Supporting Information for

A Tangled Web – Interconnecting Pathways to Amorphadiene and the Amorphene Sesquiterpenes

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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. Initial 1,6-cyclization

The potential of an alternative conformer of the bisabolyl cation, **A3** (Figure S1) to undergo rearrangements similar to **A1** was examined. In the geometry of the bisabolyl cation conformer **A3**, the acyclic chain is at a pseudo-equatorial position on the cyclohexene ring structure; note in the conformer **A1**, the acyclic chain is at a pseudo-axial position, but the primary folding of the acyclic chain is the same as for **A1**. A complete reaction pathway from the bisabolyl cation conformer **A3** to cation **H1** based on our calculations is shown in Figure S1. Although this pathway in general is extremely similar to that described in the main paper (see Figure 2), several additional mechanistic details were uncovered.

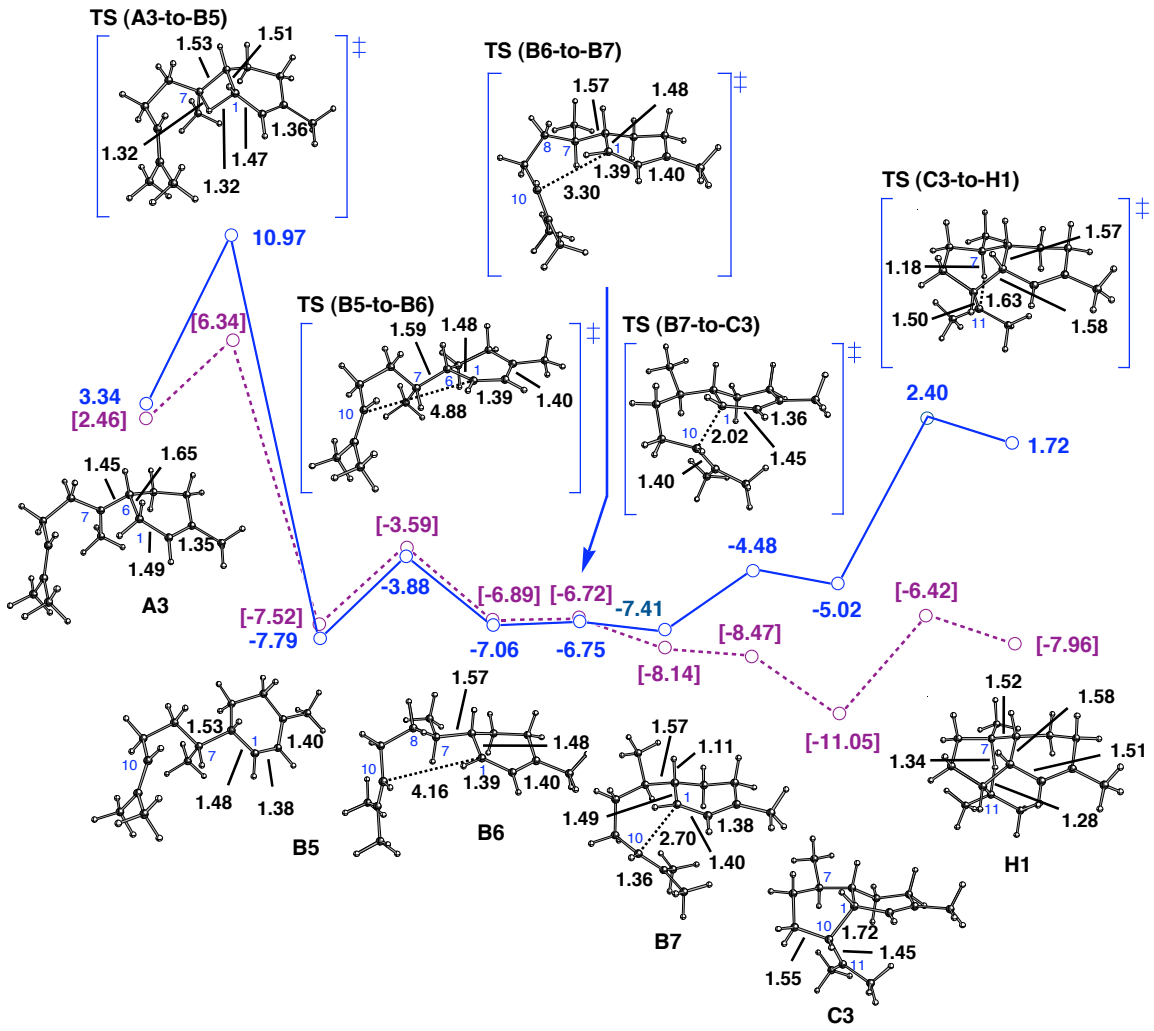


Figure S1. Conversion of **A3** to **H1** via a pathway involving a 1,3-hydride shift. Computed distances (Å) and energies (kcal/mol) are shown (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in blue and mPW1PW91/6-31+G(d,p)// B3LYP/6-31+G(d,p) in plum and brackets).

Attack by the C10=C11 π-bond on the pro-*R* face of the C1 cationic center converts **B7→C3**. The resultant structure of **C3** is a twist conformation of the cyclohexane bearing an isopropyl group at an axial and a methyl group at an equatorial position. Thus, the **B7→C3** conversion is distinguished from the **B3→C1** conversion described in the main paper where the cyclohexane is in a

chair conformation bearing both isopropyl and methyl groups at equatorial positions. In the structure of **C3**, the C1-C10 σ-bond is significantly elongated (1.72 Å) due to strong hyperconjugation (through bond coupling; Figure S1). This conversion leads directly to the conformation of cation **C** that is productive for the subsequent 1,5-hydride shift.

We were able to locate a transition structure for formation of bridged cation **H1** from **C3**. The computed barrier for the conversion of **C3** to **H1** was ~5-7 kcal/mol from **C3**.

III. A cationic two-step

The potential of an alternative conformer of the bisabolyl cation, **A4** (Figure S2), to undergo similar rearrangements was also examined. Conformer **A4** differs from conformer **A2** (Figure 3) primarily in the orientation of the C10=C11 bond and the cyclohexene ring with respect to the acyclic chain. These conformers are interconvertable by rotations about the C8-C9 bond. A complete reaction pathway from bisabolyl cation conformer **A4** to cation **C4**, based on the results of our calculations, is shown in Figure S2. A [1,2]-hydride shift (Scheme 1) converts **A4** into the cation **D2**, similar to the rearrangement of **A2** described in the main text. The barrier for the conversion of **A4** to **D2** is estimated to be ~5-7 kcal/mol from **A4**. Cation **D2** is not productive for subsequent [1,2]-hydride shift (C1-to-C6), but we found an alternative conformer, **D3**, that is productive for the [1,2]-hydride shift. We also located a transition structure connecting **D2** to **D3** (Figure S2). The computed barrier for this conformational change is ~2-3

kcal/mol from **D2**. The conversion of **D3** to cation **B8** is very similar to that of **D1→B4**. The second hydride shift is predicted to occur with a slightly higher barrier than that of the first hydride shift as observed for the pathway from **A2**. Attack of the C10=C11 π-bond on carbocationic center C1 converts **B8** to **C4** (Figure S2). In the structure of **C4**, the C1–C10 σ-bond is significantly elongated (1.72 Å) due to the strong hyperconjugation that is observed in all cation **C** structures. The newly formed cyclohexane structure is in the chair conformation with both methyl and isopropyl groups at axial position, which contrasts to the structure of **C1** bearing both at equatorial positions.

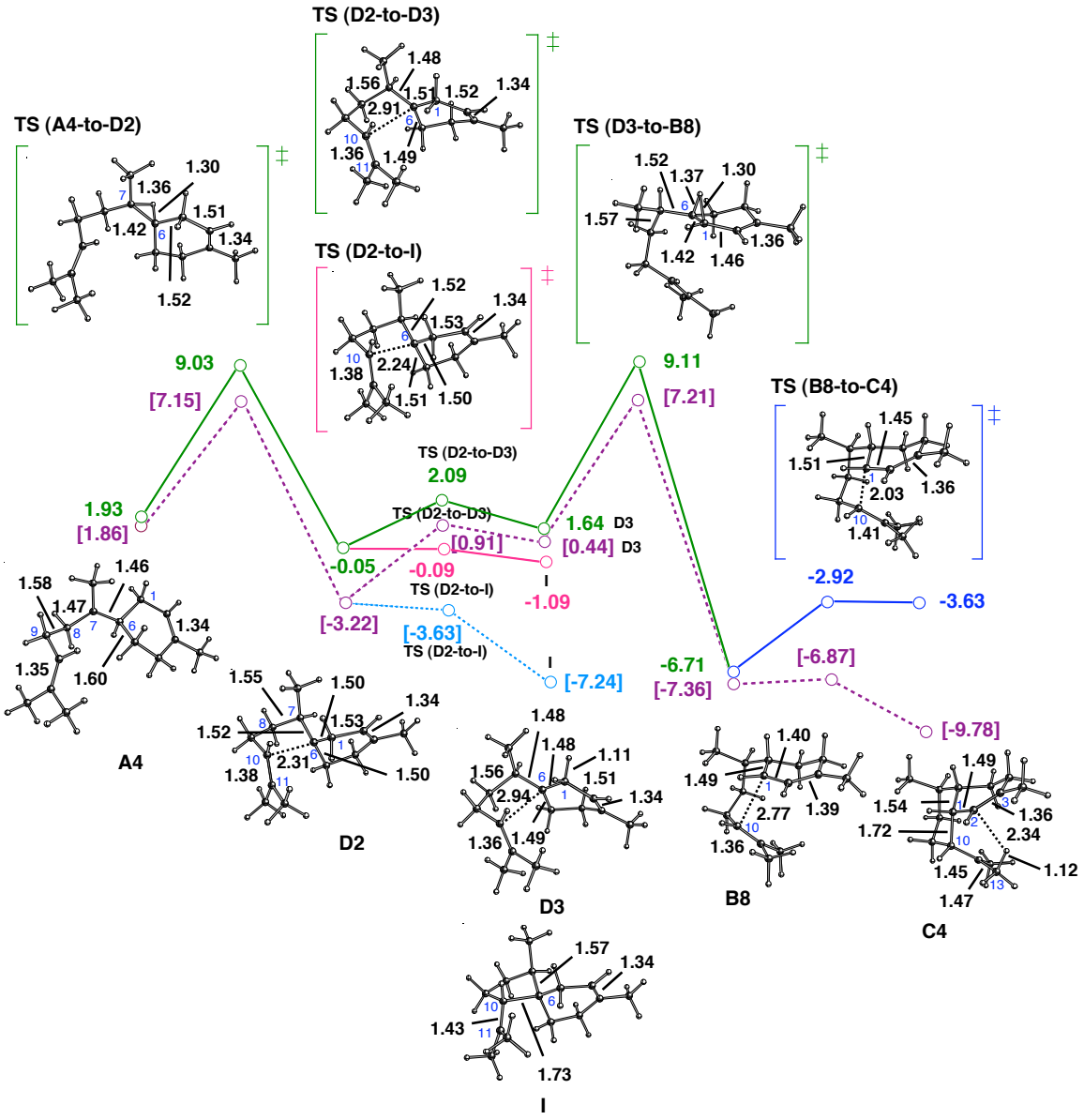


Figure S2. Conversion of **A4** to **C4** and **I**, the cation that precedes *epi*-β-acoradiene via a pathway involving two 1,2-hydride shifts. Computed distances (Å) and energies (kcal/mol) are shown (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in green and blue, and pink and mPW1PW91/6-31+G(d,p)// B3LYP/6-31+G(d,p) in plum, aqua and brackets).

Alternatively, attack by the C10=C11 π-bond on the pro-*R* face of the C6 cationic center converts **D2** directly to the acorenyl cation **I**. The transition structure for this intramolecular cation-alkene addition reaction resembles the

geometry of **D2**; note that there is little difference between the C6-C10 distances in **D2** and the transition structure (0.07 Å) and that there is almost no energetic barrier. Direct deprotonation of **I** can generate (*6R*,*7R*,*10S*)-acoradiene (*epi*-β-acoradiene).[9] Our computed results suggest that this virtually barrierless and exothermic rearrangement to acoradiene is inherently favored over the [1,2]-hydride shift to form amorphadiene. Detection of α-acoradiene related products along with amorphadiene has been reported as a product of Cop4 synthase from *Coprinus cinereus*.[13]

IV. Initial 1,10-cyclization

We further explored rearrangement of a potential alternative conformer of the germacradienyl cation **E**. A complete reaction pathway from conformer **E2** to cations that precede the amorphenes (**2,3** and **4**) and amorphadiene (**1**) is shown in Figure S3. The overall pathway from **E2** (**E2→F2→G2**) is similar to the pathway from **E1** described in the main paper (Figure 4). The energy of conformer **E2** is ~4-5 kcal/mol higher than that of **E1**. The 1,3-hydride shift converts **E2** to the cation **F2**. The barrier for the conversion of **E2→F2** is ~11-16 kcal/mol from **E2**, which is significantly higher than that for the previous case (~3-6 kcal/mol for **E1→F1**). The conversion of **E2** to **F2** is significantly exothermic (~22-23 kcal/mol from **E2**), slightly moreso than the conversion of **E1** to **F1**. Direct deprotonation of **F2** can generate germacradiene C and D.

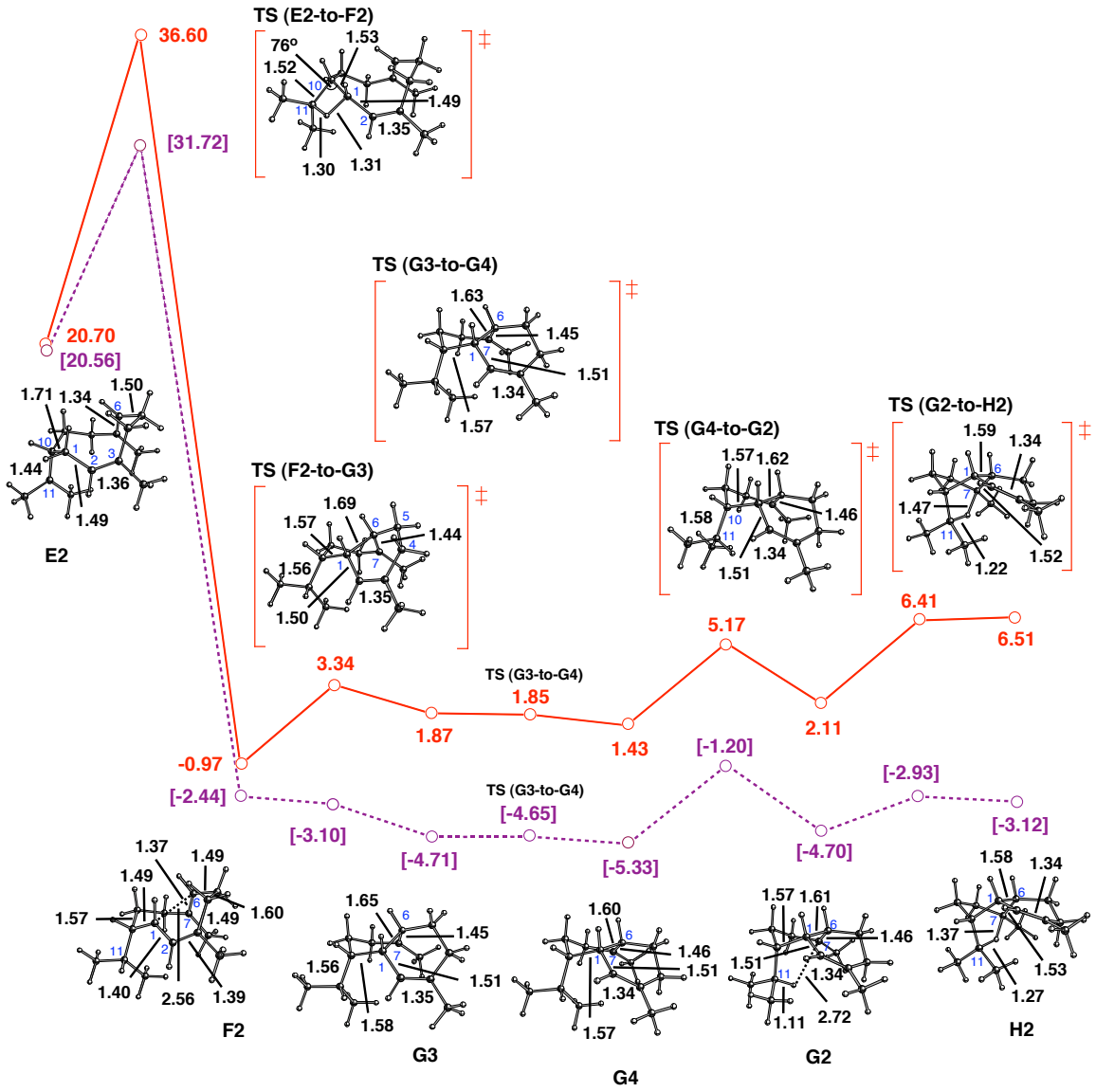


Figure S3. Conversion of **E2** to **H2**. Computed distances (Å) and energies (kcal/mol) are shown (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in red and mPW1PW91/6-31+G(d,p)// B3LYP/6-31+G(d,p) in plum and brackets).

Ring closure converts **F2** to **G3**, which is associated with a small barrier. This process generates the boat conformation of the cyclohexane ring in the structure of G3, which is ~3-4kcal/mol higher in energy than **G1**. Direct deprotonation at C8, C6 and C14 of **G1** would generate α-amorphene (**2**), γ-amorphene (**3**), and δ-amorphene (**4**), respectively.

We further explored the potential of cation **G** to undergo intramolecular 1,5-hydride shift (C11-to-C7). We were able to locate a productive conformation of cation **G** for 1,5-hydride shift (Figure S3). The conversion of the conformer **G3** to the conformer **G2** productive for 1,5-hydride shift requires two crucial conformation changes; (1) **G3→G4**, a boat-to-twist conformational change in the cyclohexane ring structure and (2) **G4→G2**, isopropyl group reorientation so as to promote 1,5-hydride shift. We were able to locate corresponding transition structures, which are shown in Figure S3. The initial ring flip to convert **G3** into **G4** occurred wth essentially no barrier, but the isopropyl group reorientation had a small barrier (~4 kcal/mol).

We also explored how the reaction sequence — for example, ring closure after isopropyl group reorientation — affects the overall rearrangement of **E2** to **H2**. Instead of ring-closure, a conformation change of **F2** generated from the 1,3-hydride shift directly leads to the conformer **F3** (Figure S4). The isopropyl reorientation process at this stage is associated with a slightly lower barrier (~2 kcal/mol from **F2**) than that of the corresponding conversion after the ring closure, **G4**-to-**G2** (~4 kcal/mol from **G4**; Figures S3 and S4). In contrast, the ring closure of **F3** leading to **G5** after isopropyl relocation faces a slightly increased barrier (~2-7 kcal/mol from **F3**) than that of the corresponding conversion, **F2**-to-**G3** (~2 kcal/mol from **F2** by B3LYP; Figure S3). As for the **G4** case described above, the conformation change of **G5**-to-**G2** (boat-to-twist conformation change in the cyclohexane ring structure bearing C2) was required, although the barrier was very small.

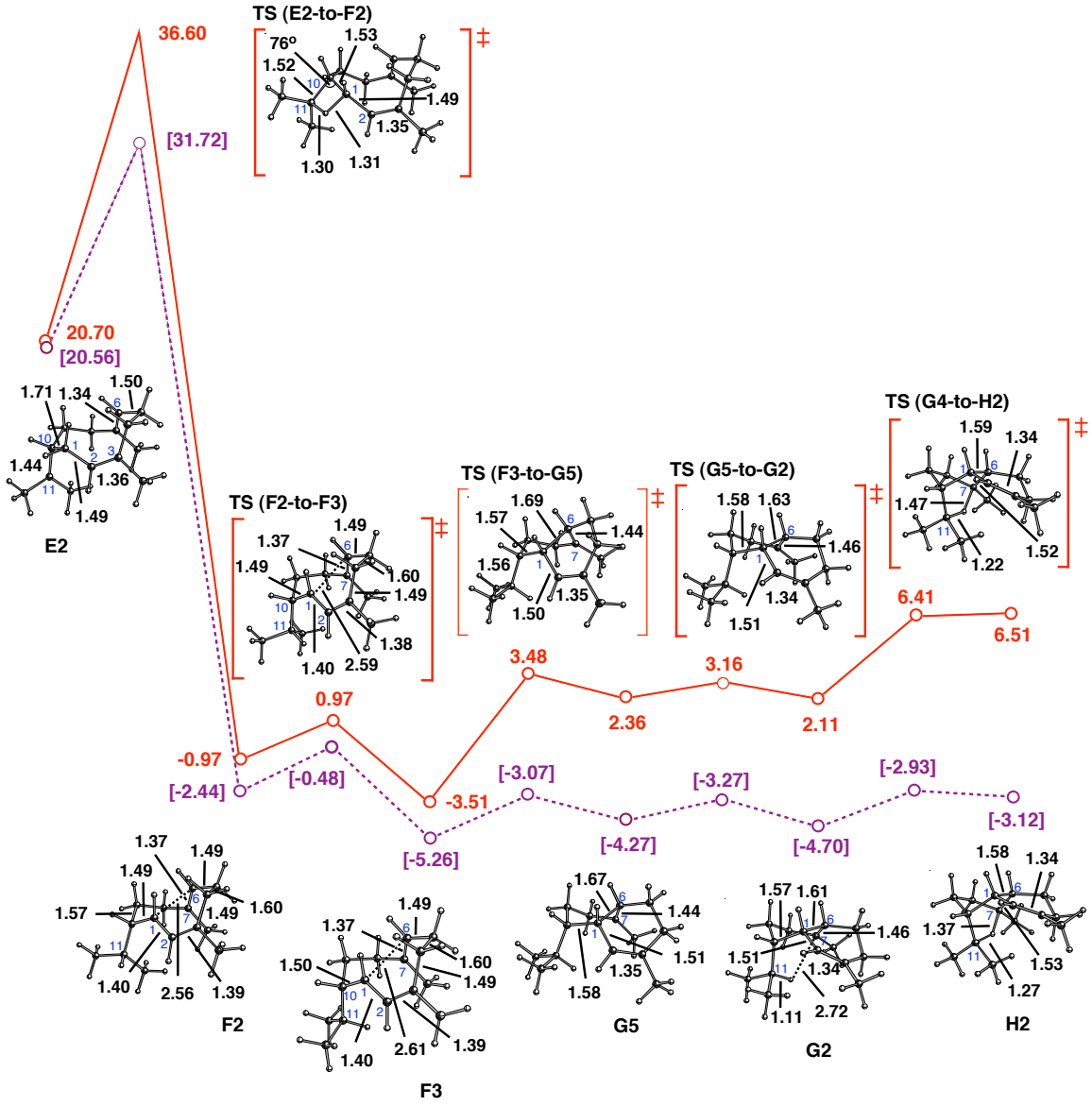


Figure S4. Alternative conversion of **E2** to **H2**. Computed distances (Å) and energies (kcal/mol) are shown (B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in red and mPW1PW91/6-31+G(d,p)// B3LYP/6-31+G(d,p) in plum and brackets).

V. Models for formation of amorphadiene (1) and amorphenene (2)

We further explored the structure of **H1**. To see if deprotonation at C8, for example, can lead to α-amorphene (**2**), we examined proton transfer from **H1** to ammonia (a simple model base; Figure S5). In the uncomplexed structure of cation **H1**, the C11-H and C7-H distances are 1.28 Å and 1.34 Å, respectively (Figure 5). Upon complexation with ammonia (C8-H•••NH_3), the bridging hydrogen shifts toward C11 as in cation **G** and deprotonation to form amorphene is essentially barrierless (top in Figure S5). In contrast, we observed that complexation with ammonia at a different site (C13-H•••NH_3) induces the structure of cation **H1** to morph toward that of cation **C** (bottom in Figure S5). Based on these results, we suggest that in a system with appropriately oriented C–H and C–C bonds, intermolecular C–H•••X interactions can promote a change in the **H1** structure towards either cation **G**, a precursor for amorphene, or cation **C**, a precursor for amorphadiene. Related to this, in a previous study, we observed that the symmetrical nonclassical 2-norbornyl cation with a cyclic 3-center 2-electron bonding array distorts towards an asymmetric classical secondary cation upon intermolecular C–H•••X interactions.[18] Conformer **H2** behaves similar to conformer **H1** upon interactions with ammonia (Figure S6).

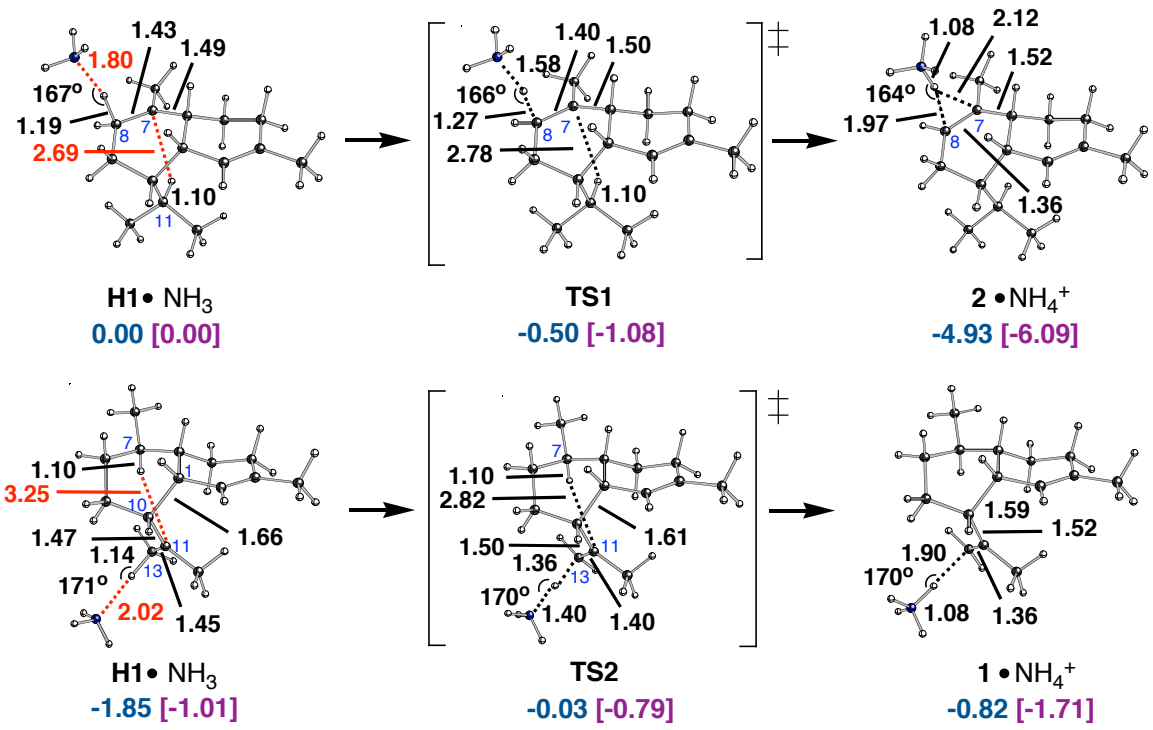


Figure S5. Model of deprotonation of **H1** and olefinic products. Computed geometries (distance in Å) and relative energies (in kcal/mol, relative to the complex **H1**•NH_3 (top)) of intermediates and transition structures are shown: B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in blue and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in plum.

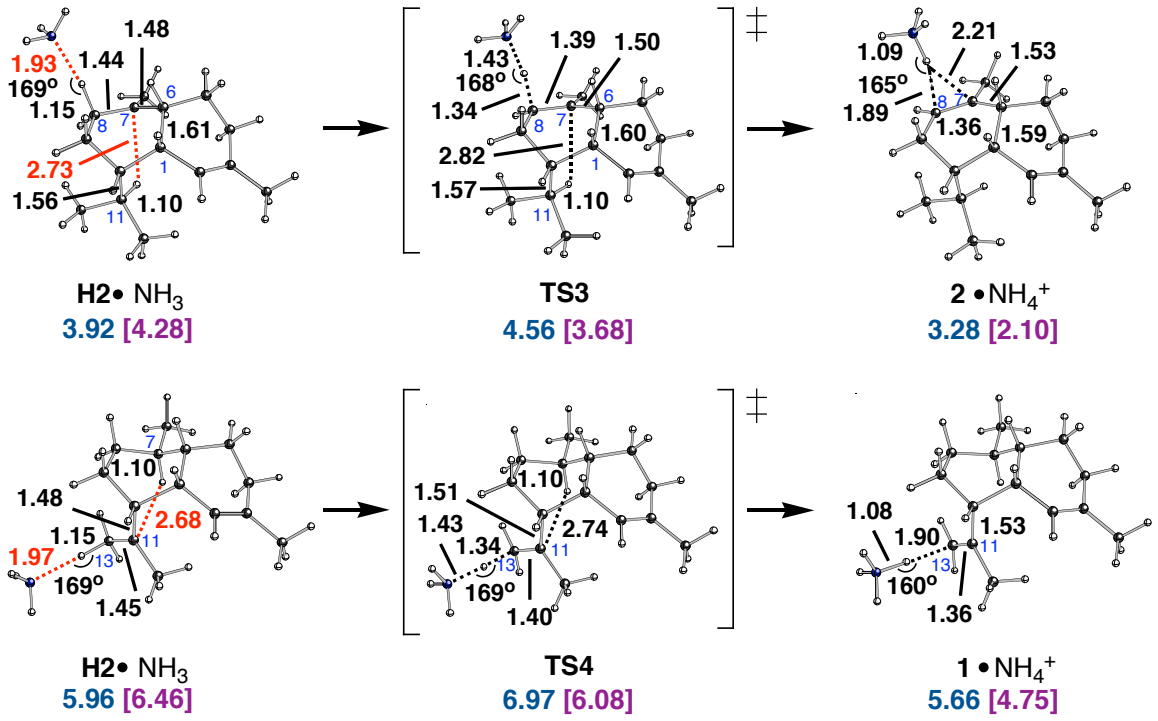


Figure S6. Model of deprotonation of **H2** and olefinic products. Computed geometries (distance in Å) and relative energies (in kcal/mol, relative to the complex **H1**•NH_3 (top in Figure S5)) of intermediates and transition structures are shown: B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in blue and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in plum.

To see if **C2** is a productive precursor for amorphadiene, we examined proton transfer from **C2** to ammonia. The C1-C10 distance (elongated to 1.77 Å) of **C2** is shortened (to 1.68 Å) upon complexation with ammonia (C2-H•••NH_3; Figure S7). This distance is further shortened to 1.59 Å in amorphadiene complexed with ammonium ion; note that this bond is longer than a typical C_{sp3}–C_{sp3} single bond due to through bond coupling involving the adjacent π-bonds. Direct deprotonation from **C2** generates (*1S, 6R, 7R, 10R*)-amorphadiene (**1**).

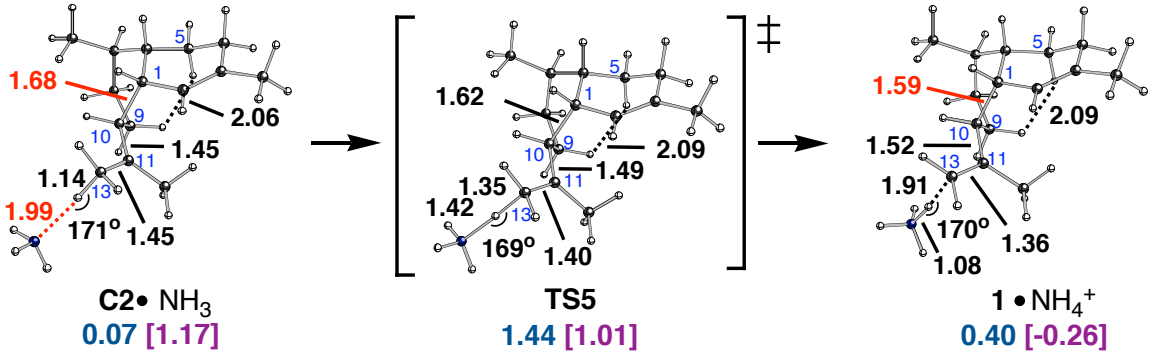
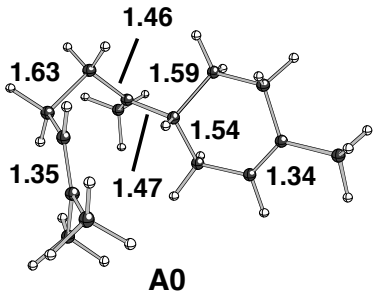


Figure S7. Model of deprotonation of **C2** to form amorphadiene (**1**). Computed geometries (distance in Å) and relative energies (in kcal/mol, relative to the complex **H1**•NH_3 (top in Figure S5)) of intermediates and transition structures are shown: B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p) in blue and mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p) in plum.

VI. Coordinates and energies

Figure 1.

A0



A0

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

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Imaginary Frequencies: none
Zero-point correction = 0.363052 (Hartree/Particle)

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HF = -586.2752278 hartrees

Coordinates:

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2	6	2.970260	0.787724	0.024316
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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
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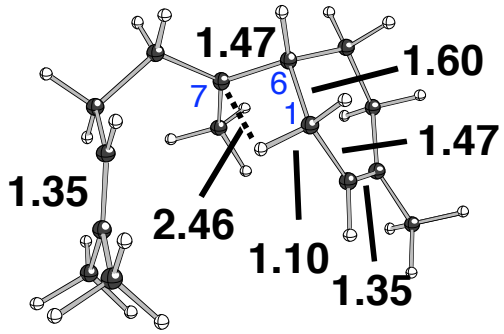
Figure 2.

A1



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Imaginary Frequencies: none found
Zero-point correction = 0.362938 (Hartree/Particle)

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

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Coordinates (from last standard orientation):

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2	6	2.710855	1.165109	0.032310
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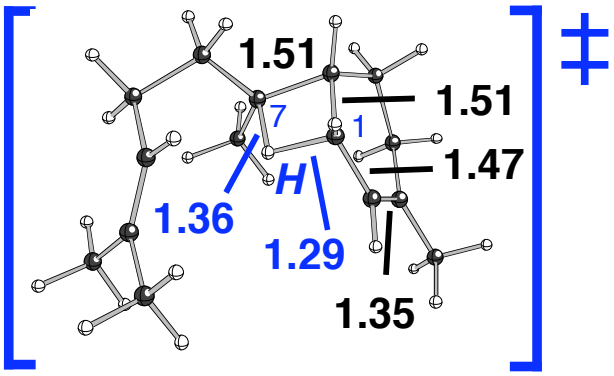

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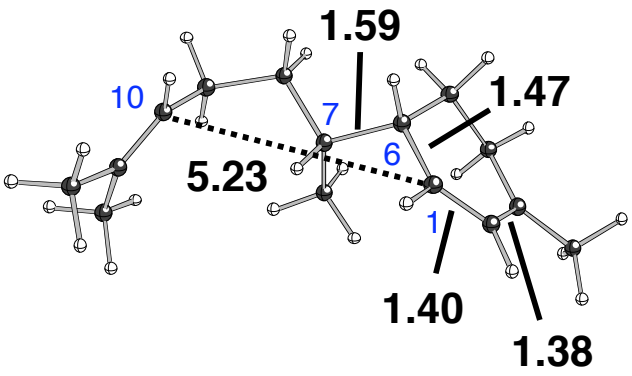
12	1	-0.210534	-0.101412	-0.400693
13	1	3.105935	-0.107252	1.588315
14	6	3.386613	2.479399	0.304831
15	1	4.378488	2.494737	-0.163557
16	1	2.831036	3.356969	-0.032367
17	1	3.552899	2.562812	1.385861
18	6	0.301521	-0.910780	1.584271
19	1	-0.677261	-0.798014	2.049562
20	1	0.848198	-1.706970	2.102775
21	1	0.855536	0.020085	1.719412
22	6	-0.996321	-2.160875	-0.309819

23	6	-2.401932	-1.634243	0.050454
24	1	-0.820749	-3.137803	0.164635
25	1	-0.929834	-2.334442	-1.390316
26	6	-2.705969	-0.309419	-0.603384
27	1	-3.117907	-2.388894	-0.300375
28	1	-2.526509	-1.590230	1.135293
29	1	1.318745	-2.143297	-1.504069
30	6	-3.128316	0.834334	-0.027029
31	6	0.180665	-1.297314	0.126475
32	6	-3.447949	2.046087	-0.870270
33	1	-4.505355	2.318264	-0.763799
34	1	-2.870267	2.919321	-0.542053
35	1	-3.249537	1.876143	-1.931947
36	6	-3.380322	1.020005	1.449382
37	1	-2.831941	1.890436	1.830005
38	1	-4.443481	1.228011	1.622466
39	1	-3.114346	0.153397	2.057655
40	1	-2.625286	-0.315020	-1.692927

B1



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

HF = -586.4256513 hartrees (-367987.960447263 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.364007 (Hartree/Particle)

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

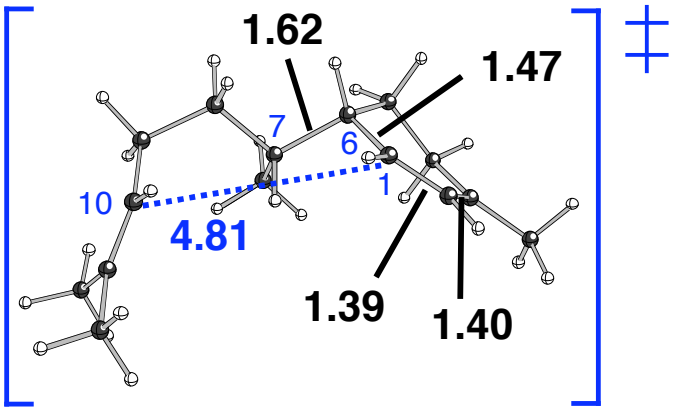
HF = -586.2857285 hartrees (-367900.157491035 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.971327	-1.380028	-0.686658

2	6	-3.756265	-0.571675	0.144446
3	6	-3.313815	0.807913	0.492670
4	6	-2.304118	1.425494	-0.487300
5	6	-1.225056	0.439654	-0.981312
6	6	-1.766656	-0.915256	-1.185116
7	1	-4.193134	1.453241	0.610293
8	1	-3.285446	-2.398826	-0.893001
9	1	-2.857715	1.788770	-1.360430
10	1	-1.842372	2.303970	-0.031055
11	1	-1.143433	-1.615302	-1.741478
12	1	0.696084	-0.492738	-0.569064
13	1	-2.899108	0.724361	1.511674
14	6	-5.018092	-1.080936	0.731428
15	1	-5.853452	-0.635320	0.166255
16	1	-5.112716	-2.166530	0.674105
17	1	-5.145907	-0.738800	1.764500
18	6	-0.133094	-0.009241	1.349929
19	1	0.815003	-0.233146	1.844345
20	1	-0.585088	0.832816	1.886073
21	1	-0.769646	-0.891246	1.480287
22	6	0.951104	1.614606	-0.308478
23	6	2.398579	1.506495	0.225306
24	1	0.451632	2.455895	0.188958
25	1	0.996917	1.862553	-1.377132
26	6	3.228244	0.480705	-0.500361
27	1	2.853434	2.498139	0.085543
28	1	2.394163	1.334374	1.305190
29	1	-0.869085	0.769156	-1.968667
30	6	4.004667	-0.491408	0.016220
31	6	0.114804	0.328691	-0.127536
32	6	4.810752	-1.394678	-0.886964
33	1	5.883873	-1.290492	-0.681679
34	1	4.563345	-2.449776	-0.712022
35	1	4.645580	-1.172712	-1.944835
36	6	4.190337	-0.758542	1.490105
37	1	3.969092	-1.807754	1.723770
38	1	5.237496	-0.594750	1.774939
39	1	3.573409	-0.127588	2.133069
40	1	3.216692	0.580933	-1.587912

TS (B1-to-B2)



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

HF = -586.4209342 hartrees (-367985.000419842 kcal/mol)
Imaginary Frequencies: 1 (-48.6724 1/cm)
Zero-point correction = 0.364203 (Hartree/Particle)

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

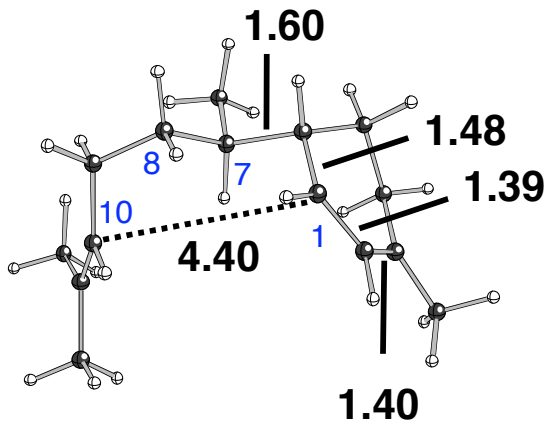
HF = -586.2808104 hartrees (-367897.071334104 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.680972	1.198441	-0.973533
2	6	3.505667	0.890508	0.111117
3	6	3.318324	-0.379434	0.870863
4	6	2.563162	-1.479603	0.108386
5	6	1.384691	-0.971787	-0.746496
6	6	1.681092	0.324112	-1.374058
7	1	4.294952	-0.742005	1.215182
8	1	2.800241	2.149436	-1.483734
9	1	3.272624	-1.964168	-0.572218
10	1	2.235775	-2.253054	0.805674
11	1	1.024082	0.641775	-2.183448
12	1	-0.394617	0.274710	-0.252995
13	1	2.797389	-0.087727	1.797626
14	6	4.562211	1.830537	0.556855
15	1	5.532913	1.430409	0.221336
16	1	4.447712	2.833729	0.143110
17	1	4.623166	1.873355	1.650188
18	6	-0.054227	-0.942886	1.455103
19	1	-1.049276	-0.723787	1.849493
20	1	0.198938	-1.967692	1.744393
21	1	0.634910	-0.255162	1.951849

22	6	-1.085534	-1.678262	-0.780684
23	6	-2.559835	-1.453841	-0.379988
24	1	-0.808352	-2.724886	-0.592566
25	1	-0.999557	-1.525296	-1.865463
26	6	-3.063565	-0.072347	-0.709078
27	1	-3.150250	-2.194517	-0.938460
28	1	-2.706401	-1.696476	0.675897
29	1	1.214244	-1.697198	-1.550905
30	6	-3.739821	0.785703	0.078278
31	6	-0.069937	-0.760046	-0.069654
32	6	-4.206690	2.119048	-0.456684
33	1	-5.299781	2.198448	-0.400491
34	1	-3.805160	2.946592	0.142627
35	1	-3.909893	2.271817	-1.498071
36	6	-4.133993	0.518721	1.510909
37	1	-3.779910	1.324485	2.166459
38	1	-5.227307	0.504326	1.604920
39	1	-3.759957	-0.429624	1.901939
40	1	-2.881590	0.239324	-1.740335

B2



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

HF = -586.4244837 hartrees (-367987.227766587 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.364283 (Hartree/Particle)

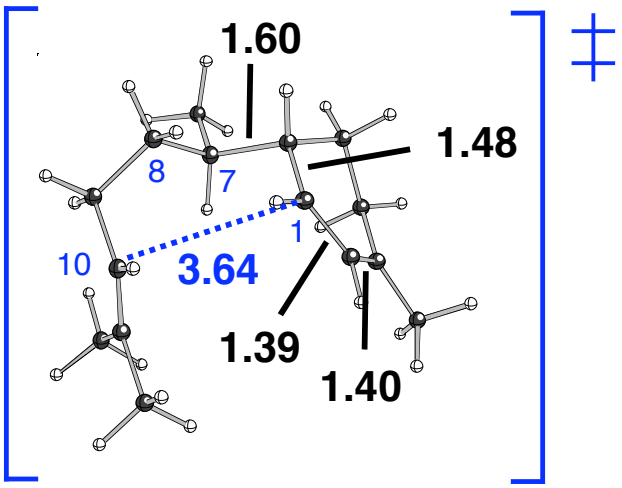
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.2846535 hartrees (-367899.482917785 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.368848	0.924399	-1.215857
2	6	2.915301	1.187953	0.046050
3	6	2.822178	0.163502	1.125752
4	6	2.616449	-1.260179	0.596429
5	6	1.498498	-1.333263	-0.460420
6	6	1.668677	-0.248533	-1.447297
7	1	3.701909	0.232647	1.776842
8	1	2.422936	1.682212	-1.991523
9	1	3.550645	-1.594976	0.129406
10	1	2.423797	-1.944559	1.423167
11	1	1.160320	-0.343545	-2.404839
12	1	-0.234100	-0.224228	0.342927
13	1	1.978458	0.484498	1.763614
14	6	3.559039	2.487629	0.345379
15	1	4.649486	2.324222	0.360941
16	1	3.341114	3.258691	-0.395147
17	1	3.301194	2.837895	1.351324
18	6	-0.158404	-2.131126	1.343606
19	1	-1.211848	-2.174173	1.632142
20	1	0.178029	-3.158913	1.166361
21	1	0.388309	-1.730161	2.201001
22	6	-1.005836	-1.710848	-1.014445
23	6	-2.466607	-1.275799	-0.754708
24	1	-0.960878	-2.803969	-1.107203
25	1	-0.714451	-1.311585	-1.993839
26	6	-2.659483	0.218550	-0.814267
27	1	-3.084641	-1.747019	-1.531331
28	1	-2.821649	-1.687515	0.193920
29	1	1.560804	-2.292686	-0.992903
30	6	-3.216435	1.033288	0.101221
31	6	-0.009755	-1.266490	0.081302
32	6	-3.371180	2.511245	-0.173992
33	1	-4.429281	2.801340	-0.151652
34	1	-2.870577	3.111852	0.596890
35	1	-2.965247	2.793030	-1.149730
36	6	-3.769087	0.588784	1.434161
37	1	-3.322819	1.170251	2.251033
38	1	-4.849391	0.776457	1.478293
39	1	-3.610686	-0.470558	1.644791
40	1	-2.334661	0.676128	-1.751967

TS (B2-to-B3)



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

HF = -586.4240271 hartrees (-367986.941245521 kcal/mol)
Imaginary Frequencies: 1 (-20.6607 1/cm)
Zero-point correction = 0.364262 (Hartree/Particle)

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

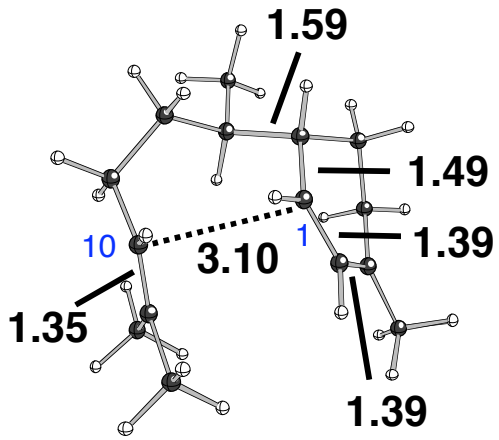
HF = -586.2844718 hartrees (-367899.368899218 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.586091	1.230864	-1.074853
2	6	2.443566	1.353372	0.022557
3	6	2.809211	0.147870	0.822879
4	6	2.659543	-1.164660	0.045606
5	6	1.315220	-1.262530	-0.697797
6	6	1.017803	0.007120	-1.394452
7	1	3.822494	0.265046	1.225090
8	1	1.297289	2.118390	-1.629502
9	1	3.463497	-1.217848	-0.698419
10	1	2.802461	-2.015684	0.712790
11	1	0.259188	-0.004831	-2.173961
12	1	-0.268830	-0.712339	0.709077
13	1	2.153048	0.171549	1.711856
14	6	2.971779	2.673586	0.440111
15	1	4.037894	2.714817	0.163577
16	1	2.461920	3.512619	-0.035634
17	1	2.948543	2.782418	1.530767
18	6	0.330588	-2.714975	1.202357
19	1	-0.601244	-3.001579	1.700702
20	1	0.741105	-3.613871	0.729121

21	1	1.023916	-2.383911	1.980344
22	6	-1.162016	-2.044240	-0.744586
23	6	-2.503428	-1.392437	-0.345779
24	1	-1.259016	-3.135479	-0.707211
25	1	-0.962302	-1.808091	-1.797811
26	6	-2.552774	0.079680	-0.669870
27	1	-3.305798	-1.900929	-0.896393
28	1	-2.700802	-1.577965	0.714885
29	1	1.378042	-2.059553	-1.452271
30	6	-2.735428	1.125163	0.162690
31	6	0.023037	-1.620756	0.167434
32	6	-2.826103	2.533781	-0.375873
33	1	-3.807176	2.970457	-0.149907
34	1	-2.083369	3.189668	0.097662
35	1	-2.684517	2.572016	-1.459767
36	6	-2.924471	1.015050	1.656163
37	1	-2.220958	1.670458	2.185779
38	1	-3.928998	1.356968	1.936053
39	1	-2.801640	0.000907	2.040201
40	1	-2.480463	0.305436	-1.736549

B3



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

HF = -586.4243569 hartrees (-367987.148198319 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.364764 (Hartree/Particle)

