
27	6	-2.795260	0.532457	0.052696
28	1	-0.232745	-0.373923	2.222284
29	1	-1.754539	-1.229245	2.063366
30	1	-2.278961	1.110828	2.054963
31	1	-1.060355	1.504515	0.869034
32	1	-3.543928	-0.701674	-1.474456
33	1	-1.450899	-1.981686	-1.602716
34	1	-2.265623	-2.586288	-0.187657
35	6	-3.814584	1.628699	-0.119015
36	1	-4.478402	1.436363	-0.965733
37	1	-4.432395	1.734395	0.781724
38	1	-3.330890	2.601498	-0.280967
39	1	2.000934	1.225373	1.533583
40	1	3.492746	1.646498	0.803041



TS (D2-to-D3)
8.53 [7.18]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3991759 hartrees (-367965.48287725 kcal/mol)
Imaginary Frequencies: 1 (-115.0768 1/cm)
Zero-point correction = 0.361134 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367772.7538 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -586.4352928 hartrees (-367994.010584928 kcal/mol)

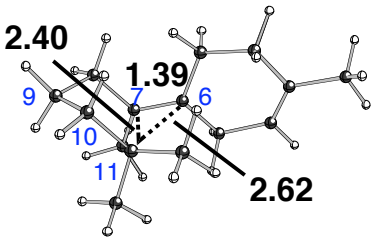
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2618644 hartrees (-367879.319911 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0482332 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.685394	-0.679494	0.768997
2	6	2.786759	0.391316	-0.033549
3	6	1.830562	0.582630	-1.190930
4	6	1.026377	-0.688563	-1.526561
5	6	0.495078	-1.377340	-0.284909
6	6	1.629562	-1.757472	0.649711
7	1	1.149007	1.423126	-0.970358
8	1	3.410638	-0.813522	1.569960
9	1	0.247938	-0.451715	-2.254694
10	1	1.707917	-1.391861	-2.025944
11	1	2.390300	0.901623	-2.080066
12	6	-1.937828	-1.367445	-1.023324
13	6	-2.958768	-0.292787	-0.572989
14	1	-2.511465	-2.291364	-1.173432
15	1	-1.561126	-1.092056	-2.011712
16	6	-2.461962	1.160134	-0.645253
17	1	-3.823203	-0.353452	-1.242249
18	1	-3.348423	-0.514897	0.426306
19	6	-1.698543	1.791668	0.440755
20	6	-0.805917	-1.677803	-0.050964
21	6	-1.461438	1.130472	1.715661
22	1	-1.053108	1.777093	2.492162
23	1	-2.328831	0.559632	2.063436
24	1	-0.719559	0.340937	1.452670
25	6	-1.167248	3.152018	0.237955
26	1	-1.288390	3.534619	-0.775611

27	1	-1.674174	3.820945	0.952690
28	1	-0.111024	3.182899	0.539715
29	1	-3.326191	1.857933	-0.723968
30	1	-1.933791	1.370281	-1.590098
31	6	-1.276151	-2.496987	1.138192
32	1	-1.427580	-3.541272	0.834453
33	1	-0.581271	-2.505724	1.978622
34	1	-2.245779	-2.150565	1.515703
35	1	2.101754	-2.682651	0.278006
36	1	1.269417	-2.009711	1.650752
37	6	3.855527	1.439926	0.138851
38	1	4.514922	1.476039	-0.737631
39	1	3.420257	2.443470	0.241315
40	1	4.473333	1.248543	1.020123



D3
1.08 [-2.47]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4148545 hartrees (-367975.32119875 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.364943 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367779.0434 kcal/mol (298 Kelvin. 1.0 atm)

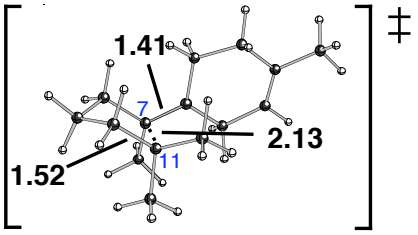
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2810515 hartrees (-367891.35981625 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0699507 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.200341	-0.753922	-0.200616

2	6	-1.709192	-2.046143	0.828698
3	1	-2.799625	-1.996338	0.872597
4	1	-1.454437	-3.071446	0.526658
5	1	-1.314746	-1.902890	1.834449
6	6	-1.147713	-1.102311	-0.213203
7	6	-2.045777	-0.913785	-1.416932
8	6	-1.439787	1.133862	0.592609
9	6	-3.074185	0.201099	-1.127574
10	1	-2.566158	-1.856005	-1.621750
11	1	-1.483201	-0.661584	-2.317370
12	6	-2.298659	1.415465	-0.610837
13	1	-3.632667	0.459149	-2.031613
14	1	-3.810255	-0.133525	-0.389174
15	6	-0.231226	2.007915	0.770964
16	1	-0.603122	2.971426	1.153880
17	1	0.472317	1.627410	1.514825
18	1	0.286921	2.217047	-0.163457
19	6	-2.118024	0.765684	1.877823
20	1	-1.434442	0.300140	2.592625
21	1	-2.436965	1.712982	2.339071
22	1	-3.005280	0.146302	1.757006
23	6	1.070077	-1.165792	0.964132
24	6	0.923197	-0.240832	-1.423317
25	6	2.511125	-0.729147	0.918945
26	6	2.241944	0.524249	-1.200957
27	6	3.063791	0.027070	-0.037711
28	1	0.264192	0.330608	-2.079824
29	1	1.162564	-1.161150	-1.983006
30	1	2.830560	0.452772	-2.123292
31	1	2.055761	1.599129	-1.072892
32	1	3.121035	-1.075106	1.750524
33	1	0.612201	-0.831849	1.907542
34	1	1.024004	-2.265774	1.032390
35	6	4.509864	0.444487	-0.012639
36	1	5.017875	0.092808	0.888623
37	1	5.045732	0.049234	-0.884512
38	1	4.604453	1.537066	-0.054112
39	1	-1.690094	1.848469	-1.411222
40	1	-3.001282	2.203739	-0.294279



TS (D3-to-E1)
1.59 [-3.10]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4144347 hartrees (-367975.05777425 kcal/mol)
Imaginary Frequencies: 1 (-113.5264 1/cm)
Zero-point correction = 0.365337 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367777.9101 kcal/mol (298 Kelvin. 1.0 atm)

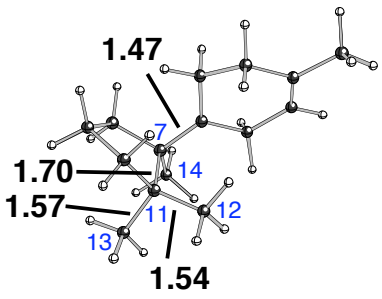
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2824575 hartrees (-367892.24208125 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0717779 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.249180	0.625432	-0.380880
2	6	1.660897	2.143116	0.249125
3	1	2.751839	2.146928	0.280637
4	1	1.359095	3.006121	-0.358009
5	1	1.289923	2.309793	1.259448
6	6	1.133804	0.884808	-0.429643
7	6	1.998386	0.460824	-1.616331
8	6	1.510209	-0.791048	0.821527
9	6	3.106181	-0.476792	-1.105543
10	1	2.418734	1.358511	-2.081999
11	1	1.420414	-0.050789	-2.388362
12	6	2.388455	-1.483844	-0.209097
13	1	3.626817	-0.970650	-1.930305
14	1	3.862047	0.081598	-0.542394
15	6	0.330151	-1.619956	1.291654
16	1	0.745251	-2.436423	1.898597
17	1	-0.359057	-1.068551	1.935270
18	1	-0.220023	-2.084550	0.473996

19	6	2.235216	-0.145333	1.979833
20	1	1.582912	0.485484	2.588789
21	1	2.564381	-0.966553	2.631837
22	1	3.121834	0.418389	1.692319
23	6	-1.116835	1.363046	0.597540
24	6	-0.960960	-0.218018	-1.394918
25	6	-2.562461	0.948666	0.674999
26	6	-2.285045	-0.881804	-0.969458
27	6	-3.113327	-0.058114	-0.014012
28	1	-0.297239	-0.945748	-1.864404
29	1	-1.190487	0.517435	-2.188857
30	1	-2.863569	-1.087067	-1.877597
31	1	-2.097368	-1.868741	-0.525700
32	1	-3.171444	1.531465	1.361837
33	1	-0.656139	1.331201	1.595874
34	1	-1.046288	2.431498	0.325337
35	6	-4.559822	-0.448459	0.125695
36	1	-5.074580	0.162458	0.870967
37	1	-5.087399	-0.341493	-0.830099
38	1	-4.654630	-1.500907	0.421654
39	1	1.781940	-2.162651	-0.818726
40	1	3.099032	-2.111909	0.346936



E1
-0.20 [-7.07]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4181428 hartrees (-367977.384607 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.366199 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367779.2009 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.289635 hartrees (-367896.7459625 kcal/mol)

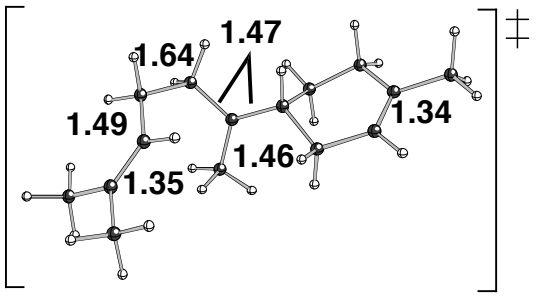
mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0819359 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.280553	-0.272378	-0.647829
2	6	-1.596000	-1.851705	-1.134618
3	1	-2.681273	-1.912128	-1.206448
4	1	-1.195362	-2.066356	-2.131013
5	1	-1.266398	-2.644125	-0.458368
6	6	-1.175050	-0.438270	-0.681039
7	6	-1.913941	0.687920	-1.479739
8	6	-1.683243	-0.101731	0.907161
9	6	-2.293128	1.841037	-0.509930
10	1	-2.809583	0.241990	-1.918464
11	1	-1.313187	1.033719	-2.325993
12	6	-1.777202	1.435354	0.884101
13	1	-1.874096	2.800020	-0.828864
14	1	-3.377984	1.975084	-0.497793
15	6	-0.760587	-0.630245	2.011180
16	1	-1.203154	-0.395971	2.984636
17	1	-0.647311	-1.718878	1.970993
18	1	0.236864	-0.178187	1.992845
19	6	-3.079975	-0.722662	1.079437
20	1	-3.053291	-1.813946	1.108757
21	1	-3.473062	-0.380403	2.043306
22	1	-3.788507	-0.409952	0.308544
23	6	1.187418	-1.432364	-0.503407
24	6	0.957222	1.026282	-0.848775
25	6	2.627486	-1.150575	-0.165377
26	6	2.197815	1.272638	0.038434
27	6	3.107033	0.068004	0.119534
28	1	-0.797119	1.878468	1.091097
29	1	0.276472	1.875010	-0.857139
30	1	1.324222	0.917103	-1.891886
31	1	2.738156	2.127805	-0.380864
32	1	1.888510	1.583864	1.046186
33	1	3.273028	-2.022988	-0.114398
34	1	0.745912	-2.168924	0.181330
35	1	1.109361	-1.951924	-1.481524
36	6	4.527087	0.314875	0.546712
37	1	5.094080	-0.615465	0.624483
38	1	5.040274	0.974023	-0.163917

39	1	4.557685	0.816955	1.521925
40	1	-2.437168	1.778126	1.687495

Figure 2b.



