10.1071/CH16504_AC

Australian Journal of Chemistry 2017, 70(4), 362-366

Supplementary Material

The Variediene-Forming Carbocation Cyclization/Rearrangement Cascade

Young J. Hong and Dean J. Tantillo*

Department of Chemistry, University of California—Davis, Davis, CA 95616, USA

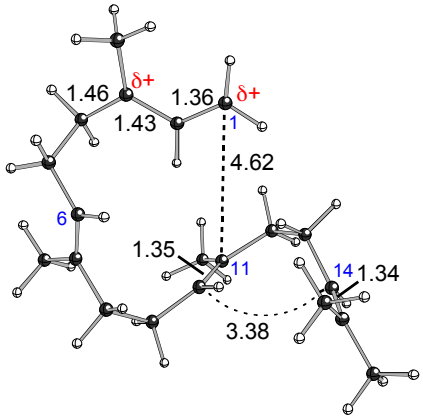
**djtantillo@ucdavis.edu*

Table of Contents

Coordinates and Energies

Figure 1

A



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7425202 hartrees (-490551.248850702 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.478476 (Hartree/Particle)

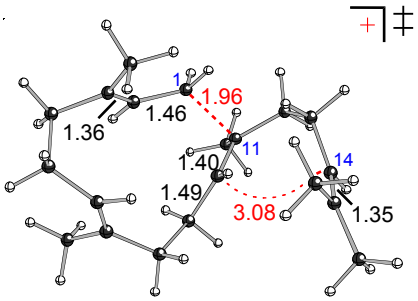
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5462074 hartrees (-490428.060605574 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.082377	0.807356	1.571209
2	6	1.015451	1.258639	0.304804
3	6	0.542529	2.600853	-0.187232
4	6	-0.516425	2.524995	-1.325868
5	1	-0.607452	3.527796	-1.763874
6	6	-1.891256	2.071745	-0.893703
7	6	-2.381182	0.882863	-1.319512
8	6	-3.730021	0.327663	-1.026110
9	1	-4.100876	-0.281239	-1.855194
10	6	-3.836235	-0.580815	0.329584
11	6	-3.170280	-1.865195	0.134737
12	6	-1.046118	-3.097521	0.325201
13	1	-1.496973	-4.066494	0.134634
14	1	0.021044	-3.088353	0.524884
15	6	-2.646804	3.024672	-0.004313
16	1	-3.655045	2.691163	0.248272

17	1	-2.106520	3.188384	0.935265
18	1	-2.729140	4.006369	-0.486398
19	1	1.423915	0.625492	-0.481149
20	6	3.738173	-0.743533	0.424408
21	1	-1.739381	0.274380	-1.955063
22	1	-0.139964	1.866929	-2.116884
23	6	-1.761045	-1.941754	0.357043
24	1	-1.247083	-1.012173	0.596586
25	6	-3.990616	-3.009893	-0.338959
26	1	-4.692925	-2.673049	-1.111421
27	1	-3.421165	-3.856873	-0.718510
28	1	-4.621010	-3.352649	0.495770
29	1	-4.904890	-0.712935	0.515419
30	1	-3.377236	0.007887	1.125956
31	1	0.173863	3.230030	0.626891
32	6	4.287752	-0.693375	-0.800998
33	6	2.417405	-1.346013	0.840623
34	6	1.684844	-0.541830	1.932324
35	1	0.887251	-1.166138	2.368914
36	6	0.615327	1.584350	2.781367
37	1	0.057018	2.488501	2.532128
38	1	-0.019506	0.961139	3.424764
39	1	1.472388	1.886278	3.396977
40	1	4.320739	-0.332938	1.250374
41	1	2.605074	-2.348014	1.257559
42	1	1.766241	-1.497060	-0.029285
43	6	3.645233	-1.231338	-2.057482
44	1	2.633946	-1.615405	-1.901792
45	1	3.600331	-0.454597	-2.831894
46	1	4.247544	-2.048270	-2.475790
47	6	5.654593	-0.085433	-1.011682
48	1	6.084976	0.286990	-0.078211
49	1	6.349054	-0.821585	-1.436885
50	1	5.608949	0.748270	-1.724602
51	1	2.384363	-0.383830	2.766300
52	1	1.408007	3.132173	-0.606468
53	1	-4.467748	1.111199	-0.839924

TS (A-C)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7343749 hartrees (-490546.137593499 kcal/mol)
Imaginary Frequencies: 1 (-222.8361 1/cm)
Zero-point correction = 0.480409 (Hartree/Particle)

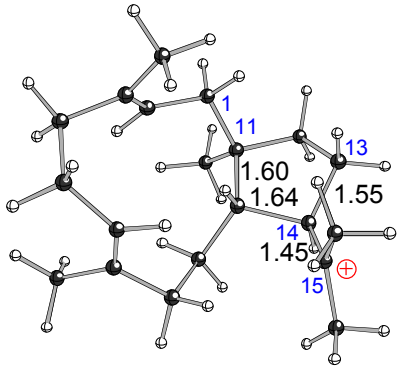
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5470248 hartrees (-490428.573532248 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	0.955760	1.748114	-0.833793
2	6	0.586029	0.396878	-0.867211
3	6	-0.086338	-0.285731	-2.002435
4	6	-0.724923	-1.668384	-1.729262
5	1	-0.772647	-2.205972	-2.683590
6	6	-2.110166	-1.551183	-1.121699
7	6	-2.271529	-1.684675	0.204539
8	6	-3.502061	-1.353132	1.014728
9	1	-3.435288	-1.840375	1.992064
10	6	-3.673485	0.196804	1.213292
11	6	-2.342584	0.868802	1.442799
12	6	-0.456154	2.184891	0.445018
13	1	0.110366	2.064313	1.362202
14	1	-0.414174	3.201291	0.055644
15	6	-3.222343	-1.222489	-2.086598
16	1	-4.191617	-1.117970	-1.596065
17	1	-3.028445	-0.292174	-2.637913
18	1	-3.314209	-2.013049	-2.841957
19	1	0.847282	-0.215217	-0.008166
20	6	3.454963	-0.036365	0.169457
21	1	-1.390727	-1.959972	0.786434
22	1	-0.064690	-2.247820	-1.074179
23	6	-1.783156	1.587635	0.434357

24	1	-2.378591	1.747595	-0.462124
25	6	-1.713588	0.626481	2.787060
26	1	-1.661107	-0.446614	3.004219
27	1	-0.712647	1.045882	2.900659
28	1	-2.345245	1.065849	3.569192
29	1	-4.352633	0.370213	2.056245
30	1	-4.144111	0.617778	0.320192
31	1	-0.788841	0.388836	-2.505338
32	6	3.513359	-1.326168	0.560080
33	6	2.847322	1.138565	0.900124
34	6	2.213524	2.169125	-0.048614
35	1	2.003100	3.104096	0.484188
36	6	0.708746	2.615108	-2.060422
37	1	-0.311734	2.538209	-2.444405
38	1	0.904052	3.666140	-1.828781
39	1	1.394454	2.328500	-2.866038
40	1	3.967563	0.226016	-0.757733
41	1	3.636345	1.668727	1.451815
42	1	2.131059	0.814054	1.664690
43	6	2.930807	-1.858875	1.845906
44	1	2.358251	-1.119782	2.410510
45	1	2.286528	-2.725877	1.652373
46	1	3.734885	-2.217735	2.500886
47	6	4.237877	-2.353276	-0.275741
48	1	4.638276	-1.926497	-1.199068
49	1	5.073502	-2.787049	0.287802
50	1	3.575831	-3.188540	-0.537581
51	1	2.954679	2.433247	-0.814807
52	1	0.734950	-0.397893	-2.737882
53	1	-4.416781	-1.730952	0.547008