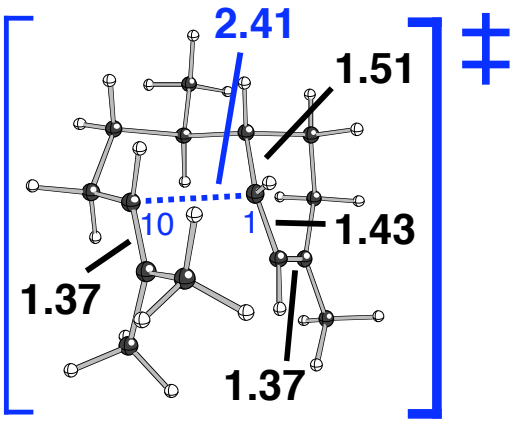
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.2849286 hartrees (-367893.7926965 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.908572	-1.422502	-0.906907
2	6	-1.913514	-1.662526	0.028838
3	6	-2.681744	-0.518567	0.608583
4	6	-2.675054	0.718276	-0.296482
5	6	-1.260550	1.090053	-0.785440
6	6	-0.566106	-0.126877	-1.278196
7	1	-3.704274	-0.838998	0.839313
8	1	-0.352067	-2.258497	-1.318647
9	1	-3.291370	0.501261	-1.177425
10	1	-3.151353	1.559318	0.207999
11	1	0.247600	-0.003116	-1.984618
12	1	-0.061462	1.141041	1.042833
13	1	-2.224693	-0.304191	1.590515
14	6	-2.236047	-3.038080	0.482253
15	1	-3.232993	-3.308948	0.101958
16	1	-1.517650	-3.784383	0.140049
17	1	-2.322422	-3.075406	1.575550
18	6	-1.093806	3.020817	0.902733
19	1	-0.420263	3.556174	1.578941
20	1	-1.446253	3.736688	0.151427
21	1	-1.950922	2.694158	1.496789
22	6	0.981802	2.371201	-0.411026
23	6	2.269238	1.637594	0.024406
24	1	1.101843	3.427601	-0.150380
25	1	0.897065	2.354840	-1.506346
26	6	2.413026	0.242266	-0.520910
27	1	3.124885	2.226250	-0.332746
28	1	2.331578	1.648141	1.117157
29	1	-1.350986	1.781207	-1.635480
30	6	2.529005	-0.925084	0.154994
31	6	-0.329887	1.853911	0.252309
32	6	2.794934	-2.215885	-0.579572
33	1	3.765249	-2.632680	-0.280788
34	1	2.048433	-2.980914	-0.326357
35	1	2.809375	-2.083086	-1.664997
36	6	2.471641	-1.057442	1.654994
37	1	1.735923	-1.818182	1.948293
38	1	3.437839	-1.407954	2.039913
39	1	2.226629	-0.127036	2.169142
40	1	2.534084	0.193784	-1.605569

TS (B3-to-C1)



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

HF = -586.4218233 hartrees (-367985.558338983 kcal/mol)
Imaginary Frequencies: 1 (-60.6549 1/cm)
Zero-point correction = 0.365177 (Hartree/Particle)

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

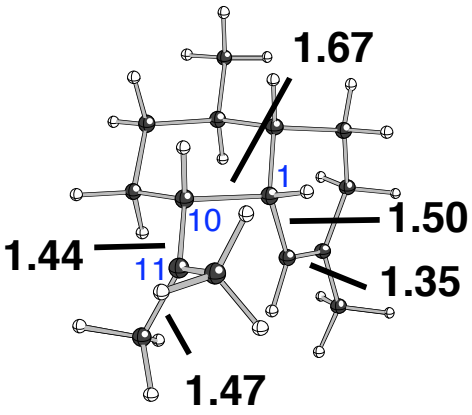
HF = -586.2854277 hartrees (-367894.10588175 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.083624	1.538662	0.191674
2	6	-1.304461	1.954163	-0.275586
3	6	-2.550765	1.179985	0.062171
4	6	-2.321192	0.170836	1.194809
5	6	-1.042499	-0.687990	0.936232
6	6	0.063513	0.338844	0.948727
7	1	-3.342388	1.889280	0.331863
8	1	0.763674	2.211819	0.097561
9	1	-2.208418	0.714304	2.140608
10	1	-3.182256	-0.488281	1.321414
11	1	0.711144	0.375348	1.817249
12	1	-1.264905	-0.903974	-1.221793
13	1	-2.912444	0.679811	-0.849005
14	6	-1.464762	3.237988	-1.022141
15	1	-2.081628	3.941200	-0.447919
16	1	-0.509756	3.713573	-1.254063
17	1	-2.006296	3.058020	-1.960151
18	6	-2.464067	-2.428094	-0.283577
19	1	-2.503108	-3.106809	-1.140230
20	1	-2.482163	-3.042907	0.624107
21	1	-3.380185	-1.833664	-0.307357
22	6	0.020879	-2.493922	-0.597266

23	6	1.326958	-1.778799	-0.962780
24	1	-0.236099	-3.167103	-1.421513
25	1	0.179553	-3.137286	0.280031
26	6	1.908729	-1.001910	0.183155
27	1	2.067558	-2.534892	-1.260897
28	1	1.172330	-1.144148	-1.842150
29	1	-0.899979	-1.367644	1.784260
30	6	2.716853	0.105647	0.108744
31	6	-1.186215	-1.571221	-0.352544
32	6	3.412329	0.629704	1.330360
33	1	4.495548	0.664632	1.156576
34	1	3.112742	1.666032	1.540289
35	1	3.232109	0.018347	2.217915
36	6	2.986713	0.843329	-1.167995
37	1	3.108102	1.917441	-0.991087
38	1	3.939092	0.492181	-1.590491
39	1	2.219621	0.688162	-1.928692
40	1	1.897825	-1.526771	1.139571

C1



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

HF = -586.4307086 hartrees (-367991.133953586 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365924 (Hartree/Particle)

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

HF = -586.3008456 hartrees (-367903.780614 kcal/mol)

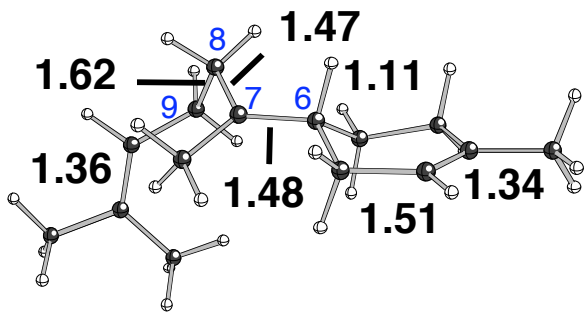
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	0.039057	1.422278	-0.077568
2	6	-1.177030	1.971470	-0.275654
3	6	-2.425209	1.355093	0.310640
4	6	-2.124510	0.269864	1.354418
5	6	-1.003859	-0.689685	0.892461
6	6	0.267288	0.188821	0.753017
7	1	-3.034868	2.147693	0.762011
8	1	0.902341	1.954651	-0.470582
9	1	-1.815556	0.747155	2.292693
10	1	-3.028540	-0.299672	1.586533
11	1	0.604875	0.468068	1.758374
12	1	-1.626833	-0.778820	-1.178304
13	1	-3.039717	0.955668	-0.509671
14	6	-1.357551	3.237829	-1.065835
15	1	-1.789784	4.027881	-0.439889
16	1	-0.416135	3.605198	-1.482950
17	1	-2.060545	3.077432	-1.893029
18	6	-2.589539	-2.403901	-0.152672
19	1	-2.791993	-3.001729	-1.046946
20	1	-2.411439	-3.098509	0.677158
21	1	-3.498924	-1.840138	0.071055
22	6	-0.179727	-2.321630	-0.885461
23	6	1.069445	-1.468764	-1.119963
24	1	-0.453105	-2.824188	-1.819463
25	1	0.049384	-3.119099	-0.163426
26	6	1.489344	-0.794874	0.190727
27	1	1.891653	-2.094282	-1.488675
28	1	0.864112	-0.715556	-1.889436
29	1	-0.817329	-1.414728	1.697699
30	6	2.692271	0.002872	0.210906
31	6	-1.373599	-1.492238	-0.382740
32	6	3.382845	0.279422	1.487274
33	1	4.407181	-0.120636	1.415145
34	1	3.517385	1.362197	1.619040
35	1	2.892867	-0.154472	2.359221
36	6	3.268325	0.557365	-1.028008
37	1	4.045381	1.302851	-0.854812
38	1	3.709566	-0.288974	-1.583356
39	1	2.490769	0.943943	-1.696711
40	1	1.543951	-1.525464	1.009066

Figure 3.

A2



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

HF = -586.4120475 hartrees (-367979.423926725 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.362970 (Hartree/Particle)

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

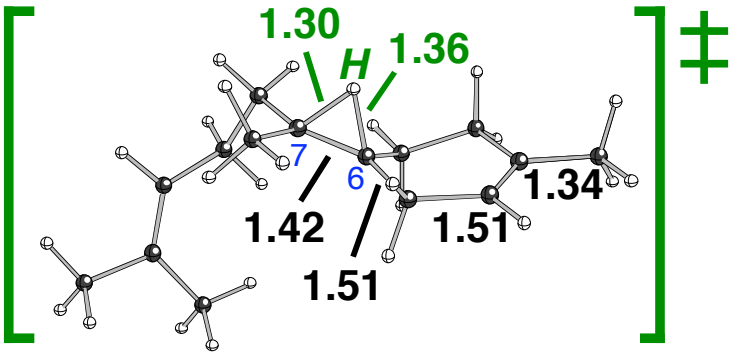
HF = -586.2731659 hartrees (-367892.274333909 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.200118	0.698818	0.313007
2	6	0.959469	1.831988	-0.562989
3	1	1.390605	2.760418	-0.164655
4	1	1.868488	1.216383	-0.763606
5	1	0.414770	2.028764	-1.482547
6	6	0.209533	1.125929	0.476327
7	6	0.929253	0.806830	1.714918
8	6	3.732097	-0.565608	-0.390403
9	6	1.988540	-0.386408	1.467841
10	1	0.250606	0.491824	2.509415
11	1	1.516830	1.663635	2.059983
12	6	3.218871	0.007752	0.727150
13	1	2.250514	-0.674448	2.492599
14	1	1.478564	-1.239568	1.018806
15	6	-1.417326	-0.847223	0.495333
16	6	-1.922774	1.165550	-0.958814
17	6	-2.911724	-1.149262	0.662939
18	6	-3.344622	0.659789	-0.997524
19	6	-3.810152	-0.368517	-0.271021
20	1	-1.925813	2.261626	-1.007927
21	1	-3.222328	-0.965677	1.702058
22	1	-1.027862	-1.342269	-0.401718
23	1	-0.864388	-1.231444	1.356161
24	6	-5.248666	-0.810118	-0.323337
25	1	-5.329009	-1.843540	-0.682897
26	1	-5.702940	-0.788000	0.675457

27	1	-5.843998	-0.172501	-0.981310
28	6	5.060036	-0.107759	-0.935777
29	1	4.964799	0.209850	-1.981443
30	1	5.485154	0.715879	-0.357462
31	1	5.778794	-0.936593	-0.930155
32	6	3.095174	-1.703831	-1.144336
33	1	3.709137	-2.607432	-1.040669
34	1	2.085852	-1.953078	-0.810567
35	1	3.059529	-1.479945	-2.216860
36	1	-1.699939	1.148499	1.194153
37	1	-3.062816	-2.224608	0.499763
38	1	-4.019847	1.188704	-1.666084
39	1	3.798497	0.807139	1.189735
40	1	-1.378749	0.818796	-1.850109

TS (A2-to-D1)



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

HF = -586.398112 hartrees (-367970.67926112 kcal/mol)
Imaginary Frequencies: 1 (-500.2709 1/cm)
Zero-point correction = 0.360474 (Hartree/Particle)

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

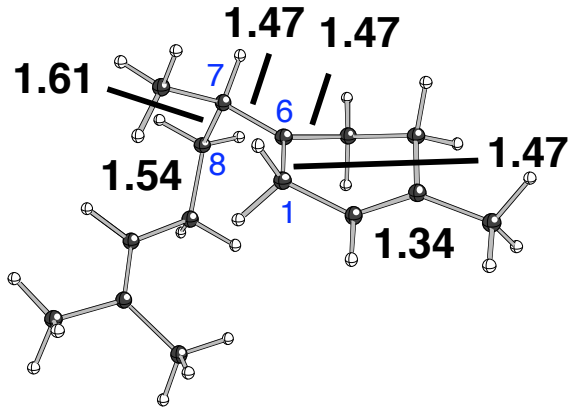
HF = -586.261833 hartrees (-367885.16282583 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.949731	0.238929	0.318496
2	6	-0.823159	0.809243	2.088549
3	1	-1.038071	1.773597	2.556032
4	1	-1.790194	0.330476	1.885005
5	1	-0.266024	0.184975	2.784182

6	6	-0.172840	1.003736	0.741889
7	6	-0.928090	1.916112	-0.212539
8	6	-3.630699	-0.658069	-0.320136
9	6	-1.971390	1.145733	-1.083339
10	1	-0.240556	2.444671	-0.877072
11	1	-1.444968	2.677605	0.378462
12	6	-3.153497	0.601986	-0.325925
13	1	-2.328142	1.881274	-1.816724
14	1	-1.464077	0.365540	-1.657866
15	6	1.508869	0.300544	-1.080546
16	6	1.625829	-0.783306	1.205086
17	6	3.039048	0.475213	-1.105210
18	6	3.088551	-1.000224	0.889994
19	6	3.752451	-0.427482	-0.123357
20	1	1.509411	-0.532511	2.263088
21	1	3.304574	1.524946	-0.911608
22	1	1.261913	-0.682860	-1.507954
23	1	1.015397	1.047085	-1.702122
24	6	5.226073	-0.631291	-0.349723
25	1	5.410244	-1.105234	-1.321610
26	1	5.755363	0.329710	-0.361371
27	1	5.673047	-1.256222	0.426808
28	6	-4.890994	-0.997304	0.439576
29	1	-4.707311	-1.794385	1.171039
30	1	-5.301508	-0.132107	0.966601
31	1	-5.661633	-1.375261	-0.243698
32	6	-3.021692	-1.820384	-1.066027
33	1	-3.718758	-2.184652	-1.830920
34	1	-2.081027	-1.582594	-1.567734
35	1	-2.845502	-2.663241	-0.386213
36	1	1.031081	1.463321	0.897376
37	1	3.389011	0.268457	-2.122886
38	1	3.611331	-1.658513	1.579028
39	1	-3.716989	1.353050	0.230120
40	1	1.054240	-1.717747	1.069325

D1



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

HF = -586.4068411 hartrees (-367976.156858661 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.362012 (Hartree/Particle)

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

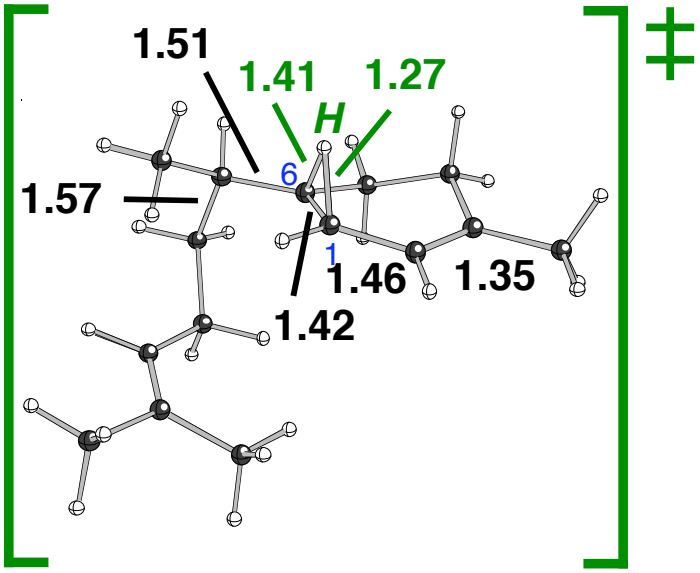
HF = -586.2687619 hartrees (-367889.510779869 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.901309	-0.997196	0.208031
2	6	0.919319	-2.021258	1.688639
3	1	1.610149	-2.868024	1.695922
4	1	1.511149	-1.111139	1.796560
5	1	0.266367	-2.126482	2.561406
6	6	0.105109	-2.051454	0.389063
7	6	1.014690	-2.048291	-0.938947
8	6	2.958391	1.134744	-0.156925
9	6	1.687600	-0.734191	-1.377697
10	1	0.402123	-2.429667	-1.760823
11	1	1.775162	-2.807578	-0.727927
12	6	2.696701	-0.161915	-0.410463
13	1	2.197728	-0.979003	-2.321597
14	1	0.933295	0.012363	-1.654230
15	6	-1.967330	-1.132912	-0.799578
16	6	-0.834294	0.267743	0.945371
17	6	-3.301619	-0.469377	-0.387178
18	6	-1.929657	1.267972	0.702178
19	6	-3.096452	0.941283	0.126011
20	1	-0.746628	0.006035	2.017735
21	1	-3.811449	-1.080203	0.371079
22	1	-1.571488	-0.545724	-1.654789
23	1	-2.087034	-2.162045	-1.147122
24	6	-4.247724	1.896286	-0.011267
25	1	-4.507914	2.048831	-1.065657
26	1	-5.142973	1.494078	0.479543
27	1	-4.022759	2.868173	0.433671
28	6	4.076908	1.524989	0.780025
29	1	3.703657	2.145794	1.604497
30	1	4.581830	0.653786	1.205510
31	1	4.827374	2.127861	0.253669
32	6	2.237394	2.302012	-0.788913
33	1	2.924587	2.857428	-1.439620
34	1	1.376744	2.017359	-1.399045
35	1	1.901458	3.013866	-0.024449
36	1	-0.425394	-3.011200	0.313295
37	1	-3.957061	-0.469359	-1.263434
38	1	-1.761593	2.267852	1.091342

39	1	3.334260	-0.903433	0.072017
40	1	0.182057	0.669814	0.752337

TS (D1-to-B4)



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

HF = -586.3972049 hartrees (-367970.110046799 kcal/mol)
Imaginary Frequencies: 1 (-691.3169 1/cm)
Zero-point correction = 0.360677 (Hartree/Particle)

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

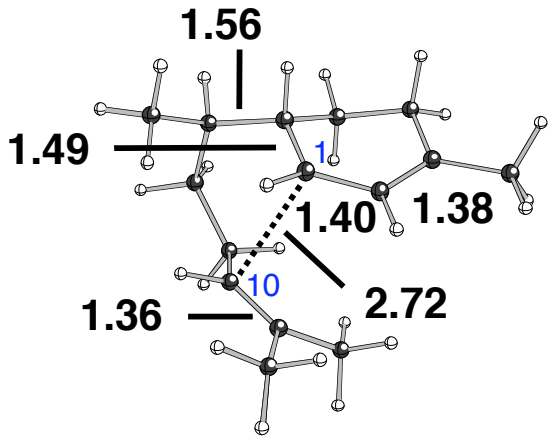
HF = -586.2607022 hartrees (-367884.453237522 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.919797	-1.050092	0.265304
2	6	1.036344	-2.026225	1.615697
3	1	1.744279	-2.858580	1.601360
4	1	1.620215	-1.107196	1.693682
5	1	0.425027	-2.140428	2.518852
6	6	0.175967	-2.084035	0.344365
7	6	1.005305	-2.014138	-0.990081
8	6	2.938715	1.155693	-0.163603
9	6	1.602805	-0.654155	-1.408351

10	1	0.373798	-2.383639	-1.805531
11	1	1.809084	-2.750339	-0.875140
12	6	2.694513	-0.121374	-0.511667
13	1	2.019895	-0.810784	-2.414131
14	1	0.805808	0.087120	-1.545572
15	6	-2.060780	-1.226722	-0.700816
16	6	-0.886781	0.180251	0.964580
17	6	-3.325419	-0.434090	-0.330337
18	6	-1.867785	1.242339	0.739239
19	6	-3.035544	0.986039	0.106077
20	1	-1.398223	-0.816902	1.569360
21	1	-3.858332	-0.938612	0.492622
22	1	-1.660591	-0.854925	-1.658724
23	1	-2.289089	-2.285513	-0.849112
24	6	-4.098661	2.017237	-0.099461
25	1	-4.300620	2.147377	-1.169923
26	1	-5.042352	1.690016	0.355762
27	1	-3.823531	2.984621	0.325390
28	6	4.143392	1.508823	0.676922
29	1	3.847601	2.037749	1.592262
30	1	4.719127	0.624347	0.962086
31	1	4.811550	2.186098	0.130213
32	6	2.107401	2.341830	-0.591883
33	1	2.694404	2.995597	-1.249451
34	1	1.197343	2.072201	-1.133353
35	1	1.827607	2.955381	0.274382
36	1	-0.322832	-3.061562	0.322588
37	1	-4.017430	-0.444092	-1.177257
38	1	-1.642704	2.219117	1.152899
39	1	3.407714	-0.874338	-0.173004
40	1	-0.005806	0.398999	1.563832

B4



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

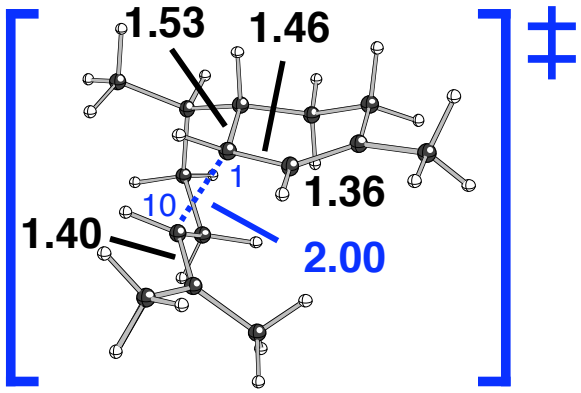
HF = -586.4256057 hartrees (-367987.931832807 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.364529 (Hartree/Particle)

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

HF = -586.2876526 hartrees (-367901.364883026 kcal/mol)
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.005512	-1.585652	-0.377699
2	6	-2.299741	-1.877250	-1.463772
3	1	-3.291313	-2.314725	-1.317305
4	1	-2.454004	-0.850559	-1.810451
5	1	-1.814905	-2.435818	-2.272614
6	6	-1.490716	-1.963921	-0.155767
7	6	-2.193933	-1.260118	1.041510
8	6	-0.933287	2.245796	0.107081
9	6	-1.811435	0.197516	1.392393
10	1	-2.038071	-1.856356	1.947009
11	1	-3.271841	-1.301303	0.848392
12	6	-1.711577	1.132106	0.219199
13	1	-2.583527	0.576055	2.077481
14	1	-0.883242	0.217554	1.970557
15	6	0.923949	-1.849743	0.827417
16	6	0.279767	-0.259520	-1.001298
17	6	2.384954	-1.515728	0.505092
18	6	1.517916	0.387893	-0.867952
19	6	2.564973	-0.193128	-0.176220
20	1	0.332933	-2.264975	-1.194779
21	1	2.809242	-2.271364	-0.179886
22	1	0.598552	-1.249418	1.682441
23	1	0.842021	-2.898103	1.128947
24	6	3.922098	0.421106	-0.161898
25	1	4.174917	0.719124	0.865627
26	1	4.682018	-0.314703	-0.453174
27	1	4.000248	1.295942	-0.809745
28	6	-1.059401	3.149626	-1.090851
29	1	-0.085723	3.316465	-1.570288
30	1	-1.756895	2.761520	-1.837510
31	1	-1.415519	4.140676	-0.781633
32	6	0.040934	2.703371	1.154211
33	1	-0.273713	3.679059	1.546460
34	1	0.133951	2.021646	2.000169
35	1	1.036404	2.860691	0.718116
36	1	-1.455452	-3.029231	0.103513
37	1	3.014496	-1.561934	1.401125
38	1	1.687236	1.314031	-1.408840
39	1	-2.446397	0.975672	-0.569876
40	1	-0.381490	0.075926	-1.792422

TS (B4-to-C2)



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

HF = -586.4218593 hartrees (-367985.580929343 kcal/mol)
Imaginary Frequencies: 1 (-186.9856 1/cm)
Zero-point correction = 0.365534 (Hartree/Particle)

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

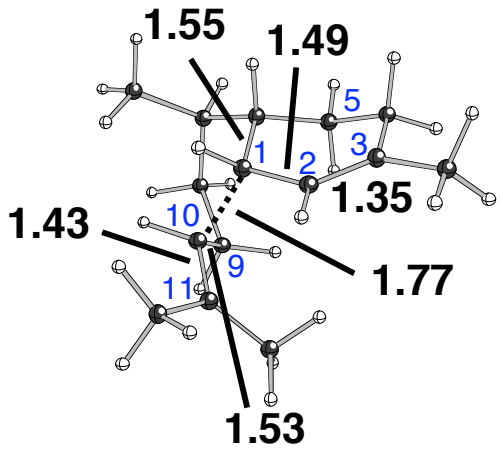
HF = -586.2890963 hartrees (-367902.270819213 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.472597	-1.432683	-0.389469
2	6	-2.828093	-1.263666	-1.404612
3	1	-3.888047	-1.448114	-1.205474
4	1	-2.751107	-0.239363	-1.786099
5	1	-2.523743	-1.940384	-2.210470
6	6	-1.998518	-1.510492	-0.130618
7	6	-2.450451	-0.629122	1.069895
8	6	-0.191139	2.352148	0.084024
9	6	-1.557851	0.594844	1.359512
10	1	-2.499099	-1.234075	1.980561
11	1	-3.474298	-0.286340	0.884282
12	6	-1.076983	1.268134	0.088506
13	1	-2.132650	1.325947	1.942680
14	1	-0.704324	0.318950	1.984605
15	6	0.359304	-2.038569	0.755856
16	6	0.071474	-0.078532	-0.845968
17	6	1.852437	-2.074215	0.423558
18	6	1.511140	0.119979	-0.719405

19	6	2.360108	-0.791040	-0.173893
20	1	-0.288692	-2.057261	-1.282438
21	1	2.064364	-2.875023	-0.303080
22	1	0.210358	-1.474157	1.681290
23	1	0.000566	-3.053746	0.953735
24	6	3.848236	-0.608929	-0.232462
25	1	4.271744	-0.591419	0.779547
26	1	4.316515	-1.458002	-0.745624
27	1	4.138072	0.309152	-0.748895
28	6	-0.081189	3.234644	-1.110582
29	1	0.966636	3.407518	-1.385463
30	1	-0.642189	2.869400	-1.973350
31	1	-0.480590	4.224406	-0.841574
32	6	0.722913	2.618374	1.223162
33	1	1.205772	3.594570	1.149615
34	1	0.222620	2.521631	2.190900
35	1	1.515229	1.847623	1.203459
36	1	-2.184756	-2.554389	0.148201
37	1	2.443031	-2.329900	1.311537
38	1	1.939219	0.996012	-1.202190
39	1	-1.832128	1.322140	-0.694065
40	1	-0.305239	0.239577	-1.816715

C2



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

HF = -586.4224377 hartrees (-367980.07965675 kcal/mol)
Imaginary Frequencies: none
Zero-point correction = 0.366088 (Hartree/Particle)

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

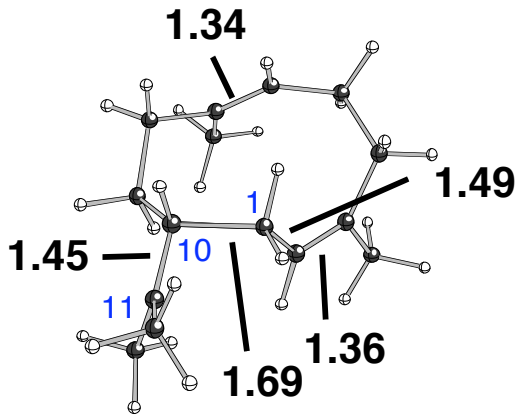
HF = -586.2918795 hartrees (-367898.15438625 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.465340	-1.432635	-0.404423
2	6	-2.847379	-1.297442	-1.362442
3	1	-3.901357	-1.485409	-1.135757
4	1	-2.782812	-0.273449	-1.748371
5	1	-2.560371	-1.973476	-2.175008
6	6	-1.980659	-1.539302	-0.112323
7	6	-2.401563	-0.656642	1.100262
8	6	-0.211712	2.357602	0.067782
9	6	-1.476967	0.549211	1.365058
10	1	-2.443367	-1.261801	2.011005
11	1	-3.421265	-0.291626	0.934994
12	6	-0.991234	1.161416	0.050432
13	1	-2.026742	1.310538	1.931057
14	1	-0.622224	0.263682	1.983862
15	6	0.387792	-2.074078	0.706217
16	6	0.031945	-0.016947	-0.789551
17	6	1.877213	-2.080851	0.359047
18	6	1.500944	0.167319	-0.653624
19	6	2.362235	-0.762364	-0.181240
20	1	-0.279469	-2.014887	-1.321421
21	1	2.090239	-2.848379	-0.401406
22	1	0.243568	-1.553490	1.658260
23	1	0.040650	-3.100695	0.863972
24	6	3.850759	-0.563326	-0.244751
25	1	4.289919	-0.604542	0.759588
26	1	4.319499	-1.371593	-0.819544
27	1	4.125747	0.388406	-0.706474
28	6	-0.205229	3.261079	-1.105445
29	1	0.808591	3.601223	-1.347882
30	1	-0.696649	2.840047	-1.984556
31	1	-0.754381	4.173097	-0.815539
32	6	0.672468	2.673900	1.203432
33	1	1.140222	3.656351	1.127352
34	1	0.162255	2.561820	2.165739
35	1	1.466956	1.901001	1.200641
36	1	-2.150857	-2.584516	0.171176
37	1	2.475861	-2.366702	1.232573
38	1	1.923563	1.071824	-1.090498
39	1	-1.806158	1.253122	-0.670376
40	1	-0.261065	0.227813	-1.813971

Figure 4.

E1



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

HF = -586.3894648 hartrees (-367965.253056648 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.363604 (Hartree/Particle)

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

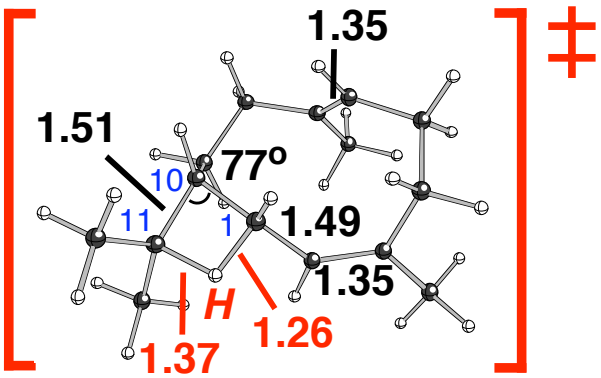
HF = -586.2505139 hartrees (-367872.19747225 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.058220	-1.409642	0.222476
2	6	-1.387753	-1.671098	0.196890
3	6	-2.312203	-1.376617	-0.971736
4	6	-2.990720	0.032193	-0.919379
5	6	-1.927729	1.085476	-1.015446
6	6	0.734948	-0.825255	-0.894833
7	1	-1.781838	-1.470523	-1.925073
8	1	0.493576	-1.753566	1.096608
9	1	-3.690747	0.092771	-1.759920
10	1	-3.582885	0.123219	-0.004964
11	1	-3.100648	-2.137458	-0.988060
12	6	-2.044085	-2.342820	1.376287
13	1	-2.423403	-3.332772	1.094905
14	1	-1.363593	-2.463998	2.222971
15	1	-2.912854	-1.763775	1.713702
16	6	-1.900210	1.816089	1.405636
17	1	-1.201236	1.410325	2.147523
18	1	-2.076128	2.863491	1.681959
19	1	-2.845005	1.283884	1.520025
20	6	-0.014876	2.430889	-0.204464
21	6	1.152384	1.593308	0.383204
22	1	0.000974	3.404905	0.299690
23	1	0.165863	2.626554	-1.268635

24	6	1.730766	0.488448	-0.523409
25	1	1.986155	2.275353	0.595987
26	1	0.846478	1.169754	1.344045
27	1	-1.472920	1.181922	-2.003975
28	6	2.901543	-0.200983	-0.026214
29	6	-1.351392	1.747818	0.000145
30	6	3.877760	-0.792130	-0.964882
31	1	4.828761	-0.252783	-0.816427
32	1	4.102270	-1.833514	-0.701258
33	1	3.591543	-0.707754	-2.013662
34	6	3.155954	-0.346115	1.421010
35	1	3.950462	-1.055845	1.653490
36	1	3.440595	0.646806	1.808268
37	1	2.237252	-0.597171	1.964381
38	1	1.938210	0.873801	-1.528627
39	1	1.375702	-1.567203	-1.382014
40	1	0.096422	-0.393780	-1.662640

TS (E1-to-F1)



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

HF = -586.3773356 hartrees (-367957.641862356 kcal/mol)
Imaginary Frequencies: 1 (-463.1760 1/cm)
Zero-point correction = 0.362501 (Hartree/Particle)

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

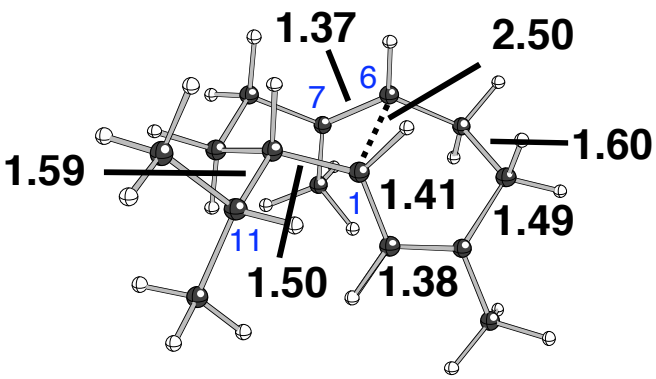
HF = -586.245112 hartrees (-367868.80778 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-0.111388	-1.265237	0.542911
2	6	-1.367650	-1.666444	0.247970
3	6	-2.008913	-1.489907	-1.108879
4	6	-2.661177	-0.069377	-1.272039
5	6	-1.628520	1.016033	-1.154887
6	6	0.846501	-0.746061	-0.468913
7	1	-1.286144	-1.632268	-1.921250
8	1	0.232756	-1.315839	1.572075
9	1	-3.140911	-0.044463	-2.256433
10	1	-3.457868	0.044051	-0.532192
11	1	-2.786669	-2.247524	-1.249186
12	6	-2.258761	-2.211648	1.333138
13	1	-2.543094	-3.244578	1.097342
14	1	-1.778259	-2.203784	2.314401
15	1	-3.192022	-1.640334	1.399575
16	6	-2.120248	1.753199	1.219353
17	1	-1.507379	1.477900	2.086856
18	1	-2.484953	2.770722	1.408681
19	1	-2.986475	1.091203	1.199840
20	6	-0.033200	2.538488	-0.014824
21	6	1.142159	1.703966	0.565643
22	1	-0.156348	3.430325	0.609285
23	1	0.240914	2.888449	-1.017358
24	6	1.577521	0.601246	-0.396273
25	1	1.999937	2.367470	0.728935
26	1	0.864987	1.295720	1.542511
27	1	-0.996650	1.144815	-2.036709
28	6	2.663450	-0.393288	-0.075588
29	6	-1.318103	1.733263	-0.058535
30	6	3.684182	-0.684870	-1.158637
31	1	4.422315	0.126045	-1.119288
32	1	4.206646	-1.629965	-0.993383
33	1	3.242970	-0.679015	-2.158132
34	6	3.111979	-0.590930	1.355747
35	1	3.626344	-1.544954	1.491278
36	1	3.827533	0.212746	1.569631
37	1	2.302356	-0.505742	2.080480
38	1	1.710713	1.012395	-1.398469
39	1	1.848704	-1.482697	-0.255844
40	1	0.683614	-1.061277	-1.499770

F1



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

HF = -586.4230259 hartrees (-367986.312982509 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366433 (Hartree/Particle)

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

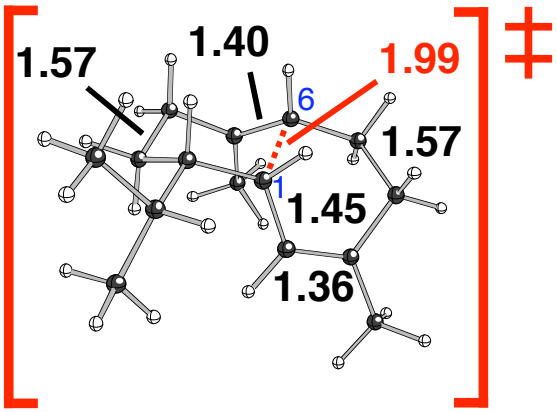
HF = -586.2864471 hartrees (-367894.74555525 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.539431	-1.246231	0.201335
2	6	-1.871961	-1.535079	-0.027621
3	6	-2.617156	-0.860928	-1.133932
4	6	-2.771618	0.708161	-0.895349
5	6	-1.473203	1.448171	-0.869172
6	6	0.182632	-0.418384	-0.680886
7	1	-2.113473	-0.997101	-2.097388
8	1	-0.082598	-1.581274	1.127504
9	1	-3.388029	1.071798	-1.722940
10	1	-3.341403	0.860703	0.024076
11	1	-3.620882	-1.280671	-1.231515
12	6	-2.647591	-2.407994	0.906099
13	1	-3.036375	-3.275829	0.356432
14	1	-2.048621	-2.767823	1.745039
15	1	-3.529306	-1.881421	1.294252
16	6	-1.398033	1.653891	1.636280
17	1	-0.672226	1.869073	2.423003
18	1	-2.248539	2.332930	1.775309
19	1	-1.778006	0.637462	1.788431
20	6	0.575823	2.419685	0.191947
21	6	1.598257	1.305435	0.543518
22	1	0.684865	3.241740	0.908351
23	1	0.790716	2.815375	-0.806312
24	6	1.551213	0.178743	-0.515801
25	1	2.605619	1.730957	0.576890
26	1	1.388836	0.908449	1.542524

27	1	-1.047062	1.728662	-1.831309
28	6	2.657482	-0.941870	-0.323430
29	6	-0.810644	1.845757	0.263437
30	6	3.985167	-0.454670	-0.930650
31	1	4.369851	0.428034	-0.408103
32	1	4.743242	-1.239606	-0.849158
33	1	3.878405	-0.205065	-1.991114
34	6	2.863129	-1.399879	1.128315
35	1	3.587369	-2.219855	1.149263
36	1	3.265346	-0.595784	1.752837
37	1	1.949919	-1.771606	1.602067
38	1	1.779976	0.652629	-1.477353
39	1	2.334262	-1.811866	-0.909741
40	1	-0.176298	-0.418759	-1.705579

TS (F1-to-G1)



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

HF = -586.4210201 hartrees (-367985.054322951 kcal/mol)
Imaginary Frequencies: 1 (-155.5173 1/cm)
Zero-point correction = 0.366447 (Hartree/Particle)

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

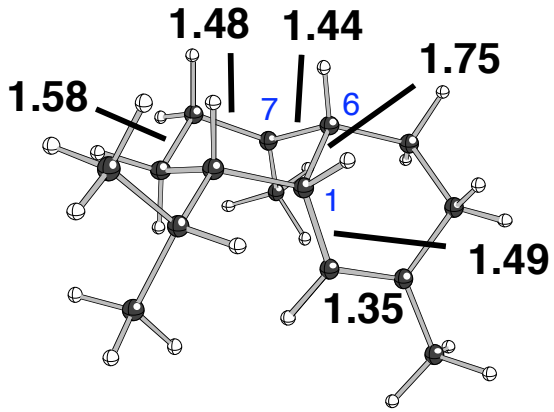
HF = -586.2887148 hartrees (-367896.168537 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.654676	-1.142072	0.327108
2	6	-1.948810	-1.473617	0.071737
3	6	-2.619837	-0.845887	-1.123458
4	6	-2.521872	0.716693	-1.100845

5	6	-1.113531	1.270202	-0.942332
6	6	0.066648	-0.295896	-0.610202
7	1	-2.158962	-1.212834	-2.050620
8	1	-0.178465	-1.457234	1.250294
9	1	-2.940623	1.097821	-2.037201
10	1	-3.165951	1.088379	-0.299872
11	1	-3.674533	-1.128191	-1.172407
12	6	-2.756180	-2.363420	0.967215
13	1	-3.116578	-3.233742	0.404059
14	1	-2.180162	-2.722304	1.823406
15	1	-3.651626	-1.846423	1.335264
16	6	-1.434251	1.860158	1.491378
17	1	-0.844825	2.187720	2.349198
18	1	-2.312875	2.515265	1.408819
19	1	-1.823391	0.850447	1.675317
20	6	0.718763	2.467729	0.260337
21	6	1.654031	1.266924	0.627292
22	1	0.807281	3.249784	1.019527
23	1	1.023623	2.876781	-0.707427
24	6	1.502650	0.180371	-0.445695
25	1	2.683851	1.631672	0.679059
26	1	1.398099	0.887764	1.622616
27	1	-0.620743	1.581358	-1.862261
28	6	2.505937	-1.030391	-0.307843
29	6	-0.661987	1.912505	0.219206
30	6	3.837778	-0.677745	-0.994040
31	1	4.324923	0.178023	-0.512409
32	1	4.530325	-1.522786	-0.935780
33	1	3.695947	-0.436902	-2.052697
34	6	2.757101	-1.495960	1.135533
35	1	3.403476	-2.378654	1.125874
36	1	3.269374	-0.726805	1.723346
37	1	1.844355	-1.776388	1.668580
38	1	1.755290	0.656745	-1.401840
39	1	2.068058	-1.872044	-0.860835
40	1	-0.126450	-0.585012	-1.644348

G1



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

HF = -586.4216473 hartrees (-367985.447897223 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366725 (Hartree/Particle)

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

HF = -586.2914138 hartrees (-367897.8621595 kcal/mol)

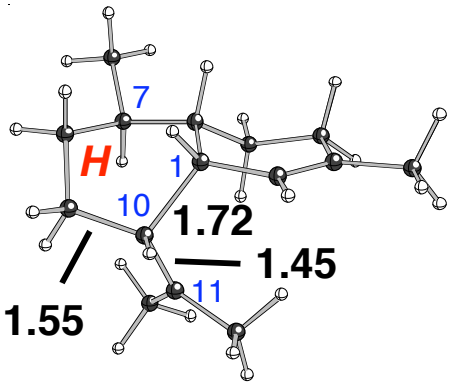
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.680555	-1.117144	0.336116
2	6	-1.970028	-1.453917	0.110319
3	6	-2.647659	-0.834412	-1.090986
4	6	-2.435085	0.705076	-1.153084
5	6	-0.979178	1.159994	-0.938386
6	6	0.020634	-0.241506	-0.636631
7	1	-2.249233	-1.288767	-2.009557
8	1	-0.160634	-1.470274	1.220855
9	1	-2.770287	1.072832	-2.127490
10	1	-3.088476	1.172110	-0.411624
11	1	-3.720608	-1.044725	-1.089815
12	6	-2.756855	-2.378083	0.992062
13	1	-3.109171	-3.242552	0.415240
14	1	-2.164912	-2.747437	1.833213
15	1	-3.654695	-1.883931	1.384281
16	6	-1.450497	1.960019	1.428898
17	1	-0.934595	2.381956	2.292245
18	1	-2.355382	2.555398	1.234984
19	1	-1.813197	0.945177	1.650756
20	6	0.747954	2.497633	0.267935
21	6	1.650045	1.251365	0.634114
22	1	0.849103	3.264229	1.039535
23	1	1.079558	2.893214	-0.696015
24	6	1.486921	0.175526	-0.444567
25	1	2.681001	1.610644	0.700762
26	1	1.374275	0.878555	1.626047
27	1	-0.510189	1.547846	-1.845063
28	6	2.455954	-1.054148	-0.284986
29	6	-0.616641	1.941702	0.209755
30	6	3.785693	-0.768402	-1.005909
31	1	4.303141	0.092562	-0.565857
32	1	4.457897	-1.627937	-0.925871
33	1	3.632807	-0.564467	-2.070862
34	6	2.729080	-1.480888	1.167863
35	1	3.333851	-2.392533	1.173239
36	1	3.295332	-0.716562	1.711619
37	1	1.822173	-1.697151	1.739528
38	1	1.770655	0.649400	-1.394116
39	1	1.980343	-1.900084	-0.798721

40	1	-0.087453	-0.664383	-1.642393

Figure 5.

C3



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

HF = -586.4259611 hartrees (-367988.154849861 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366327 (Hartree/Particle)

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

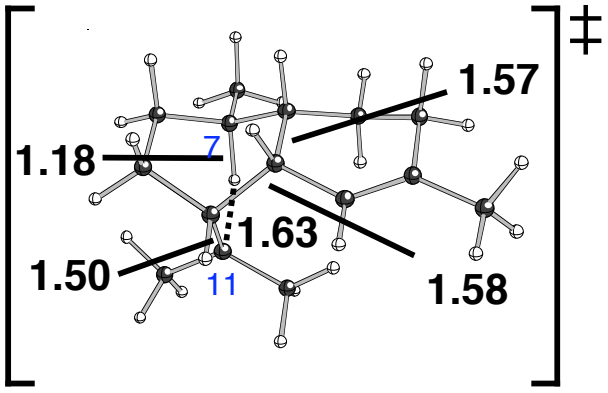
HF = -586.2961087 hartrees (-367900.80820925 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.617085	0.019149	-1.069820
2	6	2.469954	-0.658427	-0.262427
3	6	1.960098	-1.529500	0.860112
4	6	0.485361	-1.280075	1.200973
5	6	-0.378191	-1.198451	-0.065411
6	6	0.140040	-0.095245	-1.001759
7	1	2.108680	-2.578789	0.562294
8	1	2.026992	0.604461	-1.892116
9	1	0.117120	-2.071398	1.861405
10	1	0.393250	-0.345052	1.771140
11	1	2.591624	-1.391926	1.746858
12	6	3.955355	-0.642103	-0.487145
13	1	4.321638	-1.658721	-0.677720
14	1	4.240949	-0.012175	-1.333041
15	1	4.481965	-0.289203	0.408075

16	6	-2.501568	-2.529830	0.407680
17	1	-3.551364	-2.471630	0.711207
18	1	-2.454209	-3.102986	-0.525537
19	1	-1.967899	-3.097724	1.176565
20	6	-2.629100	-0.355649	-0.896168
21	6	-2.206206	1.125153	-0.979549
22	1	-3.711146	-0.395446	-0.733004
23	1	-2.455312	-0.859886	-1.855659
24	6	-0.686019	1.397899	-0.807827
25	1	-2.503348	1.535409	-1.950044
26	1	-2.765261	1.699672	-0.235071
27	1	-0.209693	-2.124801	-0.637904
28	6	-0.231418	2.075706	0.384873
29	6	-1.904689	-1.127482	0.218128
30	6	1.093430	2.713689	0.373586
31	1	1.300219	3.256392	-0.553047
32	1	1.288788	3.338987	1.245975
33	1	1.820000	1.867705	0.371103
34	6	-1.001906	2.144403	1.647909
35	1	-0.344897	2.116780	2.523006
36	1	-1.469282	3.145632	1.665254
37	1	-1.798670	1.409517	1.737248
38	1	-0.271833	1.926698	-1.671425
39	1	-2.051956	-0.581628	1.161691
40	1	-0.229714	-0.275322	-2.016178

TS (C3-to-H1)



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

HF = -586.4130762 hartrees (-367980.069446262 kcal/mol)
Imaginary Frequencies: 1 (-147.3835 1/cm)
Zero-point correction = 0.365267 (Hartree/Particle)

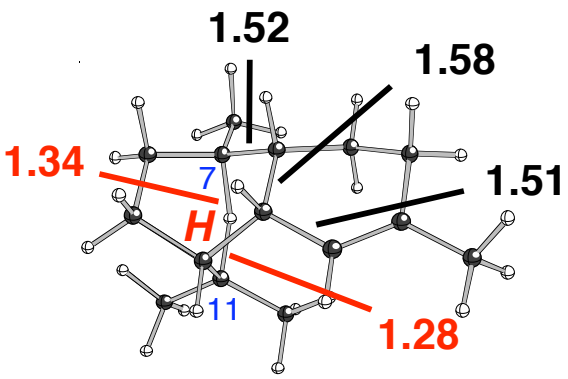
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.2876801 hartrees (-367895.51926275 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.731168	-0.866345	-0.727363
2	6	-2.769679	-0.204865	-0.188848
3	6	-2.600222	1.221808	0.282169
4	6	-1.158445	1.524835	0.707873
5	6	-0.135530	1.159689	-0.383305
6	6	-0.394323	-0.244276	-1.044086
7	1	-2.909733	1.907766	-0.520854
8	1	-1.878357	-1.884315	-1.088630
9	1	-1.066192	2.587568	0.951753
10	1	-0.940532	0.975525	1.633038
11	1	-3.279888	1.422247	1.118343
12	6	-4.136436	-0.817461	-0.049705
13	1	-4.882333	-0.216840	-0.585503
14	1	-4.173625	-1.835849	-0.445255
15	1	-4.452328	-0.839675	1.000883
16	6	1.737429	2.410458	0.947403
17	1	2.781344	2.329670	1.263316
18	1	1.644738	3.325974	0.349388
19	1	1.113483	2.526903	1.835238
20	6	2.305688	0.890706	-1.037910
21	6	2.017863	-0.517492	-1.644898
22	1	3.334601	0.965615	-0.672092
23	1	2.201949	1.664824	-1.806730
24	6	0.875315	-1.150975	-0.827348
25	1	1.698431	-0.440687	-2.686537
26	1	2.916464	-1.138877	-1.649240
27	1	-0.221779	1.911491	-1.180814
28	6	1.269713	-1.320963	0.611018
29	6	1.325454	1.216105	0.094260
30	6	0.257321	-1.699600	1.641108
31	1	0.241682	-2.802613	1.641487
32	1	0.564139	-1.400006	2.646599
33	1	-0.753025	-1.365966	1.412974
34	6	2.686021	-1.659017	0.973682
35	1	2.844965	-1.645888	2.053335
36	1	2.852731	-2.691167	0.625749
37	1	3.435668	-1.041500	0.480834
38	1	0.640789	-2.163368	-1.194597
39	1	1.385995	0.294514	0.825656
40	1	-0.393202	-0.100979	-2.132644

H1



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

HF = -586.414265 hartrees (-367980.81543015 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365371 (Hartree/Particle)

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

HF = -586.2902361 hartrees (-367897.12315275 kcal/mol)

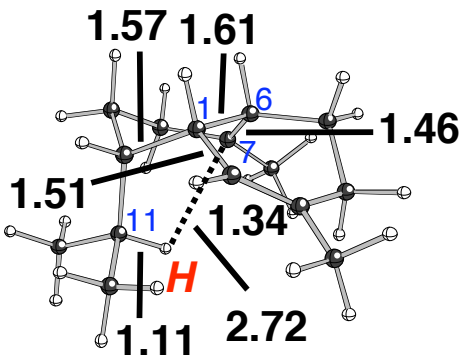
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.740010	-0.897124	-0.704517
2	6	-2.775785	-0.224063	-0.179705
3	6	-2.610237	1.220981	0.238332
4	6	-1.170689	1.534213	0.666625
5	6	-0.151489	1.135246	-0.415734
6	6	-0.406216	-0.283834	-1.059185
7	1	-2.912592	1.881439	-0.588291
8	1	-1.877910	-1.931197	-1.018813
9	1	-1.075467	2.603175	0.883281
10	1	-0.960731	1.003823	1.603090
11	1	-3.291421	1.451996	1.064970
12	6	-4.135335	-0.840627	0.007448
13	1	-4.896730	-0.266820	-0.535930
14	1	-4.170212	-1.873154	-0.349602
15	1	-4.430973	-0.828414	1.064109
16	6	1.742188	2.279322	0.997742
17	1	2.779317	2.137766	1.311298
18	1	1.687386	3.248230	0.480504
19	1	1.097433	2.340657	1.875267
20	6	2.287828	0.870473	-1.089246
21	6	1.985557	-0.543776	-1.678437
22	1	3.314398	0.954021	-0.722448
23	1	2.175787	1.642016	-1.861630
24	6	0.866243	-1.161401	-0.818376
25	1	1.653318	-0.475126	-2.716601
26	1	2.890217	-1.155040	-1.682755

27	1	-0.230212	1.873986	-1.228586
28	6	1.302021	-1.141945	0.643415
29	6	1.306672	1.222482	0.014170
30	6	0.310089	-1.585003	1.704034
31	1	0.329202	-2.683641	1.712875
32	1	0.614775	-1.254354	2.700748
33	1	-0.713458	-1.278463	1.501491
34	6	2.720708	-1.582839	0.973470
35	1	2.921100	-1.491783	2.043537
36	1	2.807634	-2.645198	0.709893
37	1	3.496532	-1.049694	0.424296
38	1	0.664732	-2.198394	-1.114614
39	1	1.369908	0.130447	0.792345
40	1	-0.431303	-0.148909	-2.148647

Figure 6.