TS (A1-to-A2)
4.22 [4.16]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4074559 hartrees (-367970.67857725 kcal/mol)
Imaginary Frequencies: 1 (-97.7772 1/cm)
Zero-point correction = 0.362544 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367777.8473 kcal/mol (298 Kelvin. 1.0 atm)

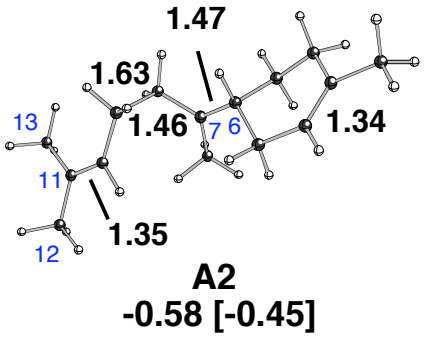
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2680972 hartrees (-367883.230993 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0509338 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.862342	1.465698	0.086356
2	6	3.832733	0.567978	-0.141967
3	6	3.559641	-0.919400	-0.100194
4	6	2.203769	-1.297618	0.509948
5	6	1.094069	-0.313974	-0.077507
6	6	1.423292	1.121447	0.382786
7	1	3.651986	-1.338308	-1.112281
8	1	3.097635	2.527007	0.050086
9	1	1.966997	-2.342354	0.288232
10	1	2.219478	-1.176606	1.597779
11	1	4.335668	-1.417902	0.496931

12	6	-0.899971	-1.802934	-0.561940
13	6	-2.324988	-1.212406	-1.118448
14	1	-1.174090	-2.710901	-0.013365
15	1	-0.280440	-2.074949	-1.417282
16	6	-2.675275	0.214641	-0.848559
17	1	-2.237834	-1.361040	-2.199091
18	1	-3.100318	-1.886833	-0.758215
19	6	-3.767147	0.677185	-0.197252
20	6	-0.182013	-0.899879	0.340562
21	6	-4.047084	2.158563	-0.139803
22	1	-5.002277	2.383047	-0.630251
23	1	-4.145925	2.500060	0.897888
24	1	-3.268311	2.748833	-0.629301
25	6	-4.809461	-0.184800	0.468697
26	1	-5.768331	-0.083153	-0.054524
27	1	-4.560354	-1.247117	0.499964
28	1	-4.983889	0.155157	1.496336
29	1	-2.015027	0.956051	-1.301693
30	1	1.182346	-0.382334	-1.168342
31	6	-0.801179	-0.572539	1.625238
32	1	-0.124156	-0.154236	2.369422
33	1	-1.535144	0.221110	1.345450
34	1	-1.401568	-1.388180	2.035379
35	1	1.217153	1.248519	1.453320
36	1	0.761369	1.822742	-0.140320
37	6	5.247444	0.967260	-0.468221
38	1	5.945885	0.592413	0.290169
39	1	5.564716	0.540767	-1.428262
40	1	5.357415	2.052859	-0.526194



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4157364 hartrees (-367975.874591 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.363176 (Hartree/Particle)

Sum of electronic and thermal Free Energies = -367783.3085 kcal/mol (298 Kelvin. 1.0 atm)

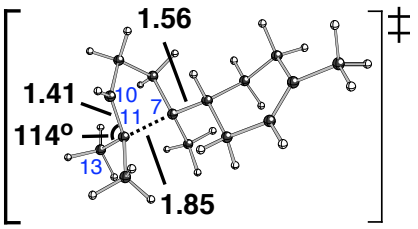
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2760635 hartrees (-367888.22984625 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0588449 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.098581	1.381004	-0.161706
2	6	3.990770	0.382409	-0.242966
3	6	3.599710	-1.051069	0.041263
4	6	2.227784	-1.209957	0.708666
5	6	1.191843	-0.258047	-0.022909
6	6	1.641987	1.208823	0.192147
7	1	3.640758	-1.632935	-0.890635
8	1	3.415221	2.399630	-0.375014
9	1	1.903165	-2.254085	0.662358
10	1	2.275472	-0.918886	1.763055
11	1	4.344865	-1.508967	0.706060
12	6	-1.057169	-1.369800	-0.354776
13	6	-1.908976	-0.315628	-1.265492
14	1	-1.782093	-1.949803	0.219051
15	1	-0.526098	-2.004898	-1.068958
16	6	-2.809779	0.617740	-0.528120
17	1	-1.193328	0.234212	-1.882063
18	1	-2.464142	-0.983545	-1.928258
19	6	-4.106373	0.398588	-0.203545
20	6	-0.136038	-0.620266	0.487052
21	6	-4.921697	1.474810	0.463882
22	1	-5.779666	1.745599	-0.163867
23	1	-5.336160	1.117658	1.414745
24	1	-4.340219	2.380041	0.655046
25	6	-4.849620	-0.880494	-0.484412
26	1	-5.711724	-0.679463	-1.132296
27	1	-4.244667	-1.653183	-0.962848
28	1	-5.257312	-1.294293	0.446001
29	1	-2.391980	1.593575	-0.282877
30	1	1.246469	-0.497637	-1.091625
31	6	-0.608915	-0.214633	1.819445
32	1	0.095956	0.373506	2.403879

33	1	-1.543148	0.359938	1.659009
34	1	-0.936855	-1.094686	2.388218
35	1	1.461406	1.522983	1.228111
36	1	1.029643	1.865798	-0.437884
37	6	5.426805	0.608052	-0.634904
38	1	6.105635	0.307847	0.172880
39	1	5.694104	0.005427	-1.512274
40	1	5.621208	1.656976	-0.871568



TS (A2-to-C1)
25.29 [19.87]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3762553 hartrees (-367951.10020075 kcal/mol)
Imaginary Frequencies: 1 (-343.5780 1/cm)
Zero-point correction = 0.364926 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367754.2147 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -586.4120675 hartrees (-367979.436476925 kcal/mol)

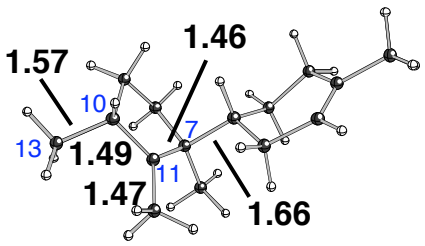
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.245441 hartrees (-367869.0142275 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0350867 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.431135	-0.182510	0.062263
2	6	-1.235507	-0.284191	2.014827
3	1	-2.241088	-0.546441	2.342898
4	1	-0.550365	-0.979996	2.512831
5	1	-0.991384	0.717710	2.377228

6	6	-1.038559	-0.433575	0.515604
7	6	-1.583800	-1.768629	-0.080097
8	6	-2.257720	0.695836	-0.292908
9	6	-1.976478	-1.423543	-1.531557
10	1	-2.432276	-2.136536	0.498107
11	1	-0.828150	-2.554761	-0.049509
12	6	-2.073950	0.049934	-1.536801
13	1	-1.236407	-1.744181	-2.274507
14	1	-2.925192	-1.869514	-1.878123
15	6	1.015960	1.228749	0.292215
16	6	1.402886	-1.192504	0.733821
17	6	2.495867	1.291452	-0.016261
18	6	2.763814	-1.174681	0.025682
19	6	3.297614	0.227365	-0.168896
20	1	0.482706	-0.372258	-1.021091
21	1	1.007179	-2.212830	0.736406
22	1	1.551372	-0.904643	1.780711
23	1	3.479977	-1.759833	0.616958
24	1	2.701654	-1.686428	-0.947117
25	1	2.908755	2.291506	-0.134423
26	1	0.514221	1.962420	-0.342850
27	1	0.837240	1.551986	1.328314
28	6	4.754250	0.349650	-0.529909
29	1	5.048132	1.390778	-0.686053
30	1	5.390609	-0.071886	0.258320
31	1	4.979770	-0.208979	-1.447526
32	6	-2.034428	2.207150	-0.253632
33	1	-1.679382	2.518659	0.732187
34	1	-1.316584	2.552156	-0.999097
35	1	-2.981290	2.726451	-0.432479
36	6	-3.624771	0.367822	0.397627
37	1	-3.629593	0.830179	1.385490
38	1	-4.414282	0.834569	-0.196708
39	1	-3.847352	-0.692370	0.492995
40	1	-1.846143	0.614292	-2.444836



C1
-3.72 [-10.02]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4236978 hartrees (-367980.8703695 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.366143 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367783.5878 kcal/mol (298 Kelvin. 1.0 atm)

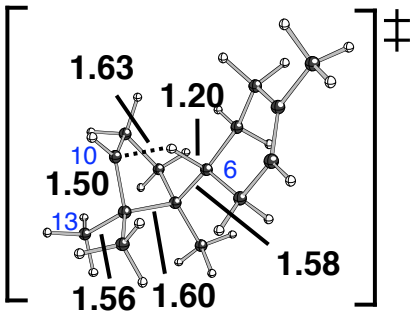
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2942943 hartrees (-367899.66967325 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0842133 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.502222	-0.170589	0.080975
2	6	-0.969004	-0.398333	2.259853
3	1	-1.984098	-0.416333	2.668651
4	1	-0.455483	-1.290095	2.623706
5	1	-0.450939	0.474601	2.664142
6	6	-1.008551	-0.414388	0.722695
7	6	-1.591353	-1.714896	0.093119
8	6	-1.805787	0.639571	0.100687
9	6	-2.068034	-1.297266	-1.312167
10	1	-2.433696	-2.055564	0.706410
11	1	-0.863489	-2.527868	0.075670
12	6	-2.480218	0.186035	-1.144016
13	1	-1.266201	-1.393455	-2.049138
14	1	-2.899771	-1.909277	-1.668236
15	6	-2.019674	1.977543	0.666196
16	1	-2.907461	1.878104	1.318501
17	1	-1.209468	2.307920	1.317239
18	1	-2.265627	2.730175	-0.086790

19	6	-4.027863	0.381171	-1.015363
20	1	-4.434913	-0.210346	-0.190489
21	1	-4.299956	1.429242	-0.873160
22	1	-4.484255	0.031522	-1.943824
23	6	1.067848	1.255283	0.172804
24	6	1.494372	-1.151449	0.734248
25	6	2.523059	1.304791	-0.240481
26	6	2.804994	-1.157245	-0.070995
27	6	3.316555	0.232445	-0.378984
28	1	0.409292	-0.429768	-0.977832
29	1	1.094264	-2.167598	0.788655
30	1	1.705359	-0.825813	1.758438
31	1	3.560301	-1.708490	0.504316
32	1	2.681249	-1.721462	-1.007444
33	1	2.919649	2.297341	-0.443547
34	1	0.504855	1.940449	-0.475344
35	1	0.968388	1.651300	1.195471
36	6	4.745614	0.333517	-0.841975
37	1	5.023074	1.362599	-1.083359
38	1	5.434213	-0.036417	-0.072182
39	1	4.911421	-0.283034	-1.734548
40	1	-2.161786	0.835124	-1.974884



TS (C1-to-E1)
26.72 [17.80]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.3726072 hartrees (-367948.811018 kcal/mol)
Imaginary Frequencies: 1 (-303.7392 1/cm)
Zero-point correction = 0.363557 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367751.5779 kcal/mol (298 Kelvin. 1.0 atm)
B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p):CPCM (solvent=benzene, radii=uaks)
HF = -586.4074442 hartrees (-367976.535309942 kcal/mol)

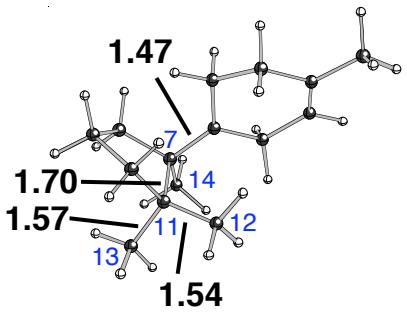
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.2473691 hartrees (-367870.22411025 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0390192 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.251328	0.069510	0.365562
2	6	1.640446	-0.480474	2.106278
3	1	2.713399	-0.380560	2.297449
4	1	1.119768	0.045561	2.913496
5	1	1.383383	-1.540848	2.179452
6	6	1.284735	0.111548	0.749892
7	6	1.736232	1.590344	0.574078
8	6	1.945516	-0.555961	-0.542078
9	6	1.515159	1.822252	-0.947458
10	1	2.782239	1.715833	0.856350
11	1	1.168150	2.282520	1.194806
12	6	1.312272	0.444565	-1.465302
13	1	0.701800	2.504082	-1.215666
14	1	2.403176	2.219393	-1.467984
15	6	1.610961	-2.016940	-0.908790
16	1	2.276338	-2.350958	-1.710180
17	1	1.775057	-2.682295	-0.056906
18	1	0.590812	-2.154642	-1.268343
19	6	3.500240	-0.434289	-0.608098
20	1	3.921743	-1.160382	0.093708
21	1	3.861009	-0.699667	-1.605780
22	1	3.891791	0.550415	-0.356504
23	6	-1.005316	-1.228093	0.689501
24	6	-1.170823	1.243716	0.716594
25	6	-2.428702	-1.257645	0.190734
26	6	-2.495984	1.206713	-0.069246
27	6	-3.121609	-0.166898	-0.166726
28	1	-0.155213	0.119771	-0.832990
29	1	-0.702356	2.217677	0.570132
30	1	-1.379527	1.166351	1.793552
31	1	-3.201389	1.899097	0.406410
32	1	-2.344449	1.607879	-1.083924
33	1	-2.894232	-2.238744	0.132917
34	1	-0.475821	-2.122872	0.370221
35	1	-0.994467	-1.276959	1.791758

36	6	-4.531622	-0.226531	-0.688601
37	1	-4.889557	-1.255522	-0.772722
38	1	-5.215915	0.321517	-0.029056
39	1	-4.605387	0.243164	-1.677771
40	1	1.028574	0.239291	-2.500474



E1
-0.20 [-7.07]