C



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

HF = -781.7635677 hartrees (-490564.456367427 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484240 (Hartree/Particle)

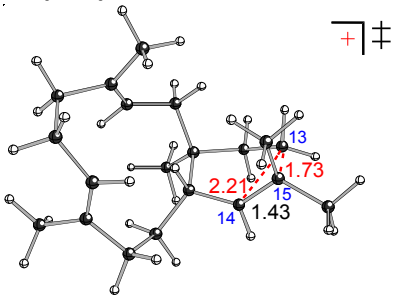
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5880485 hartrees (-490454.316314235 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.029976	-1.638371	-0.902519
2	6	-1.000407	-0.094881	-0.474676
3	6	-0.595145	0.964445	-1.513902
4	6	0.162692	2.188474	-0.928281
5	1	0.063504	3.027068	-1.628715
6	6	1.629795	1.884732	-0.680030
7	6	2.049941	1.494196	0.534932
8	6	3.392142	0.909164	0.903488
9	1	3.534706	0.990432	1.986103
10	6	3.527905	-0.588738	0.466865
11	6	2.293550	-1.411357	0.777163
12	6	0.105997	-2.403162	-0.135147
13	1	-0.193798	-2.518598	0.912095
14	1	0.134330	-3.417862	-0.557572
15	6	2.521511	1.974729	-1.894906
16	1	3.562914	1.740340	-1.668937
17	1	2.195313	1.295813	-2.694101
18	1	2.490013	2.987392	-2.316472
19	1	-0.318374	-0.014294	0.375873
20	6	-2.517822	0.147400	0.095463
21	1	1.310978	1.497801	1.338350
22	1	-0.307586	2.513169	0.011137
23	6	1.462338	-1.757146	-0.223991
24	1	1.786015	-1.504019	-1.233367
25	6	2.071350	-1.722580	2.237497
26	1	2.032277	-0.806390	2.841607
27	1	1.162626	-2.296943	2.429512
28	1	2.913446	-2.307978	2.626924
29	1	4.412735	-1.010818	0.960111
30	1	3.716008	-0.619457	-0.611115
31	1	0.054062	0.493400	-2.256288
32	6	-2.510395	1.288576	0.980414

33	6	-2.873280	-1.238472	0.681095
34	6	-2.406413	-2.176284	-0.435007
35	1	-2.350535	-3.216715	-0.100721
36	6	-0.884590	-1.853841	-2.419612
37	1	0.114593	-1.611171	-2.790925
38	1	-1.066987	-2.908766	-2.650275
39	1	-1.611180	-1.264153	-2.988277
40	1	-3.142045	0.351690	-0.780707
41	1	-3.943061	-1.314907	0.899190
42	1	-2.327193	-1.430632	1.609586
43	6	-1.988207	1.215137	2.360990
44	1	-1.408477	0.317756	2.572568
45	1	-1.424252	2.116398	2.621703
46	1	-2.867154	1.217488	3.029974
47	6	-3.107931	2.563121	0.526994
48	1	-2.961979	2.723285	-0.545881
49	1	-4.199528	2.447449	0.656869
50	1	-2.792436	3.433081	1.104702
51	1	-3.127245	-2.144719	-1.260729
52	1	-1.475680	1.294799	-2.080508
53	1	4.215644	1.469212	0.447311

TS (C-D)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7412262 hartrees (-490550.436852762 kcal/mol)
Imaginary Frequencies: 1 (-187.0670 1/cm)
Zero-point correction = 0.485154 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5656021 hartrees (-490440.230973771 kcal/mol)

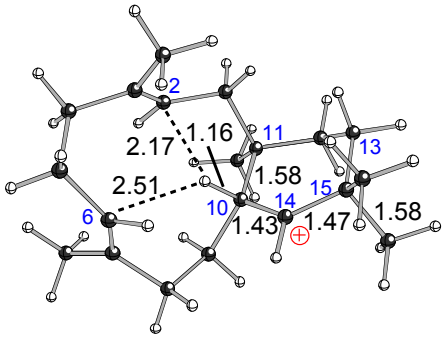
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-1.117518	-0.029256	1.603053
2	6	-0.729468	-0.825541	0.182455
3	6	-0.001529	-2.190253	0.301612
4	6	0.982312	-2.439854	-0.878951
5	1	1.236053	-3.506654	-0.882041
6	6	2.244326	-1.603775	-0.750276
7	6	2.354288	-0.427338	-1.391547
8	6	3.421289	0.627657	-1.210014
9	1	3.392198	1.314302	-2.062349
10	6	3.267812	1.443205	0.119731
11	6	1.843878	1.885920	0.388349
12	6	-0.354409	1.339266	1.606350
13	1	-0.835185	2.031419	0.909077
14	1	-0.515364	1.755864	2.612199
15	6	3.292320	-2.153709	0.187653
16	1	4.172431	-1.512540	0.259499
17	1	2.901150	-2.293454	1.204399
18	1	3.625090	-3.141993	-0.153600
19	1	-0.062643	-0.120689	-0.320660
20	6	-2.000295	-0.938228	-0.512573
21	1	1.545796	-0.157307	-2.072944
22	1	0.481688	-2.233896	-1.833420
23	6	1.115530	1.227124	1.311762
24	1	1.641360	0.473525	1.896260
25	6	1.342239	3.022265	-0.467763
26	1	1.418337	2.783603	-1.536320
27	1	0.311982	3.314228	-0.252150
28	1	1.968103	3.908699	-0.307880
29	1	3.938772	2.309712	0.067111
30	1	3.612466	0.820961	0.951365
31	1	0.562253	-2.230947	1.233802
32	6	-2.706414	0.079122	-1.220597
33	6	-3.272922	0.676975	0.300161
34	6	-2.648684	0.201929	1.620807
35	1	-2.882502	0.959088	2.379024
36	6	-0.744103	-0.852465	2.842774
37	1	0.333855	-0.972231	2.966592
38	1	-1.113602	-0.329878	3.732279
39	1	-1.201782	-1.845798	2.832015
40	1	-2.567823	-1.856363	-0.331122
41	1	-4.341118	0.463014	0.281512
42	1	-3.101193	1.742521	0.138587
43	6	-1.910826	1.173548	-1.936335

44	1	-1.076610	1.554576	-1.347714
45	1	-1.515623	0.777568	-2.877109
46	1	-2.570248	2.010529	-2.181863
47	6	-3.917698	-0.383390	-2.035903
48	1	-4.470345	-1.185838	-1.538341
49	1	-4.602839	0.451861	-2.205254
50	1	-3.591227	-0.746382	-3.015448
51	1	-3.145105	-0.718085	1.948588
52	1	-0.733659	-3.006053	0.354388
53	1	4.424562	0.187422	-1.212968

D



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.756202 hartrees (-490559.83431702 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484080 (Hartree/Particle)