G2



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

HF = -586.4138218 hartrees (-367980.537317718 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365550 (Hartree/Particle)

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

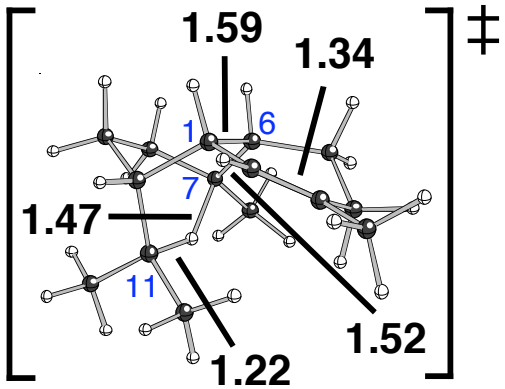
HF = -586.2852209 hartrees (-367899.838966959 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.377021	0.983556	0.820871
2	6	-2.404109	0.662494	0.021653
3	6	-2.514165	-0.723746	-0.574153
4	6	-1.819291	-1.754007	0.324724

5	6	-0.367038	-1.379270	0.649363
6	6	-0.198244	0.123909	1.205903
7	1	-3.569694	-0.998773	-0.678367
8	1	-1.364308	1.964485	1.293142
9	1	-2.363885	-1.795350	1.273643
10	1	-1.877995	-2.759709	-0.103799
11	1	-2.108697	-0.734430	-1.597351
12	6	-3.508573	1.632532	-0.302583
13	1	-4.476030	1.257266	0.053493
14	1	-3.336562	2.613992	0.146380
15	1	-3.603883	1.765377	-1.387976
16	6	0.438361	-2.609731	-1.471540
17	1	1.349569	-2.901339	-1.994346
18	1	-0.148523	-3.503284	-1.217230
19	1	-0.214319	-2.037700	-2.147807
20	6	2.081864	-1.516713	0.133355
21	6	2.225612	-0.420155	1.196615
22	1	2.668630	-1.326182	-0.774955
23	1	2.483086	-2.487095	0.487724
24	6	1.220174	0.717056	0.902286
25	1	2.031740	-0.829145	2.195811
26	1	3.257395	-0.065385	1.209700
27	1	-0.042812	-1.976065	1.532717
28	6	1.433460	1.364008	-0.504031
29	6	0.692291	-1.809257	-0.259814
30	6	0.746250	2.738186	-0.648987
31	1	1.108182	3.430575	0.120206
32	1	0.992818	3.173020	-1.622244
33	1	-0.338823	2.686174	-0.579343
34	6	2.926960	1.558688	-0.840796
35	1	3.026072	2.075635	-1.799303
36	1	3.416797	2.181642	-0.083187
37	1	3.497037	0.628941	-0.921196
38	1	1.387238	1.504018	1.648715
39	1	0.995786	0.699987	-1.271151
40	1	-0.228010	0.028051	2.299544

TS (G2-to H2)



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

HF = -586.4065703 hartrees (-367975.986928953 kcal/mol)
Imaginary Frequencies: 1 (-140.0235 1/cm)
Zero-point correction = 0.365157 (Hartree/Particle)

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

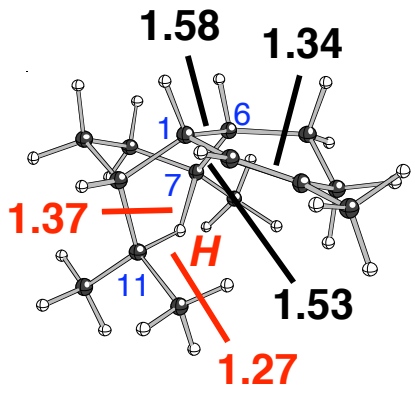
HF = -586.2819952 hartrees (-367897.814807952 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.685234	-0.703704	1.013177
2	6	2.584771	-0.242530	0.130394
3	6	2.258459	0.950899	-0.741466
4	6	1.312307	1.922347	-0.028044
5	6	0.057649	1.276859	0.590267
6	6	0.316819	-0.125522	1.285958
7	1	3.179326	1.481888	-1.006779
8	1	1.944889	-1.558979	1.636179
9	1	1.869456	2.371043	0.801769
10	1	1.034980	2.753546	-0.683780
11	1	1.834814	0.610379	-1.699951
12	6	3.931562	-0.884366	-0.063884
13	1	4.737102	-0.173015	0.156502
14	1	4.064204	-1.761027	0.575275
15	1	4.068957	-1.195872	-1.107826
16	6	-1.411234	2.077267	-1.446244
17	1	-2.345214	1.843517	-1.962181
18	1	-1.475844	3.123727	-1.111208
19	1	-0.572683	2.015630	-2.142550
20	6	-2.425607	0.932255	0.637042
21	6	-2.148783	-0.307854	1.542758
22	1	-3.317960	0.814242	0.017959
23	1	-2.600672	1.826841	1.249714
24	6	-0.913503	-1.040309	0.968198
25	1	-1.945410	-0.002450	2.572291
26	1	-3.031565	-0.948903	1.578377
27	1	-0.254202	1.945891	1.408071
28	6	-1.126910	-1.239273	-0.537955
29	6	-1.221438	1.234128	-0.221500
30	6	-0.032114	-1.901636	-1.368273
31	1	0.017650	-2.956849	-1.070029
32	1	-0.286008	-1.875950	-2.431183
33	1	0.955863	-1.480302	-1.214461
34	6	-2.493699	-1.772428	-0.969467
35	1	-2.577297	-1.791019	-2.058854
36	1	-2.572392	-2.809855	-0.620053
37	1	-3.349185	-1.232545	-0.566606
38	1	-0.777876	-2.014836	1.451485
39	1	-1.112258	-0.069515	-0.889191

40	1	0.270255	0.027609	2.371257

H2



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

HF = -586.4065995 hartrees (-367976.005252245 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365345 (Hartree/Particle)

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

HF = -586.2824858 hartrees (-367898.122664358 kcal/mol)

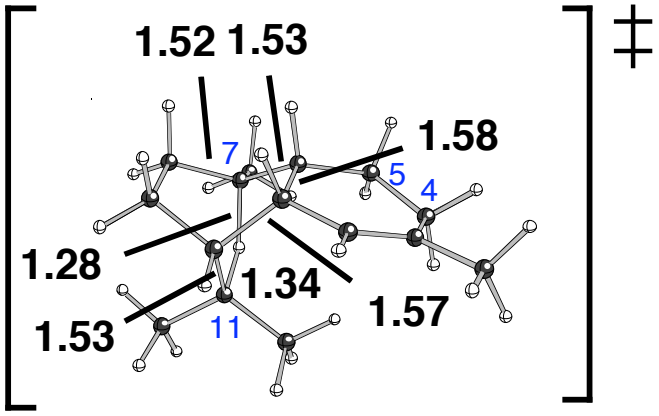
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.690787	-0.715238	-1.004865
2	6	-2.589630	-0.240714	-0.127878
3	6	-2.260696	0.961568	0.730939
4	6	-1.303986	1.919299	0.013270
5	6	-0.052117	1.262662	-0.599738
6	6	-0.322882	-0.139059	-1.285192
7	1	-3.180317	1.500552	0.984444
8	1	-1.953371	-1.577187	-1.617485
9	1	-1.856257	2.367127	-0.820407
10	1	-1.021496	2.752485	0.664235
11	1	-1.845973	0.630201	1.696596
12	6	-3.938870	-0.875910	0.071938
13	1	-4.741321	-0.164577	-0.159483
14	1	-4.073333	-1.760181	-0.556297
15	1	-4.080057	-1.173132	1.119532
16	6	1.430887	2.078732	1.428309
17	1	2.365461	1.850166	1.946214
18	1	1.501440	3.114943	1.067187

19	1	0.598346	2.037710	2.133428
20	6	2.427453	0.913505	-0.655045
21	6	2.145258	-0.332635	-1.551029
22	1	3.330831	0.801449	-0.050605
23	1	2.585344	1.807207	-1.271486
24	6	0.908069	-1.055277	-0.965953
25	1	1.935424	-0.035140	-2.581377
26	1	3.023619	-0.979853	-1.589296
27	1	0.265924	1.929389	-1.414941
28	6	1.125649	-1.241420	0.537397
29	6	1.227575	1.194851	0.227500
30	6	0.029251	-1.845820	1.399540
31	1	-0.035670	-2.910650	1.138448
32	1	0.290526	-1.787232	2.459139
33	1	-0.953520	-1.418925	1.230561
34	6	2.490754	-1.748070	0.989080
35	1	2.578641	-1.721048	2.077803
36	1	2.561163	-2.800749	0.684669
37	1	3.344345	-1.231606	0.554942
38	1	0.766524	-2.037247	-1.432937
39	1	1.116305	-0.016339	0.859406
40	1	-0.278145	0.003793	-2.371928

Figure 7.

TS (H1-to H2)



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

HF = -586.4021678 hartrees (-367973.224316178 kcal/mol)
Imaginary Frequencies: 1 (-153.4156 1/cm)
Zero-point correction = 0.365252 (Hartree/Particle)

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

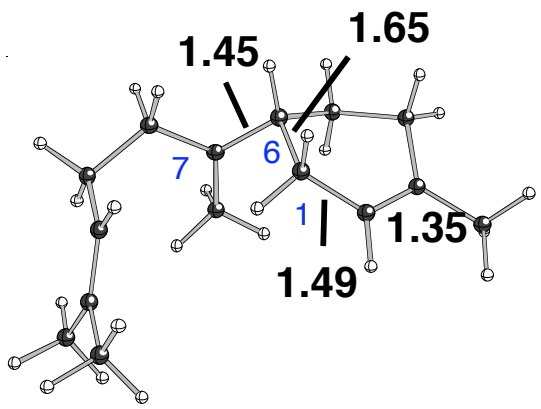
HF = -586.2776199 hartrees (-367889.20648725 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.761766	-0.761539	-0.935655
2	6	-2.710214	-0.184242	-0.186605
3	6	-2.431272	1.031395	0.658403
4	6	-1.139302	1.827933	0.350127
5	6	-0.055546	1.175222	-0.562779
6	6	-0.365668	-0.250117	-1.163422
7	1	-3.287065	1.713341	0.591840
8	1	-2.012574	-1.655683	-1.505274
9	1	-1.429942	2.766596	-0.129486
10	1	-0.697255	2.125000	1.303574
11	1	-2.425290	0.705815	1.709748
12	6	-4.103927	-0.745921	-0.084374
13	1	-4.841043	-0.023469	-0.455929
14	1	-4.213961	-1.670120	-0.657143
15	1	-4.369129	-0.954578	0.960013
16	6	1.857038	2.245551	0.919707
17	1	2.880675	2.055304	1.249978
18	1	1.861233	3.193694	0.363200
19	1	1.216920	2.386982	1.790900
20	6	2.395933	0.681166	-1.037642
21	6	2.034225	-0.740442	-1.569576
22	1	3.397553	0.711303	-0.600907
23	1	2.399327	1.412273	-1.855912
24	6	0.808740	-1.213734	-0.766190
25	1	1.787112	-0.713486	-2.633038
26	1	2.886696	-1.414428	-1.466560
27	1	0.043588	1.834222	-1.437325
28	6	1.140625	-1.138635	0.721908
29	6	1.373519	1.171246	-0.024107
30	6	0.044147	-1.415194	1.732909
31	1	-0.101874	-2.503647	1.758580
32	1	0.342976	-1.106526	2.738013
33	1	-0.912317	-0.972499	1.470749
34	6	2.486630	-1.686479	1.176575
35	1	2.629709	-1.536185	2.249150
36	1	2.484695	-2.768868	0.992026
37	1	3.343252	-1.270042	0.646650
38	1	0.538595	-2.246373	-1.018196
39	1	1.310763	0.121758	0.813096
40	1	-0.271607	-0.167646	-2.253417

Figure S1.

A3



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

HF = -586.4093687 hartrees (-367977.742952937 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.363061 (Hartree/Particle)

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

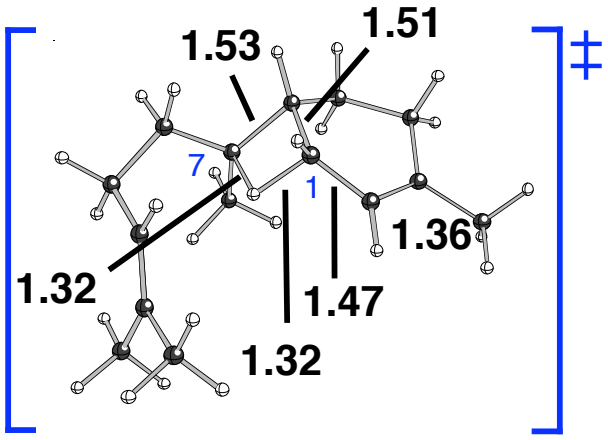
HF = -586.2713199 hartrees (-367891.115950449 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.993125	1.312430	-0.378048
2	6	3.261911	1.011338	-0.038865
3	6	3.722448	-0.425301	-0.138935
4	6	2.610498	-1.376570	0.342230
5	6	1.320139	-1.218269	-0.479034
6	6	1.057135	0.326034	-0.993420
7	1	4.002129	-0.664396	-1.175083
8	1	1.615727	2.324695	-0.255143
9	1	2.933215	-2.419754	0.259003
10	1	2.430017	-1.183174	1.402935
11	1	4.621509	-0.582161	0.464571
12	6	4.235839	2.035087	0.465311
13	1	5.124071	2.065345	-0.178216
14	1	3.801053	3.036972	0.497325
15	1	4.590052	1.774574	1.470897
16	6	-0.175409	-0.831035	1.544368
17	1	-1.185307	-0.456160	1.710579
18	1	-0.028118	-1.691077	2.219528
19	1	0.567898	-0.081167	1.826133
20	6	-1.089877	-1.975024	-0.575287
21	6	-2.543942	-1.540583	-0.292272
22	1	-0.965115	-3.041584	-0.294831
23	1	-0.870930	-1.956080	-1.650002
24	6	-2.823536	-0.124776	-0.733241
25	1	-3.181943	-2.234526	-0.855266

26	1	-2.791097	-1.701407	0.759926
27	1	1.364183	-1.835350	-1.378497
28	6	-3.437954	0.855332	-0.043217
29	6	0.025338	-1.330624	0.166118
30	6	-3.688886	2.200850	-0.681450
31	1	-3.294087	2.255316	-1.699446
32	1	-4.764521	2.412145	-0.723314
33	1	-3.237398	3.006968	-0.089600
34	6	-3.967071	0.724451	1.364284
35	1	-3.568843	1.522081	2.003537
36	1	-5.057333	0.846081	1.366776
37	1	-3.748213	-0.236336	1.835589
38	1	0.016256	0.649508	-0.844128
39	1	-2.538277	0.091929	-1.764388
40	1	1.166525	0.237508	-2.080129

TS (A3-to-B5)



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

HF = -586.3963 hartrees (-367969.542213 kcal/mol)
Imaginary Frequencies: 1 (-528.8185 1/cm)
Zero-point correction = 0.362143 (Hartree/Particle)

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

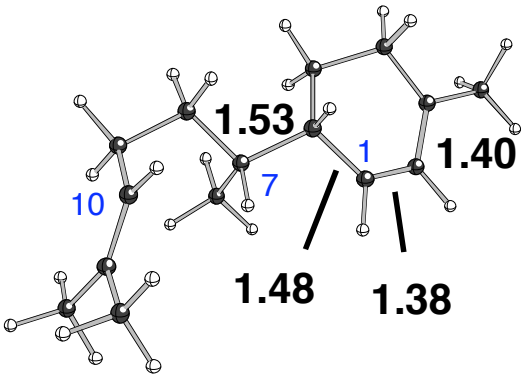
HF = -586.2642168 hartrees (-367886.658684168 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.589128	1.212781	-0.412019
2	6	2.886995	1.144239	-0.031398
3	6	3.635663	-0.169410	-0.041033

4	6	2.737432	-1.392428	0.219806
5	6	1.427528	-1.344521	-0.580406
6	6	0.909146	0.027628	-0.940056
7	1	4.139961	-0.259354	-1.014327
8	1	1.066129	2.163357	-0.451586
9	1	3.275751	-2.307945	-0.037974
10	1	2.531790	-1.451736	1.291287
11	1	4.439083	-0.140210	0.702142
12	6	3.663420	2.370629	0.341819
13	1	4.555465	2.462139	-0.290063
14	1	3.072738	3.284131	0.245823
15	1	4.023743	2.290435	1.375125
16	6	0.037011	-1.065817	1.622375
17	1	-0.964599	-0.794273	1.956038
18	1	0.325301	-2.002780	2.111905
19	1	0.733284	-0.288415	1.944868
20	6	-1.051317	-2.075693	-0.533944
21	6	-2.483455	-1.577216	-0.248325
22	1	-0.926005	-3.107972	-0.177639
23	1	-0.878140	-2.107715	-1.616450
24	6	-2.709001	-0.165287	-0.729132
25	1	-3.164408	-2.257534	-0.776395
26	1	-2.718313	-1.687955	0.813202
27	1	1.419024	-2.035334	-1.421855
28	6	-3.191487	0.889106	-0.040398
29	6	0.076343	-1.284630	0.123038
30	6	-3.412293	2.217716	-0.724106
31	1	-3.093518	2.203495	-1.769903
32	1	-4.475039	2.488762	-0.698782
33	1	-2.876452	3.022995	-0.206037
34	6	-3.607045	0.859980	1.410291
35	1	-3.093326	1.646537	1.976790
36	1	-4.679877	1.072967	1.495027
37	1	-3.424858	-0.095661	1.905762
38	1	-0.234071	-0.070327	-0.279530
39	1	-2.506322	-0.011863	-1.791801
40	1	0.404254	0.101791	-1.904691

B5



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

HF = -586.4275274 hartrees (-367989.137718774 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.363477 (Hartree/Particle)

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

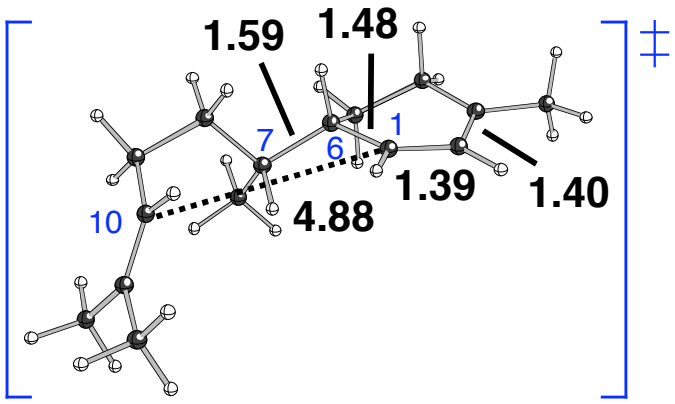
HF = -586.2876414 hartrees (-367901.357854914 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.118865	-1.461346	0.175434
2	6	-4.054078	-0.457809	-0.111151
3	6	-3.586393	0.873329	-0.593542
4	6	-2.166882	1.231372	-0.130366
5	6	-1.176218	0.080217	-0.377096
6	6	-1.769747	-1.227393	-0.021379
7	1	-3.629857	0.813275	-1.697727
8	1	-3.463104	-2.449881	0.464168
9	1	-1.834106	2.136591	-0.642576
10	1	-2.192577	1.462003	0.940574
11	1	-4.313394	1.647620	-0.324485
12	6	-5.508482	-0.711666	-0.003105
13	1	-6.047221	-0.293523	-0.861885
14	1	-5.756012	-1.766421	0.124192
15	1	-5.882675	-0.157443	0.873382
16	6	0.203898	0.261077	1.792977
17	1	1.217152	0.256503	2.201156
18	1	-0.299608	1.149806	2.188434
19	1	-0.305484	-0.623125	2.195619
20	6	0.955361	1.496895	-0.323021
21	6	2.481849	1.528092	-0.074095
22	1	0.511393	2.409016	0.096186
23	1	0.785611	1.535383	-1.408479
24	6	3.219191	0.410538	-0.764231
25	1	2.846299	2.490106	-0.461490
26	1	2.688926	1.545479	0.999711
27	1	-0.994703	-0.010089	-1.469737
28	6	4.106183	-0.460100	-0.245530
29	6	0.247297	0.255449	0.255054
30	6	4.784340	-1.484488	-1.124743
31	1	4.437163	-1.432172	-2.160373
32	1	5.872033	-1.337729	-1.123635
33	1	4.609091	-2.502097	-0.752048
34	6	4.542528	-0.493991	1.199140
35	1	4.397737	-1.496067	1.622641
36	1	5.616258	-0.280165	1.275834
37	1	4.018568	0.223337	1.833848
38	1	0.825146	-0.623632	-0.063187
39	1	3.021190	0.336797	-1.835960

40	1	-1.087720	-2.074636	0.059776

TS (B5-to-B6)



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

HF = -586.4215657 hartrees (-367985.396692407 kcal/mol)
Imaginary Frequencies: 1 (-61.4176 1/cm)
Zero-point correction = 0.363758 (Hartree/Particle)

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

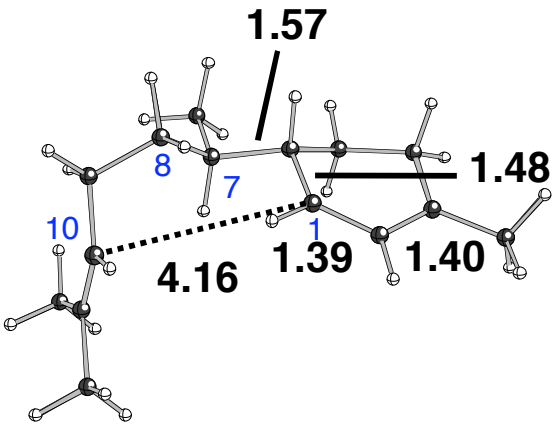
HF = -586.2816482 hartrees (-367897.597061982 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.915027	1.523594	-0.037181
2	6	3.993042	0.640212	0.099029
3	6	3.761074	-0.827955	-0.021709
4	6	2.335120	-1.251916	0.355346
5	6	1.284133	-0.396394	-0.376640
6	6	1.655468	1.034355	-0.340449
7	1	3.970985	-1.071894	-1.080821
8	1	3.088460	2.594947	-0.004024
9	1	2.195305	-2.309982	0.123513
10	1	2.210633	-1.143958	1.437706
11	1	4.517252	-1.376646	0.550499
12	6	5.372877	1.136001	0.302733
13	1	6.086281	0.585400	-0.322012
14	1	5.475870	2.209951	0.141458
15	1	5.661486	0.910292	1.342571
16	6	-0.430057	-1.535159	1.224491
17	1	-1.491179	-1.582901	1.478783
18	1	-0.093937	-2.558130	1.024250

19	1	0.088465	-1.166790	2.114669
20	6	-1.029283	-1.089985	-1.227601
21	6	-2.564707	-1.098567	-1.071273
22	1	-0.684513	-2.097752	-1.501783
23	1	-0.780972	-0.436406	-2.076714
24	6	-3.141499	0.274256	-0.834198
25	1	-2.977699	-1.504331	-2.005704
26	1	-2.862632	-1.801269	-0.288608
27	1	1.351975	-0.641060	-1.458449
28	6	-3.999683	0.674470	0.122099
29	6	-0.240958	-0.611197	0.011276
30	6	-4.502504	2.098973	0.159775
31	1	-4.070425	2.708913	-0.638633
32	1	-5.594583	2.128483	0.055149
33	1	-4.270545	2.573885	1.121971
34	6	-4.572247	-0.214262	1.200104
35	1	-4.388775	0.214918	2.193370
36	1	-5.662094	-0.285187	1.092226
37	1	-4.175236	-1.231348	1.189509
38	1	-0.651382	0.366332	0.296130
39	1	-2.839424	1.021099	-1.572418
40	1	0.881857	1.754873	-0.607451

B6



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

HF = -586.4266379 hartrees (-367988.579548629 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.363749 (Hartree/Particle)

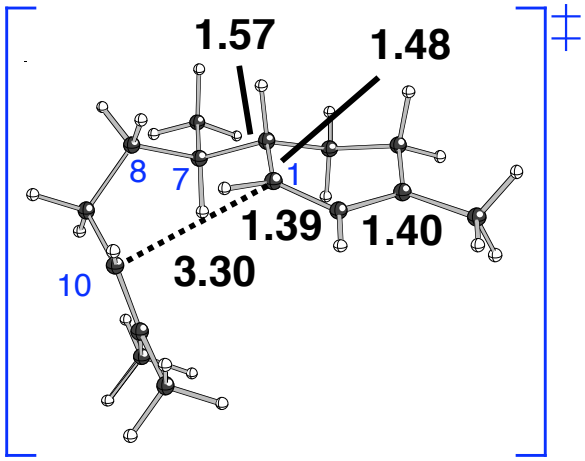
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.2868973 hartrees (-367900.890924723 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.356534	1.378123	-0.581858
2	6	3.520947	0.905466	0.036254
3	6	3.583430	-0.509088	0.501396
4	6	2.207379	-1.111251	0.815052
5	6	1.203873	-0.874207	-0.328322
6	6	1.294158	0.522162	-0.815007
7	1	4.072108	-1.067840	-0.319437
8	1	2.320705	2.398324	-0.951982
9	1	2.317154	-2.178740	1.013381
10	1	1.816523	-0.653929	1.733088
11	1	4.272072	-0.595380	1.349443
12	6	4.711528	1.769865	0.198352
13	1	5.630797	1.224520	-0.046770
14	1	4.655199	2.696820	-0.374048
15	1	4.800441	2.025040	1.267148
16	6	-0.366153	-2.575314	0.779823
17	1	-1.413841	-2.857847	0.915734
18	1	0.126235	-3.393940	0.241647
19	1	0.075104	-2.500857	1.777308
20	6	-1.136875	-1.343928	-1.297351
21	6	-2.629926	-1.013868	-1.074330
22	1	-1.037235	-2.353788	-1.716527
23	1	-0.756358	-0.665663	-2.074151
24	6	-2.868422	0.453241	-0.819501
25	1	-3.177815	-1.309590	-1.978766
26	1	-3.030336	-1.633068	-0.265956
27	1	1.497657	-1.498378	-1.199316
28	6	-3.415692	1.047647	0.258652
29	6	-0.285678	-1.257939	-0.009039
30	6	-3.619361	2.544353	0.293659
31	1	-3.252680	3.031481	-0.614356
32	1	-4.684314	2.787021	0.400016
33	1	-3.112583	2.993335	1.157841
34	6	-3.912068	0.323227	1.486438
35	1	-3.446602	0.734044	2.391531
36	1	-4.993088	0.472055	1.602890
37	1	-3.726358	-0.752220	1.467384
38	1	-0.693168	-0.455471	0.621232
39	1	-2.586579	1.102743	-1.651884
40	1	0.464918	0.900406	-1.410748

TS (B6-to-B7)



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

HF = -586.4265209 hartrees (-367988.506129959 kcal/mol)
Imaginary Frequencies: 1 (-8.6155 1/cm)
Zero-point correction = 0.364132 (Hartree/Particle)

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

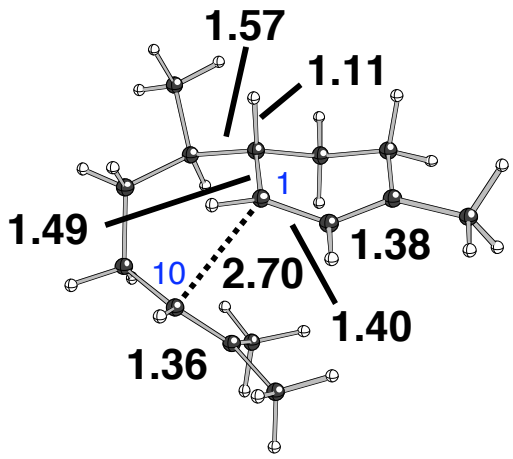
HF = -586.2870195 hartrees (-367900.967606445 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.719826	-1.234461	-0.670984
2	6	-2.957837	-0.972942	-0.079515
3	6	-3.273248	0.408018	0.387743
4	6	-2.028756	1.227561	0.752065
5	6	-0.943622	1.165179	-0.337761
6	6	-0.809402	-0.208555	-0.877796
7	1	-3.823412	0.886909	-0.443091
8	1	-1.513851	-2.223685	-1.068627
9	1	-2.324230	2.260998	0.941095
10	1	-1.607441	0.839856	1.688700
11	1	-3.989838	0.370254	1.215852
12	6	-3.997707	-2.023196	0.033283
13	1	-4.976211	-1.641236	-0.282867
14	1	-3.754262	-2.932793	-0.517540
15	1	-4.114126	-2.278338	1.098577
16	6	0.282547	3.144470	0.727127
17	1	1.265965	3.533779	1.007455
18	1	-0.158186	3.847816	0.010588
19	1	-0.330638	3.143649	1.632312
20	6	1.493221	1.765503	-1.038654
21	6	2.752196	0.916248	-0.744530
22	1	1.806297	2.800389	-1.213199

23	1	1.051103	1.440452	-1.990973
24	6	2.498697	-0.569663	-0.758870
25	1	3.504083	1.144906	-1.510940
26	1	3.181986	1.238951	0.208923
27	1	-1.256404	1.776712	-1.210271
28	6	2.580323	-1.456660	0.258437
29	6	0.444879	1.744824	0.110302
30	6	2.362849	-2.930966	0.013573
31	1	2.096498	-3.143829	-1.025812
32	1	3.272932	-3.497184	0.248833
33	1	1.576914	-3.331289	0.667391
34	6	2.948997	-1.107036	1.678704
35	1	2.189138	-1.476562	2.379049
36	1	3.886975	-1.604885	1.955687
37	1	3.078085	-0.037014	1.848764
38	1	0.808921	1.070811	0.897008
39	1	2.279755	-0.978878	-1.748473
40	1	0.050075	-0.419738	-1.507186

B7



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

HF = -586.4284784 hartrees (-367989.734480784 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365031 (Hartree/Particle)

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

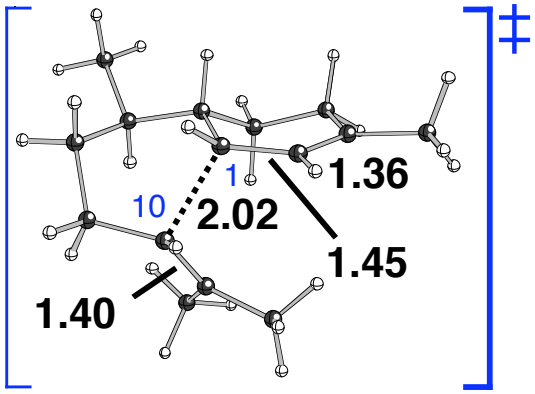
HF = -586.2901801 hartrees (-367902.950914551 kcal/mol)

Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	1.669102	0.157230	-1.031213
2	6	2.620495	-0.452138	-0.231573
3	6	2.229725	-1.570882	0.684409
4	6	0.739843	-1.573142	1.040945
5	6	-0.154444	-1.402575	-0.198967
6	6	0.340554	-0.292397	-1.054854
7	1	2.503623	-2.505698	0.163930
8	1	1.977244	0.922418	-1.736977
9	1	0.487280	-2.497260	1.566939
10	1	0.532493	-0.748320	1.733396
11	1	2.857323	-1.553700	1.583009
12	6	4.061399	-0.088146	-0.323397
13	1	4.671410	-0.982305	-0.505698
14	1	4.265147	0.650668	-1.100207
15	1	4.400439	0.309031	0.643660
16	6	-2.159008	-2.893618	0.219579
17	1	-3.160403	-2.954973	0.654757
18	1	-2.204988	-3.331097	-0.784795
19	1	-1.498794	-3.519664	0.828663
20	6	-2.605348	-0.595090	-0.750547
21	6	-2.675211	0.907390	-0.392844
22	1	-3.620504	-0.992286	-0.644658
23	1	-2.352323	-0.741325	-1.810267
24	6	-1.419606	1.710415	-0.620927
25	1	-3.467459	1.362922	-1.000197
26	1	-3.003147	0.994005	0.647819
27	1	0.007132	-2.272145	-0.873698
28	6	-0.599861	2.274435	0.310582
29	6	-1.680788	-1.431779	0.159502
30	6	0.517681	3.191092	-0.105150
31	1	0.570987	3.324449	-1.188685
32	1	0.386766	4.179627	0.352276
33	1	1.486588	2.816215	0.253667
34	6	-0.757346	2.108822	1.798100
35	1	0.194169	1.810505	2.256194
36	1	-1.019509	3.073560	2.251477
37	1	-1.521318	1.385222	2.083391
38	1	-1.759308	-1.011091	1.171712
39	1	-1.234396	1.992722	-1.658203
40	1	-0.261582	-0.009191	-1.909377

TS (B7-to-C3)



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

HF = -586.4243257 hartrees (-367987.128620007 kcal/mol)
Imaginary Frequencies: 1 (-187.9585 1/cm)
Zero-point correction = 0.365550 (Hartree/Particle)

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

HF = -586.2912303 hartrees (-367903.609925553 kcal/mol)

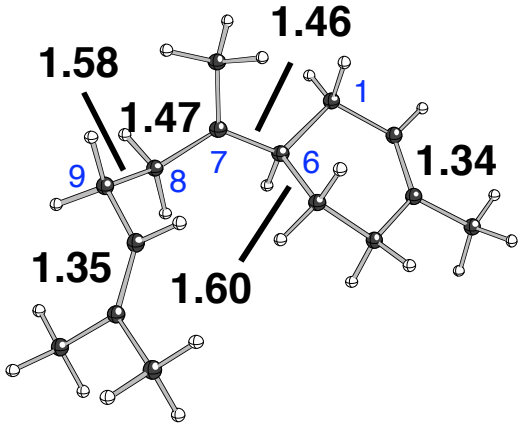
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.609185	-0.021168	-1.078010
2	6	2.462773	-0.702501	-0.262712
3	6	1.944224	-1.610405	0.821885
4	6	0.469408	-1.372974	1.168425
5	6	-0.395185	-1.238497	-0.093125
6	6	0.170564	-0.182045	-1.018736
7	1	2.093461	-2.646157	0.477014
8	1	2.017244	0.584683	-1.883835
9	1	0.099094	-2.190206	1.794336
10	1	0.376038	-0.459288	1.768581
11	1	2.575087	-1.514711	1.714111
12	6	3.947031	-0.662305	-0.469206
13	1	4.331280	-1.671764	-0.663034
14	1	4.235798	-0.017142	-1.301836
15	1	4.452392	-0.313693	0.440131
16	6	-2.544417	-2.529293	0.347756
17	1	-3.583916	-2.459126	0.681664
18	1	-2.535868	-3.064568	-0.608941
19	1	-2.005306	-3.140673	1.078685
20	6	-2.652634	-0.299552	-0.863744
21	6	-2.301435	1.200618	-0.797699
22	1	-3.733646	-0.393235	-0.716956
23	1	-2.455339	-0.708765	-1.863608

24	6	-0.811631	1.564250	-0.762952
25	1	-2.740829	1.712898	-1.660419
26	1	-2.791872	1.625503	0.083575
27	1	-0.264080	-2.158916	-0.692687
28	6	-0.191379	2.135777	0.356185
29	6	-1.921046	-1.132903	0.199829
30	6	1.140383	2.780791	0.220695
31	1	1.346730	3.139692	-0.789278
32	1	1.269687	3.594638	0.940186
33	1	1.907154	2.020941	0.461210
34	6	-0.773597	2.132065	1.731299
35	1	0.001992	1.994797	2.491883
36	1	-1.196259	3.133208	1.911764
37	1	-1.570270	1.406010	1.881443
38	1	-0.418277	1.953210	-1.701473
39	1	-2.035817	-0.615540	1.163245
40	1	-0.287941	-0.182942	-2.005102

Figure S2.

A4



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

HF = -586.4112964 hartrees (-367978.952603964 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.362748 (Hartree/Particle)

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

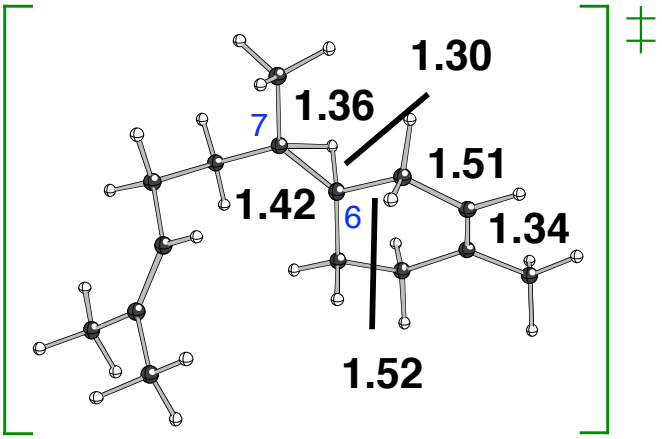
HF = -586.2719581 hartrees (-367891.516427331 kcal/mol)

Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	3.672574	0.281754	-0.167904
2	6	3.416691	-1.034537	-0.112122
3	6	2.016022	-1.560508	0.111137
4	6	0.998244	-0.499033	0.548248
5	6	1.226135	0.804108	-0.349448
6	6	2.627332	1.363449	-0.045297
7	1	1.666308	-2.073066	-0.796116
8	1	4.693182	0.621241	-0.327651
9	1	-0.020391	-0.883282	0.448873
10	1	1.157166	-0.213527	1.593072
11	1	2.034426	-2.330110	0.895588
12	6	-1.141585	1.507759	-0.909803
13	6	-2.541847	1.382556	-0.198864
14	1	-1.018561	0.714265	-1.651106
15	1	-1.169471	2.469596	-1.460784
16	6	-2.740073	0.070613	0.503180
17	1	-2.664530	2.214944	0.502026
18	1	-3.284032	1.532726	-0.985000
19	6	-3.518901	-0.957712	0.108545
20	6	0.065382	1.651545	-0.082661
21	6	-3.660848	-2.184569	0.975104
22	1	-4.709987	-2.334679	1.257915
23	1	-3.355197	-3.085739	0.428995
24	1	-3.069285	-2.116480	1.891894
25	6	-4.321939	-0.994194	-1.167025
26	1	-5.391013	-1.079329	-0.936754
27	1	-4.185492	-0.119551	-1.805429
28	1	-4.061603	-1.883655	-1.753387
29	1	-2.217877	-0.032969	1.455672
30	1	1.178422	0.448412	-1.386153
31	6	0.102848	2.657158	0.998934
32	1	0.501818	2.220507	1.923451
33	1	0.836946	3.429116	0.717478
34	1	-0.856321	3.134056	1.193590
35	1	2.659676	1.811570	0.956751
36	1	2.850329	2.172908	-0.752361
37	6	4.489002	-2.077837	-0.283360
38	1	4.578753	-2.700366	0.615374
39	1	4.249276	-2.753991	-1.113764
40	1	5.463230	-1.625912	-0.484159

TS (A4-to-D2)



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

HF = -586.3977485 hartrees (-367970.451161235 kcal/mol)
Imaginary Frequencies: 1 (-507.2847 1/cm)
Zero-point correction = 0.360513 (Hartree/Particle)

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

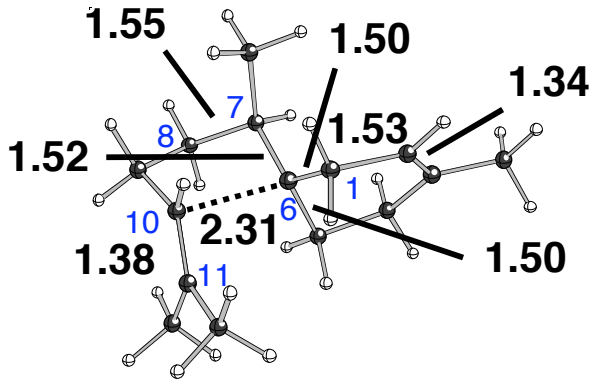
HF = -586.2612995 hartrees (-367878.96543625 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	3.223557	0.073365	0.912585
2	6	3.408996	-0.821274	-0.068291
3	6	2.289644	-1.169039	-1.025257
4	6	0.902195	-0.738903	-0.515500
5	6	0.913860	0.663439	0.053276
6	6	1.950570	0.856752	1.143257
7	1	2.488855	-0.723076	-2.011180
8	1	4.032502	0.298734	1.602816
9	1	0.138809	-0.882109	-1.278658
10	1	0.619088	-1.375390	0.333560
11	1	2.271196	-2.251826	-1.194416
12	6	-1.181917	1.442007	-1.230665
13	6	-2.538949	1.274271	-0.465057
14	1	-1.021168	0.567340	-1.860427
15	1	-1.259096	2.319153	-1.882189
16	6	-2.574842	0.119357	0.500994
17	1	-2.762606	2.208607	0.063746
18	1	-3.303922	1.175357	-1.238679
19	6	-3.218823	-1.054962	0.353830
20	6	-0.043505	1.664700	-0.265192
21	6	-3.197624	-2.086421	1.455825
22	1	-4.215913	-2.296324	1.805655

23	1	-2.792672	-3.039914	1.093880
24	1	-2.605456	-1.761855	2.315915
25	6	-4.023444	-1.451756	-0.858987
26	1	-5.068737	-1.628567	-0.577456
27	1	-4.014464	-0.710927	-1.660648
28	1	-3.651532	-2.398400	-1.270081
29	1	-2.054358	0.282848	1.446816
30	1	1.134397	1.505579	-0.915123
31	6	-0.052943	2.994187	0.453942
32	1	-0.562691	2.858362	1.415968
33	1	0.942517	3.383339	0.669692
34	1	-0.604353	3.740934	-0.118827
35	1	1.460876	0.539136	2.079484
36	1	2.188948	1.913146	1.292915
37	6	4.719966	-1.527158	-0.286708
38	1	4.604383	-2.611478	-0.168105
39	1	5.088817	-1.358357	-1.306150
40	1	5.486136	-1.185687	0.413188

D2



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

HF = -586.4172681 hartrees (-367982.699905431 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365562 (Hartree/Particle)

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

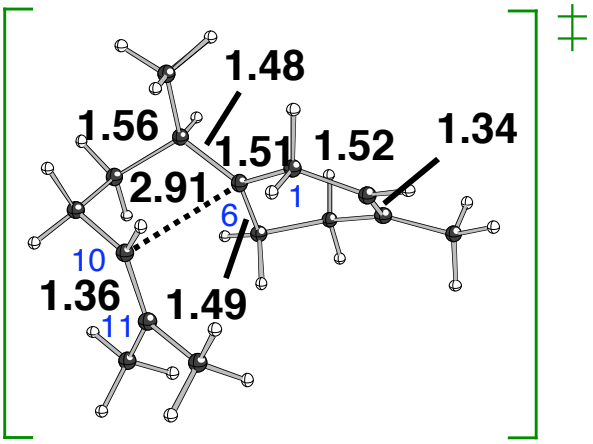
HF = -586.282867 hartrees (-367898.36187117 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	2.313395	-0.256497	1.129076
2	6	2.866953	-0.487524	-0.070752
3	6	2.020839	-0.630137	-1.313597
4	6	0.493299	-0.759913	-1.015351
5	6	0.159174	0.208851	0.084411
6	6	0.805651	-0.174838	1.381523
7	1	2.196093	0.230720	-1.973519
8	1	2.937596	-0.121935	2.009210
9	1	-0.068887	-0.574931	-1.932926
10	1	0.301385	-1.785855	-0.689277
11	1	2.331211	-1.510853	-1.888815
12	6	-1.353897	1.849662	-1.056594
13	6	-2.496209	1.386357	-0.129365
14	1	-1.355872	1.255391	-1.975943
15	1	-1.476696	2.893913	-1.357891
16	6	-2.077231	0.154914	0.641647
17	1	-2.741784	2.174706	0.587448
18	1	-3.404995	1.205059	-0.711544
19	6	-2.271343	-1.149492	0.243774
20	6	-0.010407	1.663446	-0.313498
21	6	-2.033527	-2.286366	1.189982
22	1	-2.966747	-2.851220	1.315087
23	1	-1.307749	-3.001778	0.781057
24	1	-1.704809	-1.958782	2.177748
25	6	-2.772809	-1.528429	-1.115185
26	1	-3.772594	-1.971947	-1.014165
27	1	-2.844244	-0.690854	-1.808638
28	1	-2.143634	-2.309294	-1.558904
29	1	-1.854945	0.302421	1.696707
30	1	0.783463	1.828158	-1.060360
31	6	0.183783	2.688156	0.812970
32	1	-0.552919	2.578681	1.615030
33	1	1.181359	2.619091	1.254203
34	1	0.075493	3.697038	0.405275
35	1	0.448239	-1.153174	1.722603
36	1	0.599853	0.545583	2.175096
37	6	4.356429	-0.597101	-0.265849
38	1	4.624250	-1.584334	-0.661720
39	1	4.711951	0.142464	-0.993896
40	1	4.900365	-0.444806	0.668981

TS (D2-to-D3)



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

HF = -586.4112601 hartrees (-367978.929825351 kcal/mol)
Imaginary Frequencies: 1 (-32.8123 1/cm)
Zero-point correction = 0.362957 (Hartree/Particle)