B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.4181428 hartrees (-367977.384607 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.366199 (Hartree/Particle)
Sum of electronic and thermal Free Energies = -367779.2009 kcal/mol (298 Kelvin. 1.0 atm)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.289635 hartrees (-367896.7459625 kcal/mol)

mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -586.0819359 hartrees

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.280553	-0.272378	-0.647829
2	6	-1.596000	-1.851705	-1.134618
3	1	-2.681273	-1.912128	-1.206448
4	1	-1.195362	-2.066356	-2.131013
5	1	-1.266398	-2.644125	-0.458368
6	6	-1.175050	-0.438270	-0.681039
7	6	-1.913941	0.687920	-1.479739
8	6	-1.683243	-0.101731	0.907161

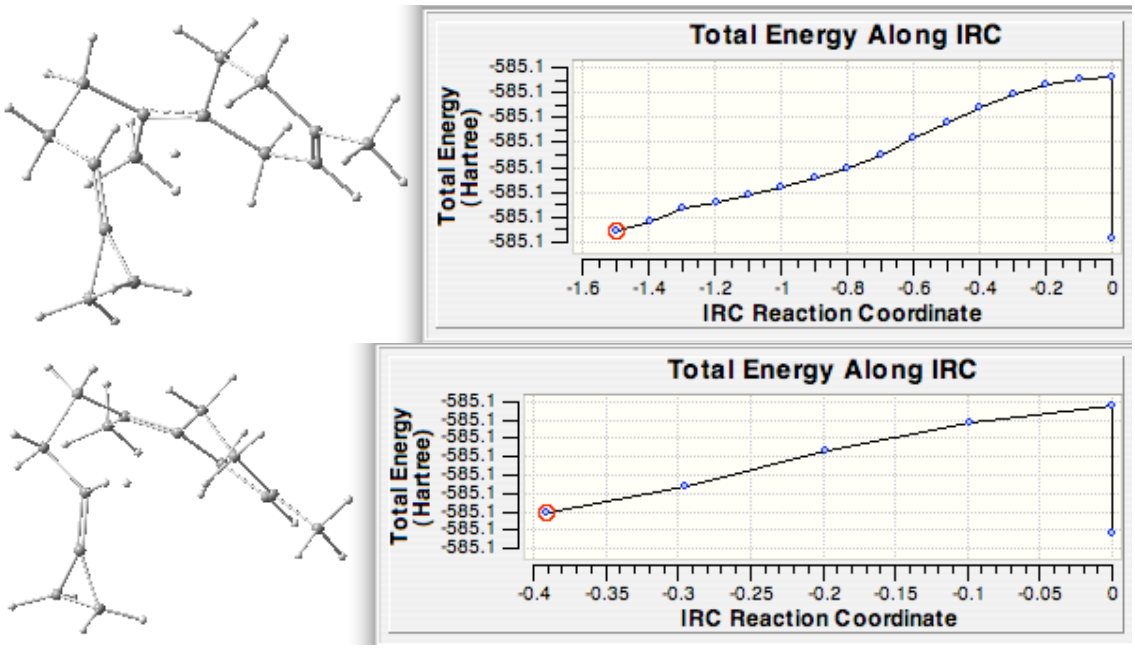
9	6	-2.293128	1.841037	-0.509930
10	1	-2.809583	0.241990	-1.918464
11	1	-1.313187	1.033719	-2.325993
12	6	-1.777202	1.435354	0.884101
13	1	-1.874096	2.800020	-0.828864
14	1	-3.377984	1.975084	-0.497793
15	6	-0.760587	-0.630245	2.011180
16	1	-1.203154	-0.395971	2.984636
17	1	-0.647311	-1.718878	1.970993
18	1	0.236864	-0.178187	1.992845
19	6	-3.079975	-0.722662	1.079437
20	1	-3.053291	-1.813946	1.108757
21	1	-3.473062	-0.380403	2.043306
22	1	-3.788507	-0.409952	0.308544
23	6	1.187418	-1.432364	-0.503407
24	6	0.957222	1.026282	-0.848775
25	6	2.627486	-1.150575	-0.165377
26	6	2.197815	1.272638	0.038434
27	6	3.107033	0.068004	0.119534
28	1	-0.797119	1.878468	1.091097
29	1	0.276472	1.875010	-0.857139
30	1	1.324222	0.917103	-1.891886
31	1	2.738156	2.127805	-0.380864
32	1	1.888510	1.583864	1.046186
33	1	3.273028	-2.022988	-0.114398
34	1	0.745912	-2.168924	0.181330
35	1	1.109361	-1.951924	-1.481524
36	6	4.527087	0.314875	0.546712
37	1	5.094080	-0.615465	0.624483
38	1	5.040274	0.974023	-0.163917
39	1	4.557685	0.816955	1.521925
40	1	-2.437168	1.778126	1.687495

III. IRC plots

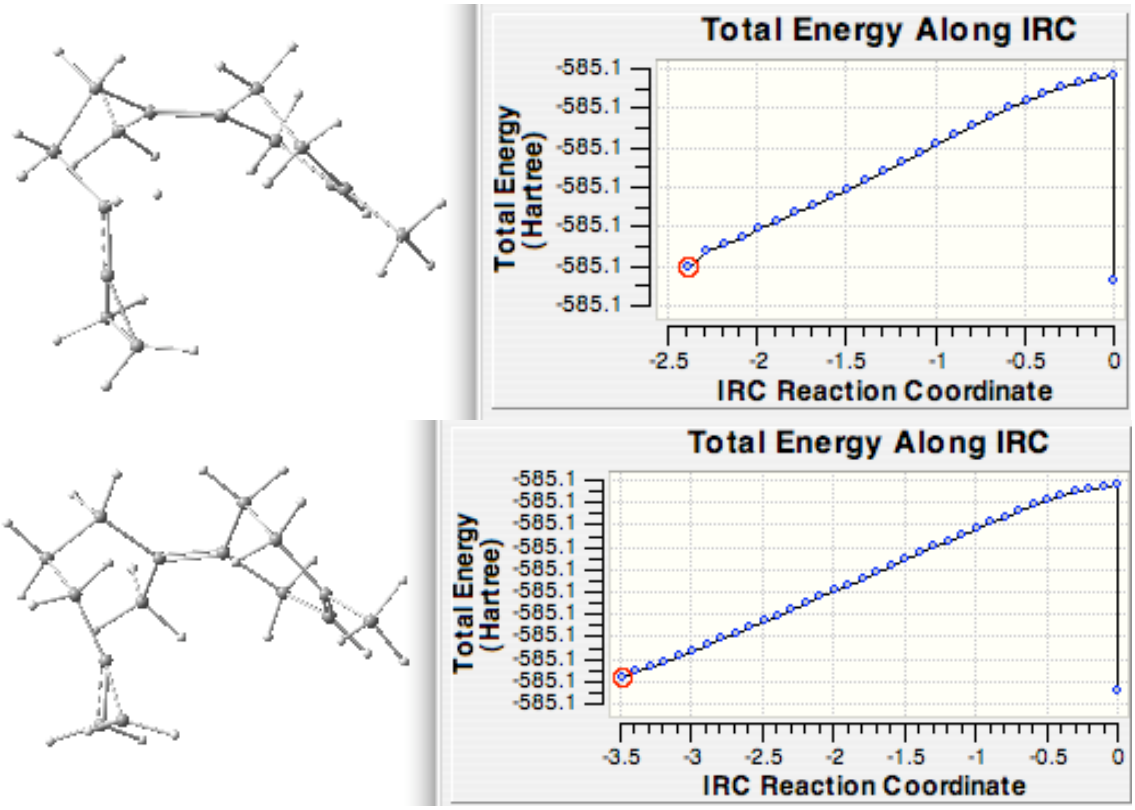
Following structures correspond to the structure at the last point from the forward and reverse IRC calculations.

Figure 1a.

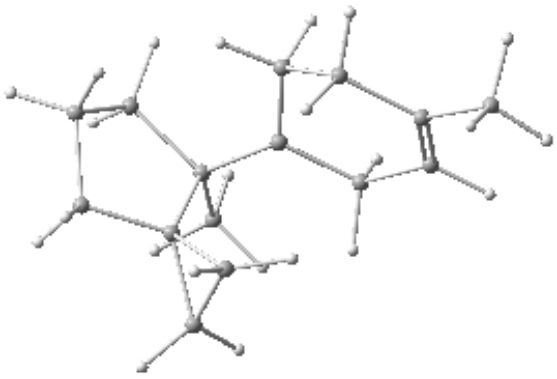
TS (A1'-to-D')

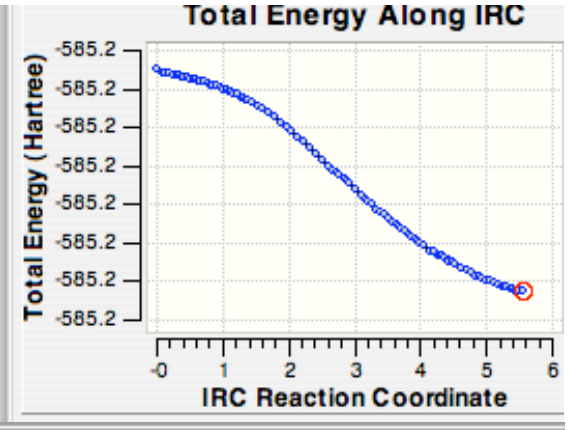


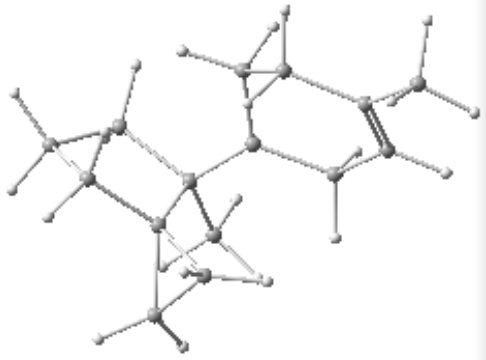
TS (D'-to-E1')

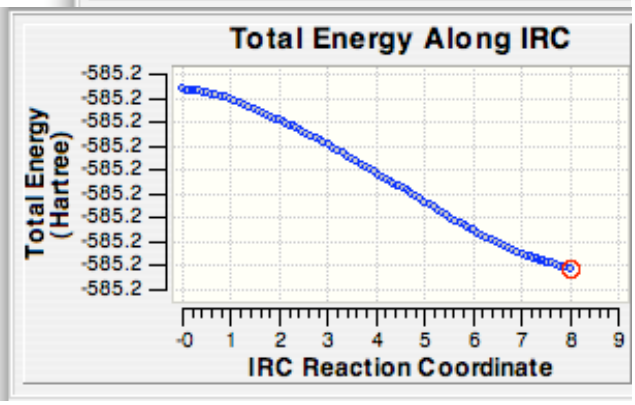


TS (E1'-to-E2')

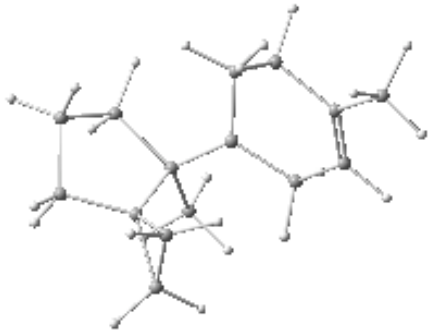


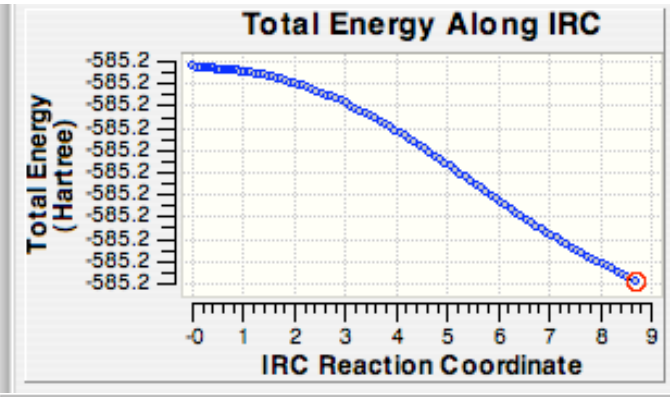


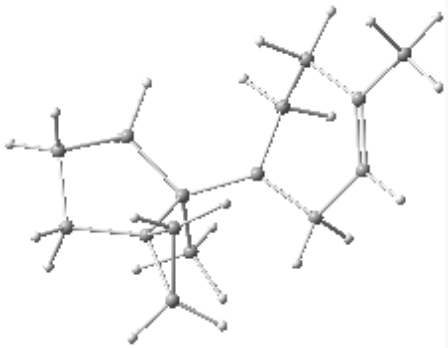


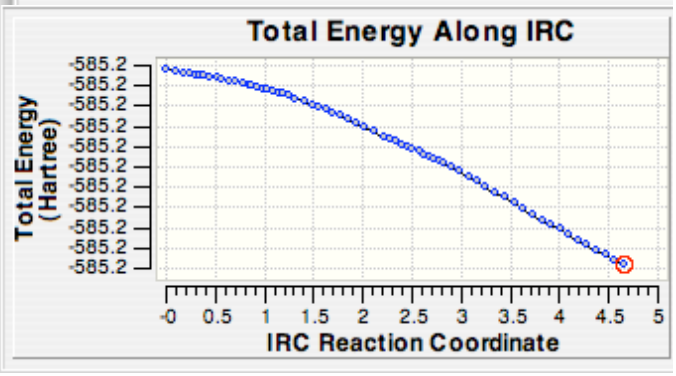


TS (E2'-to-E3')