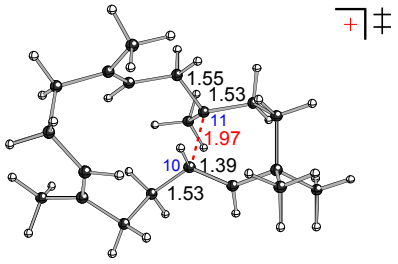
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5819841 hartrees (-490450.510842591 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.114453	0.137588	1.546892
2	6	-0.643997	-0.698571	0.287935
3	6	0.045931	-2.110482	0.475359
4	6	1.057892	-2.497226	-0.631890
5	1	1.314135	-3.552462	-0.479108
6	6	2.303973	-1.635429	-0.581424
7	6	2.399034	-0.540819	-1.360692
8	6	3.433457	0.554067	-1.279418
9	1	3.385840	1.161208	-2.188645

10	6	3.255245	1.479322	-0.024674
11	6	1.825542	1.909951	0.213740
12	6	-0.334284	1.501876	1.559282
13	1	-0.804795	2.200777	0.863389
14	1	-0.453162	1.939412	2.559047
15	6	3.347716	-2.044900	0.429104
16	1	3.689119	-3.066539	0.221253
17	1	4.223405	-1.394254	0.418430
18	1	2.950837	-2.052856	1.452490
19	6	-1.495569	-0.679175	-0.854221
20	1	1.606193	-0.380896	-2.093689
21	1	0.595059	-2.441030	-1.624666
22	6	1.122019	1.340669	1.222635
23	1	1.672310	0.655646	1.867371
24	6	1.278522	2.927117	-0.753945
25	1	0.239543	3.201436	-0.563758
26	1	1.875302	3.846013	-0.703334
27	1	1.357363	2.570192	-1.789276
28	1	3.898651	2.357139	-0.162209
29	1	3.622657	0.946668	0.857306
30	1	0.565067	-2.085976	1.433345
31	6	-2.760906	0.033316	-1.054039
32	6	-3.100128	0.977179	0.113605
33	6	-2.636501	0.422359	1.465092
34	1	-2.897317	1.133506	2.256501
35	6	-0.849938	-0.610410	2.869619
36	1	0.215129	-0.733383	3.084051
37	1	-1.279821	-0.034435	3.695015
38	1	-1.317737	-1.599678	2.882947
39	1	-1.185096	-1.303856	-1.695389
40	1	-4.180404	1.154944	0.127769
41	1	-2.638648	1.952278	-0.076957
42	6	-2.781836	0.756484	-2.425901
43	1	-2.584851	0.069012	-3.254151
44	1	-3.773141	1.194277	-2.575780
45	1	-2.045785	1.564713	-2.457591
46	6	-3.792063	-1.167684	-1.127794
47	1	-4.766813	-0.718675	-1.342787
48	1	-3.552734	-1.867112	-1.932814
49	1	-3.863857	-1.715896	-0.186254
50	1	-3.186716	-0.498989	1.697064
51	1	-0.732682	-2.875676	0.561278
52	1	4.448540	0.143780	-1.241137
53	1	0.246461	-0.100688	-0.145292

TS (D-E)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7464628 hartrees (-490553.722871628 kcal/mol)
Imaginary Frequencies: 1 (-151.4923 1/cm)
Zero-point correction = 0.483938 (Hartree/Particle)

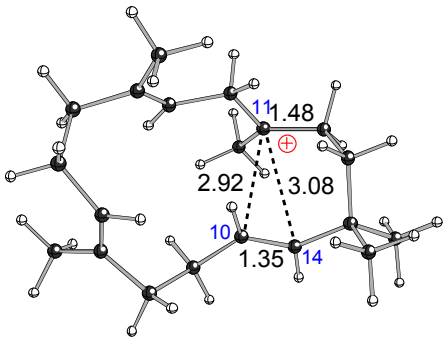
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5680682 hartrees (-490441.778476182 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.255857	0.824329	1.358049
2	6	-0.750304	-0.733614	0.267188
3	6	0.134755	-1.756235	0.976261
4	6	1.067475	-2.530972	-0.010566
5	1	1.228770	-3.535401	0.397016
6	6	2.392426	-1.811188	-0.177662
7	6	2.549353	-0.891275	-1.143228
8	6	3.656919	0.128228	-1.250625
9	1	3.679456	0.543510	-2.263178
10	6	3.476210	1.282231	-0.209150
11	6	2.068054	1.840337	-0.180882
12	6	-0.199641	1.891820	0.977164
13	1	-0.541222	2.412928	0.081275
14	1	-0.310594	2.613058	1.806481
15	6	3.428462	-2.126929	0.874015
16	1	3.694905	-3.190562	0.831509
17	1	4.346800	-1.549666	0.755073
18	1	3.049065	-1.945497	1.889002
19	6	-2.043371	-1.133785	-0.063471
20	1	1.737236	-0.780445	-1.863474
21	1	0.566892	-2.660900	-0.977028

22	6	1.244773	1.515959	0.838940
23	1	1.669264	0.936712	1.656740
24	6	1.697727	2.699394	-1.364730
25	1	0.671648	3.071436	-1.348010
26	1	2.359670	3.572832	-1.407568
27	1	1.845906	2.156147	-2.306016
28	1	4.194291	2.078624	-0.441904
29	1	3.731560	0.897297	0.783004
30	1	0.762158	-1.272673	1.726960
31	6	-3.021941	-0.404940	-0.916910
32	6	-2.913605	1.110824	-0.575055
33	6	-2.646991	1.288863	0.925373
34	1	-2.715867	2.352752	1.186541
35	6	-1.185686	0.346049	2.795327
36	1	-0.176635	0.076613	3.110039
37	1	-1.508428	1.181445	3.430765
38	1	-1.858641	-0.491177	2.992363
39	1	-2.408390	-2.047025	0.415566
40	1	-3.843888	1.606804	-0.867858
41	1	-2.114070	1.577262	-1.160309
42	6	-2.646165	-0.643790	-2.414972
43	1	-2.728012	-1.700398	-2.683944
44	1	-3.347723	-0.080885	-3.038167
45	1	-1.631917	-0.301508	-2.636393
46	6	-4.450403	-0.933077	-0.662591
47	1	-5.159950	-0.431134	-1.326113
48	1	-4.513978	-2.008351	-0.858248
49	1	-4.776066	-0.757574	0.367680
50	1	-3.419203	0.774145	1.508095
51	1	-0.509369	-2.460068	1.516183
52	1	4.642238	-0.320102	-1.084881
53	1	-0.229038	-0.091568	-0.446042

E



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7510936 hartrees (-490556.628744936 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.481778 (Hartree/Particle)

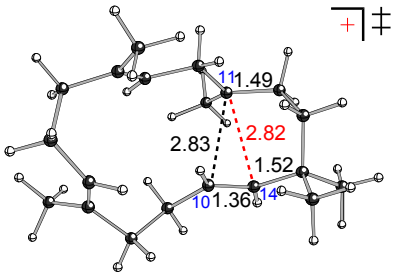
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.566531126 hartrees (-490440.8139468760 kcal/mol)

Coordinates:

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.293672	-1.430321	1.241469
2	6	0.810189	1.188551	0.050140
3	6	-0.086496	2.134447	0.809044
4	6	-1.224222	2.746714	-0.067312
5	1	-1.448036	3.746739	0.321790
6	6	-2.482671	1.900432	-0.054529
7	6	-2.703905	0.979247	-1.007378
8	6	-3.811832	-0.046929	-1.041457
9	1	-3.942814	-0.406944	-2.067259
10	6	-3.549352	-1.258076	-0.091898
11	6	-2.186120	-1.888422	-0.276994
12	6	0.189634	-2.161153	0.565121
13	1	0.479134	-2.422514	-0.454024
14	1	0.272074	-3.121746	1.129554
15	6	-3.405554	2.148413	1.115187
16	1	-4.274016	1.487509	1.126601
17	1	-2.883339	2.030608	2.074411
18	1	-3.772948	3.182224	1.092492
19	1	0.318330	0.481418	-0.619018
20	6	2.158416	1.289183	0.085462
21	1	-1.977116	0.914665	-1.818061
22	1	-0.858989	2.884616	-1.090821
23	6	-1.233277	-1.679762	0.652126
24	1	-1.505908	-1.129586	1.548356
25	6	-2.004844	-2.683772	-1.544929
26	1	-2.218356	-2.066853	-2.425614
27	1	-1.009222	-3.114134	-1.669316
28	1	-2.723114	-3.512127	-1.567255
29	1	-4.330261	-2.009789	-0.264939
30	1	-3.653394	-0.918335	0.943276
31	1	-0.552266	1.619864	1.662170

32	6	3.192525	0.512260	-0.705172
33	6	2.889142	-1.005276	-0.727252
34	6	2.655276	-1.622207	0.686572
35	1	2.771447	-2.711408	0.563733
36	6	1.097536	-0.888563	2.604981
37	1	0.168762	-0.319877	2.701064
38	1	0.987347	-1.753340	3.282516
39	1	1.945050	-0.296398	2.948276
40	1	2.569735	2.073913	0.723443
41	1	2.017854	-1.207687	-1.358230
42	6	3.188193	1.009378	-2.179161
43	1	3.412884	2.078559	-2.225302
44	1	3.950168	0.479642	-2.760767
45	1	2.214828	0.847295	-2.651840
46	6	4.592319	0.773868	-0.106271
47	1	5.361846	0.233471	-0.666349
48	1	4.835323	1.839865	-0.153364
49	1	4.664150	0.472371	0.944279
50	1	3.419220	-1.283711	1.388750
51	1	0.531230	2.932007	1.236579
52	1	-4.773115	0.391589	-0.753090
53	1	3.731741	-1.529982	-1.188541

TS (E-F)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.750907 hartrees (-490556.51165157 kcal/mol)
Imaginary Frequencies: 1 (-33.9859 1/cm)
Zero-point correction = 0.481999 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5670874 hartrees (-490441.163014374 kcal/mol)

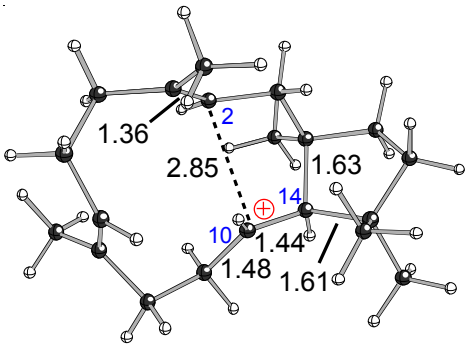
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	-1.378127	1.257598	1.300929
2	6	-0.716052	-1.161321	-0.010269
3	6	0.182971	-2.061202	0.799938
4	6	1.324496	-2.703299	-0.050670
5	1	1.561022	-3.680954	0.383970
6	6	2.563478	-1.829218	-0.070809
7	6	2.738658	-0.907399	-1.032213
8	6	3.789233	0.176854	-1.067813
9	1	3.889503	0.555896	-2.090091
10	6	3.463084	1.357633	-0.099303
11	6	2.061057	1.906823	-0.258876
12	6	-0.309248	2.057264	0.632598
13	1	-0.621046	2.335801	-0.374279
14	1	-0.420114	2.995695	1.226054
15	6	3.504866	-2.032306	1.092494
16	1	4.358951	-1.353203	1.078173
17	1	2.992381	-1.905265	2.056033
18	1	3.893986	-3.058260	1.086407
19	1	-0.236646	-0.564282	-0.785324
20	6	-2.067932	-1.196417	0.101705
21	1	2.004754	-0.879176	-1.838620
22	1	0.961528	-2.892570	-1.066783
23	6	1.134310	1.637195	0.681438
24	1	1.452261	1.094629	1.567605
25	6	1.818630	2.704466	-1.515619
26	1	0.792925	3.058798	-1.635591
27	1	2.471009	3.586068	-1.525752
28	1	2.078712	2.118691	-2.404936
29	1	4.194269	2.158245	-0.270559
30	1	3.600741	1.011904	0.929903
31	1	0.649937	-1.502003	1.622632
32	6	-3.121734	-0.527195	-0.765933
33	6	-3.030887	1.020263	-0.639310
34	6	-2.770007	1.479265	0.813767
35	1	-2.917102	2.572054	0.840173
36	6	-1.146953	0.716404	2.662578
37	1	-0.178393	0.222469	2.766829
38	1	-1.120454	1.580747	3.348431
39	1	-1.949081	0.056751	2.993466
40	1	-2.465058	-1.854080	0.878070
41	1	-2.237456	1.400604	-1.290572
42	6	-2.920918	-0.902455	-2.256730
43	1	-3.027213	-1.980800	-2.403692

44	1	-3.673381	-0.402519	-2.875485
45	1	-1.931754	-0.606027	-2.618890
46	6	-4.516637	-1.011521	-0.313186
47	1	-5.299601	-0.573510	-0.939399
48	1	-4.594222	-2.100139	-0.397003
49	1	-4.731232	-0.746255	0.728287
50	1	-3.496789	1.039288	1.500565
51	1	-0.429511	-2.839505	1.268411
52	1	4.776390	-0.209807	-0.792707
53	1	-3.963040	1.472129	-0.993632

F



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7630404 hartrees (-490564.125481404 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484016 (Hartree/Particle)

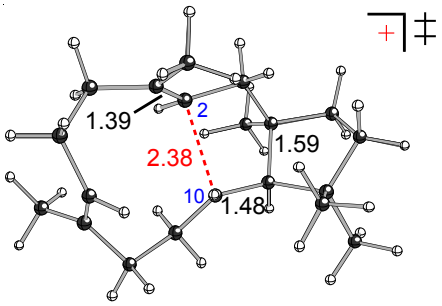
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5870946 hartrees (-490453.717732446 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.771493	-0.626134	1.222608
2	6	0.285042	1.043381	-0.109125
3	6	-0.445055	2.204741	0.442984
4	6	-1.764917	2.590372	-0.266397
5	1	-2.091715	3.555365	0.136821
6	6	-2.819883	1.525166	-0.067726
7	6	-2.961691	0.554098	-0.987475
8	6	-3.726503	-0.732336	-0.825855
9	1	-3.856699	-1.212025	-1.800435