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

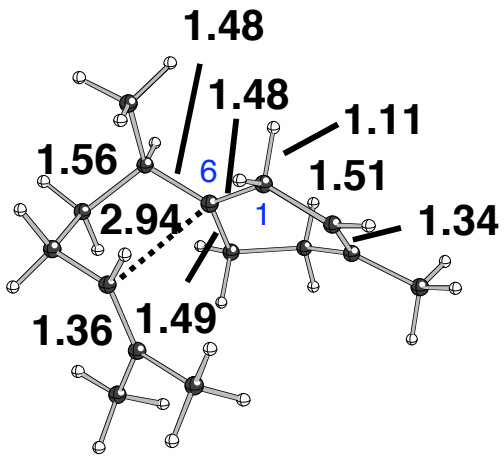
HF = -586.2736825 hartrees (-367892.598505575 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.313398	-0.777907	0.059586
2	6	-0.934588	-2.839455	-0.850172
3	1	-1.663351	-3.588158	-0.529786
4	1	-1.352496	-2.322446	-1.718588
5	1	-0.039960	-3.378874	-1.172929
6	6	-0.646597	-1.881461	0.313663
7	6	-1.947477	-1.425496	1.045915
8	6	-1.943509	1.681683	-0.288557
9	6	-2.910876	-0.661451	0.106760
10	1	-1.693217	-0.794668	1.901514
11	1	-2.437089	-2.318058	1.447629
12	6	-2.231414	0.418227	-0.692086
13	1	-3.386522	-1.367780	-0.579981
14	1	-3.716657	-0.252162	0.726376
15	6	0.798656	0.071297	1.177175
16	6	1.065849	-0.658347	-1.217236
17	6	2.342166	-0.055938	1.328315
18	6	2.419950	0.004943	-1.131548
19	6	3.052733	0.239278	0.026247
20	1	0.410008	-0.115346	-1.918633
21	1	2.619718	-1.050380	1.705601

22	1	0.608732	1.118330	0.904962
23	1	0.285082	-0.139727	2.115988
24	6	4.457646	0.768627	0.110154
25	1	4.485627	1.729579	0.638094
26	1	5.097709	0.079188	0.674939
27	1	4.897249	0.905962	-0.880367
28	6	-1.306764	2.667196	-1.231654
29	1	-0.376598	3.075422	-0.813520
30	1	-1.091330	2.230712	-2.210466
31	1	-1.970243	3.527259	-1.387493
32	6	-2.246559	2.211908	1.086135
33	1	-1.325823	2.542923	1.586691
34	1	-2.882159	3.102790	1.013220
35	1	-2.747887	1.490641	1.733451
36	1	-2.019340	0.176324	-1.733155
37	1	-0.091437	-2.442541	1.097207
38	1	2.644429	0.654744	2.104830
39	1	2.903806	0.210135	-2.082459
40	1	1.146057	-1.652500	-1.679308

D3



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

HF = -586.4116453 hartrees (-367979.171542203 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.362626 (Hartree/Particle)

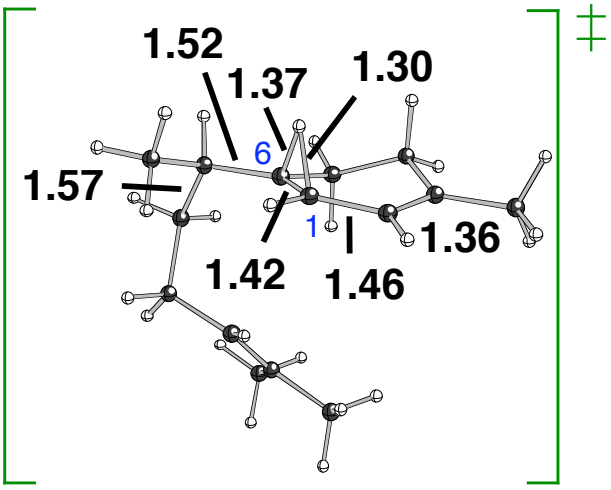
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.2740938 hartrees (-367886.9938595 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.161616	-1.044334	0.127762
2	6	-1.518088	-2.669787	-0.943842
3	1	-2.389764	-3.273630	-0.678955
4	1	-1.809605	-2.016746	-1.771097
5	1	-0.747816	-3.355008	-1.309147
6	6	-1.053146	-1.882310	0.286393
7	6	-2.219483	-1.124372	1.000874
8	6	-1.439255	1.949857	-0.278047
9	6	-2.929278	-0.112048	0.070270
10	1	-1.835390	-0.607730	1.884943
11	1	-2.933619	-1.872656	1.358800
12	6	-1.990753	0.783149	-0.696857
13	1	-3.557667	-0.656383	-0.641204
14	1	-3.616085	0.474072	0.691168
15	6	0.787667	-0.401886	1.314184
16	6	0.947534	-1.045408	-1.125998
17	6	2.331484	-0.488503	1.310705
18	6	2.223588	-0.246803	-1.128981
19	6	2.913829	-0.010370	-0.004137
20	1	0.293683	-0.824073	-1.978444
21	1	1.173615	-2.122716	-1.285569
22	1	2.655333	-1.518854	1.516953
23	1	0.522248	0.664678	1.248192
24	1	0.355195	-0.773650	2.246984
25	6	4.250782	0.672899	0.027863
26	1	4.213828	1.585302	0.635675
27	1	5.005385	0.020914	0.485919
28	1	4.594250	0.938749	-0.974653
29	6	-0.586486	2.780342	-1.200675
30	1	0.401740	2.972749	-0.763972
31	1	-0.451171	2.310497	-2.177998
32	1	-1.048272	3.763129	-1.358975
33	6	-1.642292	2.525044	1.096804
34	1	-0.680405	2.627637	1.620537
35	1	-2.046429	3.542213	1.024946
36	1	-2.313692	1.937739	1.725395
37	1	-1.810784	0.504608	-1.734737
38	1	-0.709579	-2.607739	1.052343
39	1	2.702354	0.116523	2.143745
40	1	2.606339	0.057551	-2.098754

TS (D3-to-B8)



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

HF = -586.3980352 hartrees (-367970.631068352 kcal/mol)
Imaginary Frequencies: 1 (-716.9231 1/cm)
Zero-point correction = 0.360917 (Hartree/Particle)

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

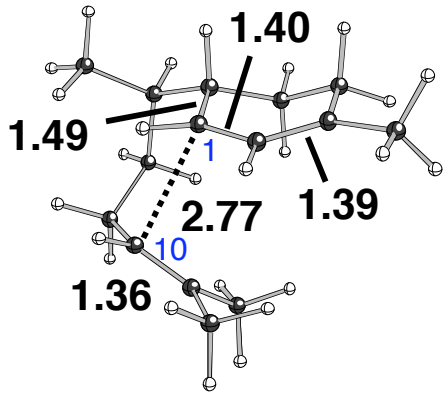
HF = -586.2615974 hartrees (-367885.014984474 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.532901	-1.263793	0.215073
2	6	-0.875430	-3.129107	-0.858839
3	1	-1.693781	-3.817791	-0.634274
4	1	-1.159024	-2.573666	-1.757552
5	1	0.002782	-3.741587	-1.093089
6	6	-0.637564	-2.218786	0.353225
7	6	-1.933550	-1.465472	0.804165
8	6	-1.935822	1.884482	-0.248635
9	6	-2.646178	-0.578626	-0.240325
10	1	-1.716304	-0.872766	1.699179
11	1	-2.625954	-2.253079	1.123250
12	6	-1.876585	0.627304	-0.730899
13	1	-2.933672	-1.192422	-1.101931
14	1	-3.590296	-0.264199	0.216112
15	6	0.970088	-0.426595	1.392370
16	6	1.217450	-1.016401	-0.998966
17	6	2.441849	0.013369	1.331276
18	6	2.269045	-0.016268	-1.128648
19	6	2.862403	0.514168	-0.032439
20	1	0.861411	-1.515218	-1.897331

21	1	1.582951	-2.012460	-0.243974
22	1	3.102870	-0.829346	1.595205
23	1	0.315358	0.456347	1.346473
24	1	0.755454	-0.935139	2.336113
25	6	3.986214	1.496534	-0.108005
26	1	3.706800	2.430764	0.394978
27	1	4.866724	1.112187	0.422910
28	1	4.269852	1.723524	-1.137533
29	6	-1.163996	3.006283	-0.901690
30	1	-0.498321	3.502614	-0.183521
31	1	-0.565033	2.658419	-1.748184
32	1	-1.849251	3.780217	-1.269535
33	6	-2.780508	2.306124	0.929092
34	1	-2.160003	2.779730	1.700742
35	1	-3.512128	3.062909	0.619587
36	1	-3.325590	1.482820	1.394266
37	1	-1.255497	0.468972	-1.613916
38	1	-0.380001	-2.857886	1.209889
39	1	2.622571	0.776230	2.094148
40	1	2.596178	0.231531	-2.132540

B8



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

HF = -586.4272775 hartrees (-367988.980904025 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.364946 (Hartree/Particle)

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

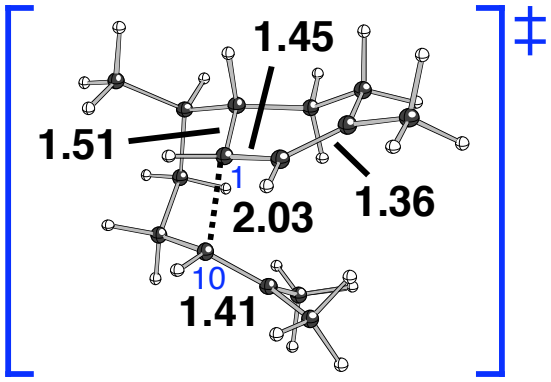
HF = -586.2888551 hartrees (-367902.119463801 kcal/mol)

Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	-0.044182	-1.594670	-0.048968
2	6	-2.277316	-2.256702	-1.132982
3	1	-3.328647	-2.486405	-0.934596
4	1	-2.261713	-1.493983	-1.919317
5	1	-1.815577	-3.163071	-1.539037
6	6	-1.578135	-1.803573	0.158517
7	6	-2.314979	-0.647084	0.868683
8	6	-0.693997	2.235090	0.012716
9	6	-2.683289	0.602610	0.037027
10	1	-1.748756	-0.347636	1.757241
11	1	-3.257103	-1.059600	1.248805
12	6	-1.553791	1.380427	-0.606637
13	1	-3.386124	0.311461	-0.749587
14	1	-3.247053	1.274183	0.696429
15	6	0.771174	-1.450861	1.246601
16	6	0.367798	-0.567358	-1.040372
17	6	2.272775	-1.362313	0.949427
18	6	1.647430	0.002705	-1.051412
19	6	2.611440	-0.385404	-0.134953
20	1	-0.247840	-0.434211	-1.923204
21	1	0.289580	-2.530839	-0.547361
22	1	2.656673	-2.341709	0.611292
23	1	0.456555	-0.546339	1.778370
24	1	0.572574	-2.297691	1.909660
25	6	4.020117	0.083135	-0.243870
26	1	4.283581	0.664131	0.651109
27	1	4.707440	-0.772798	-0.252360
28	1	4.198116	0.695843	-1.129061
29	6	0.269881	3.076362	-0.776857
30	1	1.304825	2.903545	-0.449814
31	1	0.204506	2.893118	-1.852576
32	1	0.072319	4.141436	-0.602754
33	6	-0.669005	2.464238	1.499217
34	1	0.312658	2.201865	1.917336
35	1	-0.809590	3.530834	1.714191
36	1	-1.433839	1.906329	2.040116
37	1	-1.539715	1.389743	-1.695934
38	1	-1.625406	-2.650206	0.855990
39	1	2.850044	-1.129945	1.851834
40	1	1.916963	0.682322	-1.853585

TS (B8-to-C4)



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

HF = -586.4218264 hartrees (-367985.560284264 kcal/mol)
Imaginary Frequencies: 1 (-214.3282 1/cm)
Zero-point correction = 0.365535 (Hartree/Particle)

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

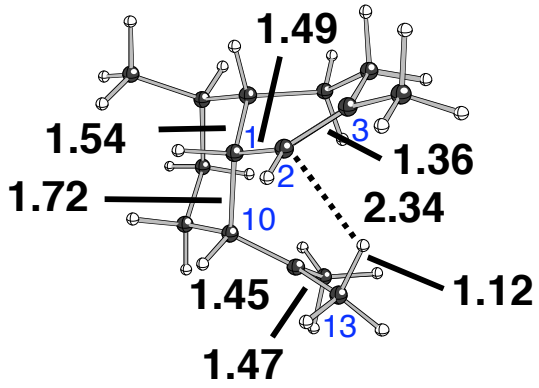
HF = -586.2886513 hartrees (-367901.991577263 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.430548	-1.369756	0.168071
2	6	-2.660596	-2.160011	-0.802648
3	1	-3.739624	-2.217448	-0.629602
4	1	-2.515277	-1.684697	-1.779161
5	1	-2.285027	-3.185639	-0.879066
6	6	-1.970282	-1.405008	0.348535
7	6	-2.576882	-0.011747	0.583284
8	6	-0.054999	2.163954	-0.029076
9	6	-2.300009	1.005137	-0.539342
10	1	-2.231749	0.372916	1.548434
11	1	-3.663320	-0.114243	0.681570
12	6	-0.832322	1.321249	-0.840676
13	1	-2.755193	0.645173	-1.467378
14	1	-2.816022	1.945063	-0.308354
15	6	0.394580	-1.121992	1.438608
16	6	0.076348	-0.487801	-0.953361
17	6	1.886871	-1.374732	1.168349
18	6	1.515064	-0.367698	-1.092871
19	6	2.382799	-0.808543	-0.139082
20	1	-0.435757	-0.641025	-1.901282
21	1	-0.158576	-2.379616	-0.189987
22	1	2.085635	-2.458302	1.145004
23	1	0.248744	-0.092915	1.787580

24	1	0.050347	-1.775699	2.246057
25	6	3.863365	-0.840222	-0.375542
26	1	4.393437	-0.275532	0.401462
27	1	4.234621	-1.870814	-0.309567
28	1	4.138061	-0.437963	-1.353169
29	6	1.251788	2.669621	-0.518791
30	1	2.028049	1.960137	-0.174607
31	1	1.320655	2.712365	-1.607409
32	1	1.501123	3.643115	-0.087524
33	6	-0.448799	2.617752	1.336317
34	1	0.403044	2.599157	2.025908
35	1	-0.733780	3.678457	1.252311
36	1	-1.289552	2.082373	1.768990
37	1	-0.619720	1.483438	-1.897320
38	1	-2.150571	-1.988174	1.260690
39	1	2.505750	-0.992516	1.989730
40	1	1.906428	0.011163	-2.033966

C4



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

HF = -586.4235339 hartrees (-367986.631757589 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366112 (Hartree/Particle)

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

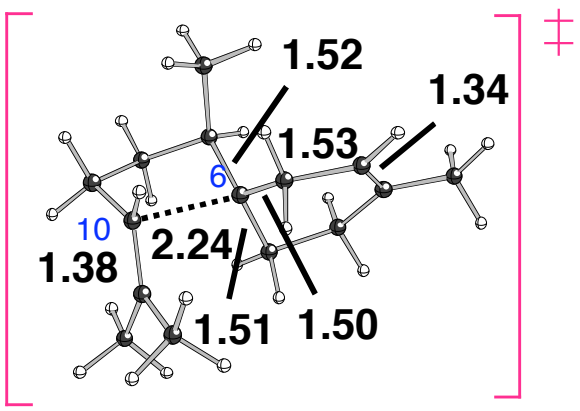
HF = -586.2938759 hartrees (-367905.270066009 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.424543	-1.315344	0.206531

2	6	-2.620215	-2.248544	-0.712010
3	1	-3.697838	-2.331610	-0.539416
4	1	-2.483152	-1.832355	-1.716207
5	1	-2.209043	-3.263150	-0.719828
6	6	-1.960482	-1.397362	0.389048
7	6	-2.603105	-0.004430	0.507393
8	6	-0.042602	2.124917	-0.029758
9	6	-2.233392	0.938204	-0.650323
10	1	-2.328935	0.435759	1.472083
11	1	-3.693426	-0.108091	0.532061
12	6	-0.720585	1.154514	-0.869261
13	1	-2.633982	0.532247	-1.585320
14	1	-2.725078	1.908866	-0.519586
15	6	0.391202	-1.010857	1.470586
16	6	0.034069	-0.389336	-0.932550
17	6	1.885515	-1.275277	1.214373
18	6	1.512880	-0.357878	-1.084596
19	6	2.373988	-0.793064	-0.132887
20	1	-0.408428	-0.718263	-1.877406
21	1	-0.109069	-2.315357	-0.128925
22	1	2.086409	-2.356058	1.269267
23	1	0.243272	0.032573	1.781954
24	1	0.045301	-1.626360	2.307501
25	6	3.852775	-0.892078	-0.385384
26	1	4.419082	-0.323152	0.362224
27	1	4.183555	-1.934182	-0.293117
28	1	4.128144	-0.534608	-1.380547
29	6	1.290174	2.603025	-0.418806
30	1	1.972639	1.753927	-0.182045
31	1	1.403615	2.748451	-1.496200
32	1	1.620139	3.483153	0.135231
33	6	-0.617041	2.702706	1.206561
34	1	0.154872	2.892731	1.960041
35	1	-0.989335	3.703356	0.920298
36	1	-1.450331	2.150820	1.630862
37	1	-0.517103	1.460256	-1.902715
38	1	-2.136022	-1.918935	1.338798
39	1	2.503450	-0.832346	2.006252
40	1	1.909444	-0.042840	-2.048755

TS (D2-to-I)



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

HF = -586.4172626 hartrees (-367982.696454126 kcal/mol)
Imaginary Frequencies: 1 (-51.0417 1/cm)
Zero-point correction = 0.365486 (Hartree/Particle)

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

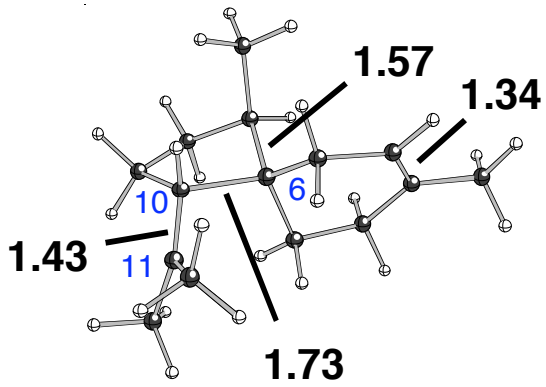
HF = -586.2834466 hartrees (-367892.8627415 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.300434	-0.272064	1.127239
2	6	2.850031	-0.493471	-0.076131
3	6	1.998889	-0.626474	-1.316882
4	6	0.474699	-0.759959	-1.015053
5	6	0.132967	0.202256	0.094008
6	6	0.795573	-0.187768	1.385280
7	1	2.173583	0.238312	-1.971900
8	1	2.928834	-0.148797	2.006136
9	1	-0.090419	-0.571733	-1.930332
10	1	0.284790	-1.788743	-0.696183
11	1	2.308722	-1.502860	-1.899159
12	6	-1.333948	1.871330	-1.055828
13	6	-2.476454	1.388986	-0.139635
14	1	-1.331282	1.293431	-1.985715
15	1	-1.456268	2.920587	-1.338898
16	6	-2.037005	0.160180	0.629099
17	1	-2.735983	2.168576	0.581867
18	1	-3.381393	1.195874	-0.723487
19	6	-2.256399	-1.146987	0.240520
20	6	-0.000649	1.665991	-0.303611
21	6	-2.031207	-2.281073	1.190859
22	1	-2.969927	-2.838126	1.311072
23	1	-1.309996	-3.003205	0.785728

24	1	-1.704623	-1.953944	2.179145
25	6	-2.766103	-1.523355	-1.114641
26	1	-3.785778	-1.919114	-1.009437
27	1	-2.798886	-0.693676	-1.820208
28	1	-2.172005	-2.339089	-1.542884
29	1	-1.828186	0.308027	1.686808
30	1	0.807065	1.820593	-1.036465
31	6	0.194747	2.682477	0.830372
32	1	-0.552583	2.580351	1.623700
33	1	1.185974	2.597646	1.282861
34	1	0.105515	3.694706	0.426194
35	1	0.439035	-1.166154	1.727524
36	1	0.594687	0.529539	2.183355
37	6	4.338722	-0.601076	-0.277678
38	1	4.605726	-1.584367	-0.683828
39	1	4.691534	0.145477	-0.999978
40	1	4.886075	-0.457286	0.656571

I



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

HF = -586.4193078 hartrees (-367983.979837578 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365938 (Hartree/Particle)

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

HF = -586.2896445 hartrees (-367896.75192375 kcal/mol)

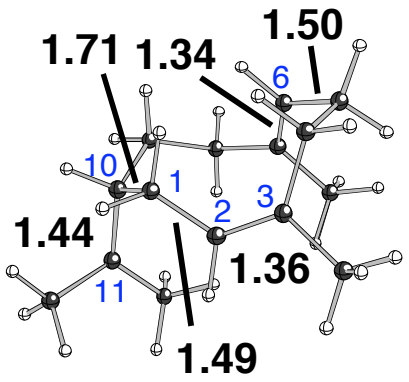
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.180499	-0.552711	1.106820

2	6	2.741284	-0.622312	-0.110036
3	6	1.901984	-0.543138	-1.365729
4	6	0.384032	-0.636477	-1.100746
5	6	-0.014590	0.184873	0.139552
6	6	0.690939	-0.415536	1.357758
7	1	2.143587	0.383538	-1.905456
8	1	2.807797	-0.609960	1.993835
9	1	-0.156964	-0.321125	-1.997881
10	1	0.135119	-1.691049	-0.928026
11	1	2.185806	-1.351970	-2.051164
12	6	-0.963099	2.147578	-1.004617
13	6	-2.215645	1.409141	-0.482166
14	1	-0.754391	1.857719	-2.038822
15	1	-1.102521	3.231730	-1.007451
16	6	-1.727706	0.229297	0.393884
17	1	-2.825833	2.055749	0.155761
18	1	-2.865542	1.088441	-1.299174
19	6	-2.262624	-1.082104	0.186198
20	6	0.187786	1.720861	-0.078841
21	6	-2.298563	-2.073173	1.286490
22	1	-3.315695	-2.485489	1.361823
23	1	-1.669611	-2.936910	1.022289
24	1	-1.994983	-1.674114	2.253259
25	6	-2.808881	-1.522802	-1.118374
26	1	-3.884328	-1.274324	-1.109249
27	1	-2.378386	-0.993757	-1.969829
28	1	-2.739812	-2.605171	-1.253459
29	1	-1.753885	0.473087	1.459078
30	1	1.147984	1.842741	-0.591441
31	6	0.243112	2.562150	1.204963
32	1	-0.664731	2.476502	1.813933
33	1	1.099415	2.299661	1.831055
34	1	0.350083	3.617713	0.937906
35	1	0.280634	-1.408388	1.585630
36	1	0.516965	0.194401	2.249351
37	6	4.226567	-0.765541	-0.311977
38	1	4.460731	-1.688125	-0.857560
39	1	4.622804	0.063524	-0.912029
40	1	4.765183	-0.785053	0.638555

Figure S3.

E2



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

HF = -586.3824331 hartrees (-367960.840594581 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.363795 (Hartree/Particle)

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

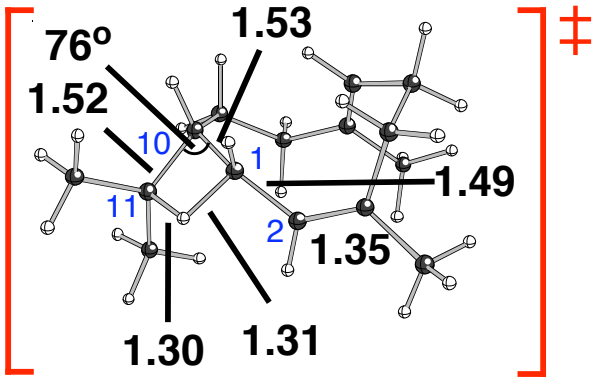
HF = -586.2431988 hartrees (-367873.469678988 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.176234	-1.579569	-0.023142
2	6	-1.530503	-1.619113	0.040246
3	6	-2.473930	-1.019566	-0.979929
4	6	-2.857875	0.460948	-0.653912
5	6	-1.621331	1.301657	-0.741537
6	6	0.663479	-1.097996	-1.150981
7	1	-2.048513	-1.053348	-1.988173
8	1	0.356401	-2.094173	0.776989
9	1	-3.606790	0.779373	-1.387962
10	1	-3.331504	0.513447	0.329809
11	1	-3.388980	-1.621081	-1.011570
12	6	-2.203557	-2.304954	1.201672
13	1	-2.766164	-3.179459	0.852050
14	1	-1.493828	-2.637023	1.963501
15	1	-2.934562	-1.638474	1.675963
16	6	-1.328329	1.877458	1.701370
17	1	-0.685832	1.289782	2.370969
18	1	-1.264724	2.916378	2.049958
19	1	-2.356769	1.546670	1.851763
20	6	0.510194	2.352909	-0.009020
21	6	1.362057	1.614021	-1.061200
22	1	1.054323	2.427774	0.938005
23	1	0.433685	3.392604	-0.357420
24	6	1.833345	0.137275	-0.941731

25	1	0.862642	1.673961	-2.033411
26	1	2.290542	2.186345	-1.189822
27	1	-1.220459	1.374404	-1.752908
28	6	2.556303	-0.367815	0.196476
29	6	-0.879875	1.792913	0.262632
30	6	3.598692	-1.400347	0.002794
31	1	4.559028	-0.940311	0.293119
32	1	3.465721	-2.238369	0.697964
33	1	3.688592	-1.754530	-1.024878
34	6	2.244833	0.042874	1.577943
35	1	2.748362	-0.565098	2.330658
36	1	2.531404	1.095504	1.714923
37	1	1.156301	0.020170	1.728167
38	1	2.421400	-0.059292	-1.843710
39	1	1.265608	-1.917999	-1.552168
40	1	0.080507	-0.661427	-1.961905

TS (E2-to-F2)



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

HF = -586.3560302 hartrees (-367944.272510802 kcal/mol)
Imaginary Frequencies: 1 (-344.0129 1/cm)
Zero-point correction = 0.362723 (Hartree/Particle)

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

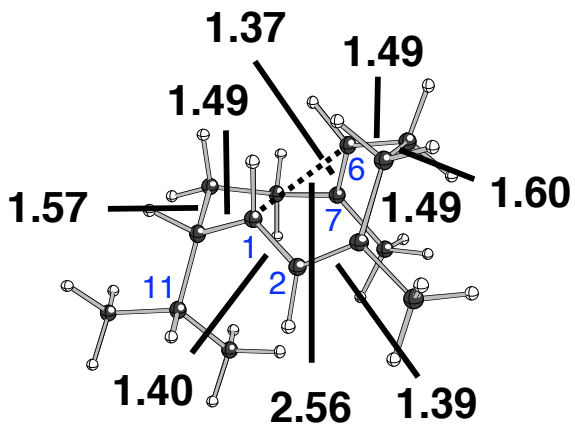
HF = -586.2243466 hartrees (-367861.639734966 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.152042	-1.186851	0.635930
2	6	-1.404632	-1.584982	0.322509

3	6	-1.961577	-1.519961	-1.080918
4	6	-2.547808	-0.089634	-1.404153
5	6	-1.482605	0.936202	-1.147117
6	6	0.891890	-0.906438	-0.394789
7	1	-1.191586	-1.745319	-1.829518
8	1	0.140052	-1.106236	1.679370
9	1	-2.871236	-0.098156	-2.450238
10	1	-3.438238	0.076169	-0.793178
11	1	-2.754496	-2.263625	-1.209763
12	6	-2.372890	-1.970939	1.408977
13	1	-2.693525	-3.010446	1.267844
14	1	-1.940077	-1.880359	2.408254
15	1	-3.279565	-1.356639	1.365820
16	6	-2.360903	1.795940	1.059962
17	1	-2.114038	1.233622	1.970192
18	1	-2.421448	2.850772	1.354523
19	1	-3.356255	1.494456	0.730866
20	6	0.037364	2.209758	0.390248
21	6	1.250922	1.849719	-0.479124
22	1	0.217223	1.909718	1.433261
23	1	-0.017485	3.306723	0.427979
24	6	1.635528	0.377611	-0.766350
25	1	1.111171	2.309554	-1.461886
26	1	2.132916	2.345462	-0.056573
27	1	-0.677021	0.929083	-1.880806
28	6	2.633163	-0.404729	0.072115
29	6	-1.303967	1.623154	-0.005011
30	6	3.821354	-1.020051	-0.654071
31	1	4.537165	-0.210965	-0.841155
32	1	4.317594	-1.786102	-0.053493
33	1	3.539913	-1.443318	-1.621362
34	6	2.855539	0.018944	1.511501
35	1	3.289675	-0.786043	2.108960
36	1	3.573832	0.846505	1.490812
37	1	1.948063	0.383992	1.993952
38	1	1.921287	0.303146	-1.815953
39	1	1.905312	-1.472003	0.205321
40	1	0.884757	-1.596449	-1.241472

F2



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

HF = -586.4196813 hartrees (-367984.214212563 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366505 (Hartree/Particle)

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

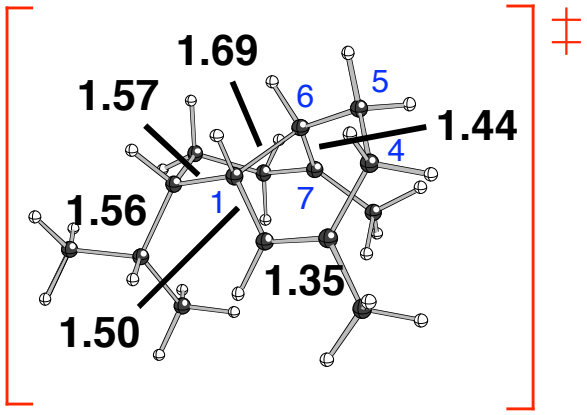
HF = -586.2825649 hartrees (-367898.172300399 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.760770	-1.392448	-0.123505
2	6	-2.144748	-1.349977	-0.156809
3	6	-2.869975	-0.315705	-0.953164
4	6	-2.656493	1.159811	-0.379572
5	6	-1.254170	1.649400	-0.515090
6	6	0.013196	-0.535003	-0.921046
7	1	-2.546459	-0.312791	-1.999693
8	1	-0.273418	-2.038931	0.600300
9	1	-3.326288	1.794834	-0.967941
10	1	-3.013055	1.183007	0.651419
11	1	-3.943674	-0.516469	-0.947133
12	6	-2.957517	-2.244643	0.721392
13	1	-3.623583	-2.861372	0.102993
14	1	-2.344059	-2.903032	1.339165
15	1	-3.617363	-1.655526	1.372568
16	6	-0.612061	1.547314	1.926209
17	1	0.115463	0.886887	2.405129
18	1	-0.517807	2.519322	2.430081
19	1	-1.615422	1.171821	2.126418
20	6	1.124070	2.101481	0.128277
21	6	1.745040	1.247710	-1.005642
22	1	1.731636	2.035708	1.033074
23	1	1.170816	3.151874	-0.190984

24	6	1.487324	-0.298710	-0.924883
25	1	1.347204	1.592074	-1.966766
26	1	2.822396	1.428335	-1.049516
27	1	-0.967243	1.967419	-1.516497
28	6	2.363000	-1.150701	0.037062
29	6	-0.307233	1.740150	0.468333
30	6	3.825158	-1.165561	-0.445978
31	1	4.302429	-0.185490	-0.337202
32	1	4.409477	-1.876508	0.145292
33	1	3.904795	-1.466697	-1.496124
34	6	2.302889	-0.794168	1.530598
35	1	2.879568	-1.525809	2.104628
36	1	2.742322	0.187510	1.733507
37	1	1.284254	-0.804532	1.928505
38	1	1.771558	-0.635797	-1.939079
39	1	1.991478	-2.180127	-0.067945
40	1	-0.471278	-0.149400	-1.811289

TS (F2-to-G3)



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

HF = -586.4125127 hartrees (-367979.715844377 kcal/mol)
Imaginary Frequencies: 1 (-104.9534 1/cm)
Zero-point correction = 0.366202 (Hartree/Particle)

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

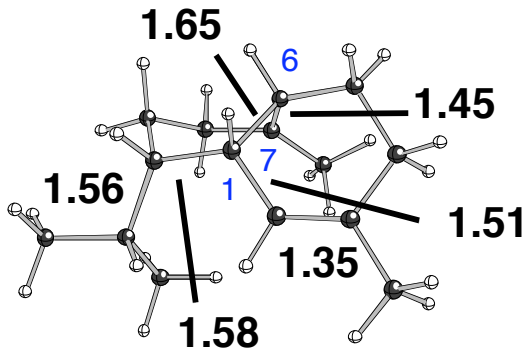
HF = -586.2833179 hartrees (-367898.644815429 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	0.752273	1.217907	-0.097839
2	6	2.096916	1.279344	-0.022458
3	6	2.958251	0.283624	-0.765969
4	6	2.350869	-1.133120	-1.006926
5	6	0.845609	-1.286371	-0.744344
6	6	0.054294	0.189205	-0.932331
7	1	3.200085	0.731084	-1.740468
8	1	0.158274	1.947414	0.440933
9	1	2.526783	-1.417371	-2.047886
10	1	2.895546	-1.870904	-0.409666
11	1	3.921800	0.183844	-0.255707
12	6	2.816550	2.358754	0.739478
13	1	3.476067	2.923747	0.068860
14	1	2.122660	3.063210	1.204720
15	1	3.459488	1.934720	1.520707
16	6	1.163615	-1.588242	1.762246
17	1	0.673986	-1.988828	2.650983
18	1	2.168222	-2.003350	1.639235
19	1	1.317695	-0.496066	1.899946
20	6	-1.092216	-1.992751	0.643561
21	6	-1.919096	-1.415924	-0.517738
22	1	-1.458750	-1.693278	1.631545
23	1	-1.167786	-3.097057	0.645809
24	6	-1.505279	0.041848	-0.885729
25	1	-1.806326	-2.054137	-1.400179
26	1	-2.979188	-1.463079	-0.257478
27	1	0.360566	-1.886119	-1.519674
28	6	-2.276262	1.138661	-0.088278
29	6	0.350567	-1.687151	0.546455
30	6	-3.722502	1.259448	-0.603180
31	1	-4.303537	0.348383	-0.420162
32	1	-4.239523	2.078551	-0.094275
33	1	-3.750886	1.466862	-1.677920
34	6	-2.277078	0.975507	1.442528
35	1	-2.718984	1.859843	1.911547
36	1	-2.885283	0.118716	1.754670
37	1	-1.273983	0.855250	1.865484
38	1	-1.829098	0.174350	-1.924197
39	1	-1.788493	2.092970	-0.324158
40	1	0.341603	0.346811	-1.979518

G3



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

HF = -586.4151705 hartrees (-367981.383640455 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366518 (Hartree/Particle)

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

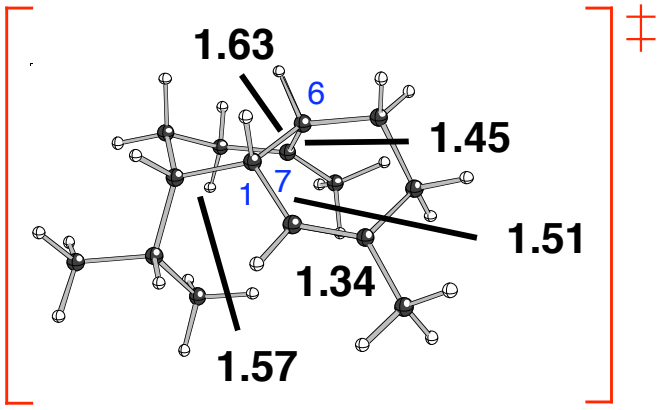
HF = -586.2862043 hartrees (-367894.59319825 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.770185	1.267602	-0.358207
2	6	2.083886	1.266825	-0.064503
3	6	2.979085	0.076448	-0.324672
4	6	2.306114	-1.111472	-1.041568
5	6	0.806720	-1.274168	-0.770657
6	6	0.033272	0.153904	-1.057108
7	1	3.837565	0.405316	-0.923948
8	1	0.196297	2.160596	-0.132373
9	1	2.405559	-0.979412	-2.124033
10	1	2.830960	-2.044588	-0.806934
11	1	3.421855	-0.239364	0.630240
12	6	2.758980	2.463460	0.554764
13	1	3.532391	2.857577	-0.116007
14	1	2.050694	3.268390	0.765092
15	1	3.264901	2.196464	1.490929
16	6	1.122278	-1.645075	1.745630
17	1	0.640112	-2.124643	2.599275
18	1	2.135616	-2.026100	1.588691
19	1	1.241463	-0.567831	1.977895
20	6	-1.130324	-1.983457	0.609185
21	6	-1.952976	-1.399702	-0.551006
22	1	-1.504307	-1.709519	1.601910
23	1	-1.191037	-3.090053	0.594891
24	6	-1.531606	0.055509	-0.912969
25	1	-1.840068	-2.034541	-1.436347

26	1	-3.013181	-1.444802	-0.292537
27	1	0.350114	-1.933511	-1.519188
28	6	-2.227642	1.154707	-0.053923
29	6	0.309082	-1.677913	0.525491
30	6	-3.730126	1.234622	-0.382082
31	1	-4.275335	0.342077	-0.055178
32	1	-4.182195	2.089898	0.129142
33	1	-3.903062	1.362206	-1.455801
34	6	-2.024325	1.055162	1.468096
35	1	-2.412686	1.954867	1.955229
36	1	-2.574841	0.208565	1.894052
37	1	-0.970661	0.966793	1.754262
38	1	-1.919424	0.216000	-1.925360
39	1	-1.799218	2.109931	-0.381794
40	1	0.242867	0.236980	-2.130928

TS (G3-to-G4)



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

HF = -586.4148659 hartrees (-367981.192500909 kcal/mol)
Imaginary Frequencies: 1 (-13.4188 1/cm)
Zero-point correction = 0.366187 (Hartree/Particle)

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

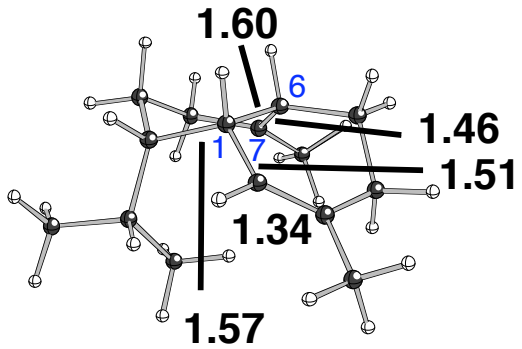
HF = -586.2857802 hartrees (-367894.3270755 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-0.912237	-1.312526	-0.563389
2	6	-2.148783	-1.210721	-0.050632

3	6	-2.884753	0.108203	0.020314
4	6	-2.244627	1.207101	-0.839873
5	6	-0.714019	1.239601	-0.774913
6	6	-0.081365	-0.205371	-1.168270
7	1	-3.919406	-0.039963	-0.312345
8	1	-0.457150	-2.299007	-0.608049
9	1	-2.507505	1.028584	-1.888046
10	1	-2.659811	2.190151	-0.589409
11	1	-2.973735	0.419128	1.071317
12	6	-2.889165	-2.406528	0.489528
13	1	-3.809977	-2.582557	-0.080041
14	1	-2.284122	-3.315567	0.448581
15	1	-3.191994	-2.244063	1.531783
16	6	-0.708454	2.135550	1.651063
17	1	-0.108102	2.799222	2.277370
18	1	-1.715853	2.530394	1.496645
19	1	-0.832419	1.188676	2.207531
20	6	1.421899	1.942524	0.278264
21	6	2.063879	1.134723	-0.858774
22	1	1.888860	1.791105	1.258308
23	1	1.552255	3.029565	0.098465
24	6	1.477125	-0.296844	-0.965199
25	1	1.908695	1.653019	-1.812694
26	1	3.145375	1.108377	-0.711056
27	1	-0.322944	1.873413	-1.590421
28	6	1.998559	-1.302704	0.108527
29	6	-0.036072	1.775363	0.394358
30	6	3.522055	-1.491746	-0.005907
31	1	4.077452	-0.614495	0.344720
32	1	3.843185	-2.337961	0.608981
33	1	3.830228	-1.697713	-1.036558
34	6	1.605778	-1.037750	1.573175
35	1	1.870285	-1.904324	2.186995
36	1	2.143730	-0.183293	1.998477
37	1	0.528766	-0.881851	1.696848
38	1	1.864950	-0.694305	-1.910625
39	1	1.554099	-2.267490	-0.163017
40	1	-0.243781	-0.222295	-2.253392

G4



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

HF = -586.4151187 hartrees (-367981.351135437 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.365762 (Hartree/Particle)

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

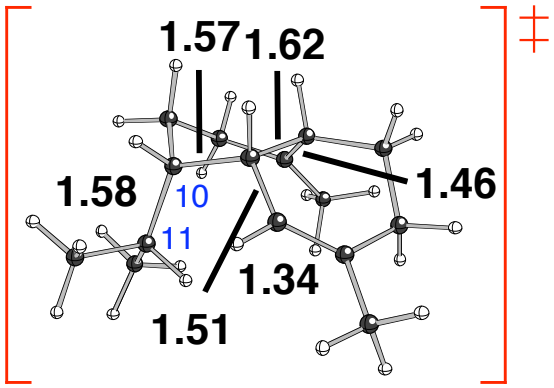
HF = -586.2864245 hartrees (-367894.73137375 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.131796	-1.259261	-0.748446
2	6	-2.248642	-1.050872	-0.037449
3	6	-2.680139	0.348082	0.344271
4	6	-2.070156	1.400429	-0.591247
5	6	-0.552929	1.242863	-0.754324
6	6	-0.140040	-0.225997	-1.236095
7	1	-3.772635	0.421761	0.293197
8	1	-0.886942	-2.276439	-1.050676
9	1	-2.513752	1.272500	-1.584206
10	1	-2.331840	2.413824	-0.269933
11	1	-2.429864	0.546364	1.397704
12	6	-3.146123	-2.175962	0.405603
13	1	-4.146490	-2.073883	-0.032827
14	1	-2.746600	-3.152936	0.122634
15	1	-3.277848	-2.164157	1.495140
16	6	-0.132709	2.672098	1.353697
17	1	0.672703	3.179988	1.885322
18	1	-0.889103	3.394586	1.022696
19	1	-0.667200	2.010288	2.053033
20	6	1.792338	1.726165	-0.001316
21	6	2.206860	0.690801	-1.050017
22	1	2.280405	1.590640	0.973136
23	1	2.114253	2.747173	-0.288802
24	6	1.357876	-0.595227	-0.955052
25	1	2.090238	1.118014	-2.054496
26	1	3.271699	0.475077	-0.938632
27	1	-0.229549	1.870318	-1.619650
28	6	1.630126	-1.495526	0.291394
29	6	0.342617	1.851672	0.225634
30	6	3.091583	-1.975015	0.322044
31	1	3.788693	-1.166587	0.571458
32	1	3.219531	-2.751527	1.082579
33	1	3.398972	-2.401382	-0.638876
34	6	1.222845	-0.949185	1.673306
35	1	1.238832	-1.762275	2.405657
36	1	1.915521	-0.187476	2.046917
37	1	0.204317	-0.544476	1.684316
38	1	1.662253	-1.216584	-1.805988

39	1	1.014176	-2.387155	0.127779
40	1	-0.230033	-0.186039	-2.329504

TS (G4-to-G2)



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

HF = -586.4096361 hartrees (-367977.910749111 kcal/mol)
Imaginary Frequencies: 1 (-66.3232 1/cm)
Zero-point correction = 0.366238 (Hartree/Particle)

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

HF = -586.2803261 hartrees (-367896.767431011 kcal/mol)

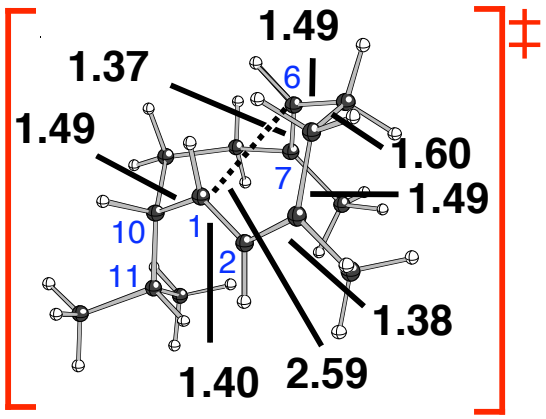
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.987378	1.334975	-0.560964
2	6	2.156735	1.212477	0.084462
3	6	2.811239	-0.136114	0.286722
4	6	2.283682	-1.190959	-0.693628
5	6	0.754878	-1.221644	-0.799581
6	6	0.144203	0.236555	-1.162634
7	1	3.894205	-0.036627	0.147407
8	1	0.586184	2.334529	-0.723702
9	1	2.664263	-0.953888	-1.692859
10	1	2.673595	-2.186028	-0.450652
11	1	2.689411	-0.456522	1.331824
12	6	2.901318	2.403189	0.628511
13	1	3.877500	2.507576	0.138945
14	1	2.346224	3.333560	0.485585
15	1	3.099581	2.285038	1.701348

16	6	0.526485	-2.416924	1.484261
17	1	-0.113082	-3.171499	1.947884
18	1	1.557321	-2.765206	1.388570
19	1	0.558241	-1.554319	2.176379
20	6	-1.469260	-2.044460	-0.039308
21	6	-2.043288	-1.030815	-1.046833
22	1	-2.023500	-2.103291	0.902254
23	1	-1.544445	-3.073345	-0.448432
24	6	-1.398214	0.365722	-0.894638
25	1	-1.870684	-1.384635	-2.070489
26	1	-3.128530	-0.988587	-0.925591
27	1	0.463744	-1.799751	-1.697410
28	6	-1.814951	1.196924	0.381927
29	6	-0.030116	-1.890822	0.229079
30	6	-2.652459	2.411656	-0.068048
31	1	-3.596906	2.092215	-0.525708
32	1	-2.896986	3.055798	0.782051
33	1	-2.116781	3.021062	-0.803800
34	6	-2.562401	0.461730	1.511094
35	1	-2.864081	1.189470	2.270059
36	1	-3.478545	-0.029371	1.164663
37	1	-1.944224	-0.278665	2.029715
38	1	-1.770851	0.939585	-1.749596
39	1	-0.896885	1.589630	0.831372
40	1	0.263854	0.284333	-2.252358

Figure S4.