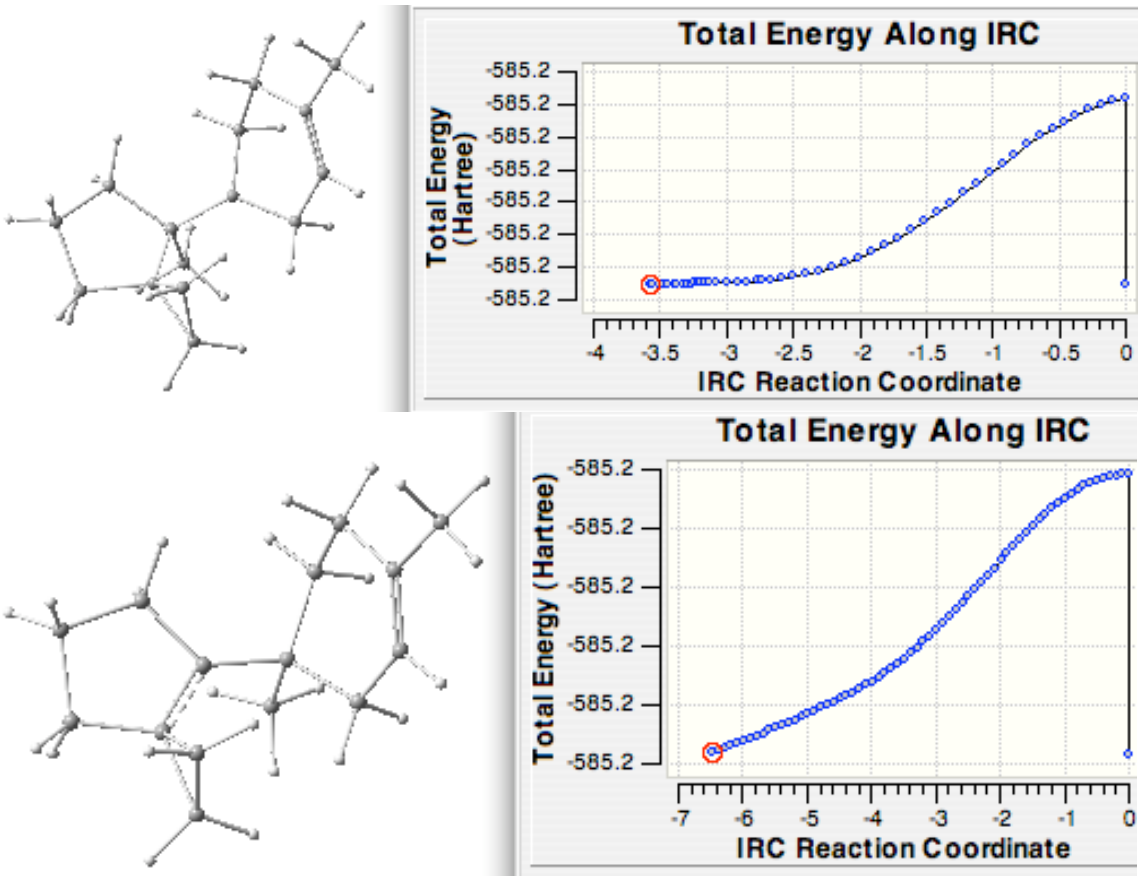




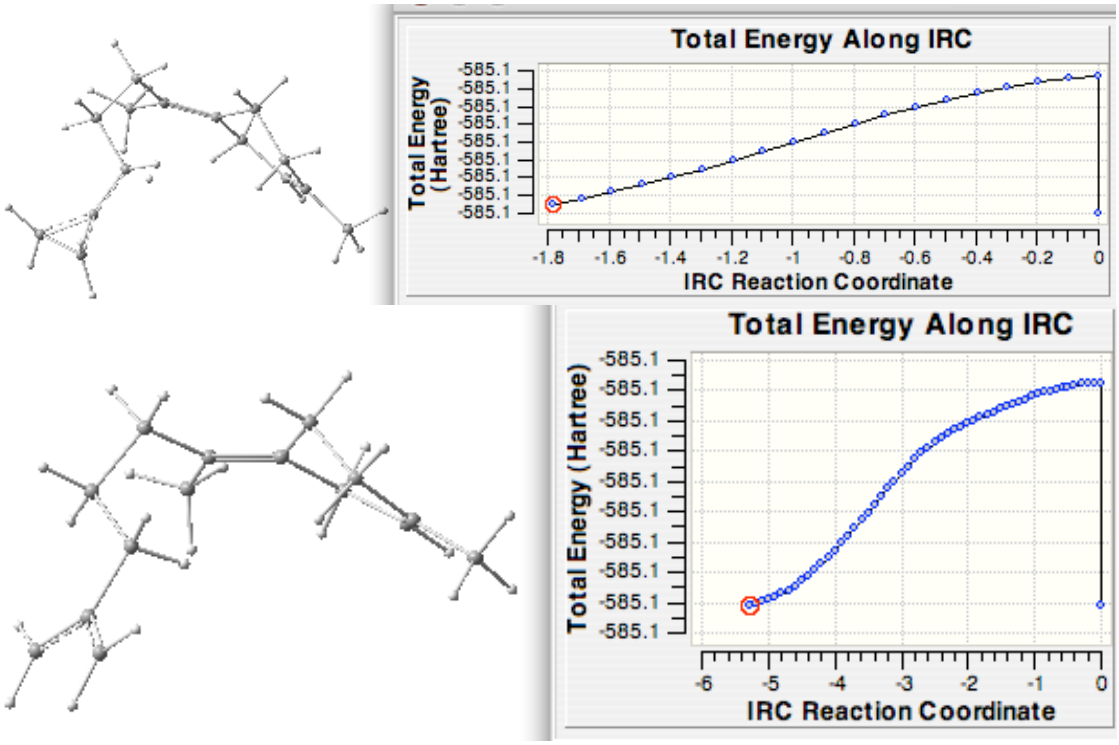




TS (E3'-to-F')


Total Energy Along IRC
Total Energy (Hartree)
-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
-4
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0
IRC Reaction Coordinate
Total Energy Along IRC
Total Energy (Hartree)
-585.2
-585.2
-585.2
-585.2
-585.2
-7
-6
-5
-4
-3
-2
-1
0
IRC Reaction Coordinate

TS (D'-to-K)


Total Energy Along IRC
Total Energy (Hartree)
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-585.1
-585.1
-585.1
-585.1
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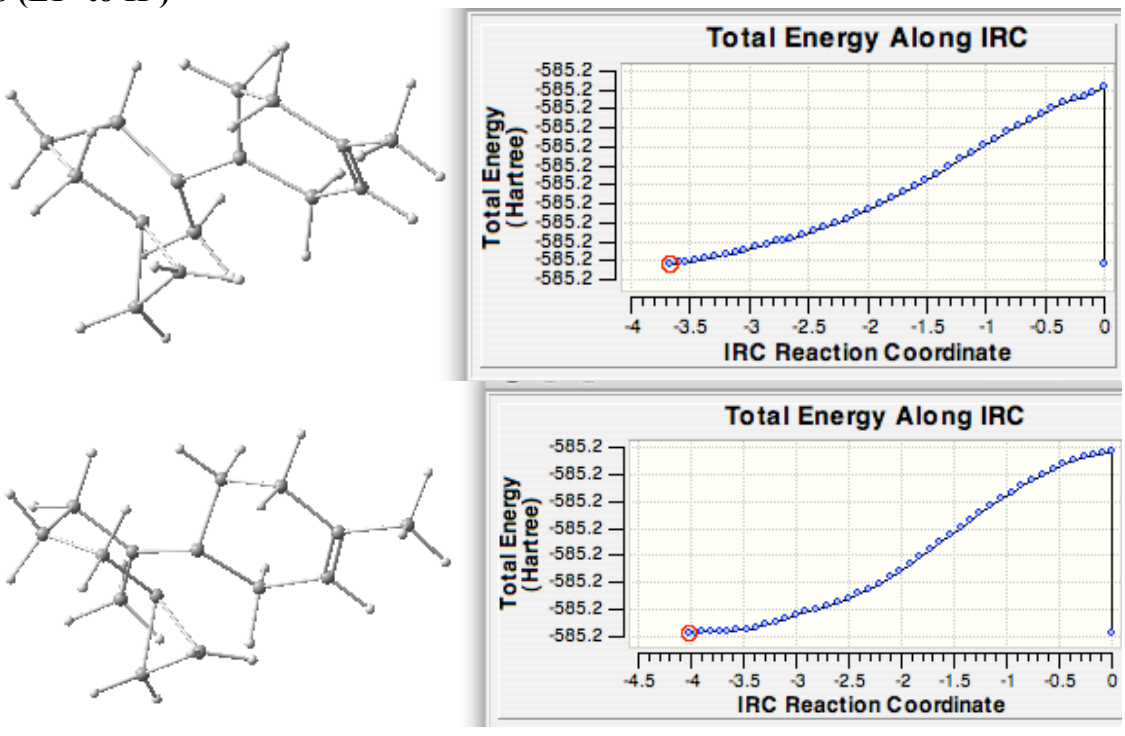
-585.1
-585.1
-1.8
-1.6
-1.4
-1.2
-1
-0.8
-0.6
-0.4
-0.2
0
IRC Reaction Coordinate
Total Energy Along IRC
Total Energy (Hartree)
-585.1
-585.1
-585.1
-585.1
-585.1
-585.1
-585.1
-585.1
-585.1
-585.1
-6
-5
-4
-3
-2
-1
0
IRC Reaction Coordinate

TS (E1'-to-H')


Total Energy Along IRC
Total Energy (Hartree)
-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
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-585.2
-585.2
-585.2
-585.2
-4
-3.5
-3
-2.5
-2
-1.5
-1
-0.5
0
IRC Reaction Coordinate
Total Energy Along IRC
Total Energy (Hartree)
-585.2
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-585.2
-585.2
-585.2
-585.2
-585.2
-585.2
-4.5
-4
-3.5
-3
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-2
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-1
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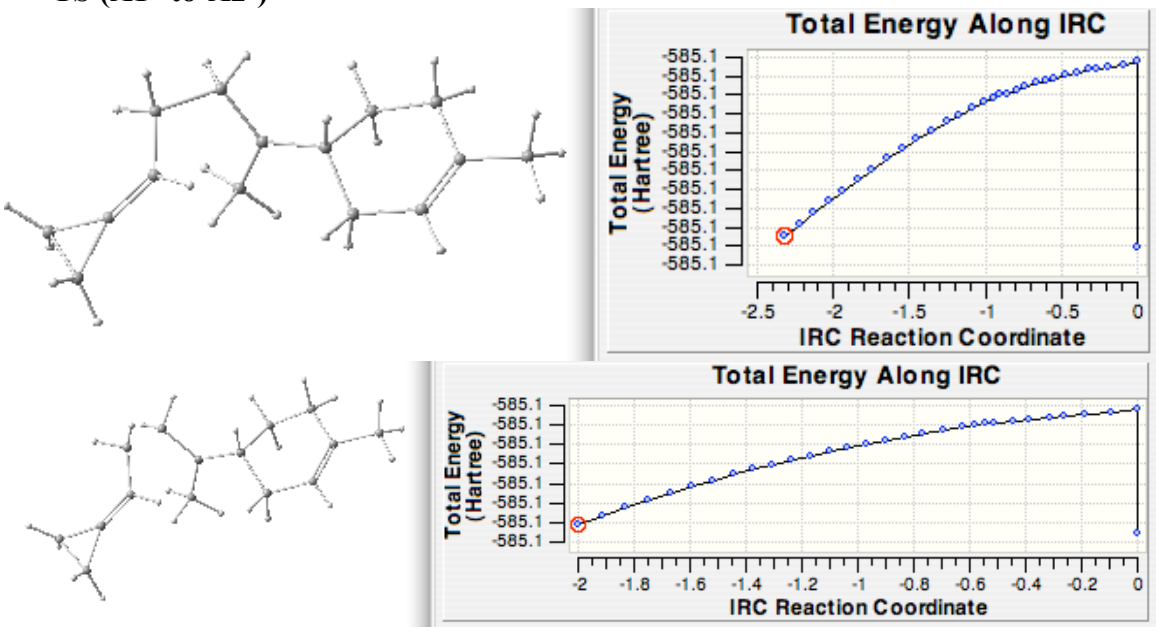
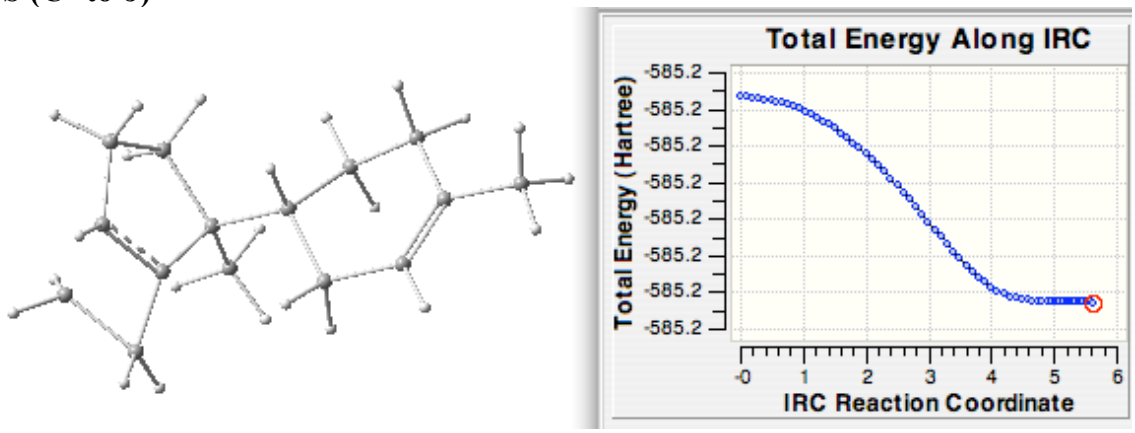
0
IRC Reaction Coordinate