10	6	-3.002576	-1.712549	0.155379
11	6	-1.538748	-1.944661	-0.136728
12	6	0.882793	-1.776780	0.701331
13	1	1.194028	-2.064946	-0.304620
14	1	1.112572	-2.641313	1.343388
15	6	-3.577387	1.588104	1.234886
16	1	-4.324497	0.798925	1.331178
17	1	-2.907289	1.519897	2.103687
18	1	-4.096097	2.550628	1.321972
19	1	-0.155729	0.531366	-0.959479
20	6	1.631193	0.710169	0.293091
21	1	-2.385291	0.649011	-1.909058
22	1	-1.563526	2.743345	-1.332319
23	6	-0.595558	-1.522361	0.751832
24	1	-0.970266	-1.088643	1.677172
25	6	-1.237423	-2.679583	-1.414542
26	1	-0.172826	-2.808993	-1.612702
27	1	-1.692598	-3.677648	-1.383646
28	1	-1.687337	-2.169215	-2.275162
29	1	-3.528265	-2.676281	0.116448
30	1	-3.109933	-1.329769	1.174230
31	1	-0.611828	2.031785	1.520754
32	6	2.688735	0.516847	-0.907609
33	6	3.534379	-0.721321	-0.482622
34	6	3.269391	-0.939153	1.006332
35	1	3.509481	-1.953263	1.343874
36	6	1.467033	-0.286091	2.686147
37	1	0.441292	0.058324	2.846760
38	1	1.611398	-1.176008	3.308730
39	1	2.144084	0.488746	3.058219
40	1	1.999046	1.504391	0.951448
41	1	3.231879	-1.601076	-1.060292
42	6	2.055399	0.293087	-2.291182
43	1	1.514366	1.174924	-2.653798
44	1	2.847912	0.082297	-3.015993
45	1	1.373367	-0.563922	-2.306911
46	6	3.554490	1.791771	-0.946942
47	1	4.298168	1.711996	-1.746803
48	1	2.952729	2.686402	-1.143686
49	1	4.094638	1.944925	-0.006565
50	1	3.872877	-0.251658	1.610561
51	1	0.273481	3.043251	0.444140
52	1	-4.734178	-0.561330	-0.432268
53	1	4.595520	-0.560088	-0.695966

TS (F-G)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7615776 hartrees (-490563.207559776 kcal/mol)
Imaginary Frequencies: 1 (-132.2461 1/cm)
Zero-point correction = 0.485006 (Hartree/Particle)

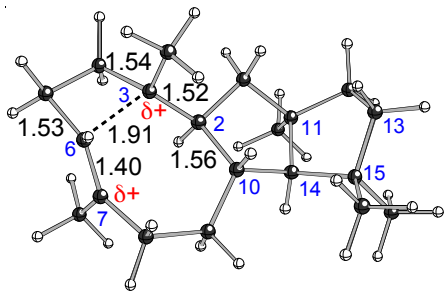
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.587814 hartrees (-490454.16916314 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.901814	0.549581	1.233025
2	6	-0.155832	-0.853812	-0.077040
3	6	0.612646	-1.981175	0.551341
4	6	1.891154	-2.456425	-0.182842
5	1	2.199532	-3.406960	0.267039
6	6	2.974629	-1.412273	-0.080009
7	6	3.054693	-0.463329	-1.027391
8	6	3.711890	0.878502	-0.866587
9	1	3.775458	1.398065	-1.826607
10	6	2.885308	1.726535	0.158635
11	6	1.409699	1.811583	-0.119160
12	6	-0.961385	1.699376	0.818026
13	1	-1.278522	2.116008	-0.140290
14	1	-1.059173	2.512015	1.552118
15	6	3.792229	-1.433032	1.187400
16	1	4.547396	-0.645967	1.222933
17	1	3.165372	-1.339676	2.085225
18	1	4.312393	-2.394479	1.276433
19	1	0.177575	-0.538902	-1.059754
20	6	-1.588411	-0.676852	0.268581

21	1	2.443340	-0.587830	-1.922097
22	1	1.645015	-2.662896	-1.230527
23	6	0.481357	1.274411	0.760433
24	1	0.895321	0.858125	1.676883
25	6	1.018197	2.592312	-1.338477
26	1	0.966558	3.659424	-1.076593
27	1	1.768989	2.503505	-2.128017
28	1	0.043491	2.314495	-1.742592
29	1	3.276536	2.754938	0.153039
30	1	3.048116	1.323160	1.160930
31	1	0.826352	-1.757200	1.606060
32	6	-2.617486	-0.572609	-0.953809
33	6	-3.503584	0.660950	-0.609144
34	6	-3.372986	0.870476	0.902188
35	1	-3.646424	1.881938	1.222915
36	6	-1.713201	0.179579	2.711167
37	1	-0.687241	-0.116831	2.953341
38	1	-1.964797	1.034650	3.347877
39	1	-2.372333	-0.647083	2.994013
40	1	-1.866187	-1.556236	0.859953
41	1	-4.540081	0.505221	-0.923495
42	1	-3.146985	1.544778	-1.150889
43	6	-1.979948	-0.408495	-2.342869
44	1	-1.397917	-1.286828	-2.645854
45	1	-2.770459	-0.276509	-3.088437
46	1	-1.334039	0.474502	-2.408222
47	6	-3.465620	-1.862651	-0.949888
48	1	-4.203262	-1.833838	-1.758534
49	1	-2.843721	-2.752791	-1.100010
50	1	-4.011223	-1.987519	-0.008250
51	1	-4.027888	0.178898	1.444991
52	1	-0.104957	-2.815037	0.607077
53	1	4.734550	0.810959	-0.482134

G



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7891927 hartrees (-490580.536311177 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.488531 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.6281576 hartrees (-490479.485175576 kcal/mol)

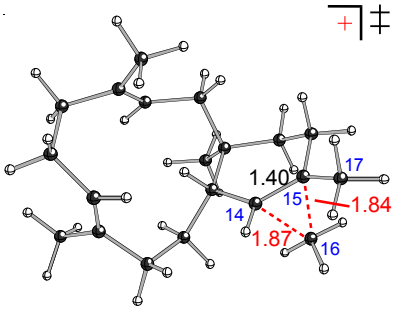
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.718540	-1.201701	0.723104
2	6	0.232589	0.643959	-0.150762
3	6	-0.333580	1.963129	0.390977
4	6	-1.775207	2.347405	-0.076139
5	1	-2.032941	3.303481	0.396500
6	6	-2.757408	1.311220	0.345412
7	6	-3.249206	0.408393	-0.601013
8	6	-4.134594	-0.798817	-0.276294
9	1	-4.722632	-1.088439	-1.149008
10	6	-2.964730	-1.770013	0.003733
11	6	-1.858418	-0.896865	-0.623889
12	6	0.430726	-1.765969	0.068297
13	1	0.622391	-1.978122	-0.988234
14	1	0.097549	-2.698080	0.537180
15	6	-3.117411	1.233391	1.789530
16	1	-3.340634	0.220869	2.130543
17	1	-2.368170	1.688882	2.439194
18	1	-4.046662	1.813747	1.911774
19	1	0.310205	0.716194	-1.241816
20	6	1.645401	0.352181	0.452359
21	1	-3.245381	0.779727	-1.623135
22	1	-1.792180	2.485052	-1.161236
23	6	-0.606987	-0.621048	0.192576
24	1	-0.902086	-0.561625	1.248595
25	6	-1.665001	-1.128893	-2.112010
26	1	-1.124298	-2.074900	-2.235385
27	1	-2.615516	-1.236243	-2.638756
28	1	-1.078767	-0.343544	-2.593974
29	1	-3.048490	-2.753246	-0.469386
30	1	-2.791282	-1.920534	1.072617
31	1	-0.303257	1.943628	1.486825