TS (F2-to-F3)



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

HF = -586.4168187 hartrees (-367982.417902437 kcal/mol)
Imaginary Frequencies: 1 (-57.4578 1/cm)
Zero-point correction = 0.366736 (Hartree/Particle)

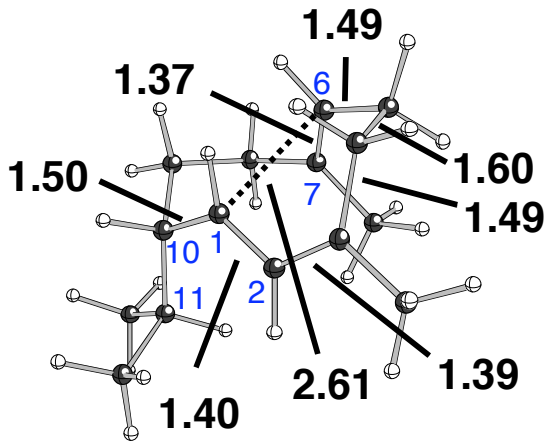
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -586.279683 hartrees (-367896.36387933 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.776980	1.383109	-0.003822
2	6	2.161087	1.369577	-0.037699
3	6	2.911207	0.382019	-0.866849
4	6	2.724014	-1.108006	-0.324838
5	6	1.349412	-1.640823	-0.544009
6	6	0.009276	0.552937	-0.836454
7	1	2.588680	0.397708	-1.913355
8	1	0.286422	1.988752	0.751839
9	1	3.443280	-1.711716	-0.887255
10	1	3.026371	-1.137344	0.723500
11	1	3.979962	0.606867	-0.851956
12	6	2.952867	2.242413	0.881018
13	1	3.608373	2.897672	0.291710
14	1	2.324463	2.861434	1.523851
15	1	3.622127	1.639141	1.509234
16	6	0.522853	-1.523330	1.845038
17	1	-0.225462	-0.821915	2.228508
18	1	0.357722	-2.468551	2.378654
19	1	1.513082	-1.158125	2.117345
20	6	-1.040029	-2.195370	-0.073209
21	6	-1.681800	-1.235166	-1.111272
22	1	-1.686484	-2.302108	0.799339
23	1	-0.983166	-3.188448	-0.537485
24	6	-1.461907	0.293032	-0.842445
25	1	-1.257347	-1.451373	-2.098288
26	1	-2.752469	-1.440316	-1.194574
27	1	1.132863	-1.954743	-1.565195
28	6	-2.344069	1.002868	0.242097
29	6	0.341627	-1.762477	0.372535
30	6	-3.364957	1.920567	-0.460341
31	1	-4.060640	1.338323	-1.076671
32	1	-3.958966	2.473014	0.273654
33	1	-2.872291	2.653386	-1.108762
34	6	-3.073548	0.083142	1.236226
35	1	-3.674645	0.694111	1.916172
36	1	-3.760707	-0.604538	0.732749
37	1	-2.391545	-0.504868	1.854971
38	1	-1.755315	0.735190	-1.812778
39	1	-1.693639	1.652571	0.838335
40	1	0.491250	0.218935	-1.749399

F3



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

HF = -586.4236037 hartrees (-367986.675557787 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366384 (Hartree/Particle)

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

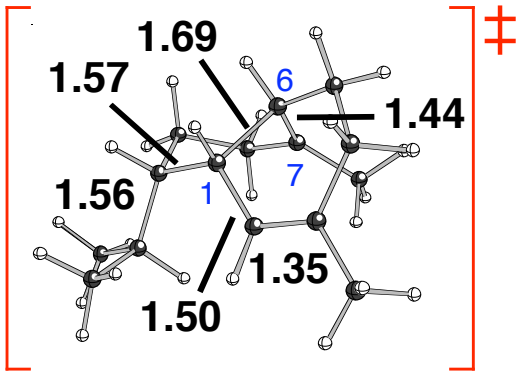
HF = -586.2869344 hartrees (-367895.051336 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.723450	1.320985	-0.083244
2	6	2.108895	1.318851	-0.114017
3	6	2.866289	0.308299	-0.904681
4	6	2.702045	-1.157547	-0.285986
5	6	1.324033	-1.703715	-0.438601
6	6	-0.037660	0.470366	-0.899530
7	1	2.534377	0.265743	-1.946992
8	1	0.226690	1.930943	0.664268
9	1	3.409256	-1.782906	-0.839564
10	1	3.035238	-1.132586	0.752976
11	1	3.932405	0.545737	-0.909433
12	6	2.890643	2.224721	0.780805
13	1	3.533743	2.875151	0.172563
14	1	2.255517	2.850727	1.410136
15	1	3.572210	1.647974	1.420561
16	6	0.558056	-1.419206	1.958442
17	1	-0.202581	-0.718872	2.319492
18	1	0.437001	-2.334162	2.553932
19	1	1.544011	-1.010265	2.179687
20	6	-1.058327	-2.200496	0.136831
21	6	-1.665393	-1.378844	-1.022796
22	1	-1.701548	-2.141554	1.019167

23	1	-1.048050	-3.256309	-0.165022
24	6	-1.502301	0.170672	-0.860105
25	1	-1.185629	-1.667697	-1.964689
26	1	-2.723920	-1.621806	-1.137663
27	1	1.083737	-2.086055	-1.430114
28	6	-2.316874	0.856685	0.272028
29	6	0.340574	-1.756341	0.510303
30	6	-2.503515	2.356661	-0.035378
31	1	-3.163213	2.486503	-0.901346
32	1	-2.969903	2.868623	0.811406
33	1	-1.566464	2.874256	-0.261024
34	6	-3.699811	0.217663	0.488289
35	1	-4.254923	0.785621	1.240567
36	1	-4.293103	0.232970	-0.433409
37	1	-3.644018	-0.816158	0.839876
38	1	-1.881372	0.564737	-1.821817
39	1	-1.756433	0.760845	1.212488
40	1	0.446347	0.106018	-1.800215

TS (F3-to-G5)



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

HF = -586.4123157 hartrees (-367979.592224907 kcal/mol)
Imaginary Frequencies: 1 (-108.1787 1/cm)
Zero-point correction = 0.366237 (Hartree/Particle)

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

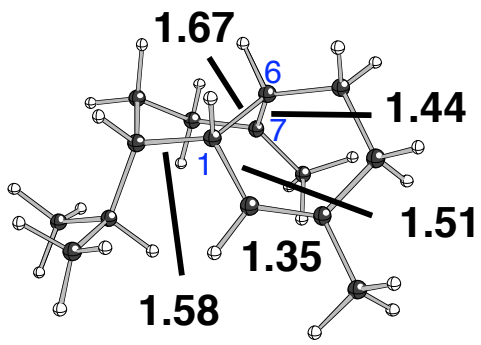
HF = -586.2833044 hartrees (-367892.773511 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	0.680861	1.167189	0.076516
2	6	2.022395	1.288602	0.134007
3	6	2.921456	0.415887	-0.710632
4	6	2.364196	-0.986009	-1.105913
5	6	0.881661	-1.244180	-0.805004
6	6	0.003533	0.197080	-0.844911
7	1	3.152206	0.973841	-1.628823
8	1	0.072465	1.797022	0.713523
9	1	2.500547	-1.129464	-2.181183
10	1	2.965684	-1.767666	-0.630844
11	1	3.885770	0.297047	-0.205429
12	6	2.701892	2.320707	0.993207
13	1	3.314922	2.987541	0.373921
14	1	1.983158	2.934574	1.541585
15	1	3.384512	1.853837	1.713947
16	6	1.306748	-1.742089	1.654504
17	1	0.867687	-2.233335	2.524115
18	1	2.321087	-2.104148	1.461295
19	1	1.424908	-0.658918	1.874323
20	6	-0.974222	-2.146652	0.580550
21	6	-1.830878	-1.564765	-0.547314
22	1	-1.333460	-1.874065	1.582528
23	1	-1.012753	-3.252141	0.571047
24	6	-1.548311	-0.047160	-0.750148
25	1	-1.625182	-2.097336	-1.481819
26	1	-2.885374	-1.746040	-0.339674
27	1	0.405481	-1.805882	-1.612638
28	6	-2.298338	0.895112	0.242898
29	6	0.453970	-1.775587	0.463462
30	6	-2.364070	2.323701	-0.335944
31	1	-3.028015	2.343783	-1.208305
32	1	-2.769944	3.022545	0.401768
33	1	-1.392058	2.707982	-0.657607
34	6	-3.730006	0.430182	0.564494
35	1	-4.243061	1.200852	1.147384
36	1	-4.316219	0.269170	-0.348169
37	1	-3.760970	-0.489070	1.157416
38	1	-1.953215	0.189821	-1.742053
39	1	-1.751196	0.924779	1.195462
40	1	0.247703	0.463166	-1.880399

G5



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

HF = -586.4145465 hartrees (-367980.992074215 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.366673 (Hartree/Particle)

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

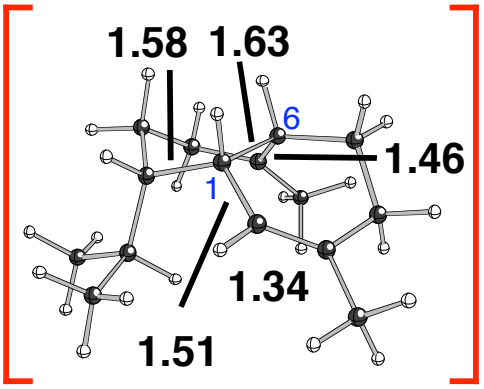
HF = -586.2856588 hartrees (-367894.250897 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.756917	1.240221	-0.216500
2	6	2.070144	1.247946	0.085414
3	6	2.994239	0.098688	-0.238737
4	6	2.352620	-1.057683	-1.028583
5	6	0.855150	-1.274168	-0.791528
6	6	0.037242	0.166931	-0.990562
7	1	3.849811	0.481815	-0.809222
8	1	0.169851	2.099459	0.083697
9	1	2.462862	-0.862871	-2.100526
10	1	2.892274	-1.992908	-0.840115
11	1	3.435905	-0.262925	0.700455
12	6	2.711184	2.417181	0.787878
13	1	3.474875	2.875531	0.147486
14	1	1.981740	3.187358	1.049574
15	1	3.222947	2.100407	1.705014
16	6	1.086485	-1.689803	1.721465
17	1	0.588866	-2.196672	2.549925
18	1	2.120879	-2.028050	1.607469
19	1	1.153223	-0.608919	1.962427
20	6	-1.098501	-2.121473	0.473327
21	6	-1.875386	-1.489060	-0.690628
22	1	-1.531660	-1.898757	1.456273
23	1	-1.125449	-3.225789	0.401399
24	6	-1.525274	0.017539	-0.828110
25	1	-1.639600	-2.003896	-1.627884
26	1	-2.945244	-1.635868	-0.539045

27	1	0.430280	-1.885636	-1.593641
28	6	-2.170064	0.936350	0.262472
29	6	0.331045	-1.746736	0.465910
30	6	-2.396968	2.352944	-0.309015
31	1	-3.209525	2.330964	-1.044628
32	1	-2.687834	3.050614	0.482147
33	1	-1.520512	2.767943	-0.814367
34	6	-3.514608	0.423796	0.810108
35	1	-3.934322	1.164944	1.496915
36	1	-4.247553	0.275980	0.008481
37	1	-3.428696	-0.513291	1.369134
38	1	-1.961999	0.329337	-1.784983
39	1	-1.480742	1.009584	1.115409
40	1	0.244263	0.305603	-2.058863

TS (G5-to-G2)



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

HF = -586.4125695 hartrees (-367979.751486945 kcal/mol)
Imaginary Frequencies: 1 (-54.5493 1/cm)
Zero-point correction = 0.365968 (Hartree/Particle)

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

HF = -586.2833596 hartrees (-367898.670982596 kcal/mol)

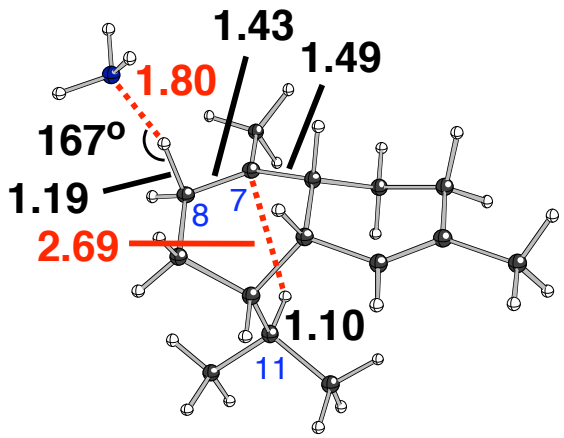
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.031162	1.263647	-0.571776
2	6	2.200295	1.107849	0.068073
3	6	2.813528	-0.255704	0.289380
4	6	2.232764	-1.302415	-0.667661

5	6	0.703518	-1.276563	-0.746523
6	6	0.132089	0.195703	-1.148548
7	1	3.896439	-0.192752	0.129755
8	1	0.694936	2.276179	-0.769564
9	1	2.606614	-1.094362	-1.675774
10	1	2.585403	-2.309366	-0.416230
11	1	2.701080	-0.555749	1.340999
12	6	2.996906	2.283910	0.569977
13	1	3.970633	2.336385	0.067387
14	1	2.476741	3.231088	0.407931
15	1	3.202965	2.187566	1.643509
16	6	0.475341	-2.363814	1.593224
17	1	-0.204914	-3.034453	2.122400
18	1	1.465790	-2.811433	1.474036
19	1	0.623750	-1.473934	2.230779
20	6	-1.528404	-1.981424	0.078160
21	6	-2.047353	-1.054571	-1.029364
22	1	-2.066489	-1.884041	1.029317
23	1	-1.679194	-3.046309	-0.191667
24	6	-1.416073	0.352409	-0.895541
25	1	-1.804468	-1.467792	-2.015850
26	1	-3.136654	-1.013813	-0.982019
27	1	0.372035	-1.872626	-1.617472
28	6	-1.839263	1.116899	0.407752
29	6	-0.082476	-1.870159	0.323917
30	6	-1.863360	2.645397	0.182162
31	1	-2.642007	2.903602	-0.545126
32	1	-2.102110	3.161585	1.116857
33	1	-0.922896	3.056855	-0.182138
34	6	-3.236920	0.734942	0.939582
35	1	-3.479159	1.358867	1.804775
36	1	-4.011148	0.918286	0.185683
37	1	-3.331203	-0.303916	1.267554
38	1	-1.798702	0.938945	-1.739879
39	1	-1.101952	0.903192	1.197146
40	1	0.253988	0.211357	-2.239292

Figure S5 (top).

H1•NH_3



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

HF = -643.004552 hartrees (-403491.78642552 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.402245 (Hartree/Particle)

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

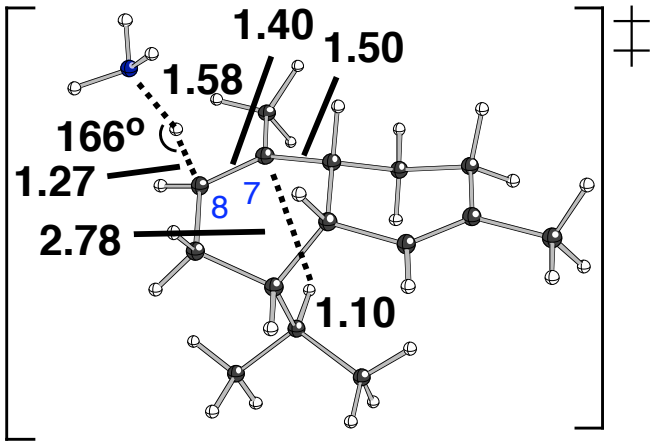
HF = -642.8594157 hartrees (-403394.28335175 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.828719	-0.219522	-1.166287
2	6	2.732025	-0.936538	-0.481877
3	6	2.339209	-1.706441	0.758994
4	6	1.034756	-1.202095	1.383921
5	6	-0.073666	-1.067011	0.302593
6	6	0.342492	-0.170137	-0.902556
7	1	2.257390	-2.777925	0.520807
8	1	2.151281	0.334907	-2.046510
9	1	0.721800	-1.883599	2.179433
10	1	1.204261	-0.221537	1.840910
11	1	3.139309	-1.633191	1.505967
12	6	4.179172	-1.017168	-0.890441
13	1	4.483423	-2.059906	-1.047945
14	1	4.373084	-0.465084	-1.813561
15	1	4.832351	-0.615325	-0.105337
16	6	-1.865504	-1.361403	2.127284
17	1	-2.949983	-1.326705	2.250615
18	1	-1.496289	-2.382745	2.257357
19	1	-1.422629	-0.768962	2.943119
20	6	-2.352667	0.024637	0.095135
21	6	-1.830792	0.990967	-0.987403
22	1	-3.173534	0.404035	0.714528
23	1	-2.907674	-0.866856	-0.458240

24	6	-0.317440	1.246924	-0.837383
25	1	-2.019237	0.568968	-1.981183
26	1	-2.409986	1.914035	-0.937142
27	1	-0.220479	-2.097002	-0.084960
28	6	0.045689	2.127726	0.396245
29	6	-1.425363	-0.755034	0.844209
30	6	1.501971	2.628291	0.344963
31	1	1.654799	3.266687	-0.533468
32	1	1.725603	3.231126	1.230889
33	1	2.228429	1.816263	0.295729
34	6	-0.889600	3.342731	0.553754
35	1	-0.523518	3.995634	1.351755
36	1	-0.921156	3.938391	-0.366702
37	1	-1.916766	3.067651	0.812894
38	1	0.008157	1.793573	-1.732611
39	1	-0.063770	1.521067	1.310675
40	1	-0.112642	-0.625493	-1.796243
41	7	-3.944024	-1.907959	-1.489885
42	1	-4.433026	-2.628260	-0.961106
43	1	-4.655533	-1.323926	-1.926417
44	1	-3.439504	-2.375661	-2.240964

TS1



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

HF = -643.0043509 hartrees (-403491.660233259 kcal/mol)
Imaginary Frequencies: 1 (-195.8823 1/cm)
Zero-point correction = 0.401240 (Hartree/Particle)

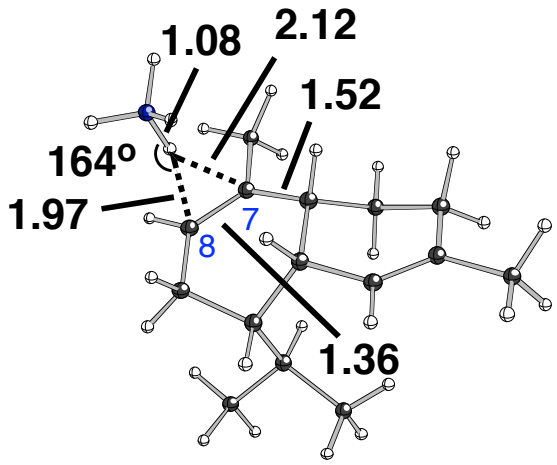
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -642.8601304 hartrees (-403394.731826 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.804906	-0.215266	-1.160001
2	6	2.705997	-0.922509	-0.462058
3	6	2.311798	-1.677502	0.787736
4	6	0.987838	-1.192430	1.387297
5	6	-0.100493	-1.084779	0.283462
6	6	0.318649	-0.160867	-0.897765
7	1	2.256244	-2.754320	0.566136
8	1	2.132279	0.330086	-2.044251
9	1	0.671019	-1.878295	2.177859
10	1	1.132928	-0.209828	1.847314
11	1	3.101719	-1.575201	1.542300
12	6	4.155285	-1.004455	-0.863210
13	1	4.464043	-2.048334	-1.003619
14	1	4.351663	-0.465361	-1.793536
15	1	4.803604	-0.588668	-0.081297
16	6	-1.938678	-1.492116	2.045514
17	1	-3.024491	-1.450464	2.157751
18	1	-1.592933	-2.529263	2.094978
19	1	-1.500794	-0.978329	2.913442
20	6	-2.362315	0.018788	0.096138
21	6	-1.848483	1.020742	-0.949786
22	1	-3.252963	0.315702	0.659509
23	1	-2.869674	-0.938685	-0.558686
24	6	-0.330180	1.261083	-0.810593
25	1	-2.053221	0.647628	-1.961374
26	1	-2.419524	1.945396	-0.853611
27	1	-0.196901	-2.112980	-0.117390
28	6	0.051395	2.136229	0.423086
29	6	-1.472302	-0.796705	0.811075
30	6	1.508371	2.632065	0.351822
31	1	1.652022	3.271855	-0.527320
32	1	1.746221	3.232335	1.235851
33	1	2.231250	1.817733	0.291496
34	6	-0.875379	3.356260	0.593811
35	1	-0.492405	4.007971	1.384853
36	1	-0.920174	3.952189	-0.326139
37	1	-1.898662	3.085792	0.872415
38	1	-0.009485	1.813223	-1.704485
39	1	-0.050647	1.528975	1.335541
40	1	-0.138055	-0.594601	-1.802595
41	7	-3.700584	-1.848375	-1.542928
42	1	-4.157342	-2.616806	-1.053256
43	1	-4.430309	-1.290347	-1.984871
44	1	-3.129783	-2.250004	-2.285680

2•NH_4^+



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

HF = -643.0166229 hartrees (-403499.361035979 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.406458 (Hartree/Particle)

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

HF = -642.8733386 hartrees (-403403.0199715 kcal/mol)

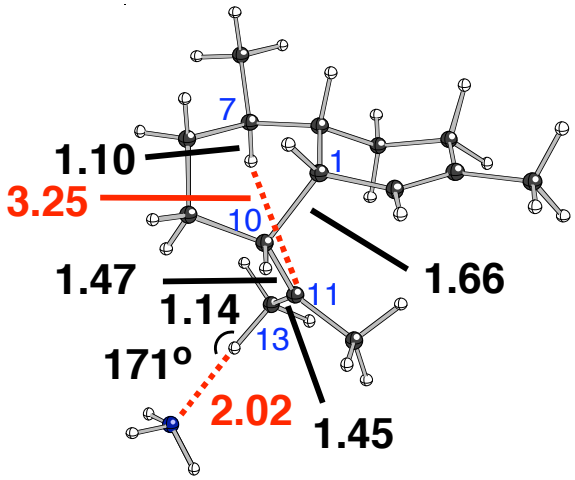
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.712811	-0.365254	-1.112550
2	6	2.550565	-1.088644	-0.353188
3	6	2.094749	-1.721189	0.943303
4	6	0.769898	-1.149974	1.462340
5	6	-0.266137	-1.054782	0.317664
6	6	0.237696	-0.167094	-0.857578
7	1	2.008857	-2.810224	0.803669
8	1	2.092379	0.095183	-2.024366
9	1	0.391949	-1.785628	2.268874
10	1	0.939703	-0.158251	1.892491
11	1	2.872747	-1.588488	1.705933
12	6	3.993615	-1.304174	-0.727554
13	1	4.230223	-2.375000	-0.773438
14	1	4.235295	-0.860951	-1.697303
15	1	4.663296	-0.868864	0.025301
16	6	-2.264727	-1.497309	1.910527
17	1	-3.336775	-1.310622	2.023895
18	1	-2.101836	-2.574797	1.778794
19	1	-1.789559	-1.231461	2.861264
20	6	-2.374342	0.301339	0.182825
21	6	-1.809221	1.228951	-0.871731
22	1	-3.378342	0.516356	0.554707

23	1	-2.816930	-1.281546	-0.905804
24	6	-0.267844	1.315699	-0.800329
25	1	-2.093675	0.889354	-1.883588
26	1	-2.277653	2.210202	-0.773359
27	1	-0.335364	-2.087735	-0.074436
28	6	0.247038	2.207775	0.375105
29	6	-1.670380	-0.692239	0.778342
30	6	1.730130	2.585297	0.201440
31	1	1.871616	3.177648	-0.711215
32	1	2.064387	3.198729	1.044425
33	1	2.383875	1.714939	0.138774
34	6	-0.570035	3.505353	0.535367
35	1	-0.091155	4.155885	1.273528
36	1	-0.621345	4.065779	-0.406794
37	1	-1.591908	3.327962	0.884084
38	1	0.072102	1.800158	-1.726779
39	1	0.144155	1.650130	1.313765
40	1	-0.254463	-0.556398	-1.770815
41	7	-3.163639	-1.931646	-1.696309
42	1	-3.464332	-2.828596	-1.305783
43	1	-3.951465	-1.494591	-2.182279
44	1	-2.403198	-2.090186	-2.363279

Figure S5 (bottom).

H1•NH_3



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

HF = -643.0083177 hartrees (-403494.149439927 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.403057 (Hartree/Particle)

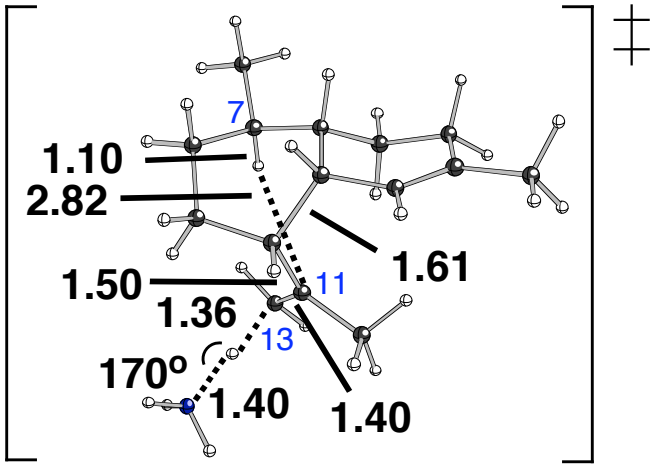
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)

HF = -642.8618352 hartrees (-403395.801588 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.718999	-0.979089	1.033238
2	6	2.662197	-1.199343	0.090501
3	6	2.758115	-0.331920	-1.143063
4	6	1.513631	0.535809	-1.367743
5	6	1.063812	1.218069	-0.068031
6	6	0.762654	0.167446	1.020863
7	1	3.650402	0.304566	-1.043016
8	1	1.705376	-1.613781	1.919185
9	1	1.716708	1.285654	-2.139211
10	1	0.696415	-0.086451	-1.760327
11	1	2.952130	-0.962770	-2.020003
12	6	3.703260	-2.274179	0.242873
13	1	4.708238	-1.833623	0.244956
14	1	3.579369	-2.841820	1.168614
15	1	3.674387	-2.972233	-0.602925
16	6	0.475080	3.621084	-0.692931
17	1	-0.335879	4.314816	-0.936279
18	1	1.066914	4.068286	0.114262
19	1	1.118368	3.544552	-1.575515
20	6	-0.940051	2.360759	0.996042
21	6	-1.669317	1.046562	1.349721
22	1	-1.687512	3.151833	0.872433
23	1	-0.304884	2.680262	1.832349
24	6	-0.844415	-0.250696	1.109727
25	1	-1.953297	1.063865	2.407047
26	1	-2.609942	0.992128	0.793818
27	1	1.929572	1.773828	0.324709
28	6	-1.249986	-1.118898	0.002411
29	6	-0.077250	2.251578	-0.271578
30	6	-0.802227	-2.524207	0.024171
31	1	-0.906809	-2.982986	1.012055
32	1	-1.270121	-3.142167	-0.743301
33	1	0.293344	-2.493049	-0.155136
34	6	-2.089853	-0.696480	-1.106669
35	1	-1.897645	-1.262652	-2.022861
36	1	-3.144092	-1.006930	-0.807066
37	1	-2.125244	0.375708	-1.289753
38	1	-0.839714	-0.875646	2.009777
39	1	-0.718602	1.894493	-1.090552
40	1	0.833276	0.652451	2.001301
41	7	-5.091381	-1.475521	-0.587223
42	1	-5.629167	-0.882038	-1.216284
43	1	-5.293651	-2.438207	-0.850402
44	1	-5.476157	-1.338416	0.345490

TS2



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

HF = -643.0035774 hartrees (-403491.174854274 kcal/mol)
Imaginary Frequencies: 1 (-922.9661 1/cm)
Zero-point correction = 0.401226 (Hartree/Particle)

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

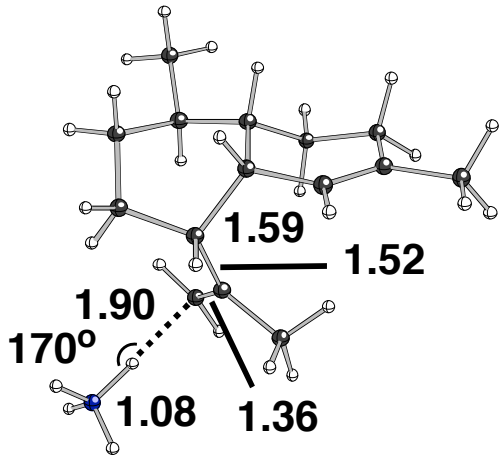
HF = -642.859658 hartrees (-403394.435395 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.708734	-0.932865	1.043763
2	6	2.718129	-1.050749	0.160323
3	6	2.832984	-0.126771	-1.031331
4	6	1.543423	0.656079	-1.305683
5	6	0.969341	1.260749	-0.015085
6	6	0.668371	0.154101	1.025537
7	1	3.666742	0.569170	-0.853807
8	1	1.674489	-1.614057	1.894842
9	1	1.736078	1.444631	-2.041033
10	1	0.799193	-0.011222	-1.763154
11	1	3.123968	-0.706711	-1.916985
12	6	3.806888	-2.078523	0.321420
13	1	4.787795	-1.591664	0.392187
14	1	3.666773	-2.689266	1.217377
15	1	3.853713	-2.743815	-0.550036
16	6	0.228047	3.619221	-0.657018
17	1	-0.622828	4.255078	-0.923063
18	1	0.756868	4.099465	0.174677

19	1	0.906365	3.599697	-1.515920
20	6	-1.155026	2.249672	0.965325
21	6	-1.768232	0.875620	1.327287
22	1	-1.963827	2.971271	0.804538
23	1	-0.579616	2.635108	1.816708
24	6	-0.857685	-0.347732	1.013922
25	1	-1.991367	0.858555	2.399463
26	1	-2.735296	0.762923	0.825333
27	1	1.766517	1.869053	0.438438
28	6	-1.228718	-1.165826	-0.186780
29	6	-0.234849	2.208082	-0.266331
30	6	-0.687741	-2.555165	-0.249857
31	1	-0.889136	-3.103934	0.677421
32	1	-1.064344	-3.119545	-1.105311
33	1	0.409133	-2.492770	-0.313583
34	6	-2.111197	-0.748302	-1.184377
35	1	-2.091820	-1.305404	-2.122908
36	1	-3.295953	-1.208887	-0.705971
37	1	-2.331911	0.311622	-1.288963
38	1	-0.896854	-1.048379	1.858793
39	1	-0.811347	1.808389	-1.113396
40	1	0.705823	0.620548	2.019306
41	7	-4.614616	-1.598295	-0.427175
42	1	-5.252368	-1.173420	-1.100919
43	1	-4.720911	-2.611182	-0.487641
44	1	-4.898383	-1.302730	0.507143

1•NH_4^+



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

HF = -643.0103773 hartrees (-403495.441859523 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.406765 (Hartree/Particle)

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

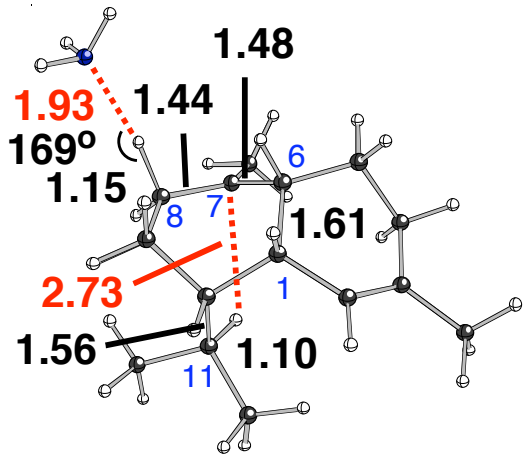
HF = -642.8666558 hartrees (-403398.8265145 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.616374	-1.003983	-1.042853
2	6	-2.675402	-1.111746	-0.222102
3	6	-2.896627	-0.135109	0.911362
4	6	-1.646638	0.690139	1.237538
5	6	-0.999520	1.252954	-0.038767
6	6	-0.602389	0.113549	-1.016287
7	1	-3.730068	0.531897	0.643020
8	1	-1.504551	-1.728379	-1.851049
9	1	-1.909543	1.506342	1.919596
10	1	-0.921975	0.061888	1.771764
11	1	-3.236374	-0.679790	1.802316
12	6	-3.715232	-2.188900	-0.392130
13	1	-4.709679	-1.747572	-0.536292
14	1	-3.503611	-2.832113	-1.250995
15	1	-3.782618	-2.818478	0.504539
16	6	-0.345798	3.646321	0.573486
17	1	0.475364	4.309249	0.866777
18	1	-0.837849	4.090378	-0.300042
19	1	-1.070363	3.636833	1.393850
20	6	1.150544	2.260703	-0.928645
21	6	1.812778	0.889380	-1.203641
22	1	1.931117	3.010157	-0.752853
23	1	0.612421	2.597169	-1.824116
24	6	0.909543	-0.345871	-0.901399
25	1	2.109727	0.849080	-2.258093
26	1	2.744801	0.826491	-0.626781
27	1	-1.777570	1.826845	-0.564747
28	6	1.260552	-1.130970	0.356788
29	6	0.166101	2.234655	0.252124
30	6	0.785233	-2.562026	0.398340
31	1	1.104577	-3.114642	-0.494422
32	1	1.133661	-3.087855	1.291657
33	1	-0.309633	-2.586544	0.385986
34	6	1.990461	-0.644662	1.394038
35	1	2.120766	-1.239848	2.296831
36	1	3.569556	-1.271444	0.551828
37	1	2.282688	0.399071	1.460118
38	1	1.033320	-1.066484	-1.722487
39	1	0.704442	1.871056	1.139252
40	1	-0.620053	0.545439	-2.027619
41	7	4.567328	-1.542472	0.222879
42	1	5.256999	-1.190645	0.892897
43	1	4.651453	-2.560560	0.156982
44	1	4.748308	-1.126853	-0.695180

Figure S6 (top).

H2•NH_3



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

HF = -642.9986444 hartrees (-403488.079347444 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.402589 (Hartree/Particle)

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

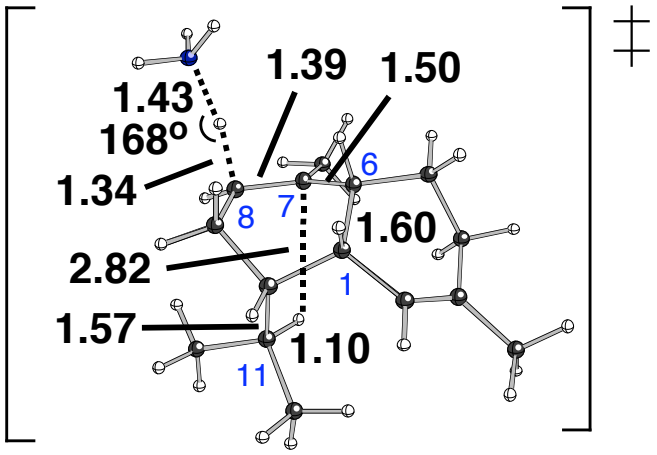
HF = -642.8529436 hartrees (-403390.222109 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.971393	-0.003895	-0.985872
2	6	2.705514	-0.815159	-0.211505
3	6	2.052184	-1.932032	0.572015
4	6	0.766653	-2.400335	-0.121721
5	6	-0.214519	-1.255910	-0.420421
6	6	0.473212	-0.006881	-1.163132
7	1	2.742675	-2.779603	0.650437
8	1	2.480352	0.742269	-1.593468
9	1	1.047840	-2.846254	-1.081551
10	1	0.275493	-3.195390	0.449099
11	1	1.864558	-1.615062	1.609122
12	6	4.201611	-0.690311	-0.099292
13	1	4.699031	-1.603037	-0.450518
14	1	4.586989	0.153047	-0.678156
15	1	4.503312	-0.552022	0.947097

16	6	-1.235783	-1.533546	1.947528
17	1	-2.040736	-1.154872	2.578164
18	1	-1.346392	-2.617807	1.814564
19	1	-0.274878	-1.409966	2.466013
20	6	-2.149122	0.137815	0.282228
21	6	-1.766493	1.041503	-0.899453
22	1	-2.523504	0.661419	1.168855
23	1	-3.055796	-0.508134	-0.019794
24	6	-0.251508	1.348611	-0.854410
25	1	-2.003505	0.546514	-1.849676
26	1	-2.371372	1.949390	-0.870562
27	1	-0.932313	-1.620601	-1.182843
28	6	0.179905	2.097067	0.448492
29	6	-1.169735	-0.858934	0.632665
30	6	1.534819	2.821059	0.302468
31	1	1.492296	3.551598	-0.514260
32	1	1.763613	3.370530	1.220892
33	1	2.365211	2.143489	0.111935
34	6	-0.854499	3.146919	0.904344
35	1	-0.475161	3.685574	1.777407
36	1	-1.030241	3.889398	0.116665
37	1	-1.823809	2.726711	1.186312
38	1	-0.028464	2.014563	-1.698180
39	1	0.290960	1.356675	1.259620
40	1	0.289060	-0.177535	-2.232640
41	7	-4.693461	-1.291353	-0.683485
42	1	-5.337388	-1.432790	0.092901
43	1	-5.140972	-0.634645	-1.320411
44	1	-4.624416	-2.179813	-1.176238

TS3



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

HF = -642.9959186 hartrees (-403486.368880686 kcal/mol)

Imaginary Frequencies: 1 (-740.4245 1/cm)
Zero-point correction = 0.400886 (Hartree/Particle)

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

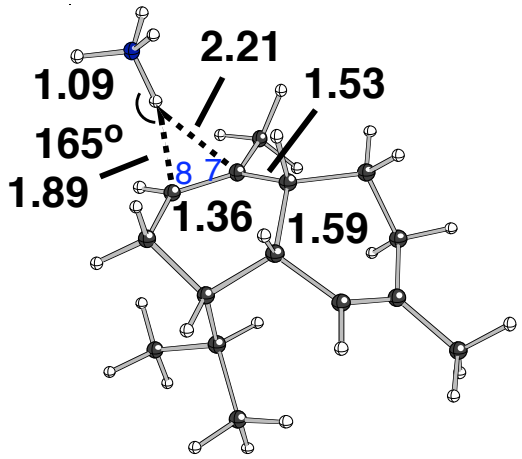
HF = -642.8521928 hartrees (-403389.750982 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.940786	0.001493	-0.988121
2	6	2.670102	-0.790123	-0.189115
3	6	2.005085	-1.886886	0.612741
4	6	0.747303	-2.388557	-0.107363
5	6	-0.250830	-1.267287	-0.452074
6	6	0.441368	-0.013240	-1.162406
7	1	2.701539	-2.723436	0.742746
8	1	2.453719	0.735369	-1.606896
9	1	1.065346	-2.846184	-1.050283
10	1	0.255920	-3.183180	0.463596
11	1	1.777821	-1.535919	1.630706
12	6	4.165711	-0.665937	-0.070428
13	1	4.663814	-1.588620	-0.394200
14	1	4.556452	0.161277	-0.669051
15	1	4.461636	-0.500506	0.973747
16	6	-1.338185	-1.622647	1.902509
17	1	-2.139883	-1.239864	2.537266
18	1	-1.486801	-2.696548	1.736445
19	1	-0.390305	-1.538591	2.448278
20	6	-2.148953	0.123920	0.293498
21	6	-1.793406	1.054423	-0.865829
22	1	-2.695614	0.552259	1.137872
23	1	-3.128388	-0.658186	-0.172539
24	6	-0.272196	1.347996	-0.839558
25	1	-2.038054	0.592448	-1.833512
26	1	-2.386263	1.968947	-0.804358
27	1	-0.917119	-1.676192	-1.232412
28	6	0.186809	2.090872	0.458950
29	6	-1.238699	-0.881514	0.612263
30	6	1.500222	2.873186	0.251524
31	1	1.374738	3.633683	-0.528832
32	1	1.775634	3.393583	1.174343
33	1	2.337850	2.235411	-0.025765
34	6	-0.861563	3.089329	0.990778
35	1	-0.456048	3.625828	1.853630
36	1	-1.110431	3.840566	0.231410
37	1	-1.794045	2.620668	1.318336
38	1	-0.060654	2.016848	-1.684129
39	1	0.368512	1.341109	1.244706
40	1	0.262190	-0.160454	-2.237045
41	7	-4.305261	-1.234983	-0.751286

42	1	-4.845066	-1.730107	-0.041437
43	1	-4.894371	-0.495129	-1.133631
44	1	-4.096617	-1.890373	-1.504202

2•NH_4^+



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

HF = -643.0035571 hartrees (-403491.162115821 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.406480 (Hartree/Particle)

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

HF = -642.8603051 hartrees (-403394.84145025 kcal/mol)

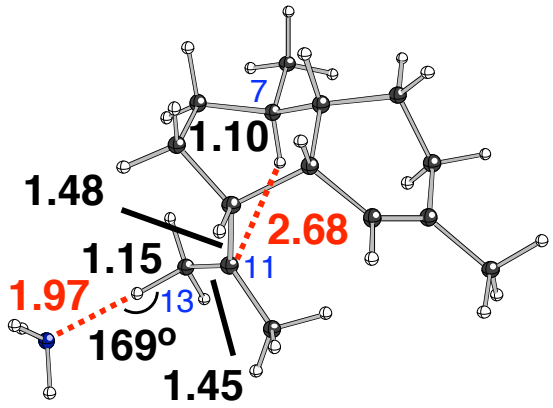
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.845727	-0.327271	-1.086146
2	6	2.479879	-1.109027	-0.201213
3	6	1.670954	-1.954408	0.758485
4	6	0.367619	-2.393079	0.081152
5	6	-0.497625	-1.207705	-0.402656
6	6	0.353932	-0.099859	-1.169644
7	1	2.246065	-2.839585	1.054124
8	1	2.433235	0.232416	-1.811929
9	1	0.638662	-2.991092	-0.795807
10	1	-0.212035	-3.053933	0.732651
11	1	1.469951	-1.402859	1.689565
12	6	3.978760	-1.225890	-0.137234
13	1	4.302336	-2.258529	-0.320809

14	1	4.471052	-0.578053	-0.867688
15	1	4.348005	-0.955737	0.860852
16	6	-1.821926	-1.443313	1.864943
17	1	-2.581915	-0.933576	2.464176
18	1	-2.179045	-2.453748	1.628260
19	1	-0.937640	-1.578283	2.497574
20	6	-2.068883	0.545017	0.381957
21	6	-1.597301	1.421134	-0.756244
22	1	-2.746091	0.965663	1.127455
23	1	-3.405335	-0.508743	-0.428511
24	6	-0.051251	1.380844	-0.824983
25	1	-1.983989	1.075981	-1.731549
26	1	-1.968195	2.440925	-0.632096
27	1	-1.156587	-1.639356	-1.177094
28	6	0.652217	2.001838	0.431273
29	6	-1.474978	-0.648564	0.631509
30	6	1.987492	2.669897	0.045812
31	1	1.808304	3.525561	-0.617101
32	1	2.497425	3.047092	0.938395
33	1	2.671424	1.988179	-0.459834
34	6	-0.190829	3.048704	1.185109
35	1	0.391210	3.455389	2.017979
36	1	-0.457484	3.893697	0.538492
37	1	-1.111994	2.639746	1.610582
38	1	0.244406	1.988261	-1.690336
39	1	0.874451	1.188712	1.135407
40	1	0.087181	-0.206636	-2.231173
41	7	-4.271320	-0.865800	-0.981686
42	1	-4.804857	-1.522831	-0.406325
43	1	-4.869351	-0.071763	-1.226280
44	1	-3.972672	-1.336203	-1.839903

Figure S6 (bottom).

H2•NH_3



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

HF = -642.9961945 hartrees (-403486.542010695 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.403388 (Hartree/Particle)

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

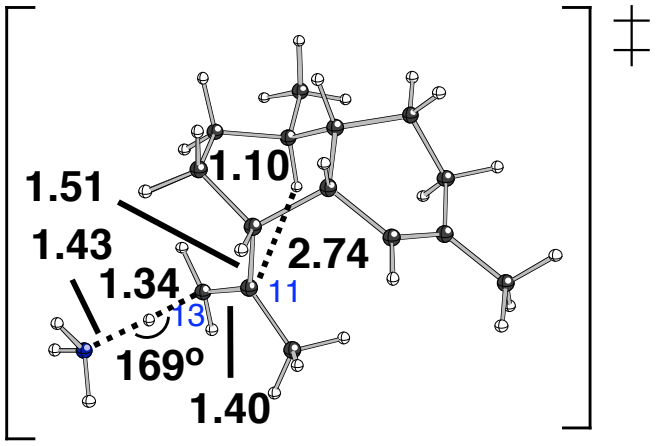
HF = -642.8502629 hartrees (-403388.53996975 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.434079	-1.359640	0.856847
2	6	2.418513	-1.452047	-0.059637
3	6	2.878820	-0.211954	-0.791610
4	6	2.714791	1.016056	0.111823
5	6	1.267743	1.222978	0.602136
6	6	0.693688	-0.104972	1.213222
7	1	3.928195	-0.326862	-1.085398
8	1	1.176708	-2.245422	1.437113
9	1	3.360740	0.876820	0.987008
10	1	3.070523	1.920276	-0.388438
11	1	2.319758	-0.091728	-1.732150
12	6	3.148796	-2.737349	-0.334101
13	1	4.207126	-2.641843	-0.060667
14	1	2.728752	-3.582370	0.218575
15	1	3.129129	-2.976229	-1.405229
16	6	0.884161	3.059392	-1.186280
17	1	0.104754	3.546475	-1.781912
18	1	1.283709	3.808037	-0.492113
19	1	1.685010	2.773387	-1.873024
20	6	-0.980434	2.283450	0.315722
21	6	-1.514154	1.205540	1.296487
22	1	-1.748070	2.570335	-0.411851
23	1	-0.762084	3.196944	0.881182
24	6	-0.947185	-0.198402	1.025018
25	1	-1.227314	1.464011	2.320932
26	1	-2.609078	1.181167	1.294107
27	1	1.325038	1.944544	1.428679
28	6	-1.462121	-0.887078	-0.177061
29	6	0.302885	1.857424	-0.427990
30	6	-1.110656	-2.300510	-0.409816
31	1	-1.091891	-2.893339	0.508169
32	1	-1.735068	-2.775068	-1.168265
33	1	-0.059462	-2.294776	-0.761051
34	6	-2.406128	-0.288244	-1.099093
35	1	-2.389734	-0.747856	-2.091597
36	1	-3.429460	-0.589196	-0.679421
37	1	-2.410470	0.797435	-1.144174
38	1	-1.217015	-0.881777	1.844928
39	1	0.049414	1.091844	-1.179187
40	1	0.736307	-0.014350	2.304755

41	7	-5.323939	-0.957349	-0.273925
42	1	-5.885783	-0.349346	-0.867194
43	1	-5.601912	-1.913495	-0.487144
44	1	-5.607043	-0.774036	0.686842

TS4



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

HF = -642.9928239 hartrees (-403484.426925489 kcal/mol)
Imaginary Frequencies: 1 (-834.4384 1/cm)
Zero-point correction = 0.401628 (Hartree/Particle)

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

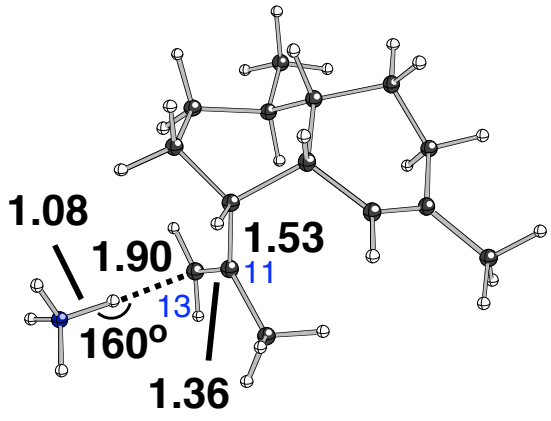
HF = -642.8491029 hartrees (-403387.81206975 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.346126	-1.377462	0.806002
2	6	2.390920	-1.439061	-0.037055
3	6	2.936472	-0.173295	-0.659778
4	6	2.697462	1.015432	0.277081
5	6	1.214660	1.209490	0.645223
6	6	0.596549	-0.126730	1.192900
7	1	4.009681	-0.291235	-0.849926
8	1	1.028463	-2.291551	1.307259
9	1	3.262575	0.835545	1.199885
10	1	3.098500	1.938531	-0.150183
11	1	2.478408	-0.001276	-1.645727
12	6	3.102385	-2.728277	-0.349646

13	1	4.146661	-2.684625	-0.015795
14	1	2.628643	-3.590488	0.128881
15	1	3.132235	-2.906192	-1.432609
16	6	0.969641	3.040812	-1.173528
17	1	0.240140	3.524787	-1.832268
18	1	1.314258	3.793222	-0.454203
19	1	1.822512	2.749922	-1.792461
20	6	-0.998885	2.272957	0.196974
21	6	-1.561284	1.219816	1.187501
22	1	-1.728658	2.519713	-0.583150
23	1	-0.829580	3.209732	0.741407
24	6	-1.001924	-0.197627	0.959102
25	1	-1.289695	1.499763	2.210663
26	1	-2.657897	1.215093	1.169351
27	1	1.201083	1.928470	1.476756
28	6	-1.524077	-0.898242	-0.268077
29	6	0.331816	1.842713	-0.457042
30	6	-1.194966	-2.339598	-0.476466
31	1	-1.202104	-2.908101	0.457681
32	1	-1.856274	-2.809942	-1.207883
33	1	-0.164522	-2.398403	-0.853667
34	6	-2.442478	-0.318169	-1.146612
35	1	-2.601794	-0.830661	-2.097493
36	1	-3.602319	-0.637873	-0.551512
37	1	-2.526013	0.763787	-1.192412
38	1	-1.345978	-0.852593	1.776078
39	1	0.123524	1.077364	-1.220685
40	1	0.643260	-0.070896	2.288713
41	7	-4.946291	-0.864070	-0.135474
42	1	-5.587668	-0.408474	-0.785138
43	1	-5.170770	-1.859005	-0.117730
44	1	-5.117134	-0.482683	0.795010

1•NH_4^+



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

HF = -643.0004034 hartrees (-403489.183137534 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.407119 (Hartree/Particle)

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

HF = -642.8567261 hartrees (-403392.59562775 kcal/mol)

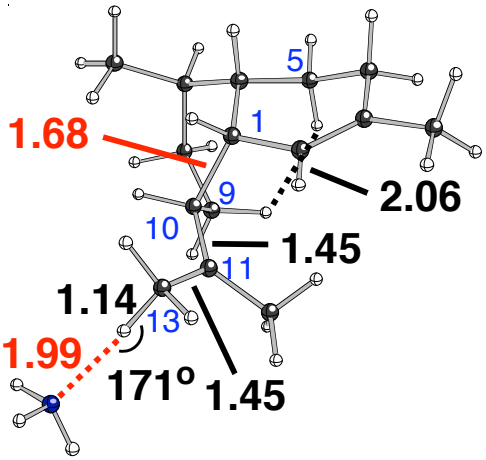
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.272196	-1.398329	0.760554
2	6	2.344311	-1.453452	-0.045685
3	6	2.965359	-0.179207	-0.573402
4	6	2.701736	0.975326	0.398819
5	6	1.204828	1.188672	0.687841
6	6	0.540941	-0.145276	1.184037
7	1	4.045360	-0.323762	-0.698370
8	1	0.907096	-2.325858	1.200477
9	1	3.206876	0.742604	1.344624
10	1	3.148978	1.904751	0.034777
11	1	2.579594	0.050438	-1.578148
12	6	3.014997	-2.751198	-0.411595
13	1	4.050716	-2.770455	-0.049481
14	1	2.493687	-3.618170	0.005526
15	1	3.065814	-2.871845	-1.501753
16	6	1.089681	3.048374	-1.111070
17	1	0.409903	3.547347	-1.811087
18	1	1.390967	3.788479	-0.359818
19	1	1.980501	2.759009	-1.674930
20	6	-0.967588	2.277543	0.117450
21	6	-1.584992	1.233788	1.083661
22	1	-1.653403	2.518392	-0.703659
23	1	-0.828742	3.218365	0.664523
24	6	-1.036621	-0.199700	0.917354
25	1	-1.370703	1.529938	2.116327
26	1	-2.682519	1.244236	1.003741
27	1	1.156596	1.900965	1.524879
28	6	-1.541330	-0.943083	-0.320542
29	6	0.397895	1.843991	-0.457758
30	6	-1.406806	-2.449505	-0.340345
31	1	-1.588971	-2.892515	0.644838
32	1	-2.083183	-2.905294	-1.070102
33	1	-0.387155	-2.725644	-0.622455
34	6	-2.186543	-0.345878	-1.355287
35	1	-2.490597	-0.934665	-2.220190
36	1	-3.832610	-0.585731	-0.429322
37	1	-2.246741	0.731393	-1.461837
38	1	-1.426538	-0.800591	1.753178
39	1	0.229898	1.092722	-1.241457
40	1	0.590210	-0.121927	2.282452

41	7	-4.853645	-0.632781	-0.069965
42	1	-5.469953	-0.141931	-0.723945
43	1	-5.154194	-1.608282	0.008041
44	1	-4.913763	-0.184891	0.848746

Figure S7.