Figure 1b.

TS (A1'-to-A2')



TS (C'-to-J)



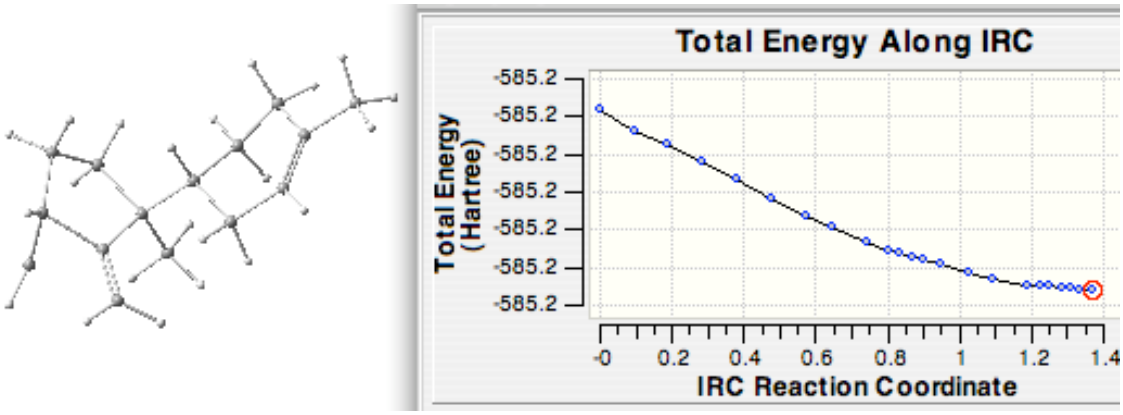
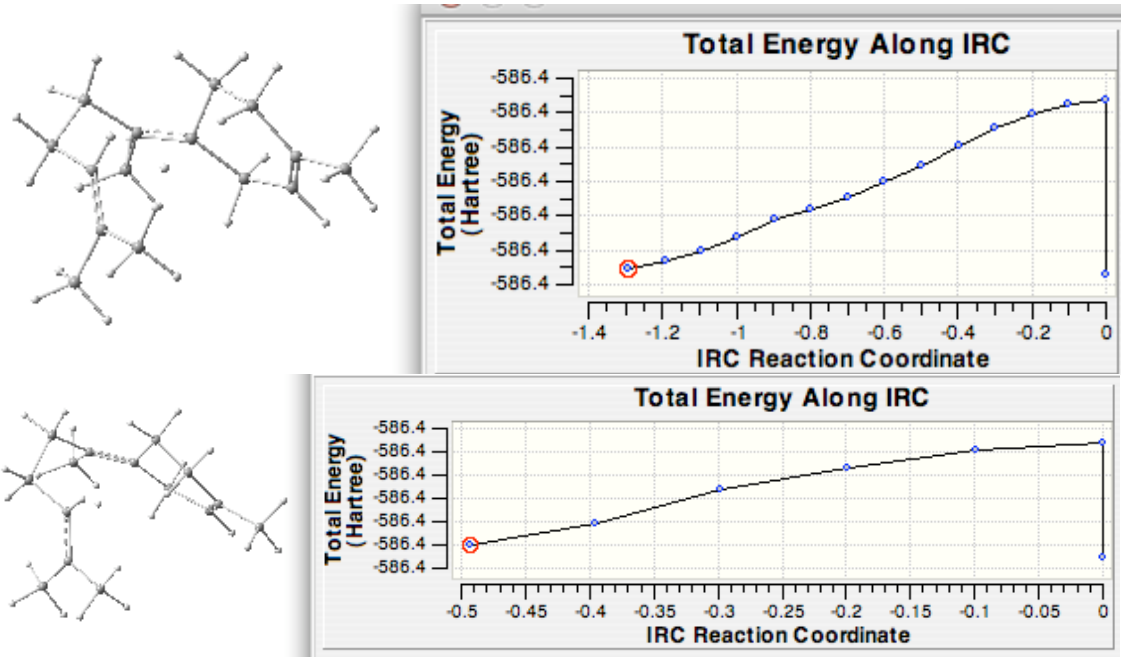
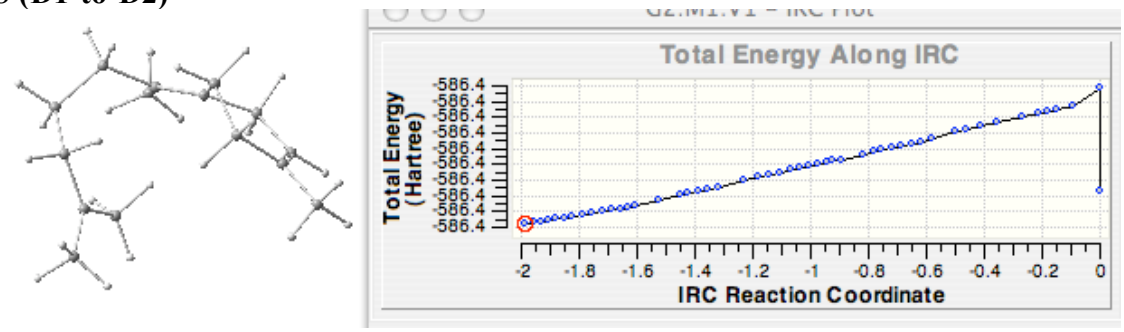


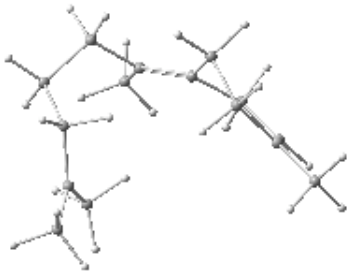
Figure 2a.

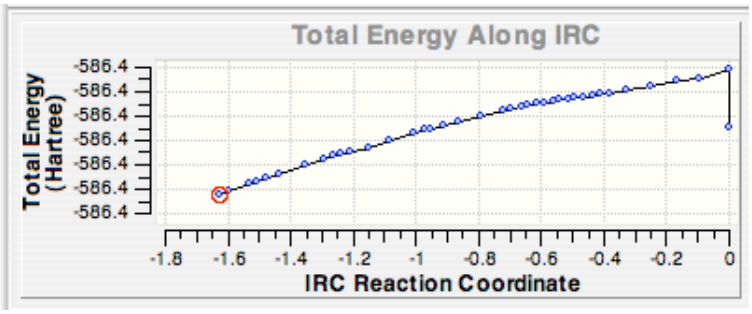
TS (A1-to-D1)



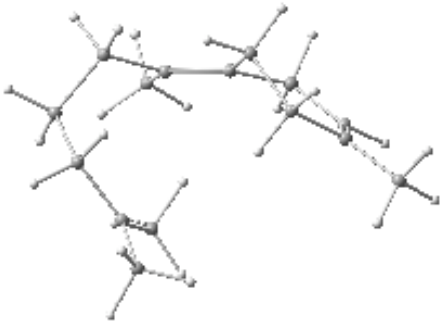
TS (D1-to-D2)

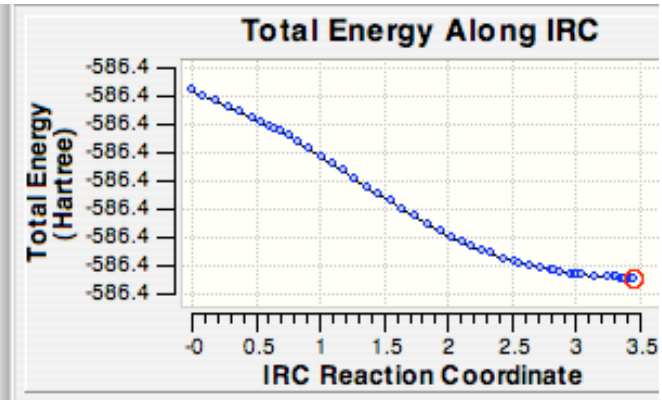


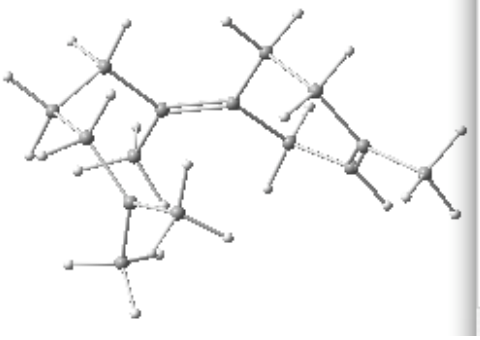


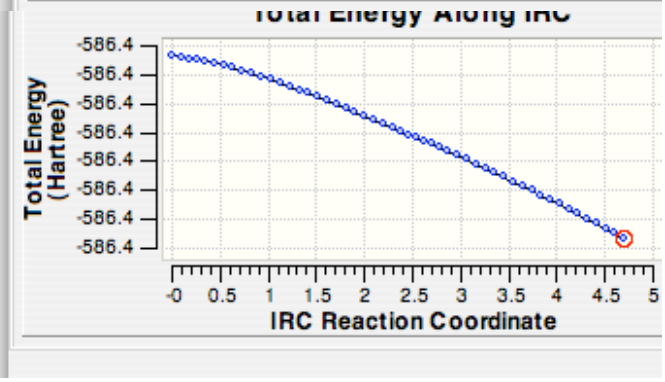


TS (D2-to-D3)

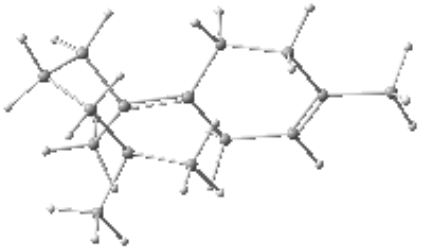


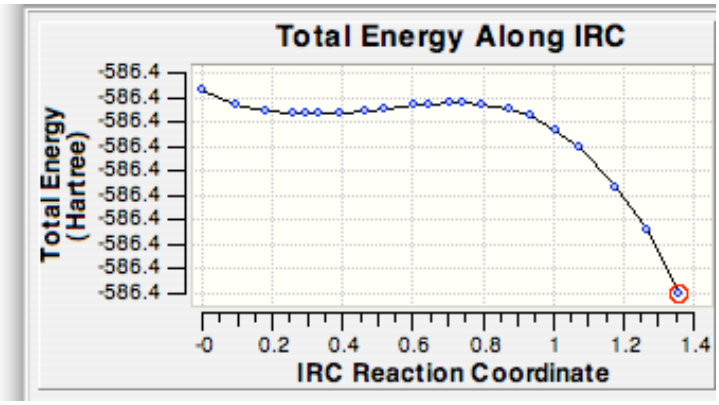




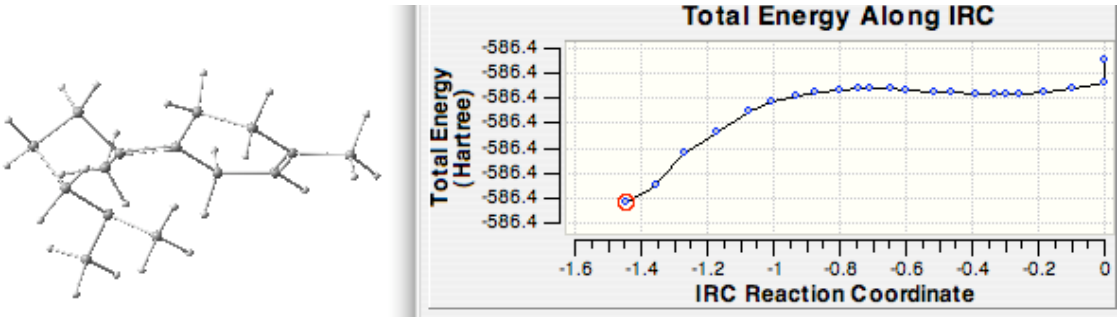


TS (D3-to-E1)