32	6	2.903100	0.715837	-0.422819
33	6	3.242043	-0.634280	-1.105244
34	6	2.985847	-1.694029	-0.025804
35	1	2.857064	-2.703006	-0.433097
36	6	1.761406	-1.551476	2.219212
37	1	0.850741	-1.238206	2.744468
38	1	1.873139	-2.632157	2.362517
39	1	2.607577	-1.062120	2.712286
40	1	1.714364	0.893273	1.404203
41	1	4.264033	-0.658072	-1.497878
42	1	2.571817	-0.791606	-1.962482
43	6	2.702896	1.837789	-1.454687
44	1	2.441364	2.790233	-0.979167
45	1	3.634843	2.003035	-2.005651
46	1	1.934853	1.599971	-2.198428
47	6	4.051557	1.140061	0.521126
48	1	4.981486	1.282228	-0.039762
49	1	3.813986	2.087207	1.018900
50	1	4.245828	0.399102	1.302185
51	1	3.833737	-1.743525	0.665417
52	1	0.314088	2.788906	0.081978
53	1	-4.826143	-0.653762	0.556220

Figure 3

TS (D-H)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7477821 hartrees (-490554.550745571 kcal/mol)
Imaginary Frequencies: 1 (-271.6965 1/cm)
Zero-point correction = 0.485231 (Hartree/Particle)

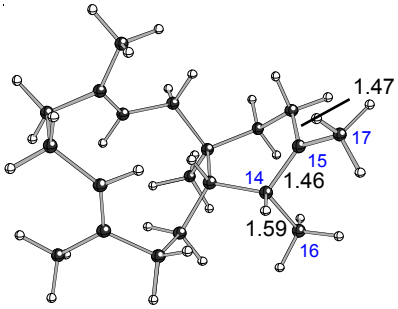
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5754256 hartrees (-490446.395318256 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.082231	-0.415463	1.420144
2	6	0.686749	0.585225	0.252567
3	6	0.079227	1.974052	0.611256
4	6	-0.934921	2.511624	-0.440300
5	1	-1.112137	3.571344	-0.221019
6	6	-2.244653	1.742560	-0.409084
7	6	-2.451071	0.717678	-1.255009
8	6	-3.568041	-0.300086	-1.227094
9	1	-3.628529	-0.787213	-2.205788
10	6	-3.383894	-1.388318	-0.114804
11	6	-1.966079	-1.914257	-0.017968
12	6	0.279405	-1.757630	1.229035
13	1	0.695831	-2.315715	0.384178
14	1	0.464260	-2.370039	2.122313
15	6	-3.222227	2.161362	0.662664
16	1	-3.515552	3.209057	0.519518
17	1	-4.131345	1.557808	0.661707
18	1	-2.783104	2.096897	1.666779
19	6	1.680376	0.693091	-0.864363
20	1	-1.685282	0.540628	-2.012974
21	1	-0.502500	2.477882	-1.448856
22	6	-1.197049	-1.544020	1.024825
23	1	-1.685754	-0.952603	1.798307
24	6	-1.512619	-2.779753	-1.168418
25	1	-0.493154	-3.155464	-1.057314
26	1	-2.171969	-3.651316	-1.261506
27	1	-1.578304	-2.243405	-2.124306
28	1	-4.087592	-2.205188	-0.319969
29	1	-3.668948	-0.954628	0.848911
30	1	-0.440242	1.890857	1.565648
31	6	2.818632	-0.106412	-1.051113
32	6	3.166739	-1.109278	0.024717
33	6	2.600554	-0.739885	1.399128
34	1	2.791778	-1.567974	2.089439
35	6	0.777810	0.148572	2.823486
36	1	-0.289870	0.297595	2.998723
37	1	1.131560	-0.558007	3.581372
38	1	1.284928	1.102335	3.002771
39	1	1.349308	1.278333	-1.721741
40	1	4.252548	-1.251430	0.067239

41	1	2.757960	-2.067073	-0.323689
42	6	3.431560	-0.310077	-2.416077
43	1	3.132930	0.458735	-3.132638
44	1	4.522901	-0.351194	-2.361246
45	1	3.087031	-1.278442	-2.796196
46	6	3.288403	1.595261	-0.530181
47	1	4.203410	1.193593	-0.093087
48	1	3.490586	2.180658	-1.421779
49	1	2.794318	2.178589	0.246243
50	1	3.160096	0.113808	1.803674
51	1	0.869600	2.719011	0.773661
52	1	-4.541115	0.177272	-1.068026
53	1	-0.140433	0.079824	-0.280822

H



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7549992 hartrees (-490559.079547992 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484670 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5801343 hartrees (-490449.350074593 kcal/mol)

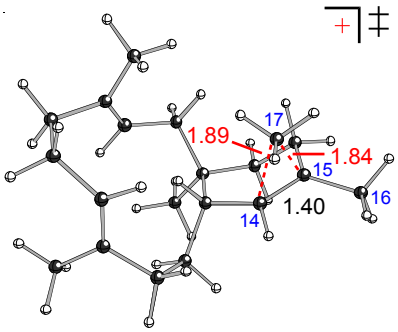
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.185172	-0.543827	1.333131
2	6	0.821489	0.535607	0.223110
3	6	0.067567	1.800536	0.710107
4	6	-0.855702	2.456205	-0.361640
5	1	-0.970060	3.518822	-0.116779
6	6	-2.214537	1.779857	-0.394280
7	6	-2.448742	0.756270	-1.232357

8	6	-3.606629	-0.212300	-1.193229
9	1	-3.680215	-0.730120	-2.155353
10	6	-3.455238	-1.262521	-0.041430
11	6	-2.062655	-1.854537	0.040435
12	6	0.228987	-1.789518	1.193912
13	1	0.564474	-2.404692	0.350727
14	1	0.383440	-2.402917	2.093224
15	6	-3.202329	2.270227	0.637216
16	1	-3.418656	3.334113	0.476930
17	1	-4.149756	1.729611	0.606913
18	1	-2.804188	2.186310	1.657348
19	6	2.007095	0.954149	-0.718585
20	1	-1.666263	0.518115	-1.955073
21	1	-0.390162	2.418214	-1.354601
22	6	-1.230871	-1.465376	1.025793
23	1	-1.647432	-0.800584	1.781820
24	6	-1.705636	-2.809804	-1.073152
25	1	-0.701002	-3.230083	-0.988326
26	1	-2.408436	-3.651929	-1.083553
27	1	-1.792608	-2.327011	-2.055478
28	1	-4.203291	-2.051412	-0.192592
29	1	-3.692144	-0.772781	0.908397
30	1	-0.559631	1.520509	1.557684
31	6	2.800073	-0.169752	-1.200184
32	6	3.062198	-1.289558	-0.292200
33	6	2.637199	-1.076273	1.159402
34	1	2.732127	-2.027925	1.691744
35	6	1.094437	0.000009	2.775101
36	1	0.066461	0.200448	3.084713
37	1	1.498777	-0.740957	3.472956
38	1	1.669154	0.923116	2.903355
39	1	1.612351	1.515809	-1.572359
40	1	4.098988	-1.638438	-0.405571
41	1	2.480131	-2.112332	-0.762455
42	6	3.293108	-0.203422	-2.589108
43	1	3.583506	0.793761	-2.937804
44	1	4.089406	-0.929363	-2.760823
45	1	2.427109	-0.481819	-3.215603
46	6	3.108864	1.905719	-0.079697
47	1	3.554838	1.497643	0.825901
48	1	3.899794	2.142289	-0.795502
49	1	2.597357	2.837082	0.169612
50	1	3.352179	-0.398975	1.637405
51	1	0.769382	2.541252	1.108474