C2•NH_3



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

HF = -643.0051781 hartrees (-403492.179309531 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.402978 (Hartree/Particle)

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

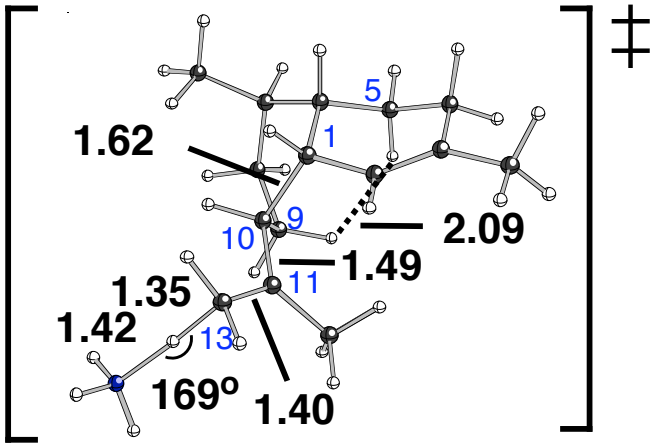
HF = -642.8582895 hartrees (-403393.57666125 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.547928	1.106689	-0.444040
2	6	-0.286525	3.164273	-1.320555
3	1	0.039529	4.178175	-1.067922
4	1	0.596716	2.622430	-1.678097
5	1	-0.985114	3.242572	-2.160570
6	6	-0.960205	2.496852	-0.106376
7	6	-0.034640	2.442788	1.146480
8	6	1.703177	-0.874005	0.157772
9	6	0.592315	1.058689	1.416510
10	1	-0.590183	2.747033	2.038959

11	1	0.767715	3.179528	1.026290
12	6	0.929580	0.356306	0.094206
13	1	1.504286	1.183787	2.012038
14	1	-0.080751	0.432834	2.009045
15	6	-2.568302	0.638853	0.611427
16	6	-0.476085	0.023210	-0.759363
17	6	-3.233892	-0.682675	0.224022
18	6	-1.001959	-1.377878	-0.637810
19	6	-2.245470	-1.719240	-0.246178
20	1	-2.103354	1.214149	-1.387915
21	1	-3.964030	-0.520086	-0.583874
22	1	-2.093445	0.525274	1.591710
23	1	-3.331033	1.416492	0.729285
24	6	-2.738016	-3.139716	-0.311487
25	1	-3.037152	-3.494379	0.682586
26	1	-3.630807	-3.206677	-0.945569
27	1	-1.984629	-3.823319	-0.712184
28	6	2.609875	-1.219749	-0.919645
29	1	2.718796	-2.297572	-1.072787
30	1	2.425940	-0.681011	-1.852428
31	1	3.640249	-0.880375	-0.561070
32	6	1.564348	-1.786125	1.309477
33	1	2.212315	-2.660963	1.249336
34	1	1.725470	-1.254987	2.255116
35	1	0.509390	-2.112127	1.338927
36	1	-1.817079	3.132010	0.148050
37	1	-3.815370	-1.080097	1.065078
38	1	-0.354687	-2.171030	-1.014558
39	1	1.453231	1.050800	-0.569731
40	1	-0.131693	0.152828	-1.791581
41	7	5.537173	-0.406041	-0.215194
42	1	6.088738	-0.762375	-0.993700
43	1	5.712413	0.595832	-0.166306
44	1	5.926696	-0.816102	0.631589

TS5



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

HF = -643.0014496 hartrees (-403489.839638496 kcal/mol)
Imaginary Frequencies: 1 (-863.6319 1/cm)
Zero-point correction = 0.401441 (Hartree/Particle)

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

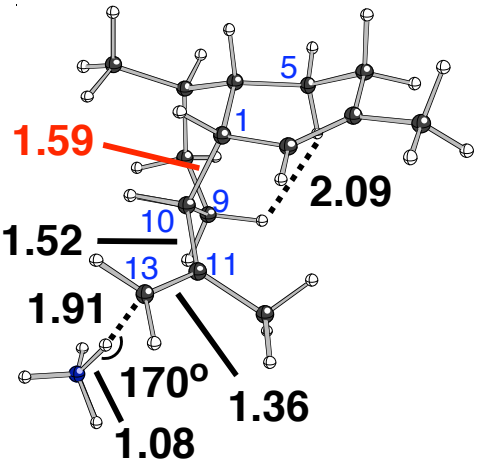
HF = -642.8570066 hartrees (-403392.7716415 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.477947	1.174914	-0.416022
2	6	-0.141098	3.184430	-1.286093
3	1	0.245590	4.174964	-1.024618
4	1	0.699483	2.602338	-1.681739
5	1	-0.860622	3.316319	-2.101362
6	6	-0.808828	2.524245	-0.064512
7	6	0.161110	2.391491	1.148610
8	6	1.701860	-1.019331	0.077709
9	6	0.724948	0.969902	1.364107
10	1	-0.341374	2.705161	2.069111
11	1	0.995372	3.089593	1.010636
12	6	0.945033	0.263747	0.015251
13	1	1.669997	1.037869	1.917819
14	1	0.049001	0.375543	1.985888
15	6	-2.491660	0.736441	0.659351
16	6	-0.455018	0.051374	-0.768066
17	6	-3.230338	-0.544002	0.264028
18	6	-1.055335	-1.330338	-0.658689
19	6	-2.301123	-1.619220	-0.244052
20	1	-2.058150	1.331747	-1.336653
21	1	-3.971346	-0.328986	-0.521117
22	1	-1.995902	0.578351	1.623507
23	1	-3.212545	1.547295	0.814871
24	6	-2.860939	-3.016152	-0.306311
25	1	-3.151275	-3.367341	0.691836
26	1	-3.770443	-3.039551	-0.919803
27	1	-2.148215	-3.729135	-0.730401
28	6	2.604388	-1.352292	-0.934171
29	1	2.887200	-2.401853	-1.034954
30	1	2.536026	-0.799163	-1.873287
31	1	3.762099	-0.857264	-0.455369
32	6	1.520288	-1.924506	1.246875
33	1	2.090549	-2.850902	1.157065
34	1	1.791806	-1.414533	2.179129
35	1	0.452470	-2.164839	1.339921
36	1	-1.618900	3.199308	0.237504
37	1	-3.809543	-0.926934	1.113825
38	1	-0.450354	-2.146352	-1.056462

39	1	1.521671	0.938055	-0.628430
40	1	-0.170451	0.176430	-1.821196
41	7	5.082349	-0.430851	-0.174120
42	1	5.693387	-0.656306	-0.959552
43	1	5.124043	0.576863	-0.021208
44	1	5.451928	-0.894943	0.655802

1•NH_4^+



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

HF = -643.0084493 hartrees (-403494.232020243 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.406780 (Hartree/Particle)

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

HF = -642.8643683 hartrees (-403397.39110825 kcal/mol)

Coordinates (from last standard orientation):

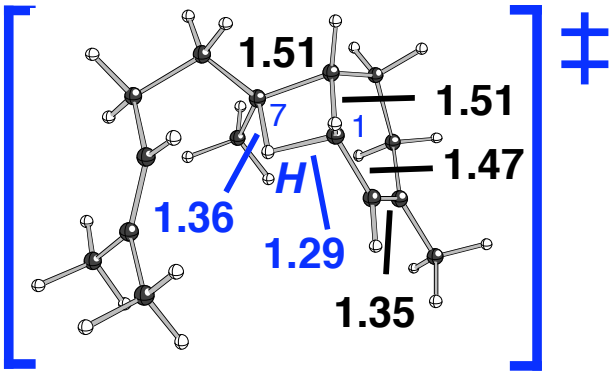
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.365867	1.294142	-0.335443
2	6	0.083335	3.176036	-1.304121
3	1	0.595807	4.115058	-1.068132
4	1	0.812412	2.520531	-1.794884
5	1	-0.697284	3.403245	-2.038080
6	6	-0.523605	2.554757	-0.031226
7	6	0.546725	2.285636	1.068784
8	6	1.616412	-1.265904	-0.169057
9	6	0.974542	0.806268	1.188730
10	1	0.177569	2.620412	2.043736

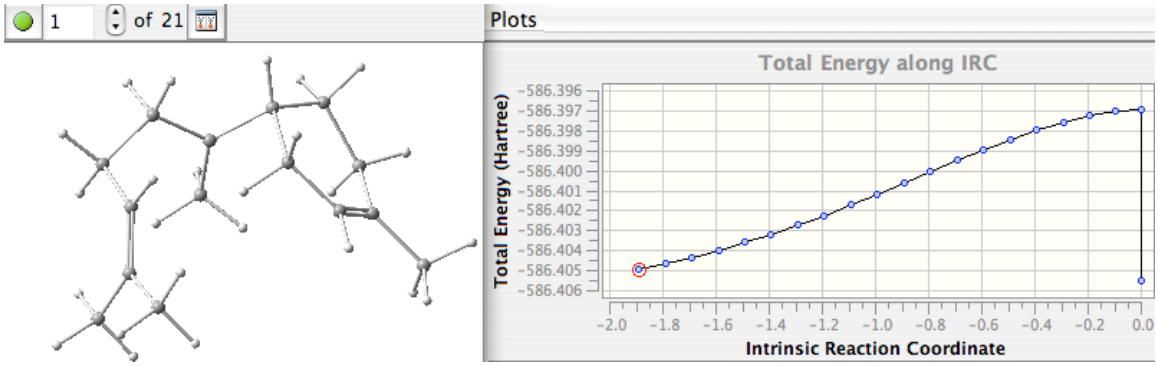
11	1	1.429324	2.902705	0.857189
12	6	0.960800	0.102650	-0.180830
13	1	1.979400	0.756489	1.637694
14	1	0.319313	0.270888	1.882387
15	6	-2.300634	0.926931	0.834030
16	6	-0.503054	0.085055	-0.811031
17	6	-3.216787	-0.247517	0.481089
18	6	-1.247939	-1.226692	-0.690444
19	6	-2.471034	-1.394262	-0.160176
20	1	-2.023275	1.541829	-1.180719
21	1	-4.009025	0.083549	-0.207861
22	1	-1.725362	0.670842	1.731149
23	1	-2.904927	1.803505	1.096108
24	6	-3.189609	-2.717988	-0.205191
25	1	-3.415269	-3.078616	0.806606
26	1	-4.153275	-2.618407	-0.720975
27	1	-2.607277	-3.485205	-0.723518
28	6	2.429402	-1.645948	-1.187851
29	1	2.814723	-2.662368	-1.253074
30	1	2.553835	-1.017543	-2.069156
31	1	3.871553	-0.889380	-0.186943
32	6	1.352856	-2.192012	0.990171
33	1	1.832709	-3.164520	0.852024
34	1	1.695792	-1.759020	1.937711
35	1	0.274810	-2.348698	1.101043
36	1	-1.218907	3.304070	0.367359
37	1	-3.740712	-0.603427	1.377706
38	1	-0.774634	-2.084069	-1.169475
39	1	1.558468	0.722726	-0.861445
40	1	-0.323502	0.218586	-1.886973
41	7	4.792462	-0.485891	0.216063
42	1	5.436410	-0.264701	-0.548692
43	1	4.589572	0.367160	0.744938
44	1	5.231253	-1.171321	0.837232

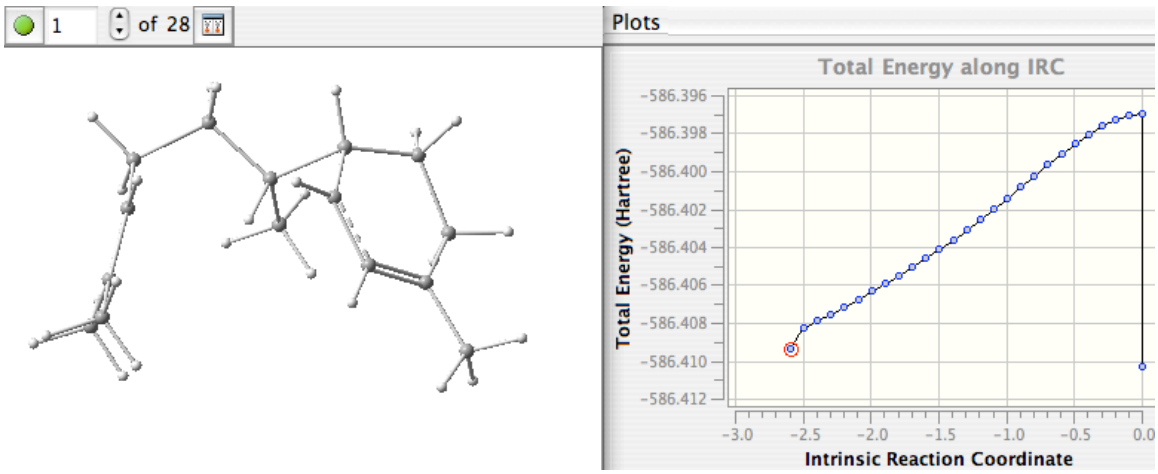
VII. IRC Plots

Figure 2.

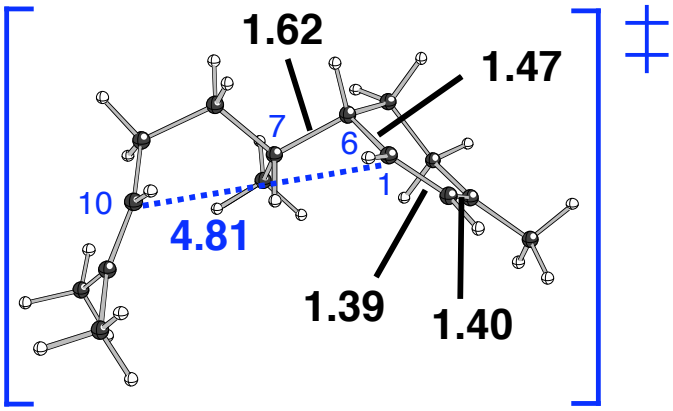
TS (A1-to-B1)

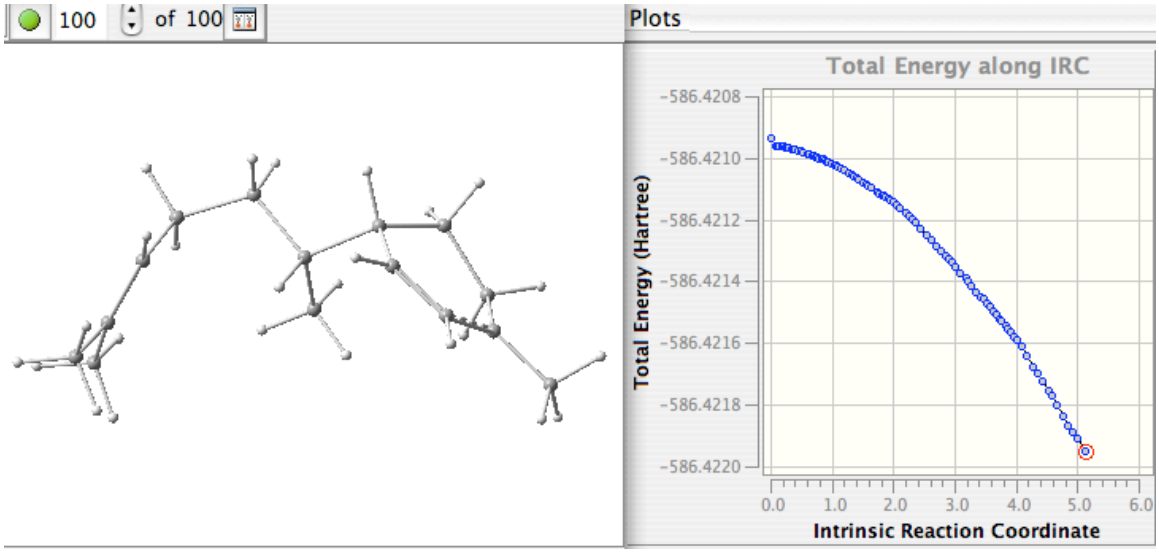


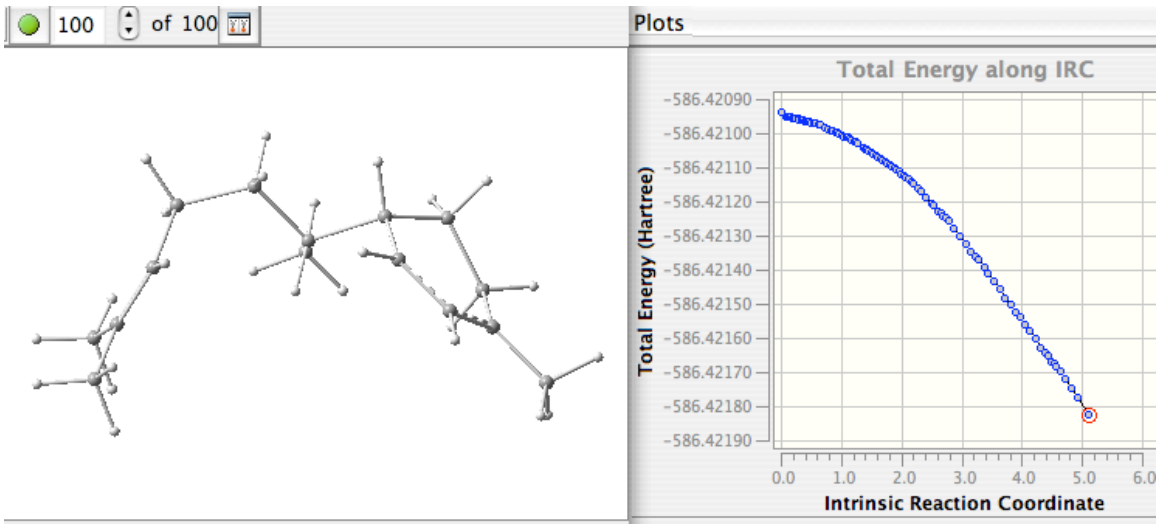




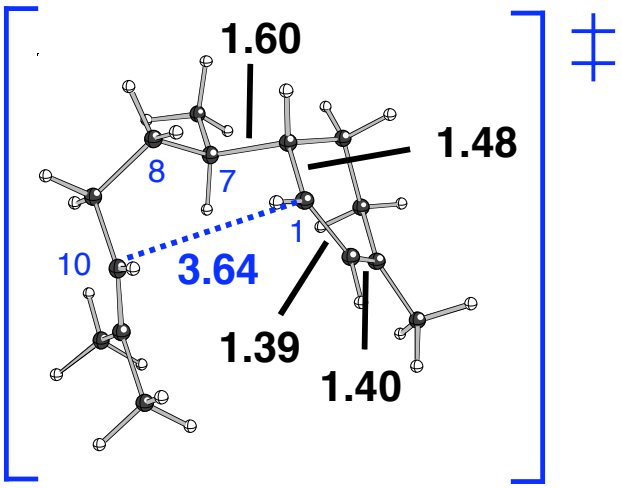
TS (B1-to-B2)

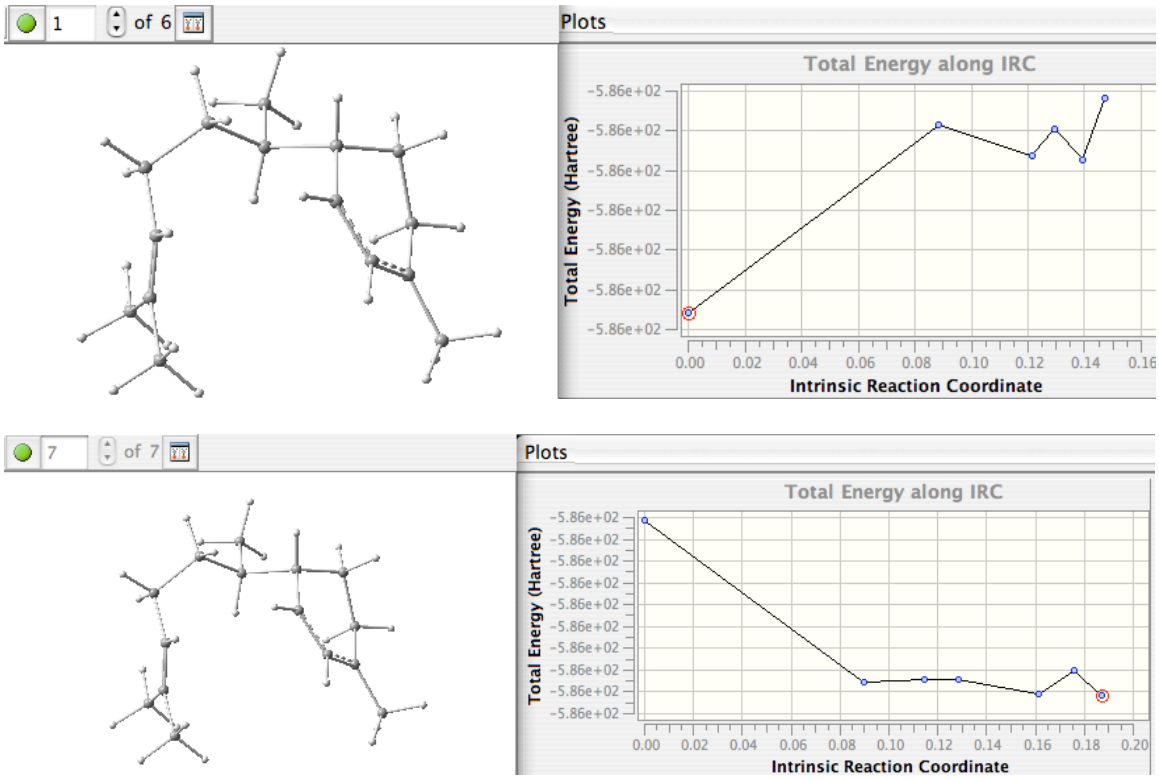

1.62
1.47
7
6
1
10
4.81
1.39
1.40


100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4208
-586.4210
-586.4212
-586.4214
-586.4216
-586.4218
-586.4220
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Intrinsic Reaction Coordinate

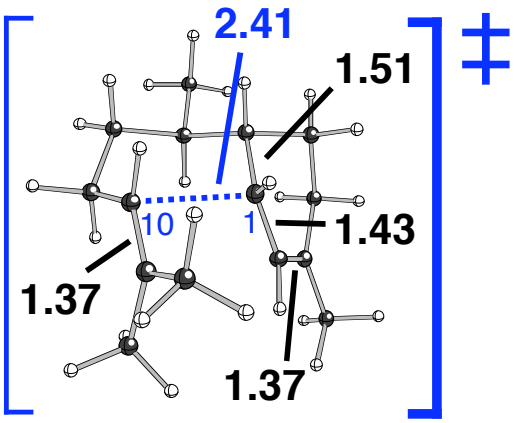

100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.42090
-586.42100
-586.42110
-586.42120
-586.42130
-586.42140
-586.42150
-586.42160
-586.42170
-586.42180
-586.42190
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Intrinsic Reaction Coordinate

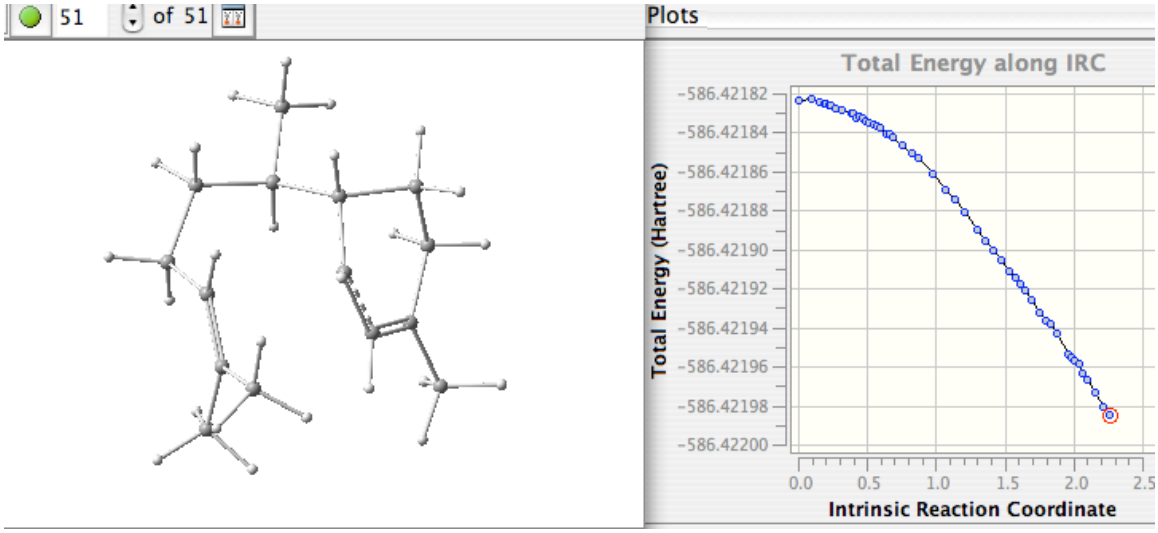
TS (B2-to-B3)


1.60
1.48
8
7
1
10
3.64
1.39
1.40


1
of 6
Plots
Total Energy along IRC
Total Energy (Hartree)
-5.86e+02
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
Intrinsic Reaction Coordinate
7
of 7
Plots
Total Energy along IRC
Total Energy (Hartree)
-5.86e+02
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
Intrinsic Reaction Coordinate

TS (B3-to-C1)





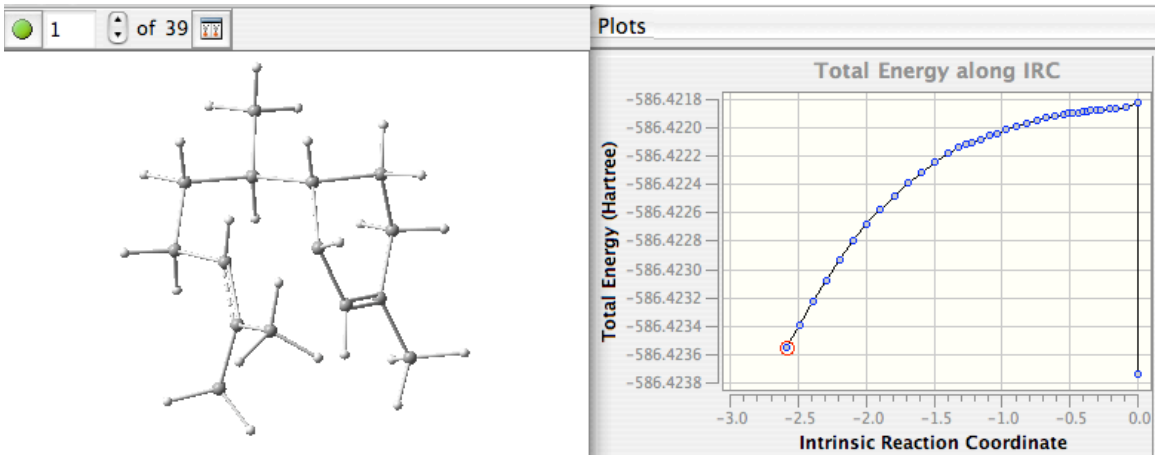
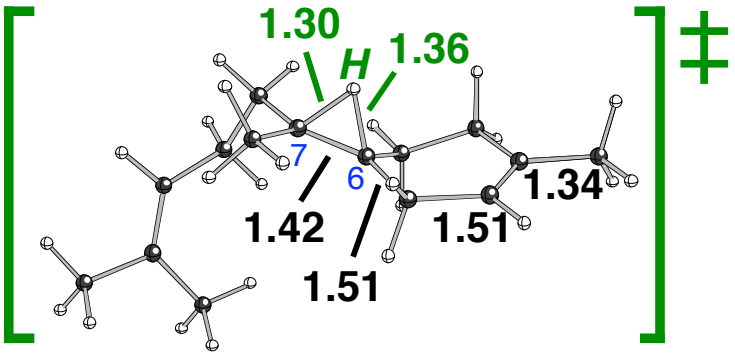
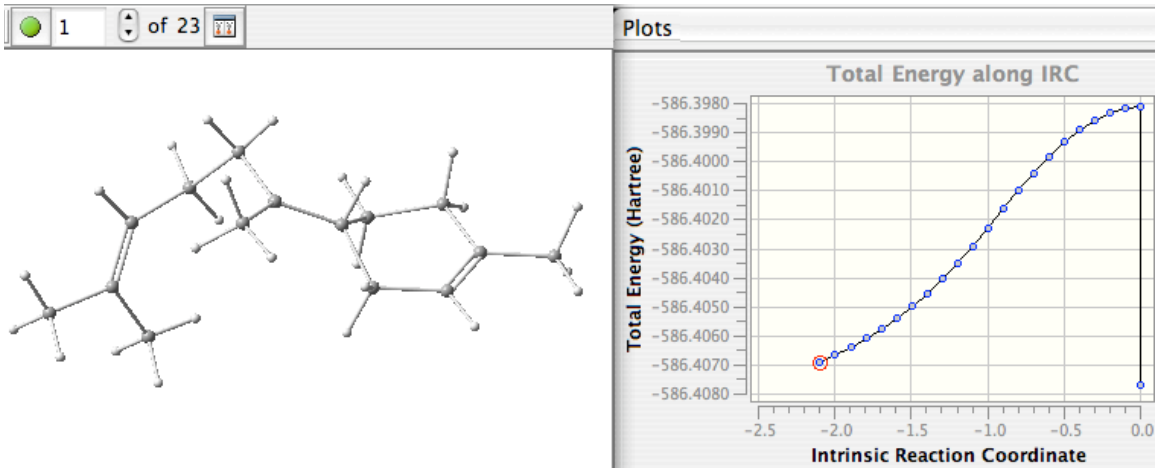
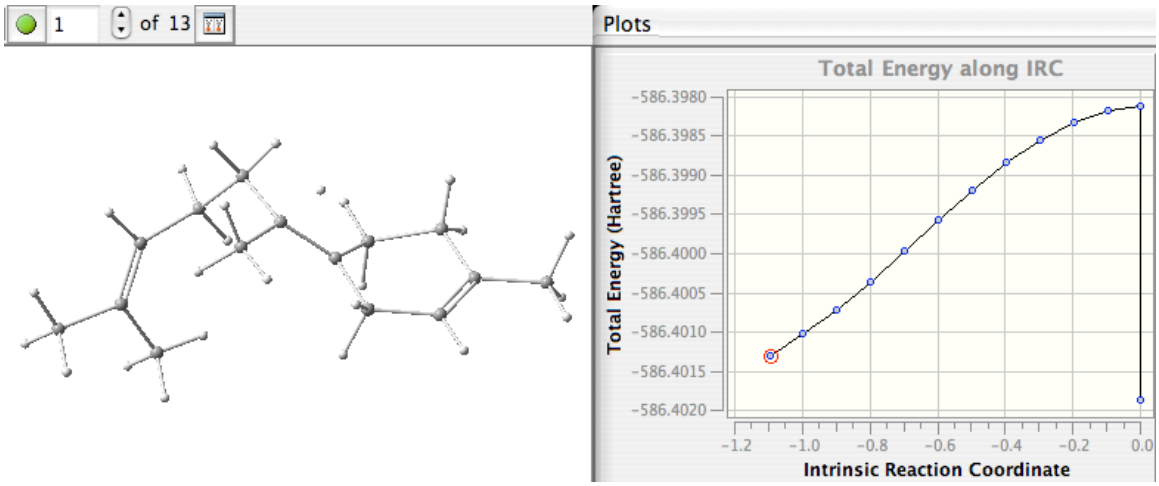


Figure 3.

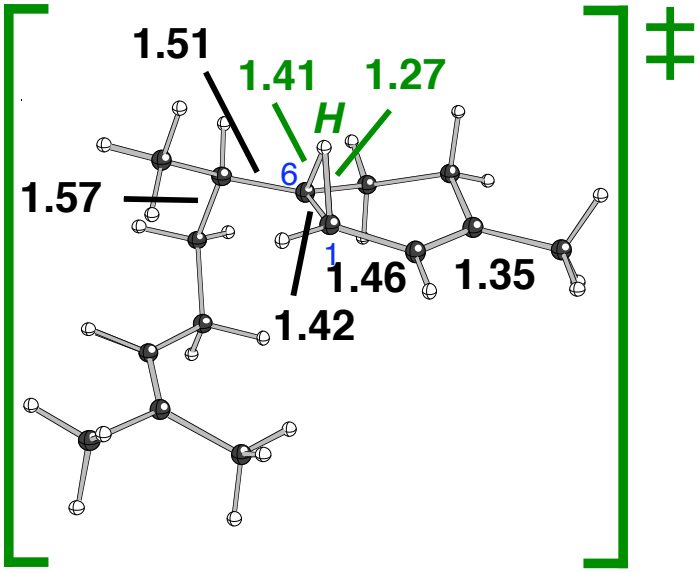
TS (A2-to-D1)

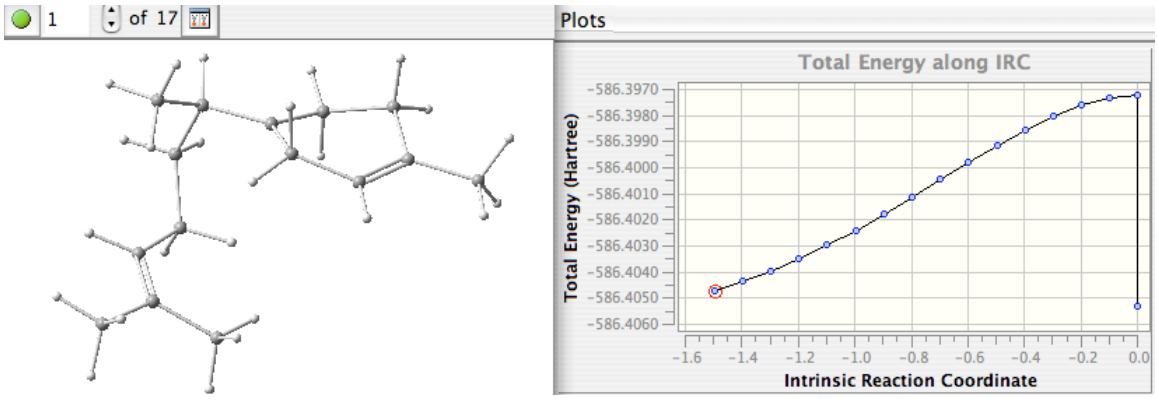

1.30
H
1.36
7
6
1.34
1.42
1.51
1.51
‡

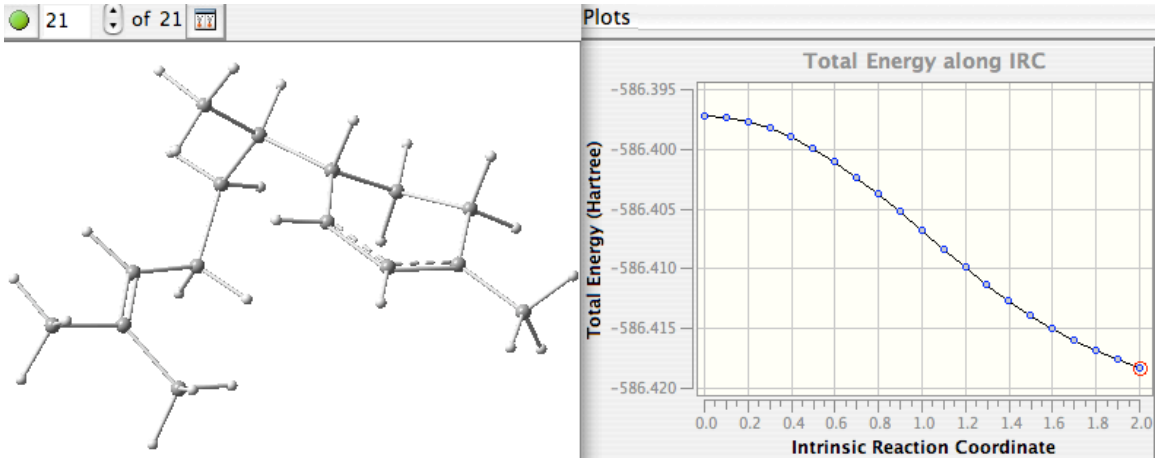

1
of 23
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3980
-586.3990
-586.4000
-586.4010
-586.4020
-586.4030
-586.4040
-586.4050
-586.4060
-586.4070
-586.4080
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate


1
of 13
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3980
-586.3985
-586.3990
-586.3995
-586.4000
-586.4005
-586.4010
-586.4015
-586.4020
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate

TS (D1-to-B4)


1.51
1.41
1.27
H
6
1.57
1
1.46
1.35
1.42
‡


1
of 17
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3970
-586.3980
-586.3990
-586.4000
-586.4010
-586.4020
-586.4030
-586.4040
-586.4050
-586.4060
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate


21
of 21
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.395
-586.400
-586.405
-586.410
-586.415
-586.420
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
2.0
Intrinsic Reaction Coordinate

TS (B4-to-C2)

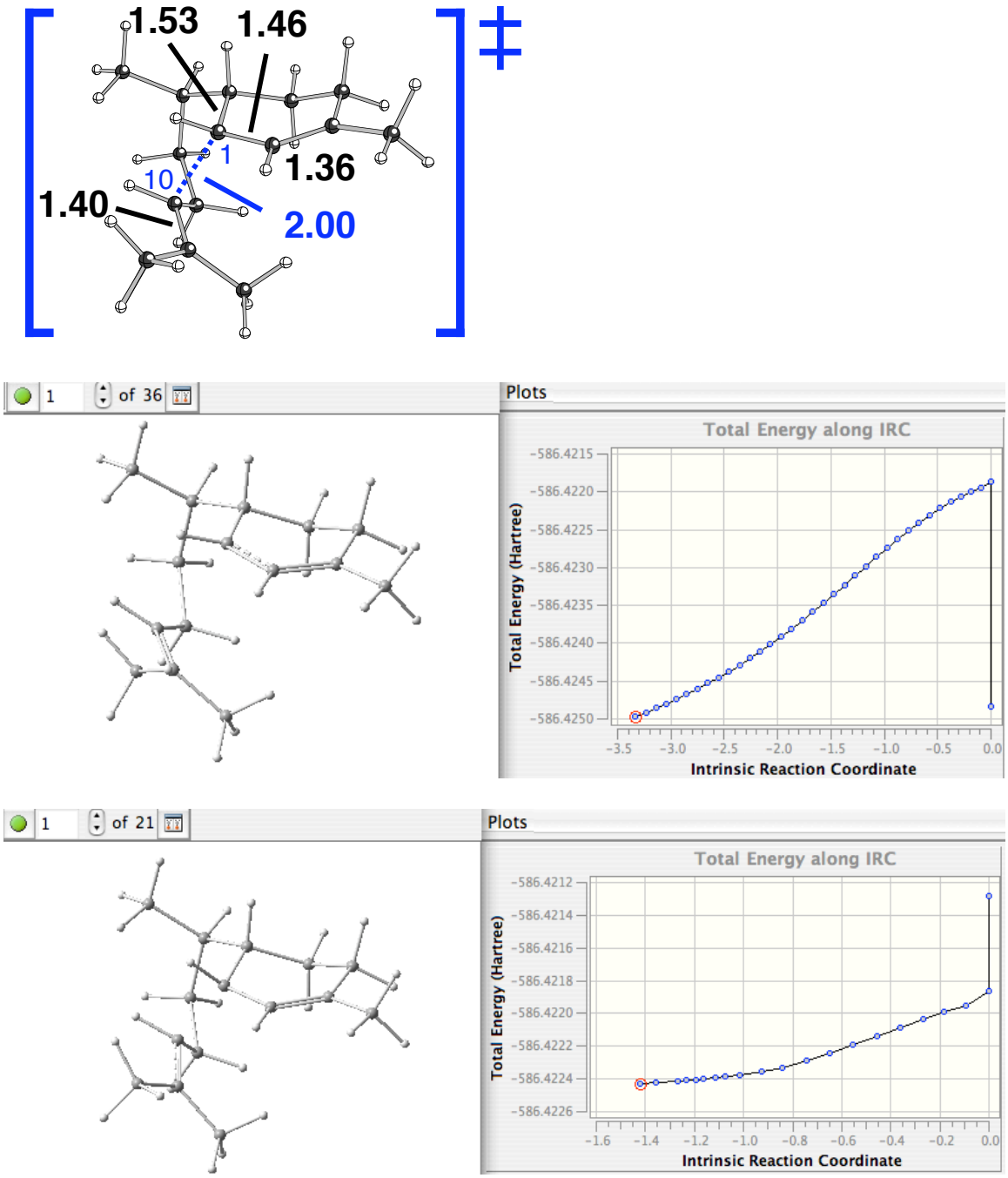
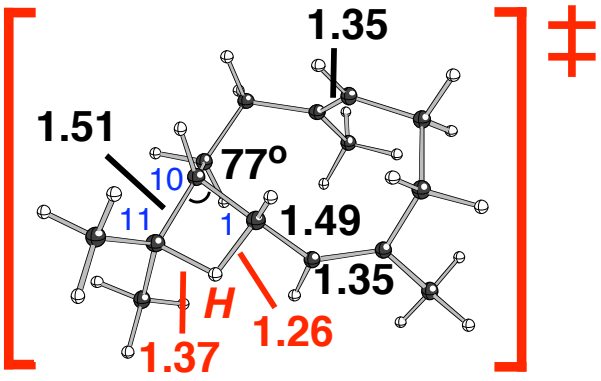
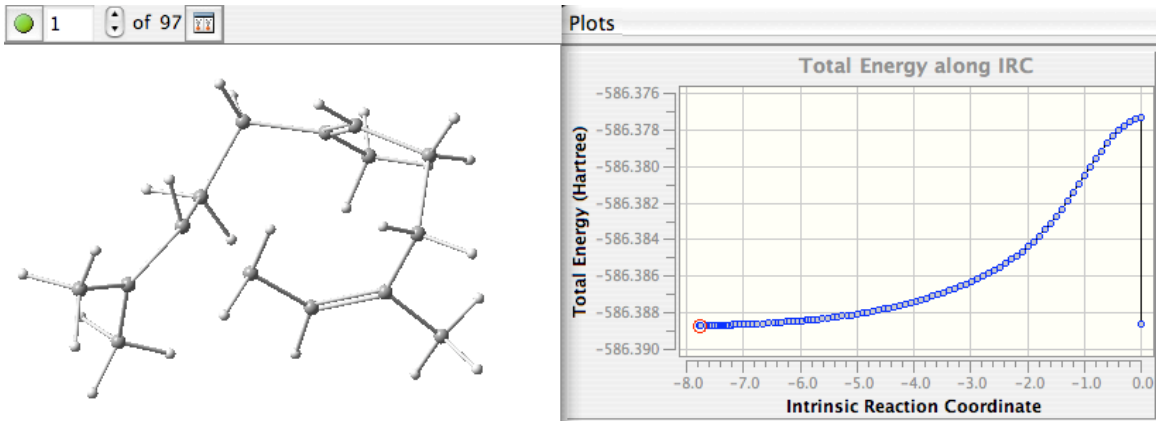
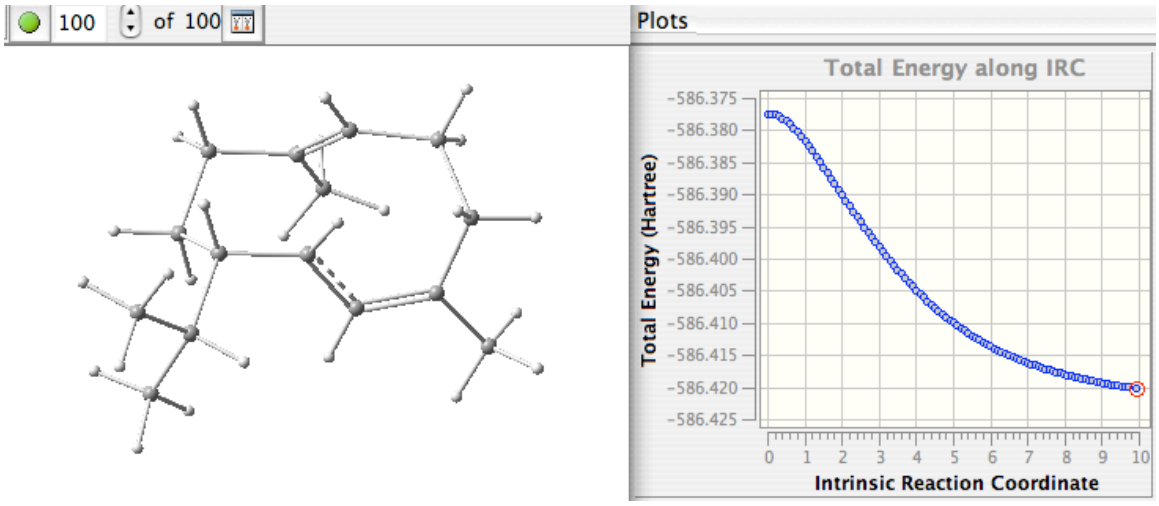


Figure 4.

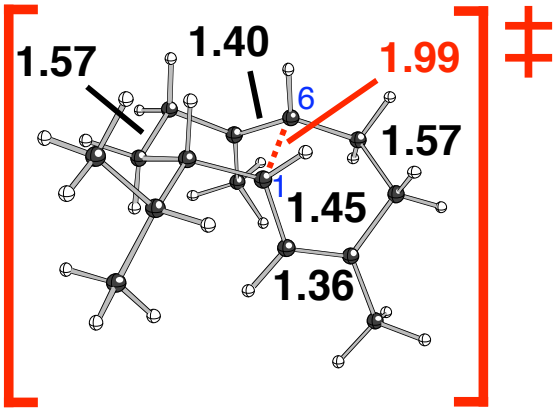
TS (E1-to-F1)

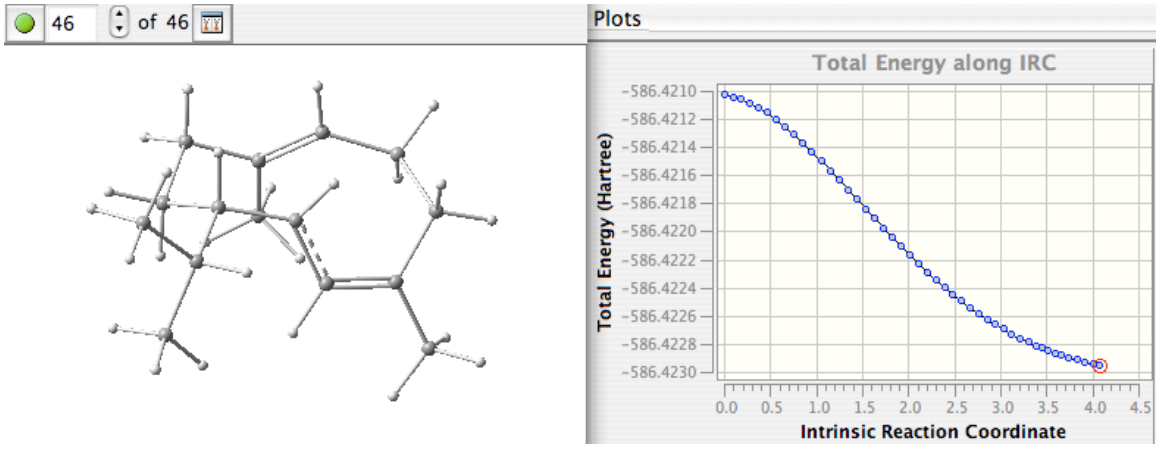

1.35
1.51
77°
10
11
1
1.49
1.35
H
1.26
1.37
‡


1
of 97
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.376
-586.378
-586.380
-586.382
-586.384
-586.386
-586.388
-586.390
-8.0
-7.0
-6.0
-5.0
-4.0
-3.0
-2.0
-1.0
0.0
Intrinsic Reaction Coordinate


100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.375
-586.380
-586.385
-586.390
-586.395
-586.400
-586.405
-586.410
-586.415
-586.420
-586.425
0
1
2
3
4
5
6
7
8
9
10
Intrinsic Reaction Coordinate

TS (F1-to-G1)





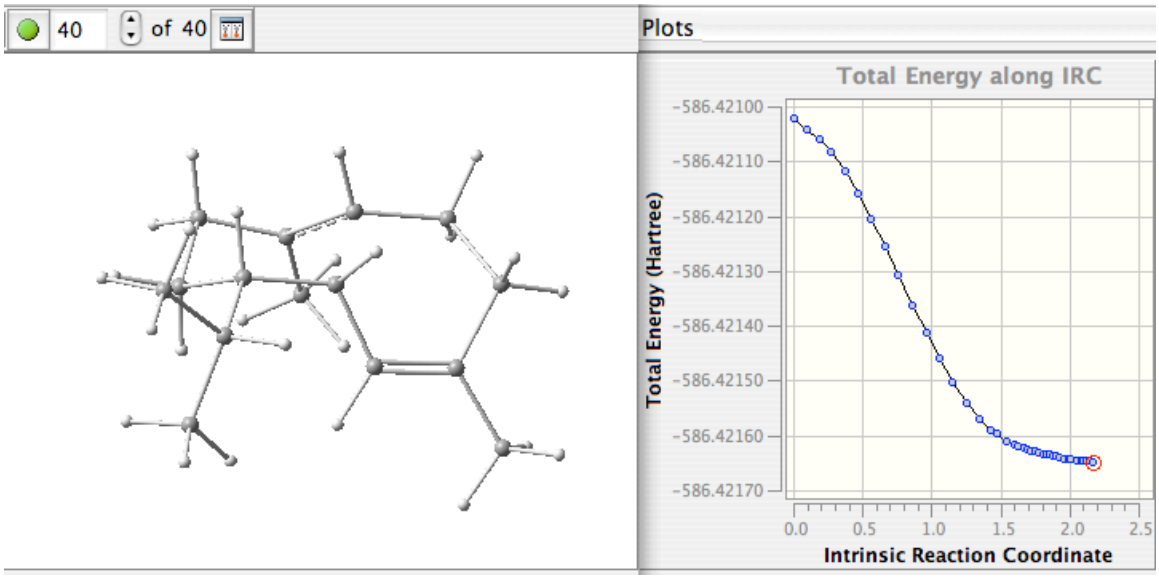


Figure 5.