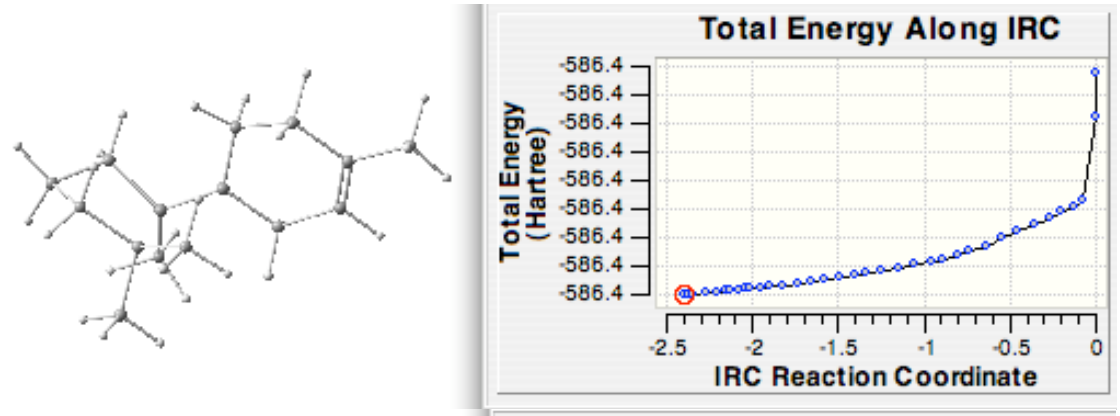




additional point calculations



additional point calculations



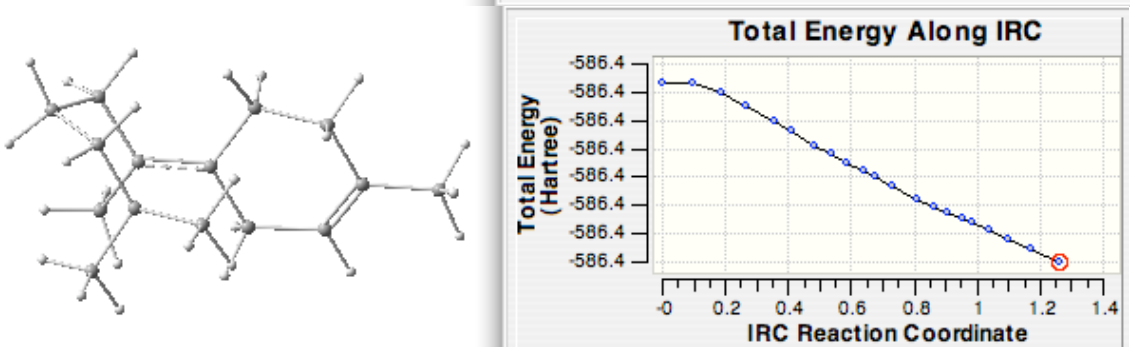
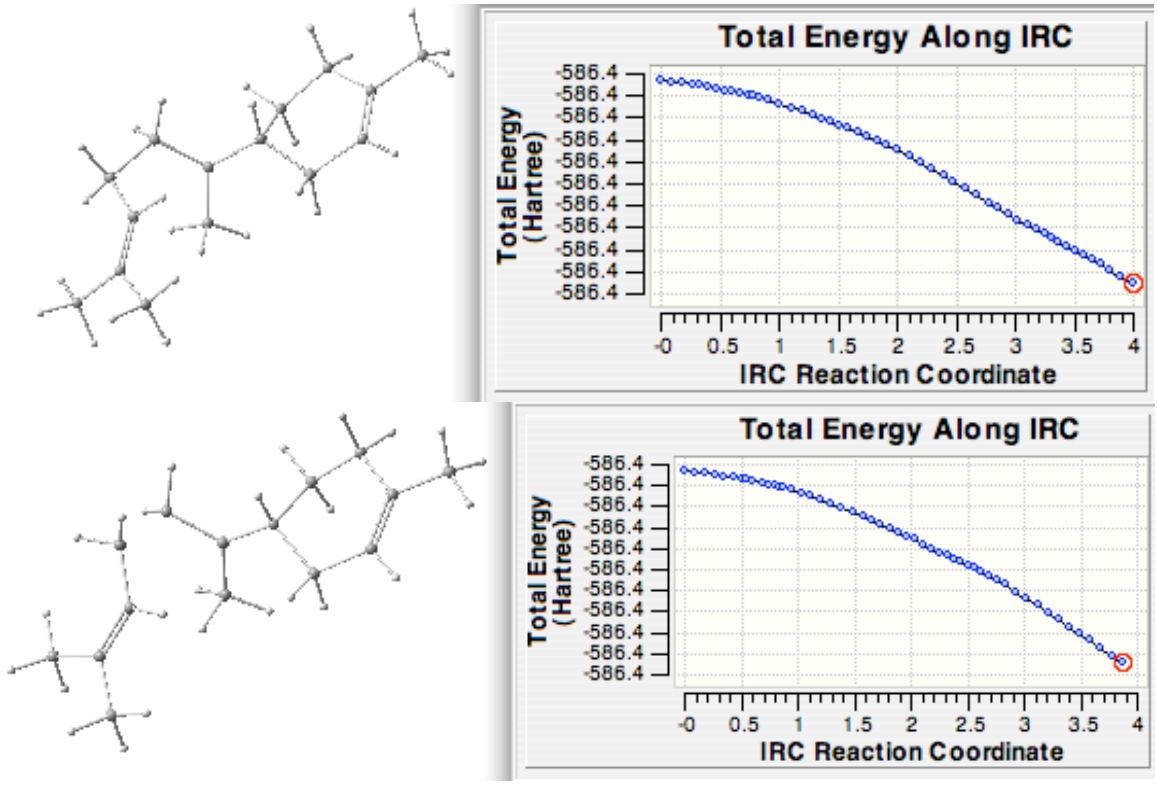
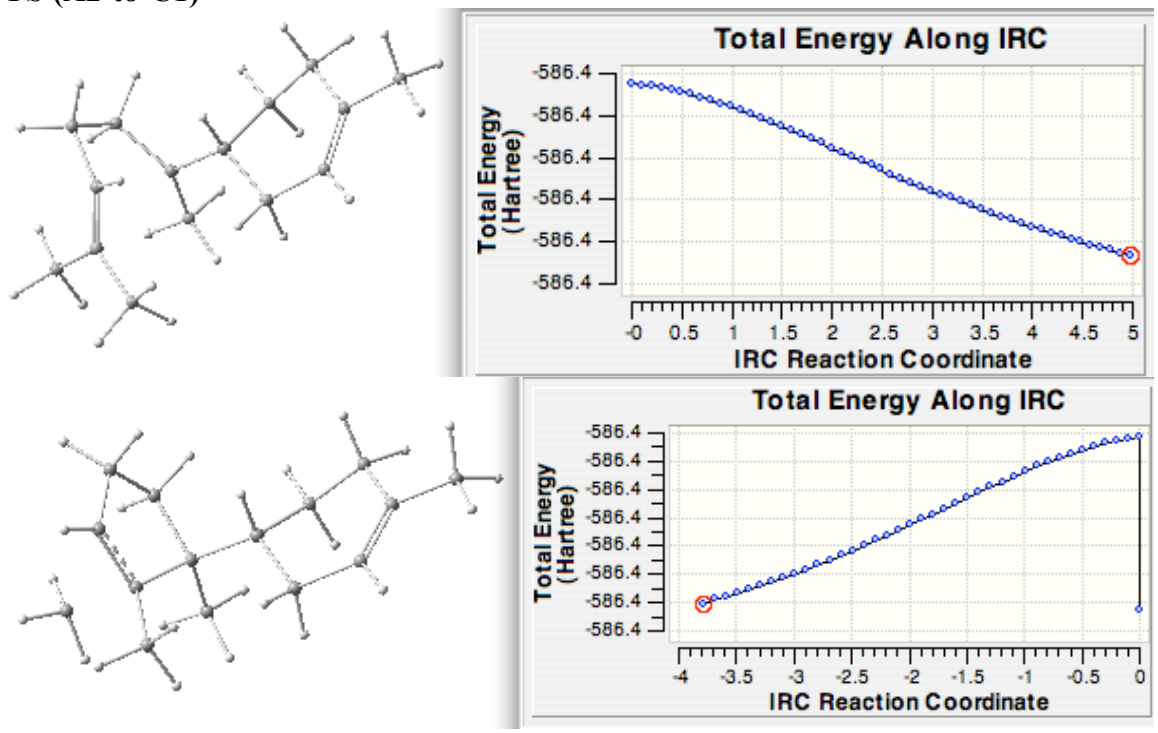


Figure 2b.

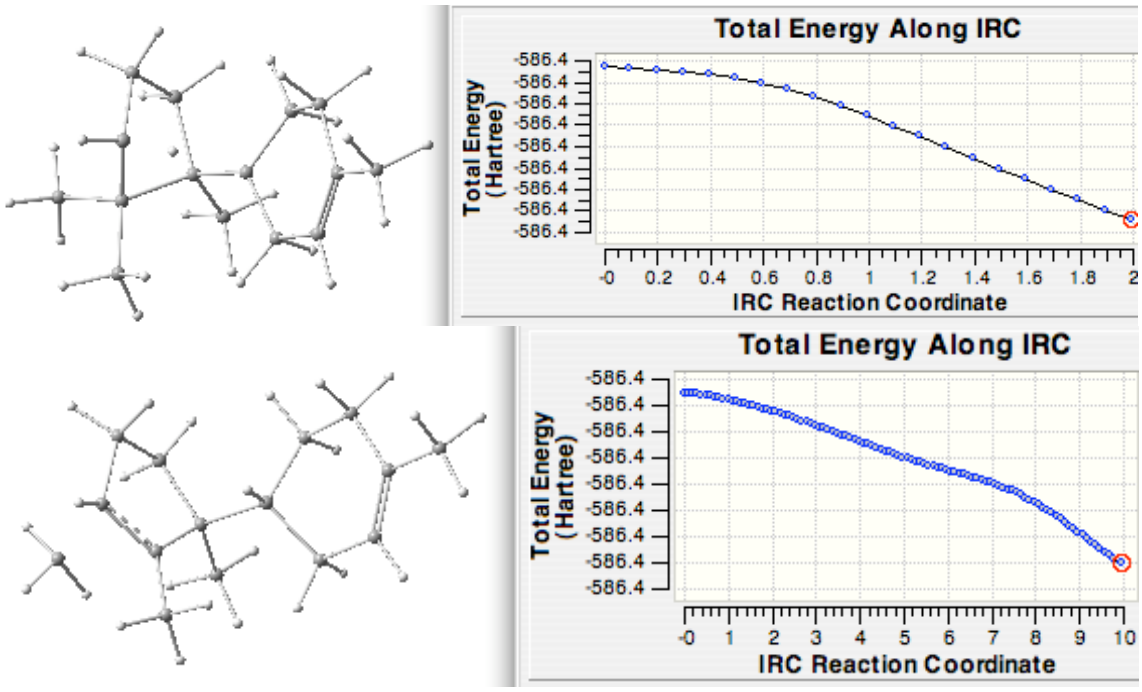
TS (A1-to-A2)



TS (A2-to-C1)



TS (C1-to-E1)