52	1	-4.562866	0.303522	-1.054244
53	1	0.124138	0.030560	-0.455154

TS (D-I)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7430958 hartrees (-490551.610045458 kcal/mol)
Imaginary Frequencies: 1 (-275.5847 1/cm)
Zero-point correction = 0.485969 (Hartree/Particle)

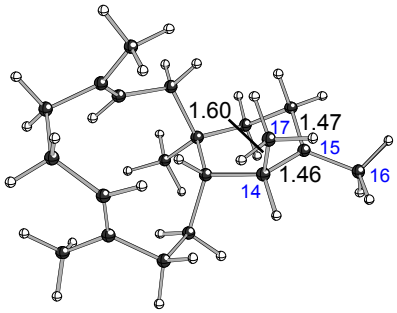
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5704584 hartrees (-490443.278350584 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.087678	-0.252489	1.478258
2	6	0.685267	0.674061	0.249196
3	6	0.126592	2.110454	0.523311
4	6	-0.939201	2.547361	-0.522992
5	1	-1.154692	3.609455	-0.355320
6	6	-2.215271	1.727946	-0.428254
7	6	-2.409681	0.677822	-1.247093
8	6	-3.498370	-0.370138	-1.186954
9	1	-3.551703	-0.876136	-2.156622
10	6	-3.293235	-1.437304	-0.056854
11	6	-1.864663	-1.929569	0.061755
12	6	0.369464	-1.647114	1.325269
13	1	0.830117	-2.222731	0.514820
14	1	0.567988	-2.213207	2.245474
15	6	-3.176941	2.132165	0.663134
16	1	-3.501760	3.170038	0.517589
17	1	-4.069147	1.504200	0.690352

18	1	-2.711489	2.089441	1.656409
19	6	1.756359	0.828086	-0.795578
20	1	-1.659116	0.515967	-2.023723
21	1	-0.525709	2.476315	-1.538201
22	6	-1.113211	-1.508783	1.097369
23	1	-1.629376	-0.912708	1.848219
24	6	-1.383806	-2.822576	-1.056245
25	1	-0.360408	-3.180927	-0.917508
26	1	-2.025059	-3.709533	-1.127079
27	1	-1.450990	-2.322504	-2.032122
28	1	-3.977740	-2.272003	-0.254786
29	1	-3.596033	-0.996035	0.897804
30	1	-0.331341	2.128275	1.511820
31	6	2.982026	0.147156	-0.857461
32	6	3.288491	-0.872780	0.227853
33	6	2.621015	-0.458067	1.547654
34	1	2.846115	-1.214187	2.307185
35	6	0.678653	0.356973	2.837410
36	1	-0.399287	0.504243	2.932383
37	1	0.983929	-0.320046	3.641924
38	1	1.168230	1.319106	3.016584
39	1	1.653870	1.695359	-1.446125
40	1	4.374160	-0.931431	0.349798
41	1	2.967504	-1.874412	-0.076891
42	6	1.787195	-0.583860	-2.053848
43	1	1.367550	0.023442	-2.854154
44	1	2.627363	-1.143886	-2.467927
45	1	1.072277	-1.257537	-1.593977
46	6	4.139110	0.717773	-1.643352
47	1	4.781658	-0.073762	-2.039095
48	1	3.815109	1.366356	-2.461558
49	1	4.745713	1.317857	-0.955145
50	1	3.090409	0.472303	1.894153
51	1	0.935923	2.851183	0.558769
52	1	-4.482204	0.087031	-1.033616
53	1	-0.166703	0.167766	-0.224912

I



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7528916 hartrees (-490557.757007916 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.485332 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5779747 hartrees (-490447.994903997 kcal/mol)

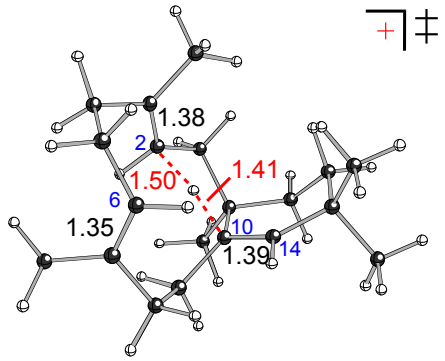
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.089890	-0.479474	1.355215
2	6	0.732504	0.555951	0.204013
3	6	0.287332	1.986749	0.619666
4	6	-0.819924	2.563019	-0.313502
5	1	-0.961936	3.619551	-0.054880
6	6	-2.134776	1.809485	-0.181906
7	6	-2.466744	0.861420	-1.076632
8	6	-3.610615	-0.127132	-1.031131
9	1	-3.791086	-0.496422	-2.046124
10	6	-3.367367	-1.348193	-0.075129
11	6	-1.949153	-1.881064	-0.120476
12	6	0.353368	-1.841526	1.049352
13	1	0.754460	-2.288619	0.131739
14	1	0.597717	-2.536536	1.865088
15	6	-2.969378	2.149113	1.029771
16	1	-3.225755	3.215950	1.029869
17	1	-3.900975	1.581614	1.069257
18	1	-2.427862	1.960283	1.966154
19	6	1.802897	0.695030	-0.941602
20	1	-1.794565	0.737261	-1.927513
21	1	-0.481573	2.544678	-1.357840
22	6	-1.138879	-1.665515	0.933506
23	1	-1.605670	-1.215878	1.807840

24	6	-1.543991	-2.563261	-1.403428
25	1	-0.528218	-2.965259	-1.378498
26	1	-2.218808	-3.403428	-1.607364
27	1	-1.627916	-1.887873	-2.265155
28	1	-4.088547	-2.131616	-0.341565
29	1	-3.595373	-1.039378	0.949963
30	1	-0.110640	1.975108	1.634328
31	6	3.145459	0.177769	-0.720651
32	6	3.320807	-1.009272	0.119174
33	6	2.607774	-0.729828	1.477842
34	1	2.799402	-1.593171	2.123913
35	6	0.653512	-0.003141	2.761689
36	1	-0.415407	0.206647	2.822586
37	1	0.873933	-0.785254	3.496133
38	1	1.191107	0.898576	3.069348
39	1	1.875246	1.739824	-1.264502
40	1	4.372495	-1.278077	0.242818
41	1	2.810416	-1.858017	-0.360359
42	6	1.391286	-0.099641	-2.267003
43	1	0.456994	0.353623	-2.602760
44	1	2.129242	-0.000091	-3.067067
45	1	1.218317	-1.154938	-2.055138
46	6	4.318453	0.849719	-1.303630
47	1	5.072663	0.137185	-1.654051
48	1	4.070089	1.588221	-2.067655
49	1	4.793881	1.387676	-0.461743
50	1	3.097003	0.127831	1.955122
51	1	1.141538	2.676700	0.644507
52	1	-4.543084	0.355023	-0.718085
53	1	-0.151828	0.127552	-0.269176