TS (C3-to-H1)

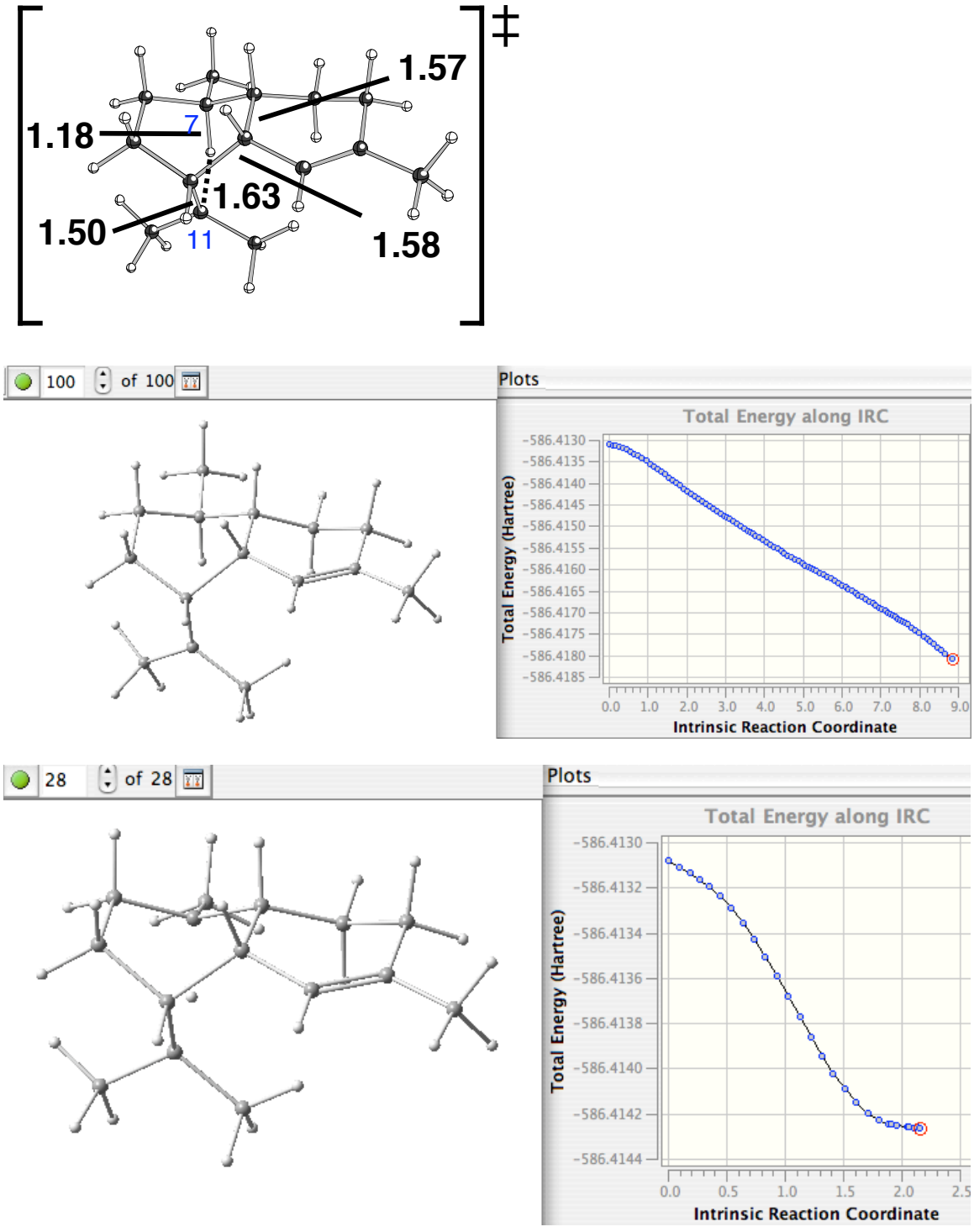


Figure 6.

TS (G2-to H2)

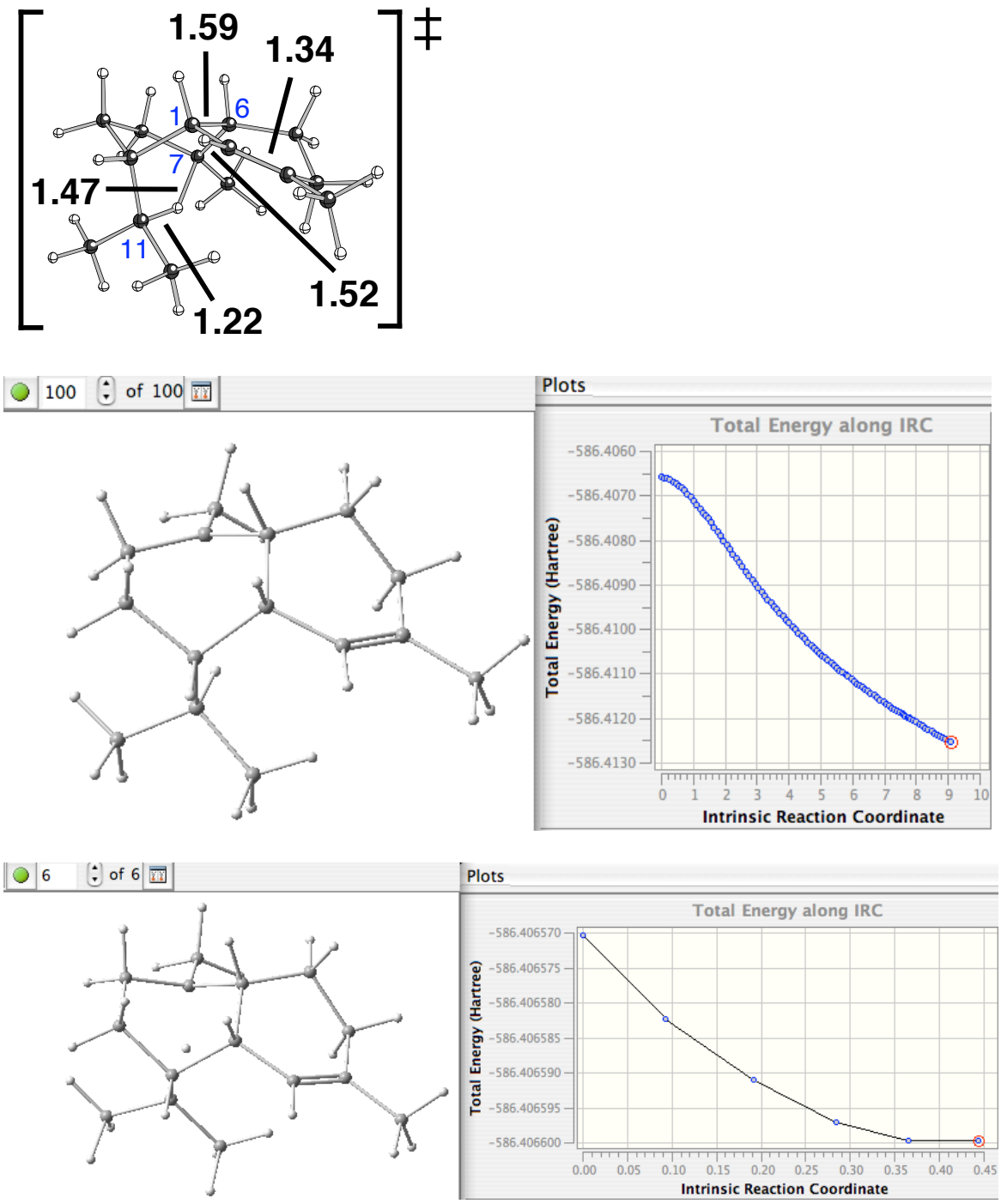
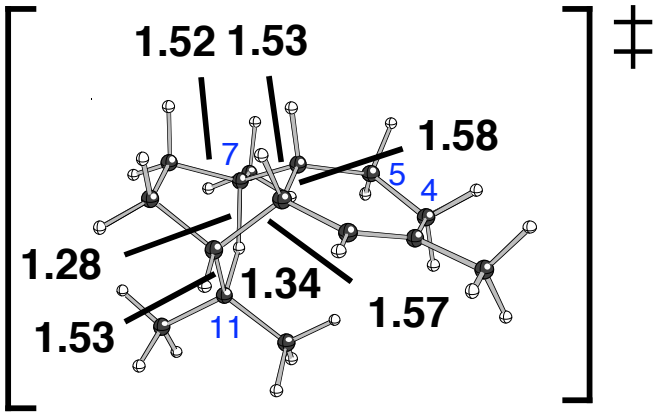
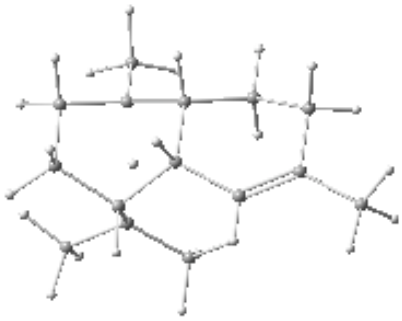
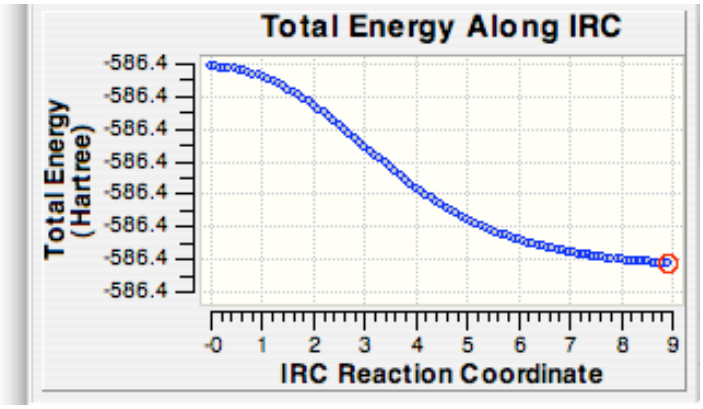


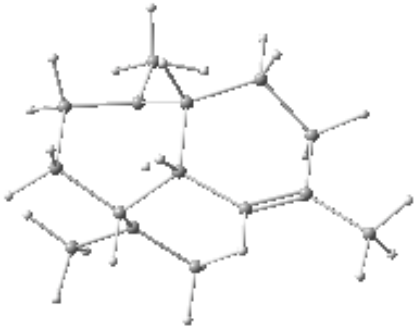
Figure 7.

TS (H1-to H2)









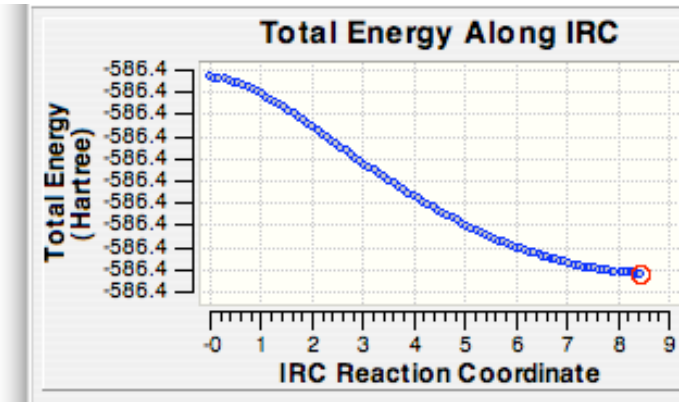
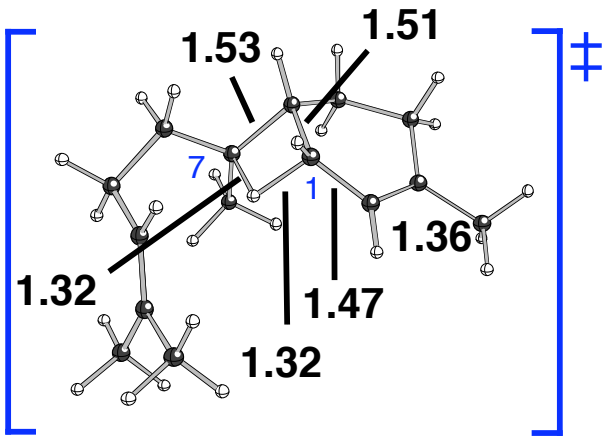
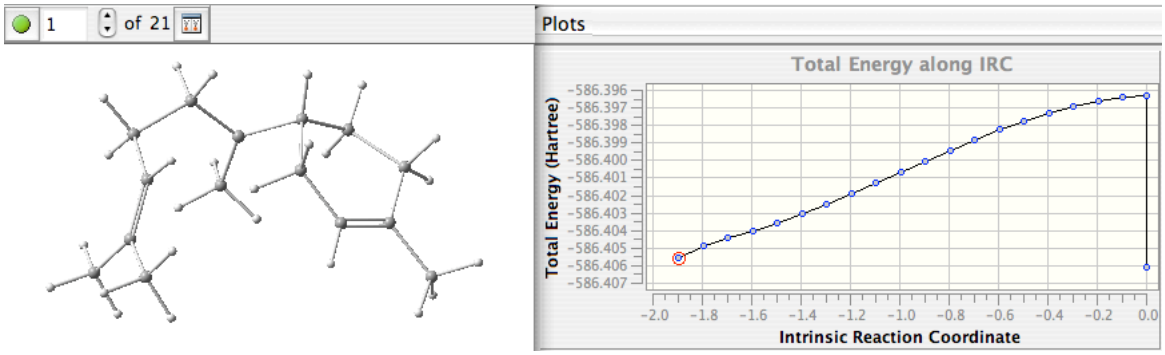
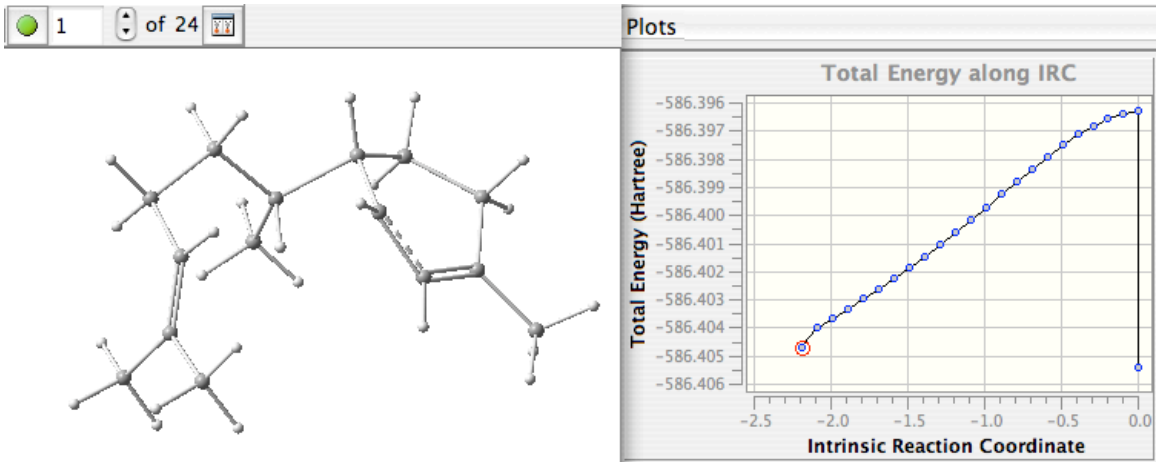


Figure S1.

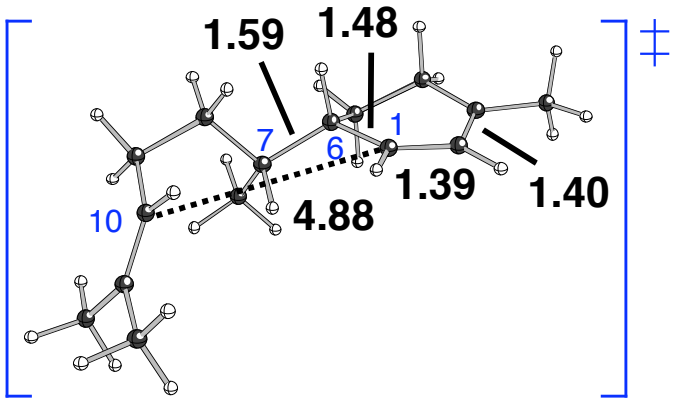
TS (A3-to-B5)

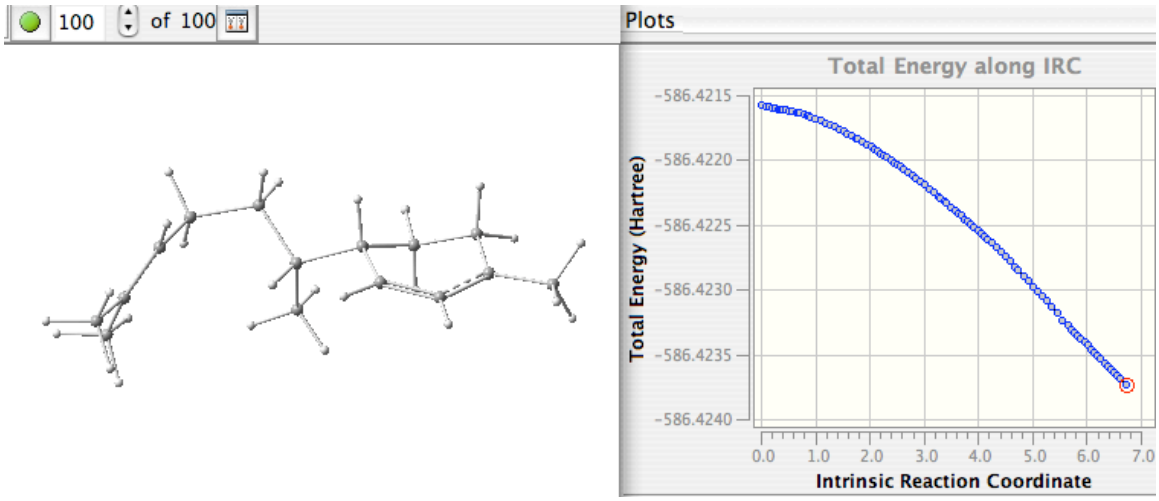

1.53
1.51
7
1
1.36
1.32
1.47
1.32
‡

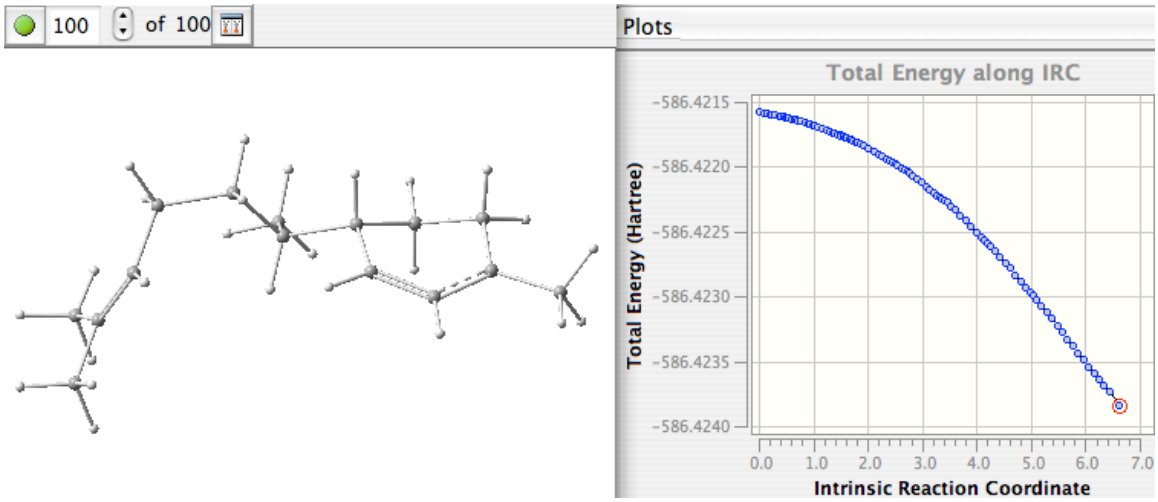

1
of 21
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.396
-586.397
-586.398
-586.399
-586.400
-586.401
-586.402
-586.403
-586.404
-586.405
-586.406
-586.407
-2.0
-1.8
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate


1
of 24
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.396
-586.397
-586.398
-586.399
-586.400
-586.401
-586.402
-586.403
-586.404
-586.405
-586.406
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate

TS (B5-to-B6)


1.59
1.48
7
6
1
1.39
1.40
10
4.88


100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4215
-586.4220
-586.4225
-586.4230
-586.4235
-586.4240
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Intrinsic Reaction Coordinate


100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4215
-586.4220
-586.4225
-586.4230
-586.4235
-586.4240
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Intrinsic Reaction Coordinate

TS (B6-to-B7)

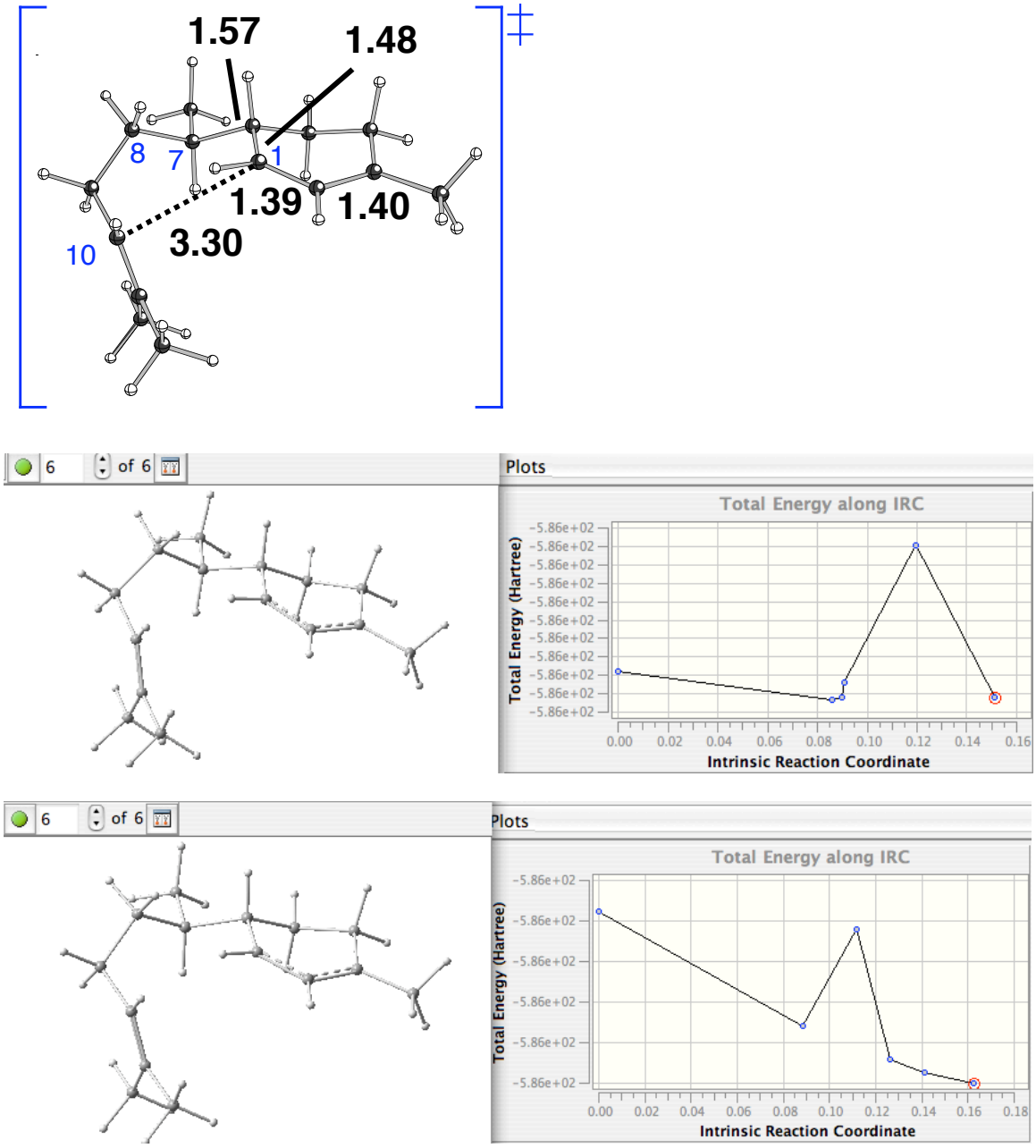
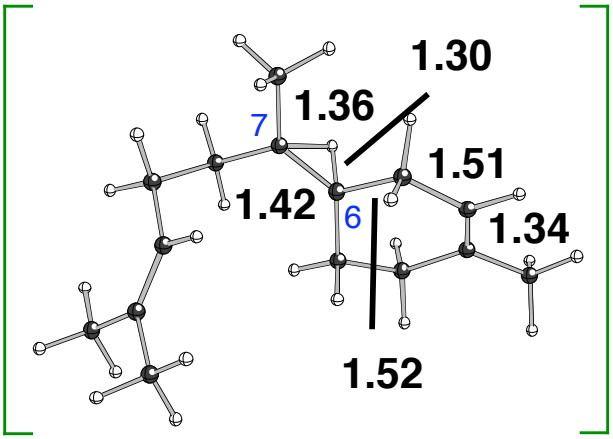
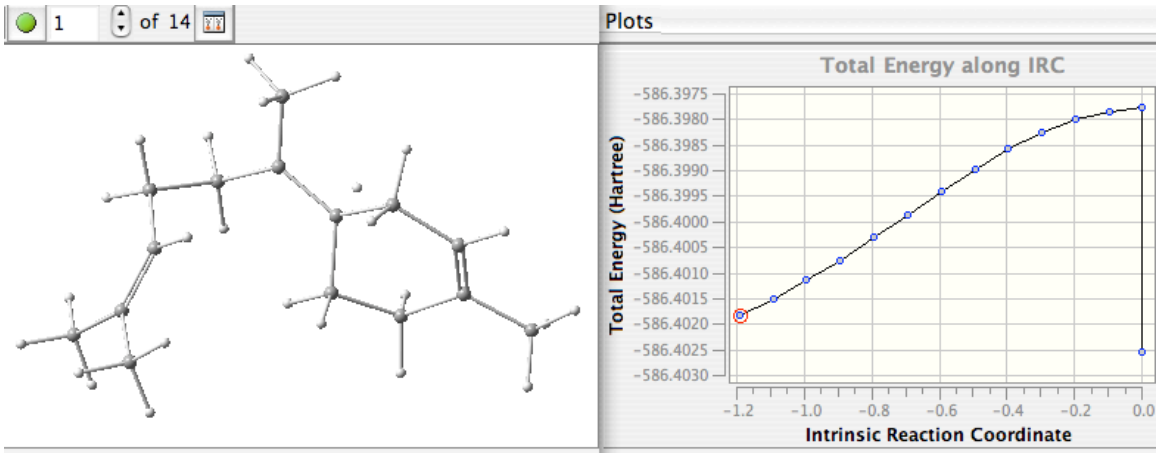
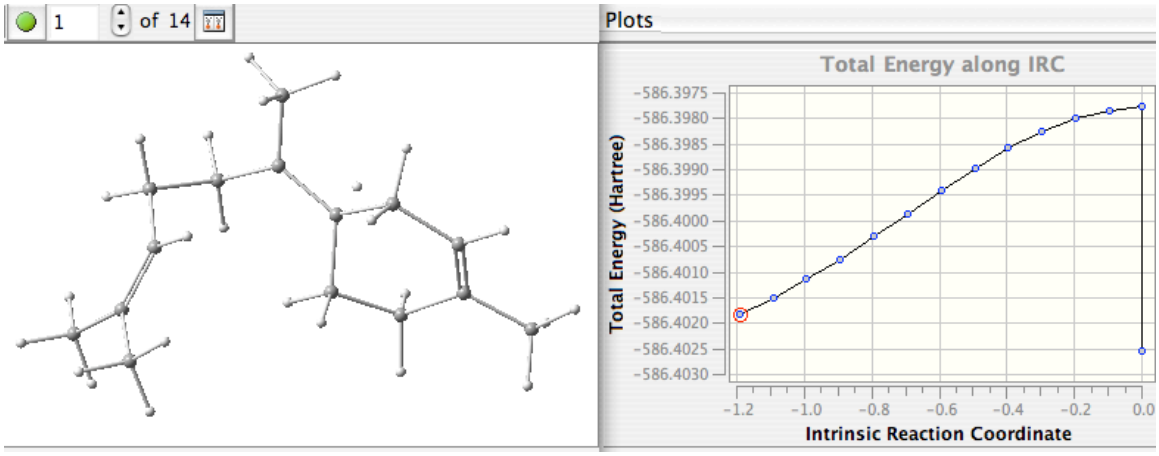


Figure S2.

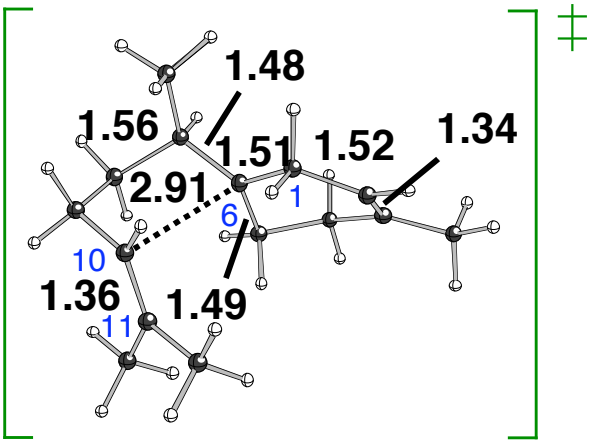
TS (A4-to-D2)

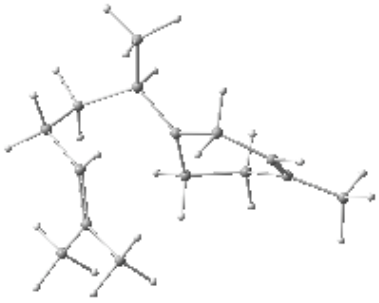

1.30
1.36
7
1.51
1.42
6
1.34
1.52

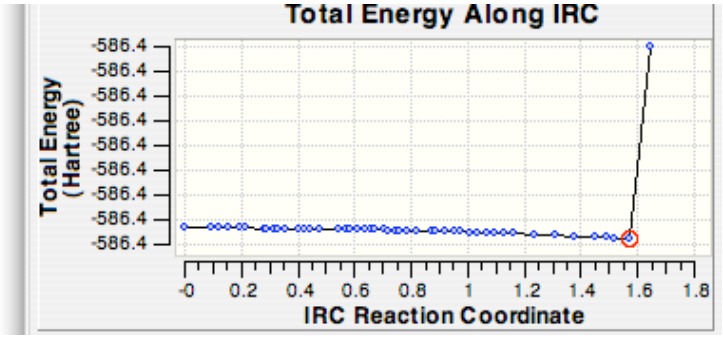

1
of 14
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3975
-586.3980
-586.3985
-586.3990
-586.3995
-586.4000
-586.4005
-586.4010
-586.4015
-586.4020
-586.4025
-586.4030
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate

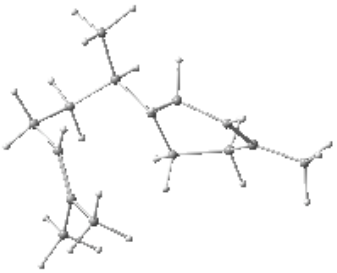

1
of 14
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3975
-586.3980
-586.3985
-586.3990
-586.3995
-586.4000
-586.4005
-586.4010
-586.4015
-586.4020
-586.4025
-586.4030
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate

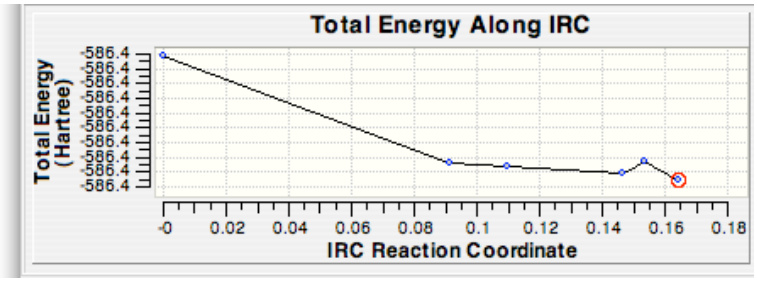
TS (D2-to-D3)


1.48
1.56
1.51
1.52
1.34
2.91
1
6
10
1.36
1.49
11

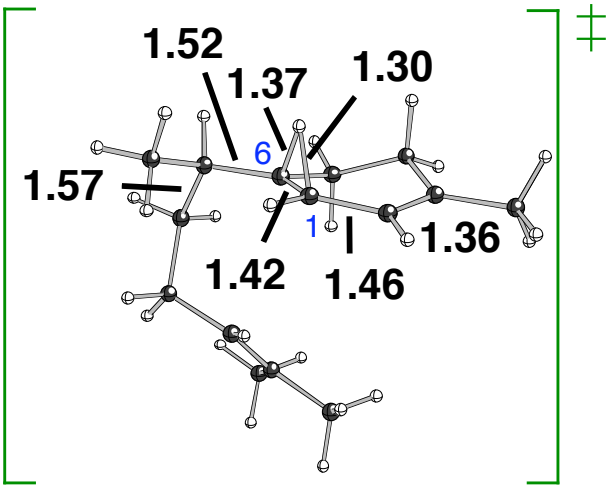


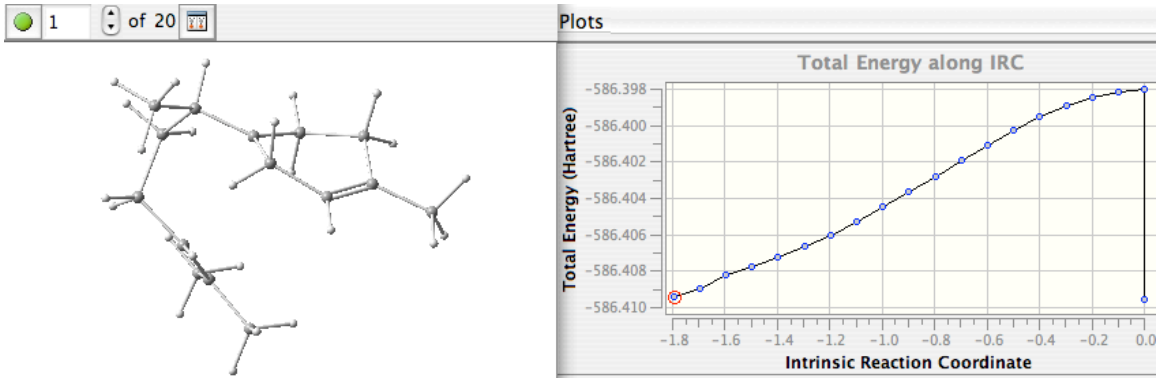

Total Energy Along IRC
Total Energy (Hartree)
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-0
0.2
0.4
0.6
0.8
1
1.2
1.4
1.6
1.8
IRC Reaction Coordinate

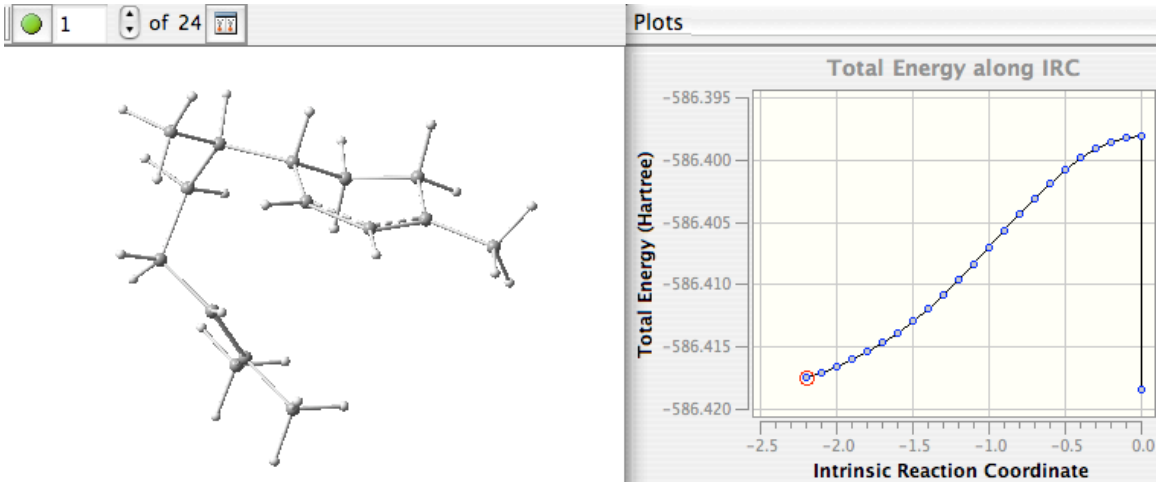



Total Energy Along IRC
Total Energy (Hartree)
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
IRC Reaction Coordinate

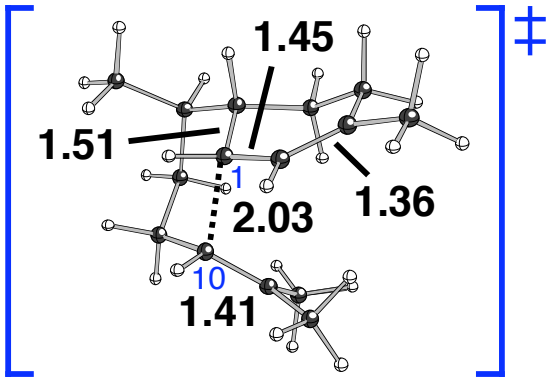
TS (D3-to-B8)

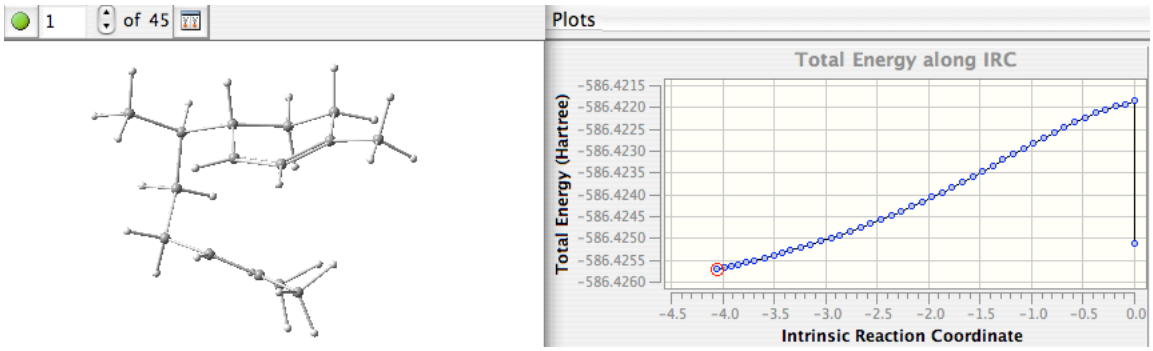

1.52
1.37
1.30
6
1.57
1
1.36
1.42
1.46

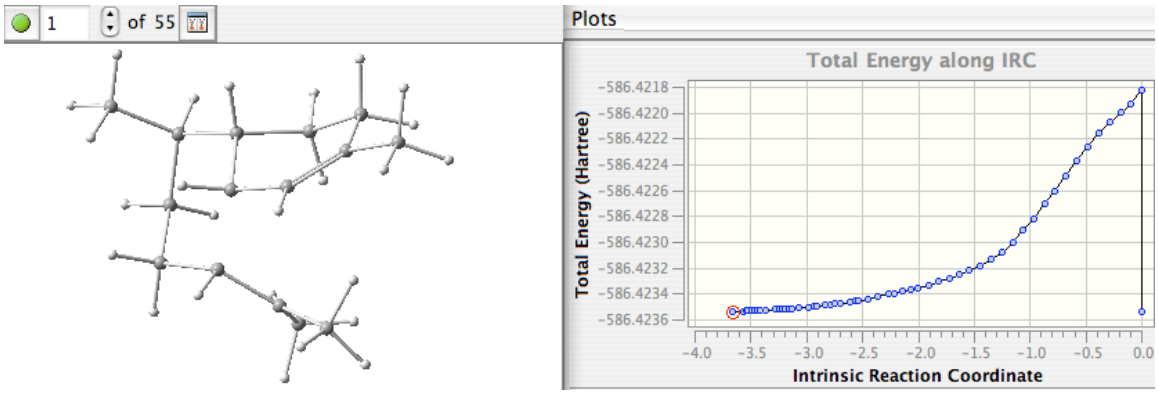

1
of 20
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.398
-586.400
-586.402
-586.404
-586.406
-586.408
-586.410
-1.8
-1.6
-1.4
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate


1
of 24
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.395
-586.400
-586.405
-586.410
-586.415
-586.420
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate

TS (B8-to-C4)


1.45
1.51
1
1.36
2.03
10
1.41
‡


1
of 45
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4215
-586.4220
-586.4225
-586.4230
-586.4235
-586.4240
-586.4245
-586.4250
-586.4255
-586.4260
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate


1
of 55
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4218
-586.4220
-586.4222
-586.4224
-586.4226
-586.4228
-586.4230
-586.4232
-586.4234
-586.4236
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate

TS (D2-to-I)

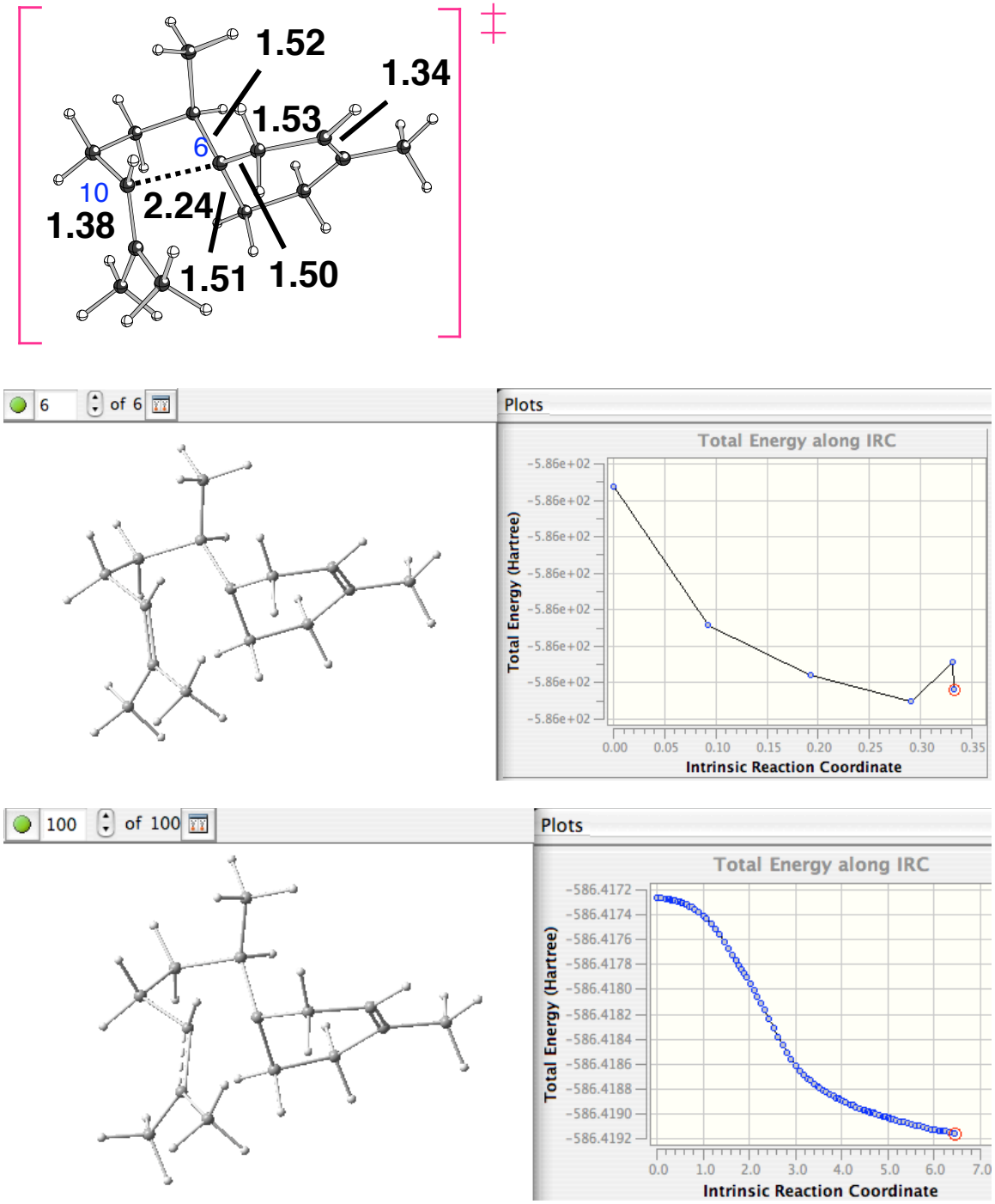
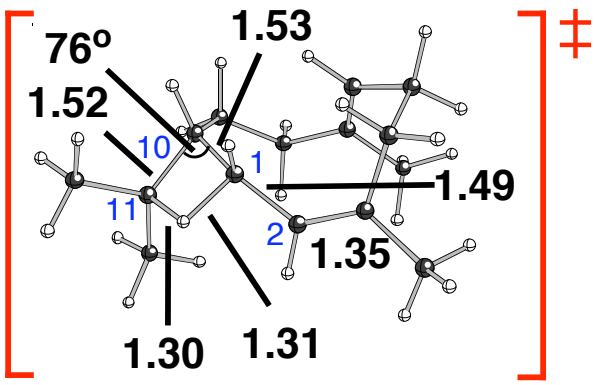
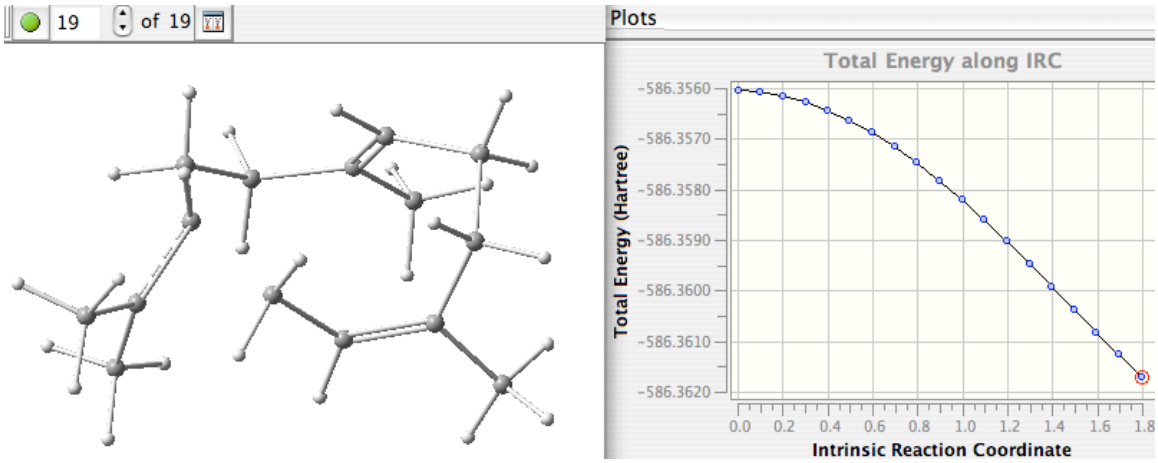
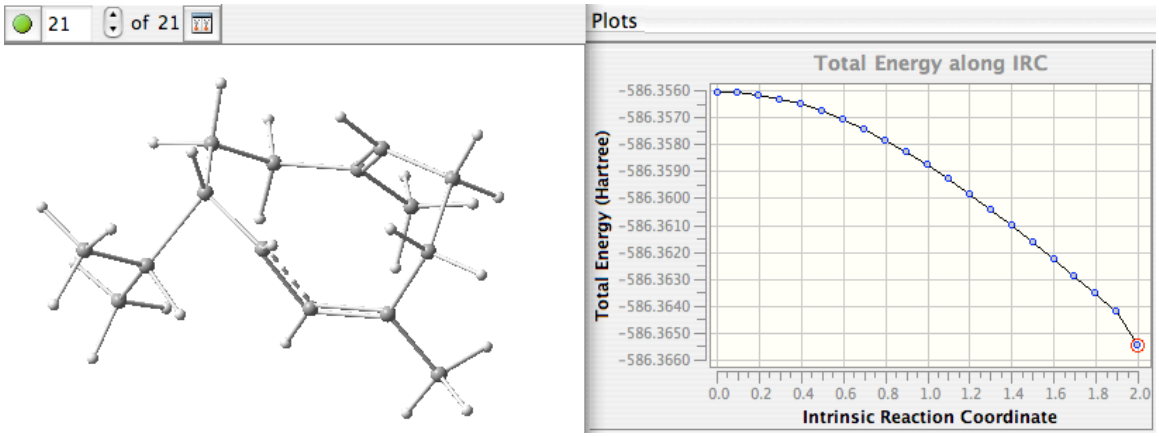


Figure S3.