IV. Reaction Energetics

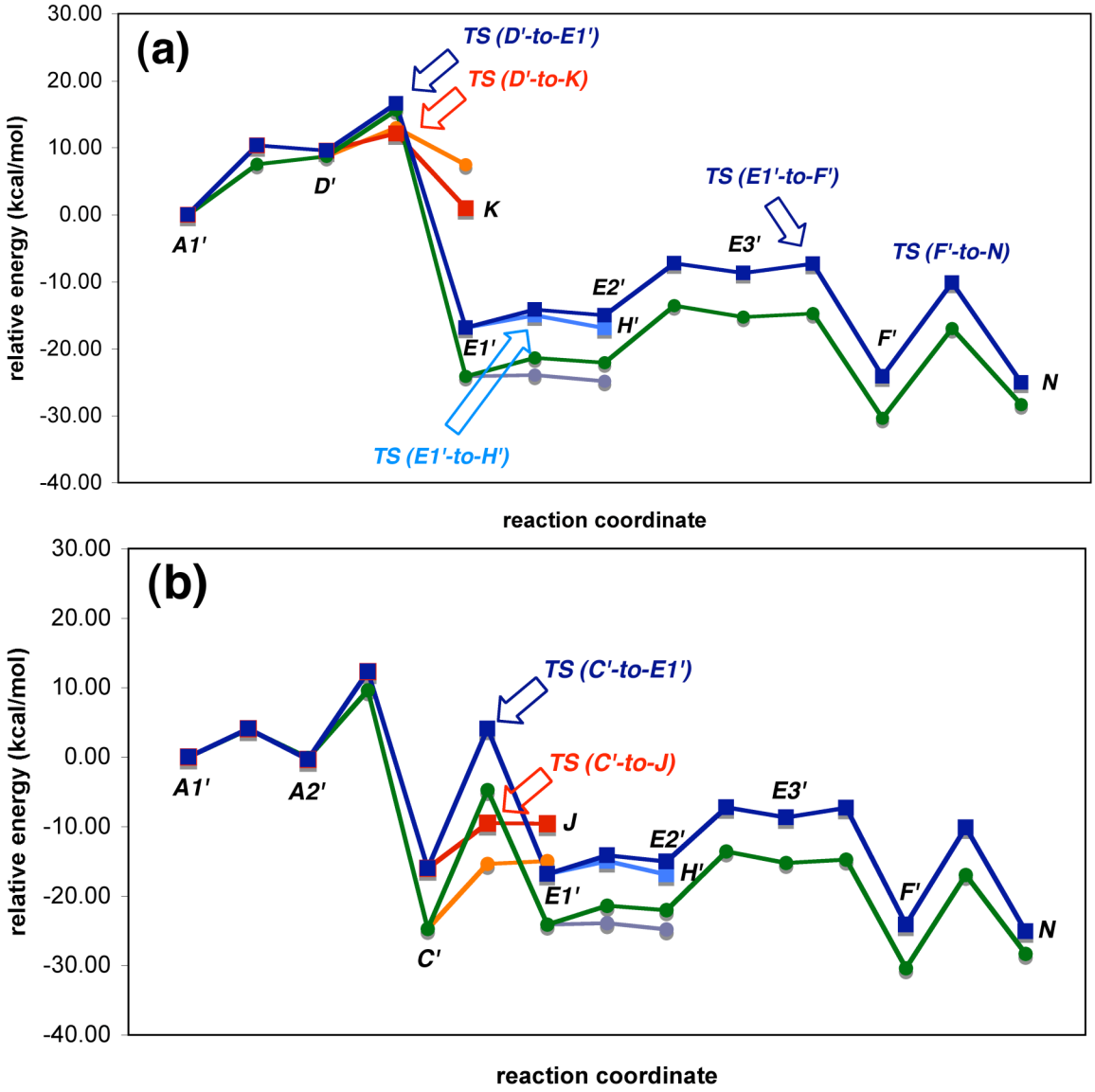


Figure S1. Overall energetics for the rearrangement of bisabolyl cation analog **A'**: (a) the proton transfer, (b) the hydride transfer pathway. B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p): ——, ——and——; mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p): ——, ——and——

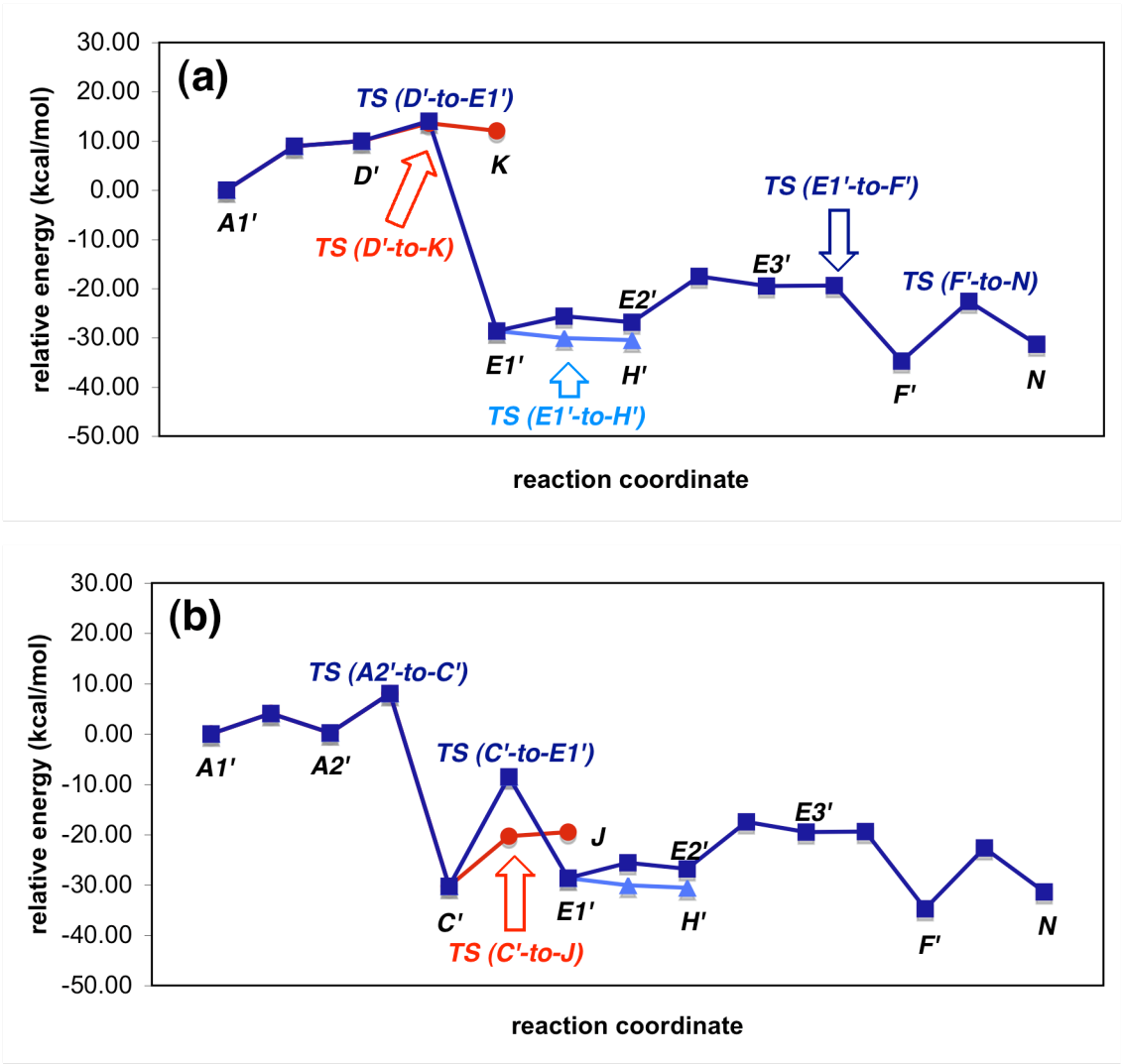
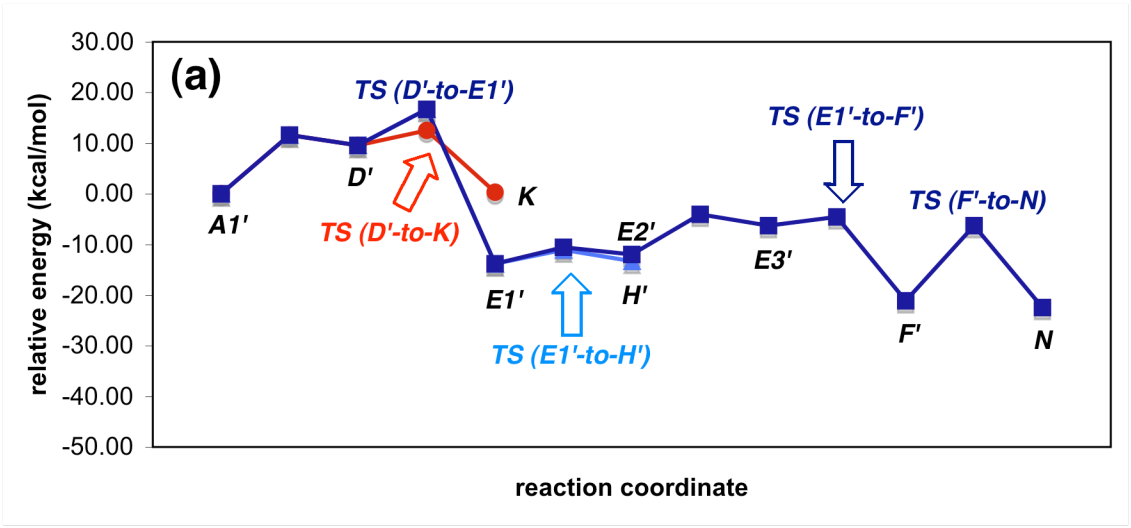


Figure S2. Overall energetics for the rearrangement of bisabolyl cation analog **A'**: (a) the proton transfer, (b) the hydride transfer pathway. mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p).



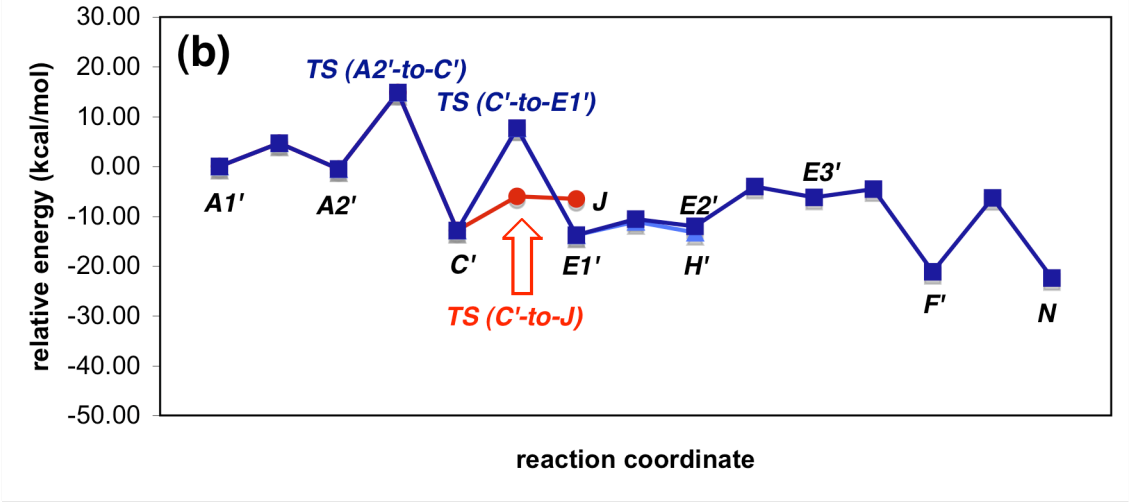


Figure S3. Overall energetics for the rearrangement of bisabolyl cation analog **A'**: (a) the proton transfer, (b) the hydride transfer pathway. Free energy by B3LYP/6-31+G(d,p)// B3LYP/6-31+G(d,p), 298° K, 1.0 atm.