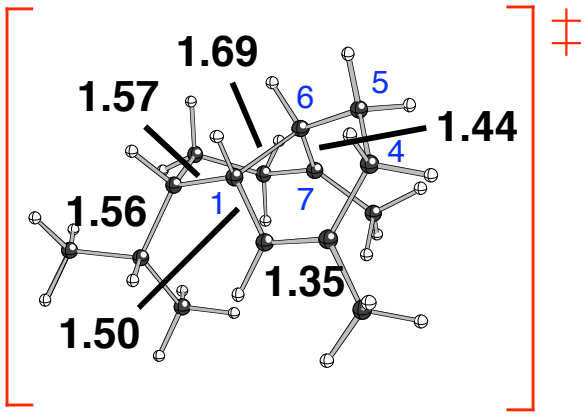
TS (E2-to-F2)

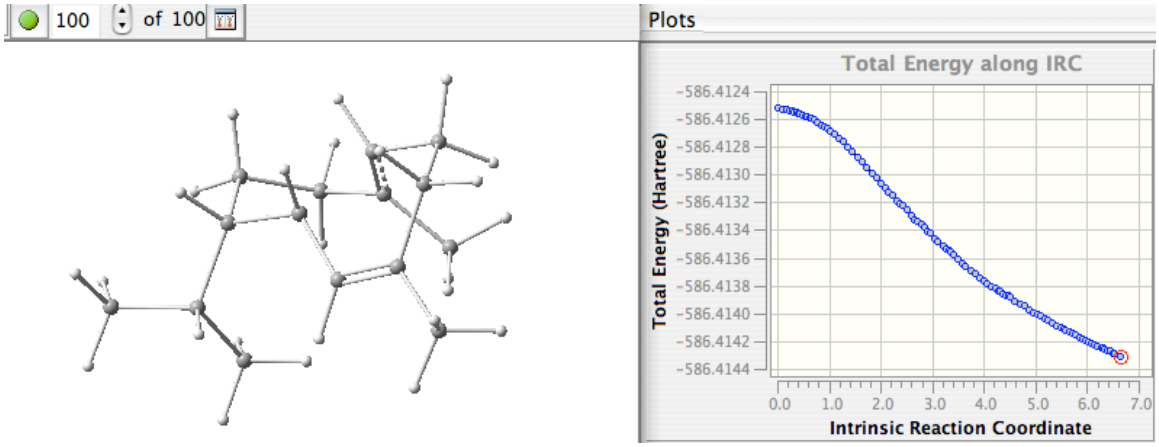

76°
1.53
1.52
10
1
1.49
11
2
1.35
1.30
1.31
‡

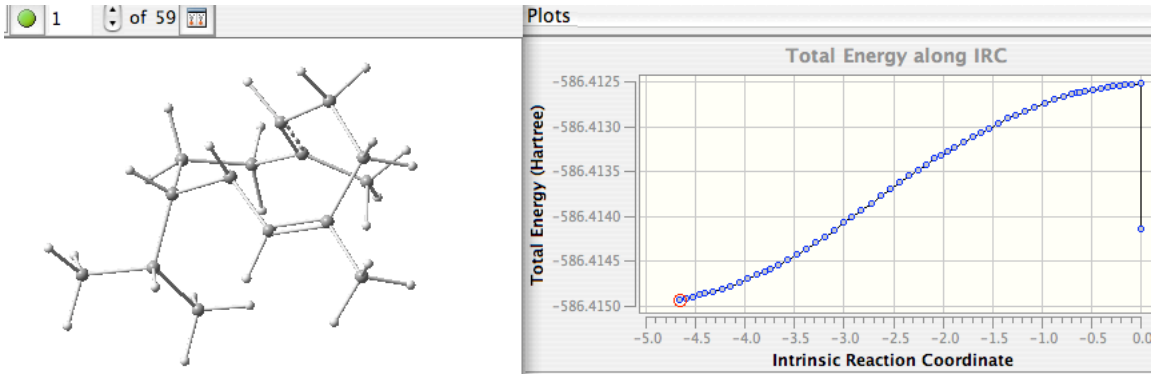

19
of 19
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3560
-586.3570
-586.3580
-586.3590
-586.3600
-586.3610
-586.3620
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8
Intrinsic Reaction Coordinate


21
of 21
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.3560
-586.3570
-586.3580
-586.3590
-586.3600
-586.3610
-586.3620
-586.3630
-586.3640
-586.3650
-586.3660
0.0 0.2 0.4 0.6 0.8 1.0 1.2 1.4 1.6 1.8 2.0
Intrinsic Reaction Coordinate

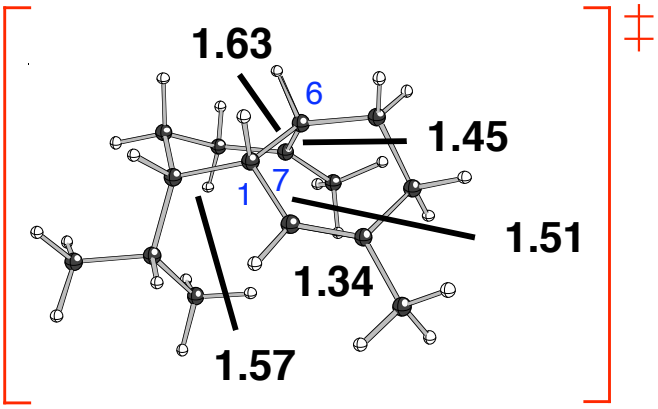
TS (F2-to-G3)

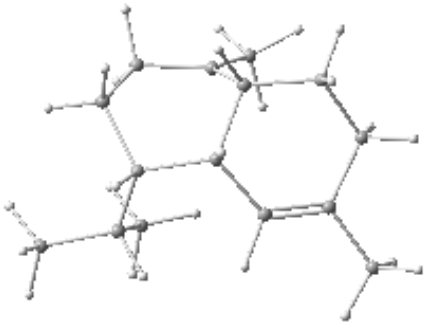

1.69
1.57
1.44
1.56
1.35
1.50
1
4
5
6
7

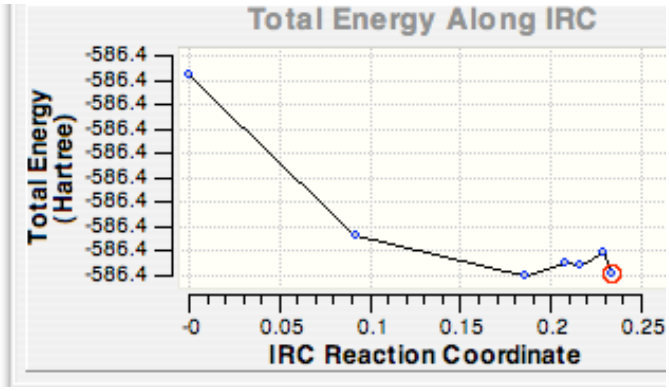

100
of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4124
-586.4126
-586.4128
-586.4130
-586.4132
-586.4134
-586.4136
-586.4138
-586.4140
-586.4142
-586.4144
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Intrinsic Reaction Coordinate

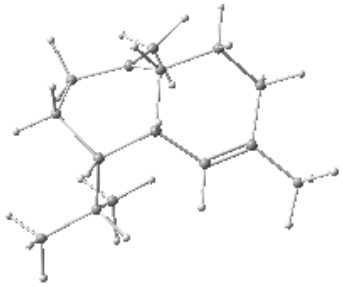

1
of 59
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4125
-586.4130
-586.4135
-586.4140
-586.4145
-586.4150
-5.0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
Intrinsic Reaction Coordinate

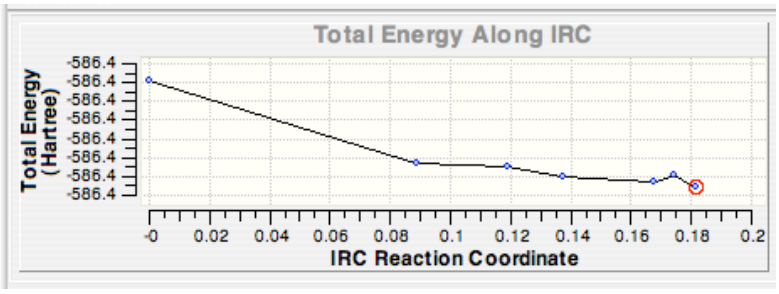
TS (G3-to-G4)


1.63
6
1.45
7
1
1.51
1.34
1.57

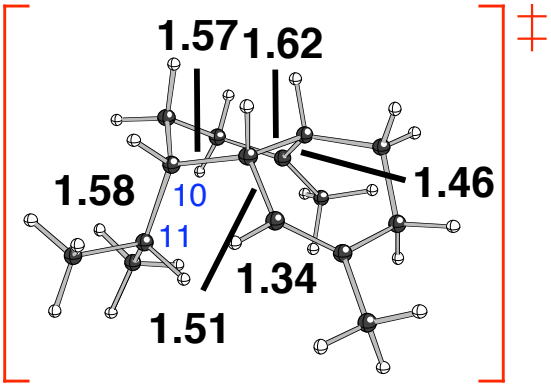



Total Energy Along IRC
Total Energy (Hartree)
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-0
0.05
0.1
0.15
0.2
0.25
IRC Reaction Coordinate




Total Energy Along IRC
Total Energy (Hartree)
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-586.4
-0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
IRC Reaction Coordinate

TS (G4-to-G2)


1.57
1.62
1.58
10
1.46
11
1.34
1.51

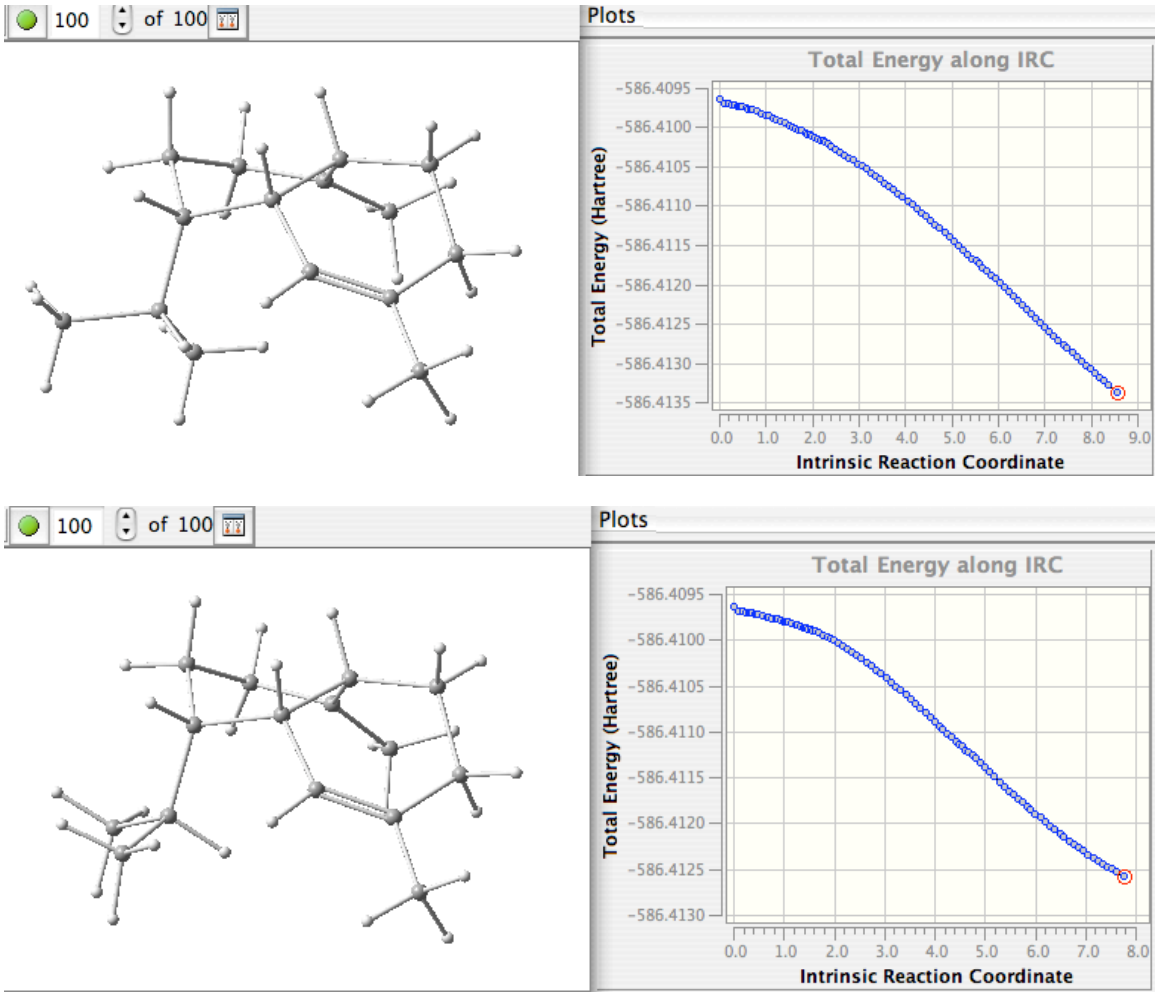
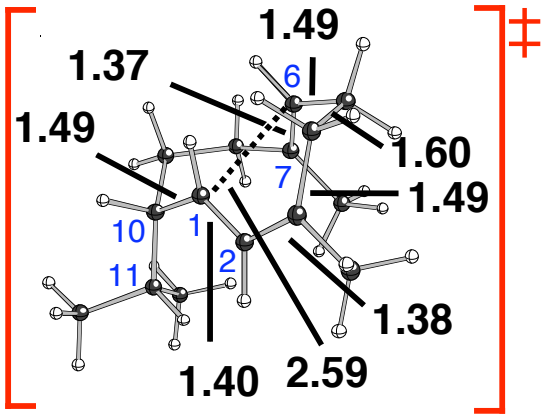
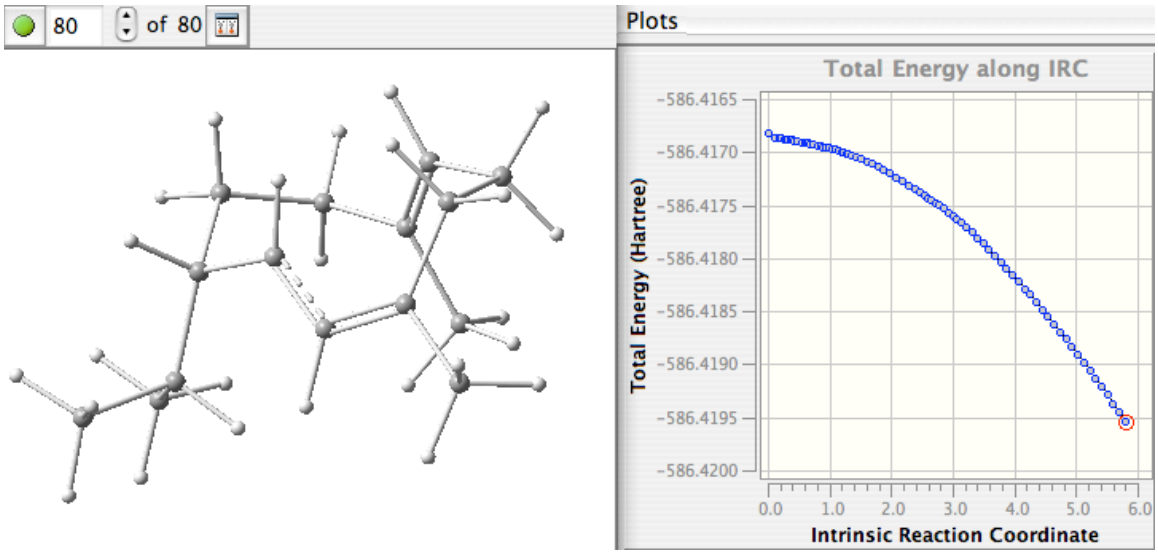
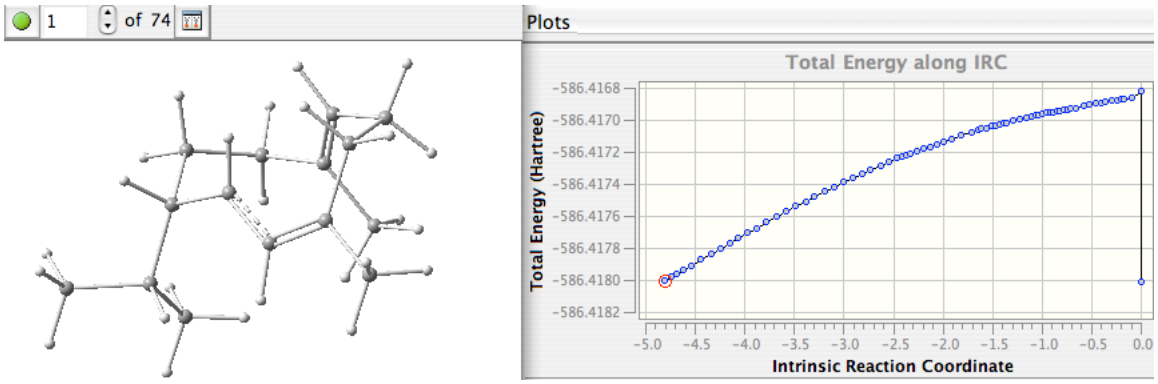


Figure S4.

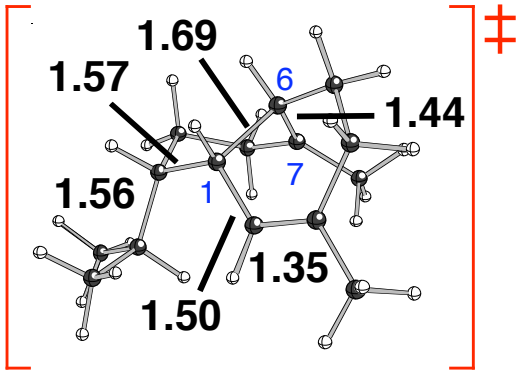
TS (F2-to-F3)

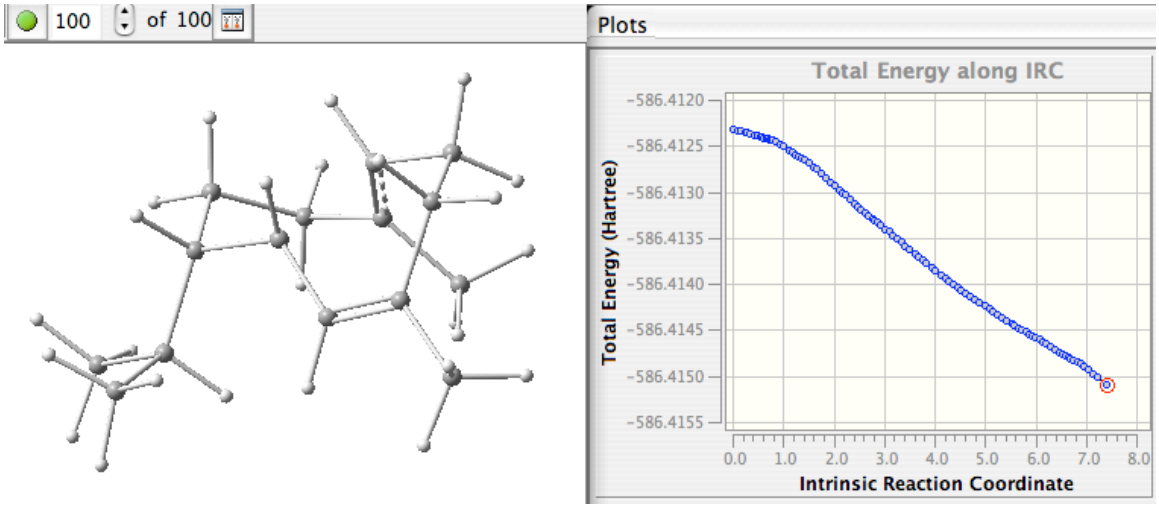


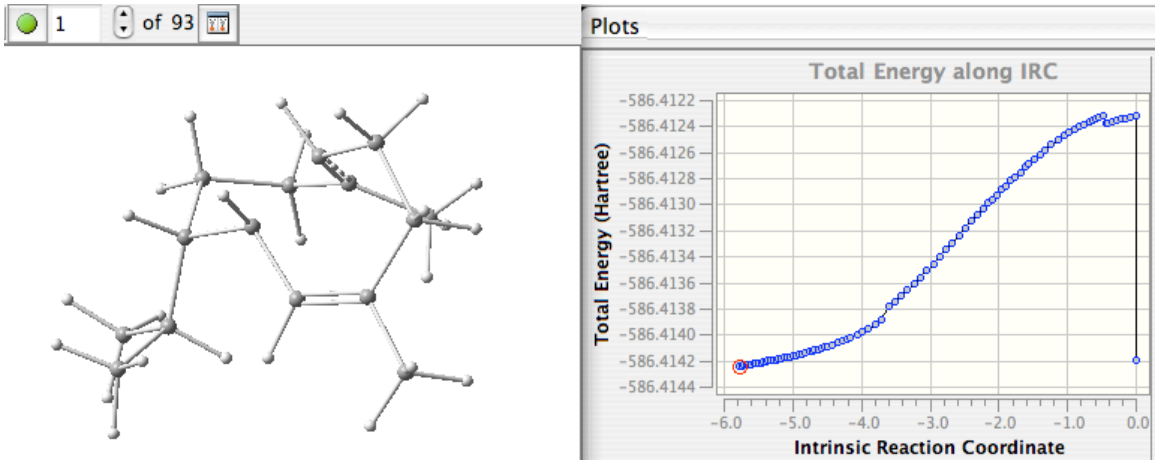

80
of 80
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4165
-586.4170
-586.4175
-586.4180
-586.4185
-586.4190
-586.4195
-586.4200
0.0
1.0
2.0
3.0
4.0
5.0
6.0
Intrinsic Reaction Coordinate


1
of 74
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4168
-586.4170
-586.4172
-586.4174
-586.4176
-586.4178
-586.4180
-586.4182
-5.0
-4.5
-4.0
-3.5
-3.0
-2.5
-2.0
-1.5
-1.0
-0.5
0.0
Intrinsic Reaction Coordinate

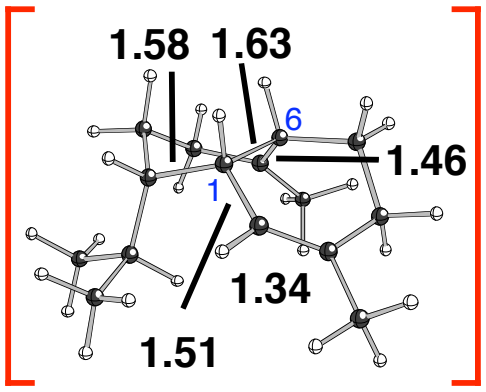
TS (F3-to-G5)

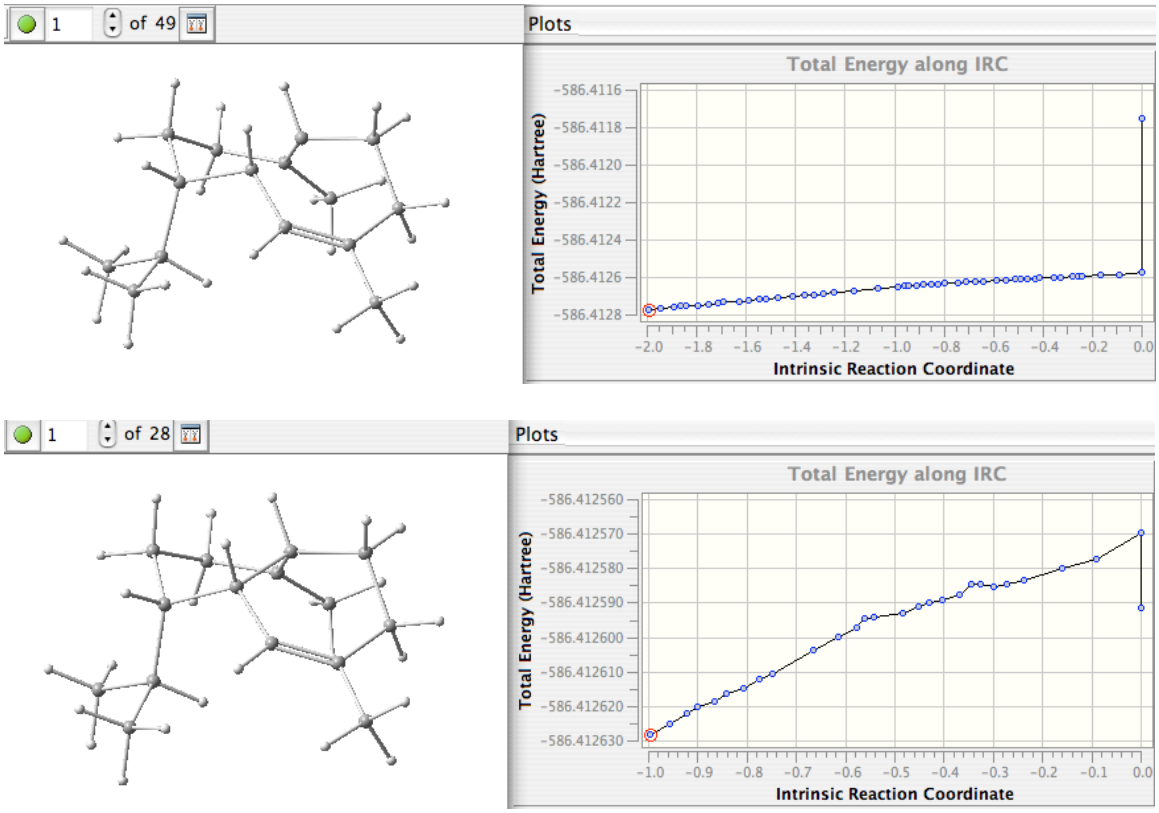

1.69
1.57
6
1.44
7
1.56
1
1.35
1.50
‡


100 of 100
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4120
-586.4125
-586.4130
-586.4135
-586.4140
-586.4145
-586.4150
-586.4155
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0
Intrinsic Reaction Coordinate


1 of 93
Plots
Total Energy along IRC
Total Energy (Hartree)
-586.4122
-586.4124
-586.4126
-586.4128
-586.4130
-586.4132
-586.4134
-586.4136
-586.4138
-586.4140
-586.4142
-586.4144
-6.0 -5.0 -4.0 -3.0 -2.0 -1.0 0.0
Intrinsic Reaction Coordinate

TS (G5-to-G2)


1.58
1.63
6
1.46
1
1.34
1.51



Extended IRC calculation from the above.

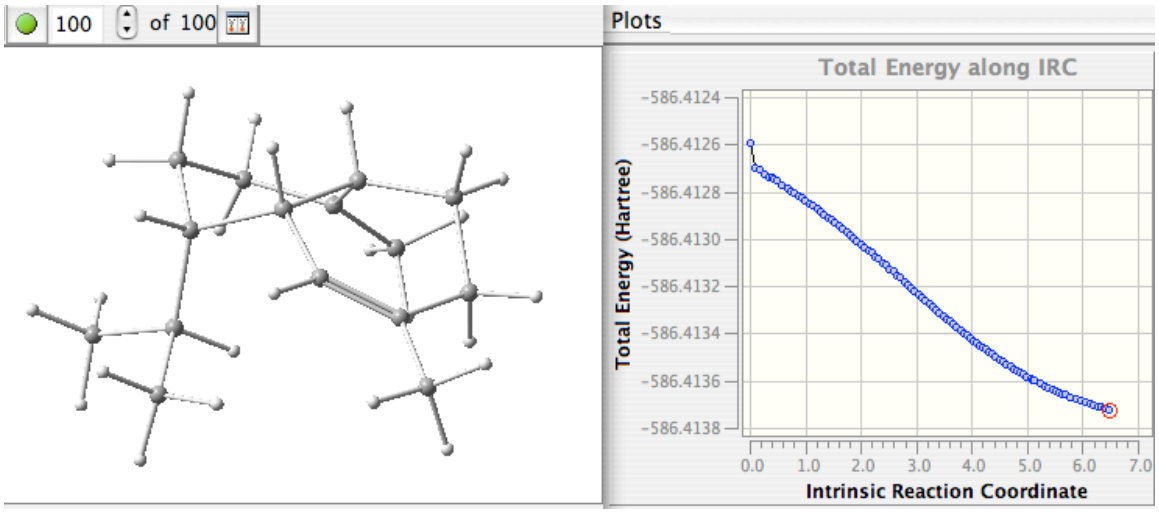
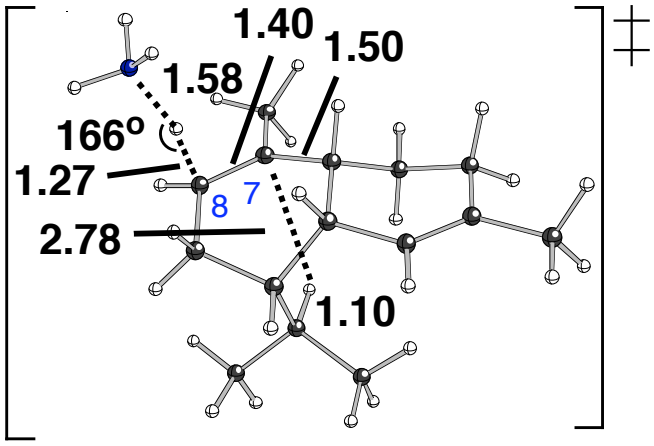
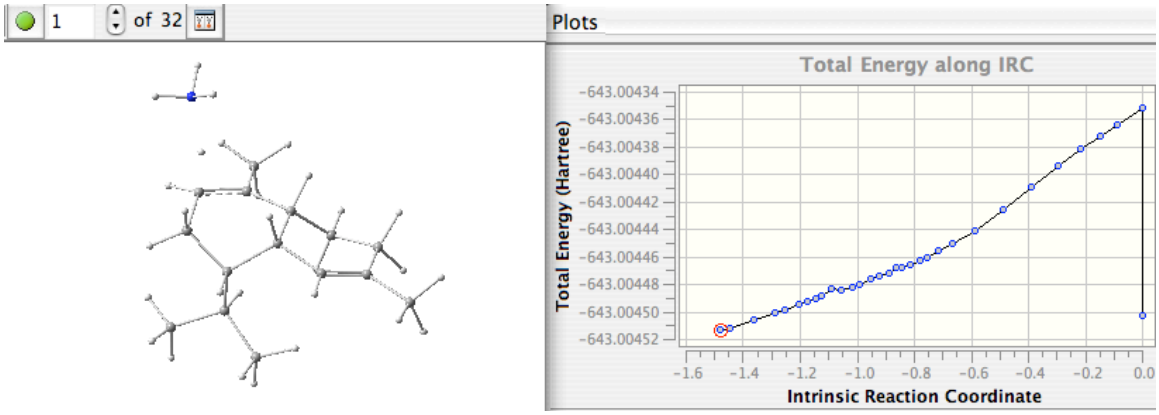


Figure S5 (top).

TS1





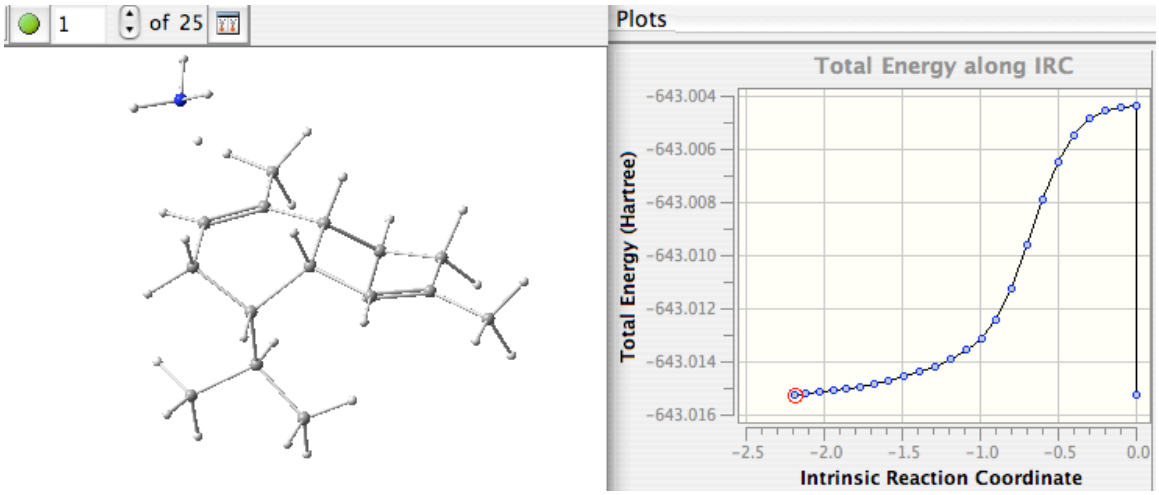


Figure S5 (bottom).

TS2

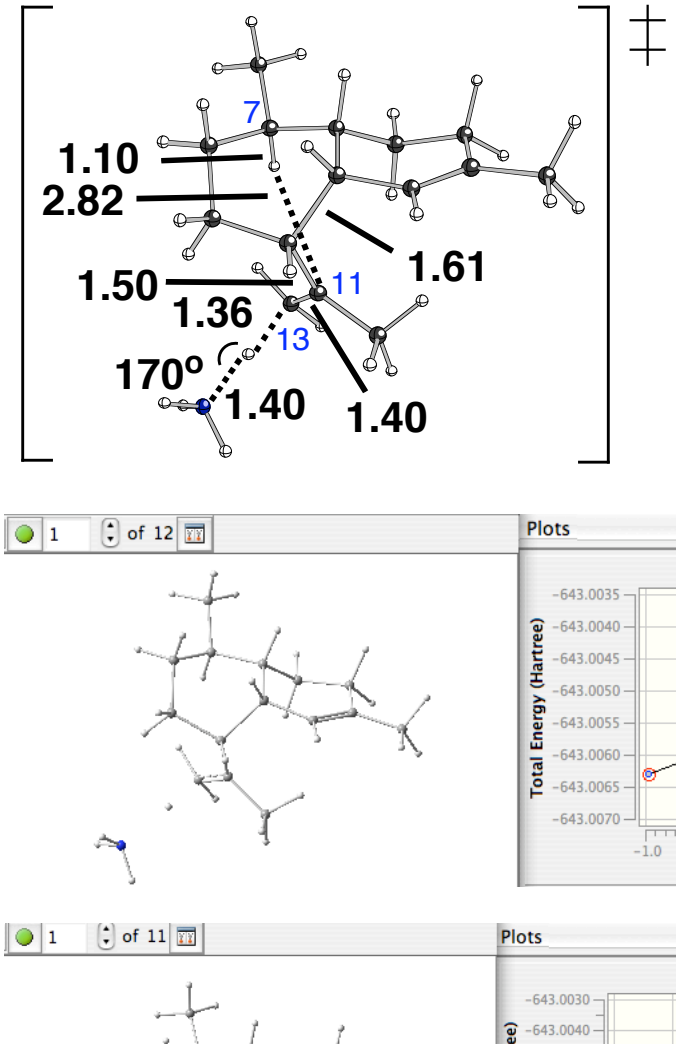
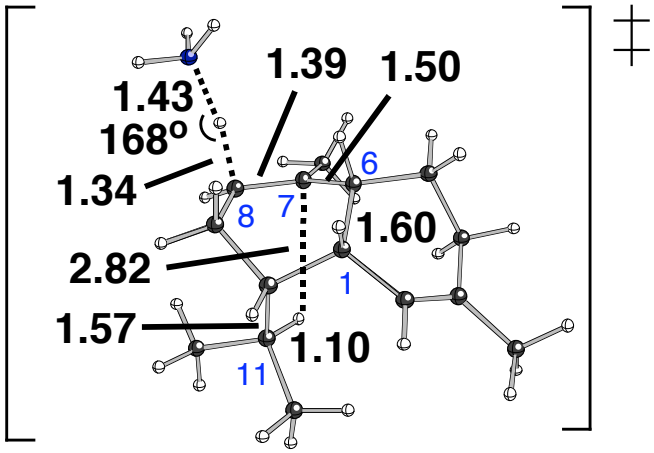
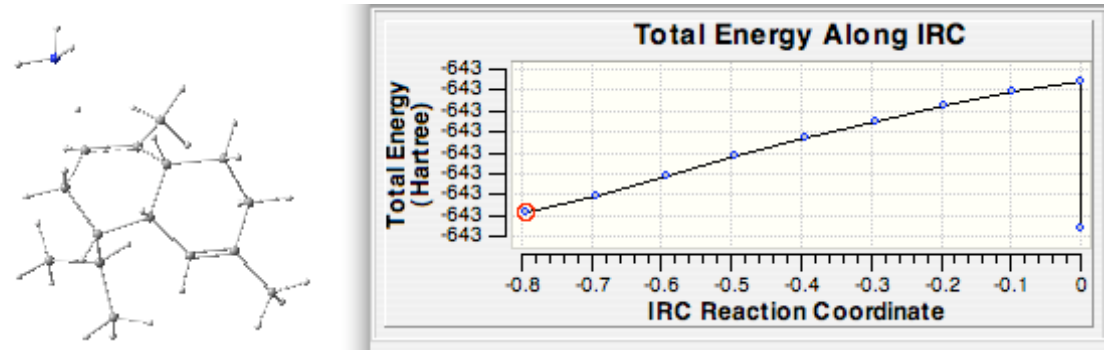


Figure S6 (top).

TS3





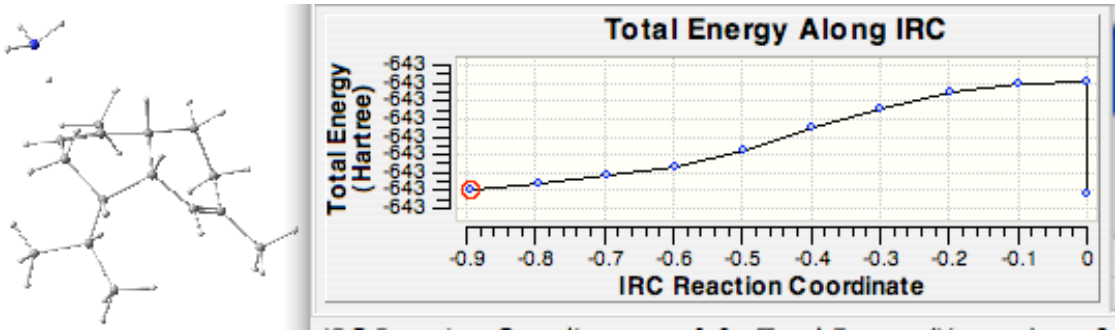


Figure S5 (bottom).

TS4

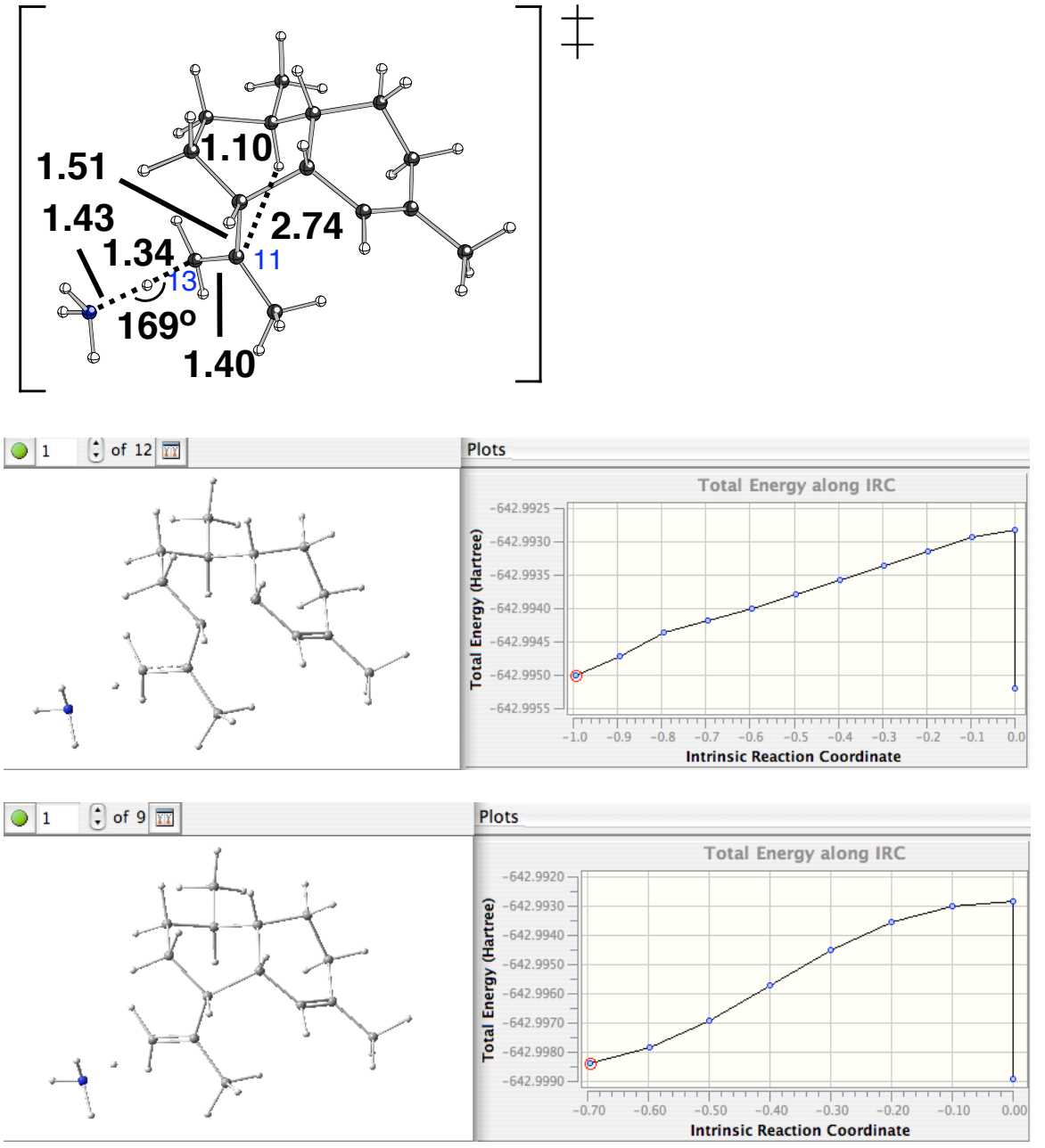
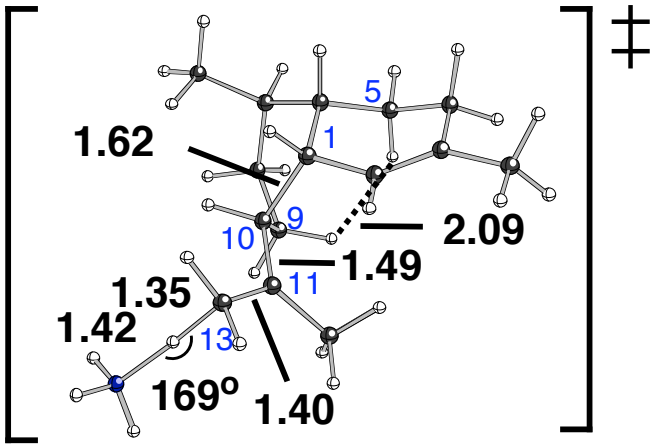
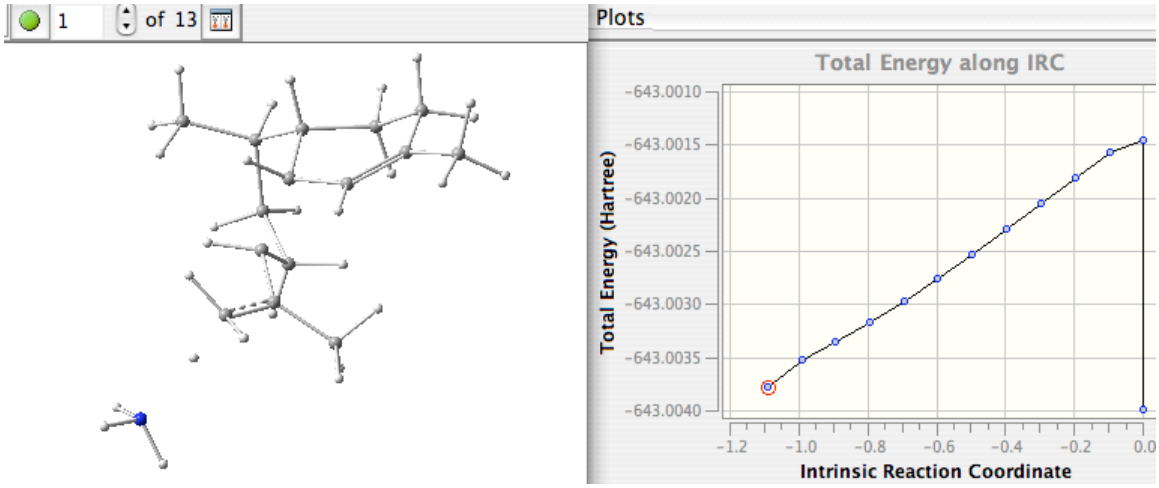
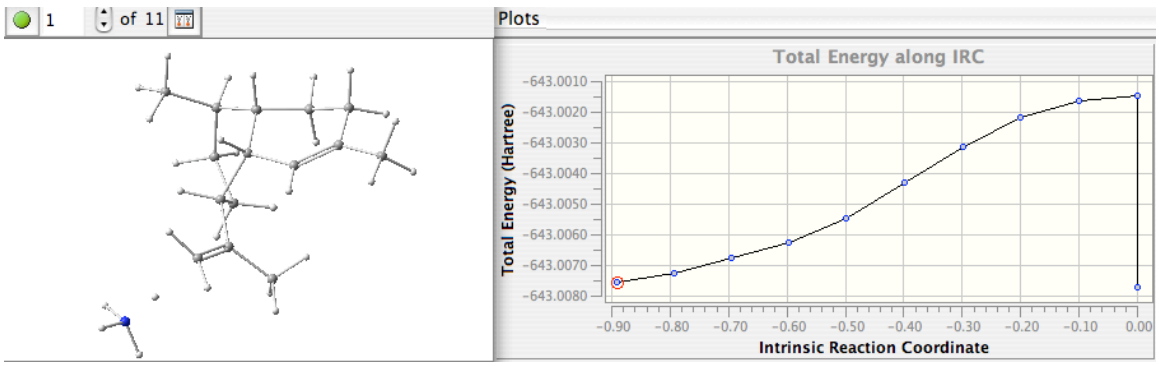


Figure S7.

TS5


1.62
5
1
9
10
2.09
1.49
11
1.35
1.42
13
169°
1.40


1
of 13
Plots
Total Energy along IRC
Total Energy (Hartree)
-643.0010
-643.0015
-643.0020
-643.0025
-643.0030
-643.0035
-643.0040
-1.2
-1.0
-0.8
-0.6
-0.4
-0.2
0.0
Intrinsic Reaction Coordinate


1
of 11
Plots
Total Energy along IRC
Total Energy (Hartree)
-643.0010
-643.0020
-643.0030
-643.0040
-643.0050
-643.0060
-643.0070
-643.0080
-0.90
-0.80
-0.70
-0.60
-0.50
-0.40
-0.30
-0.20
-0.10
0.00
Intrinsic Reaction Coordinate