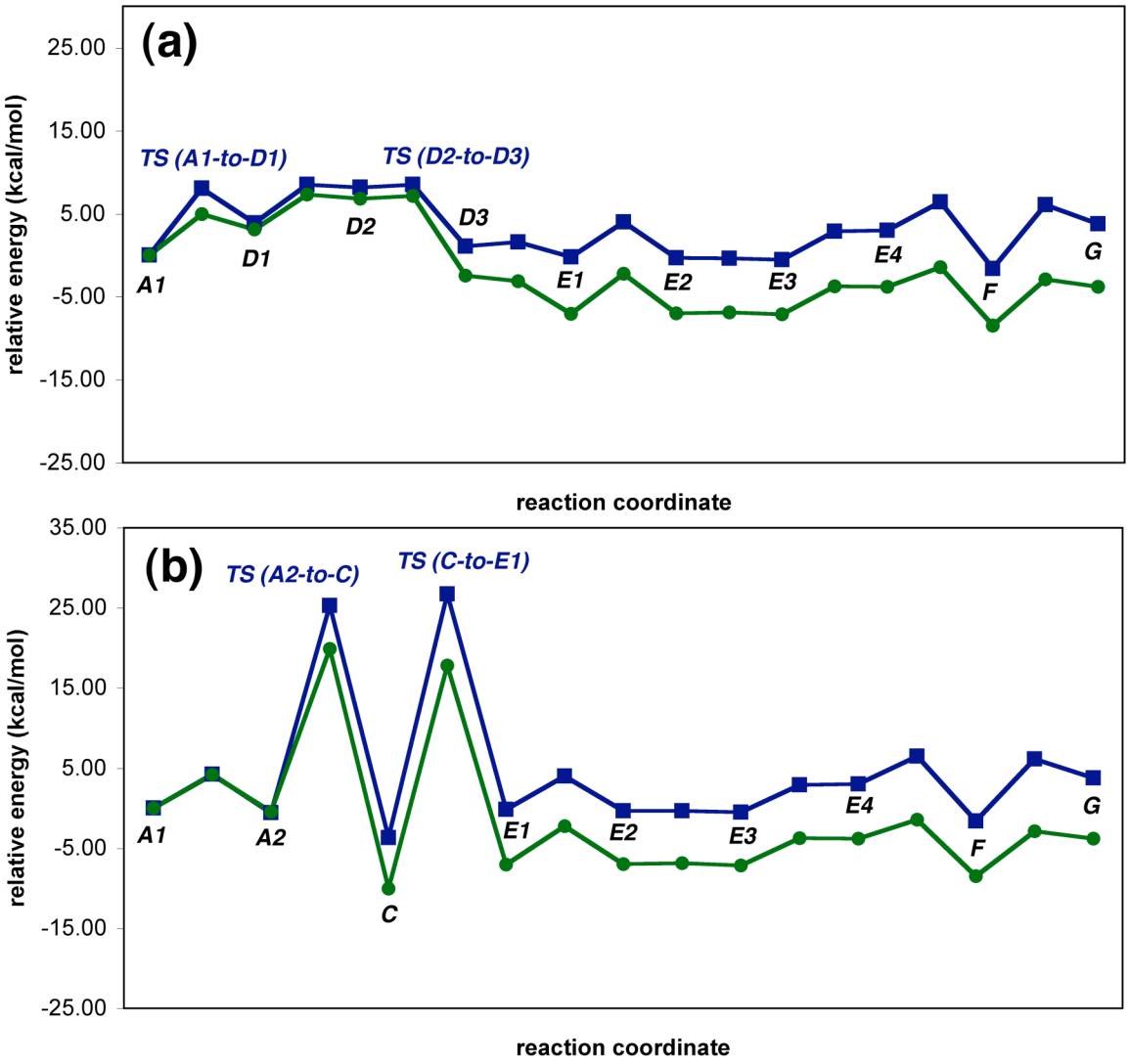


Figure S4. Overall energetics for the rearrangement of the bisabolyl cation: (a) the proton transfer, (b) the hydride transfer pathway. B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p): —■— ; mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p): —●—

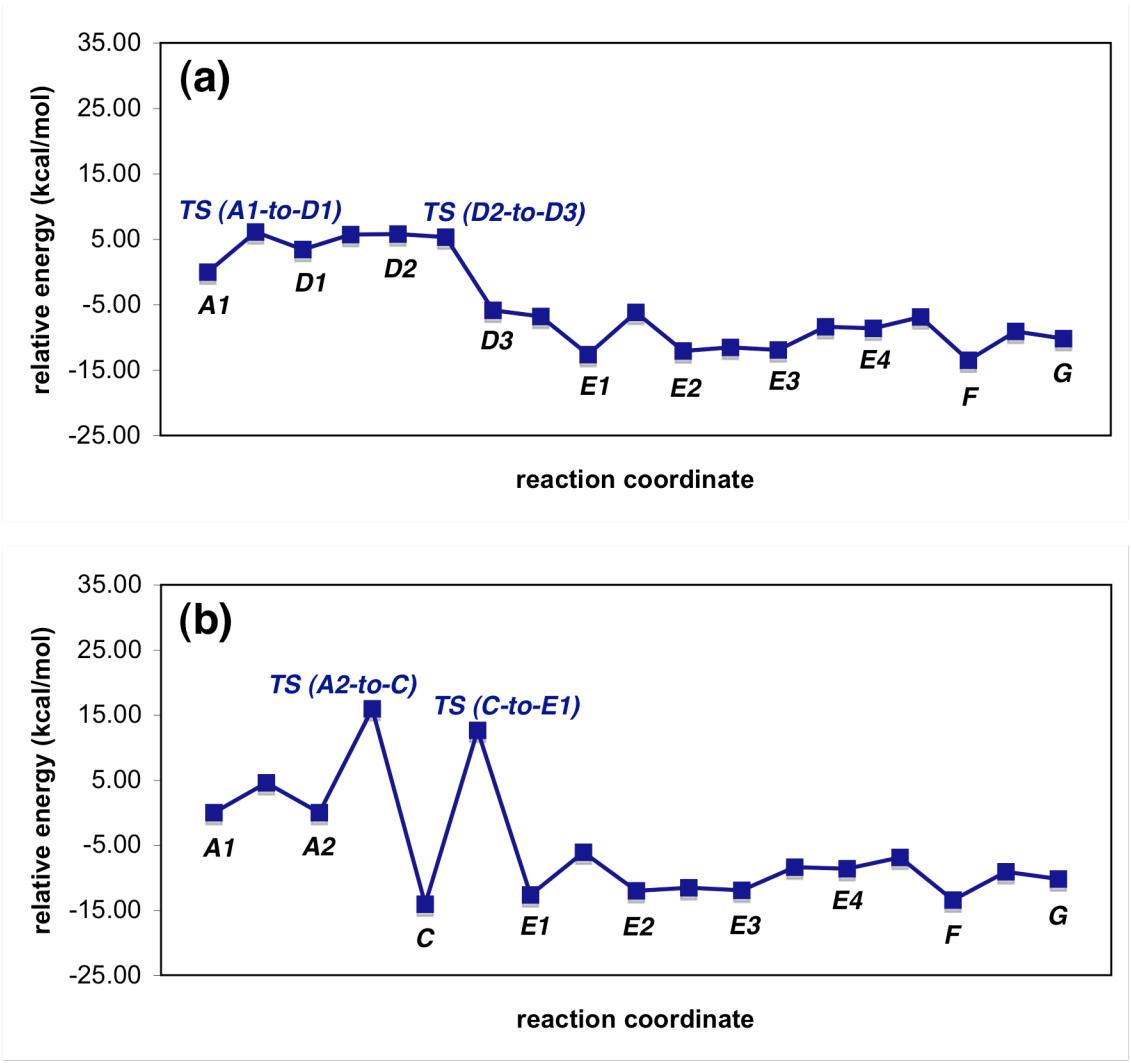


Figure S5. Overall energetics for the rearrangement of bisabolyl cation: (a) the proton transfer, (b) the hydride transfer pathway. mPWB1K/6-31+G(d,p)//B3LYP/6-31+G(d,p).

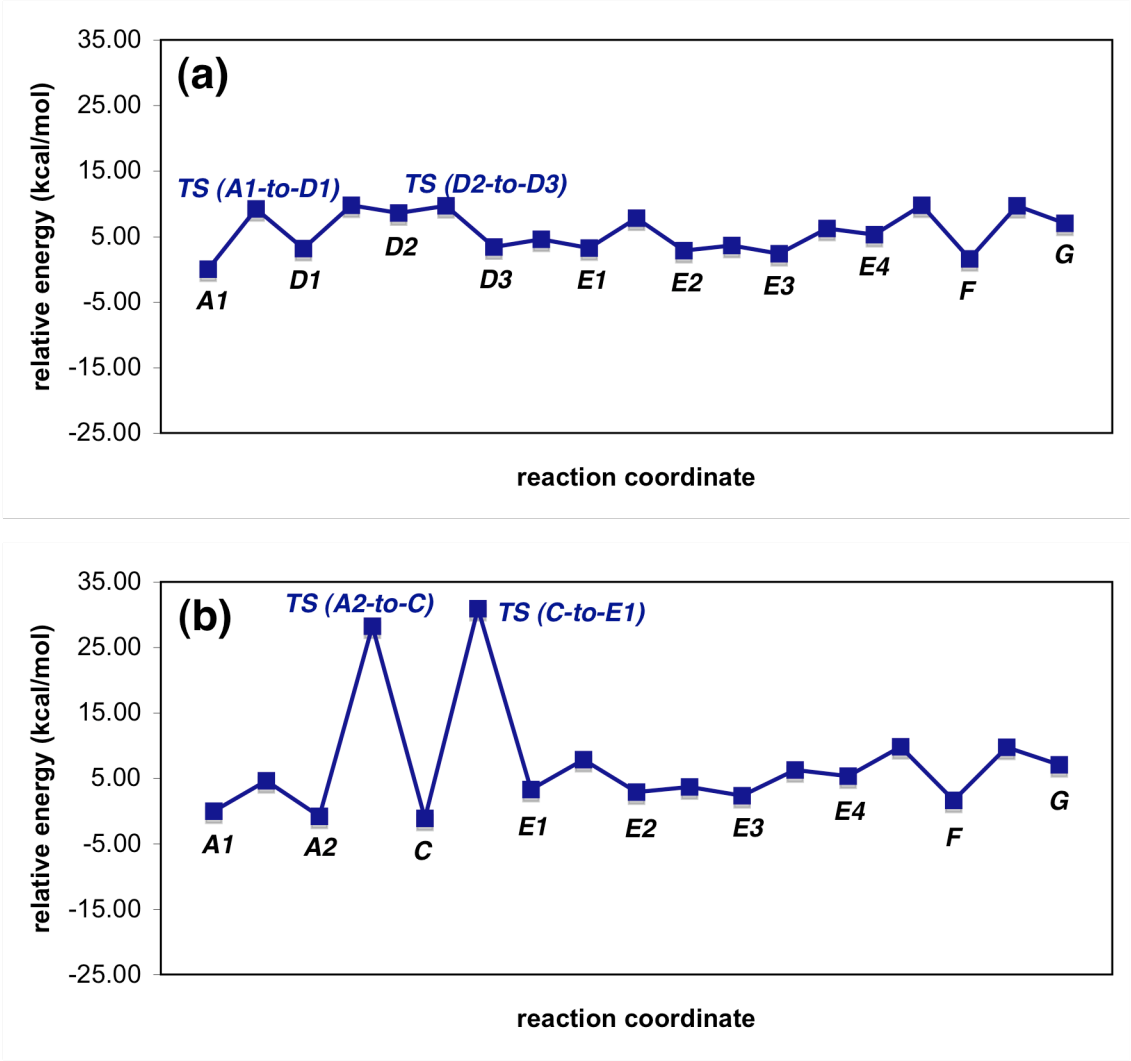


Figure S6. Overall energetics for the rearrangement of bisabolyl cation: (a) the proton transfer, (b) the hydride transfer pathway. Free energy by B3LYP/6-31+G(d,p)// B3LYP/6-31+G(d,p), 298° K, 1.0 atm.

IV. Solvation Calculations

Test calculations were performed on selected transition state structures shown in Figures 2 and 4 with CPCM (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) with UAKS radii) using benzene as solvent (since the active sites of terpene synthases are largely hydrophobic and often lined with aromatic residues).

Table S1. Relative Energies (in kcal/mol)

Transition structure	CPCM[a,b,e]	CPCM[b,e]-ZPEcrxn[c]	B3LYP[a]	B3LYP-ZPEcrxn[c]	Free Energy[d]	mPW1PW91[a,e]	mPW1PW91-ZPEcrxn[c,e]	mPWB1K[a,e]	mPWB1K-ZPEcrxn[c,e]
TS (A1'-to-D')	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TS (D'-to-E1')	4.24	3.36	5.42	6.30	5.16	7.24	8.11	4.17	5.05
TS (A2'-to-C')	-2.67	1.23	-1.94	1.96	3.23	-1.78	2.11	-4.83	-0.93
TS (C'-to-E1')	-8.35	-5.38	-9.24	-6.27	-3.83	-15.21	-12.25	-20.41	-17.44
TS (A1-to-D1)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TS (D2-to-D3)	-1.51	-3.17	-1.18	0.48	0.47	2.22	0.57	-2.46	-0.80
TS (A2-to-C1)	11.4	15.44	13.2	17.24	19.01	14.91	10.87	5.79	9.83
TS (C1-to-E1)	14.31	17.48	15.49	18.67	21.65	12.84	9.66	3.33	6.5

[a] These energies do not include zero-point energy corrections.
[b] B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p), solvent=benzene, radii=uaks.
[c] These energies include unscaled zero-point energy corrections from B3LYP/6-31+G(d,p) frequency calculations.
[d] These free energies are from B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) calculations.
[e] These energies are from single point calculations on the B3LYP/6-31+G(d,p) optimized geometries.