Figure 4

TS (D-J)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.749382 hartrees (-490555.55469882 kcal/mol)
Imaginary Frequencies: 1 (-967.9116 1/cm)
Zero-point correction = 0.480863 (Hartree/Particle)

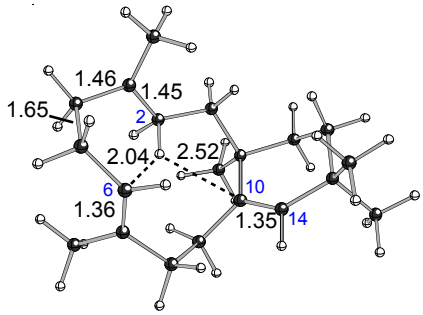
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5778372 hartrees (-490447.908621372 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.312407	-0.618991	1.479652
2	6	-0.647220	-0.939586	0.092032
3	6	0.253431	-2.195066	-0.054492
4	6	1.270978	-2.213064	-1.228253
5	1	1.651064	-3.237814	-1.306004
6	6	2.413511	-1.244342	-0.990799
7	6	2.311231	0.030392	-1.410202
8	6	3.173576	1.194485	-0.999603
9	1	2.954277	2.058926	-1.633196
10	6	2.968144	1.593421	0.511986
11	6	1.528933	1.724396	0.926480
12	6	-0.489947	0.567631	2.119035
13	1	-1.021057	1.511942	1.984257
14	1	-0.394882	0.417108	3.199755
15	6	3.573005	-1.781520	-0.188276
16	1	4.022457	-2.633512	-0.713105
17	1	4.360805	-1.043907	-0.024672
18	1	3.254610	-2.160459	0.791975
19	6	-1.236925	-0.442529	-1.057737
20	1	1.448470	0.287770	-2.024189
21	1	0.775391	-2.004471	-2.181798
22	6	0.886376	0.635841	1.489387
23	1	1.544839	-0.190450	1.757276
24	6	0.861110	3.029359	0.627600
25	1	-0.225263	3.002379	0.716600
26	1	1.232478	3.785802	1.333068
27	1	1.134185	3.388139	-0.371610
28	1	3.480919	2.548149	0.677263
29	1	3.458619	0.841168	1.134458
30	1	0.802704	-2.345776	0.877721
31	6	-2.440294	0.433720	-1.182900

32	6	-2.964362	0.887340	0.194674
33	6	-2.784745	-0.184517	1.273985
34	1	-3.173396	0.186240	2.229639
35	6	-1.296439	-1.833926	2.428434
36	1	-0.287936	-2.111823	2.747412
37	1	-1.862961	-1.588397	3.332411
38	1	-1.765921	-2.712392	1.975439
39	1	-0.807999	-0.745532	-2.012596
40	1	-4.021503	1.159402	0.107000
41	1	-2.446237	1.807502	0.489755
42	6	-2.130525	1.646671	-2.093100
43	1	-1.799743	1.331150	-3.088004
44	1	-3.035571	2.249726	-2.216301
45	1	-1.356875	2.287886	-1.658955
46	6	-3.501510	-0.457534	-1.908116
47	1	-4.388899	0.152841	-2.103612
48	1	-3.130134	-0.828581	-2.868217
49	1	-3.803356	-1.315191	-1.301110
50	1	-3.384358	-1.069072	1.025469
51	1	-0.413722	-3.059905	-0.148438
52	1	4.241803	0.986310	-1.121280
53	1	0.341671	0.051741	0.214852

J



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7681178 hartrees (-490567.311600678 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484127 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5937728 hartrees (-490457.908369728 kcal/mol)

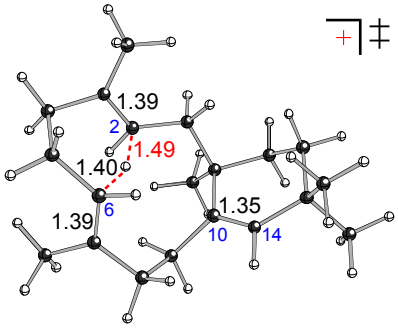
Coordinates (from last standard orientation):

Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z
1	6	-1.124935	0.431111	1.414959
2	6	-0.982594	-0.804040	0.487622
3	6	-0.036291	-1.958479	0.865584
4	6	0.863003	-2.560200	-0.268120
5	1	1.060649	-3.609325	-0.022804
6	6	2.179567	-1.828490	-0.394785
7	6	2.316387	-0.808867	-1.283897
8	6	3.456810	0.146293	-1.387751
9	1	3.420222	0.689816	-2.333578
10	6	3.556166	1.270033	-0.188350
11	6	2.243501	1.884626	-0.001082
12	6	-0.148095	1.588210	1.007613
13	1	-0.511259	2.032137	0.077603
14	1	-0.196479	2.372031	1.774696
15	6	3.261584	-2.251951	0.560663
16	1	3.541700	-3.291423	0.348489
17	1	4.168146	-1.647334	0.500190
18	1	2.904560	-2.241432	1.597891
19	6	-1.809677	-0.971649	-0.562067
20	1	1.476380	-0.621885	-1.951366
21	1	0.325956	-2.549616	-1.219735
22	6	1.296953	1.149694	0.809692
23	1	1.778765	0.759001	1.714543
24	6	1.838024	3.041243	-0.831632
25	1	1.001011	2.760847	-1.488250
26	1	1.433757	3.832889	-0.185443
27	1	2.652810	3.441126	-1.435906
28	1	4.316513	1.983249	-0.511734
29	1	3.889194	0.738941	0.705247
30	1	0.607931	-1.673113	1.701173
31	6	-2.975002	-0.106258	-0.992829
32	6	-3.027938	1.192759	-0.158434
33	6	-2.571299	0.981609	1.288300
34	1	-2.645715	1.924140	1.845488
35	6	-0.895185	0.070473	2.900782
36	1	0.143141	-0.185839	3.135517
37	1	-1.169119	0.920126	3.535318
38	1	-1.517730	-0.778484	3.199828
39	1	-1.707334	-1.884507	-1.151975
40	1	-4.047766	1.593986	-0.168316
41	1	-2.407347	1.958669	-0.640944
42	6	-2.850478	0.230727	-2.495066

43	1	-2.843848	-0.677380	-3.108130
44	1	-3.696781	0.845471	-2.821104
45	1	-1.929643	0.787627	-2.704299
46	6	-4.270369	-0.933471	-0.782968
47	1	-5.136959	-0.380690	-1.161852
48	1	-4.222439	-1.887744	-1.318698
49	1	-4.442167	-1.154032	0.275129
50	1	-3.247167	0.277270	1.787714
51	1	-0.652973	-2.776181	1.256671
52	1	4.430419	-0.346013	-1.321614
53	1	1.302788	0.207417	0.160847

TS (J-K)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7580286 hartrees (-490560.980526786 kcal/mol)
Imaginary Frequencies: 1 (-934.7170 1/cm)
Zero-point correction = 0.480708 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5862705 hartrees (-490453.200601455 kcal/mol)

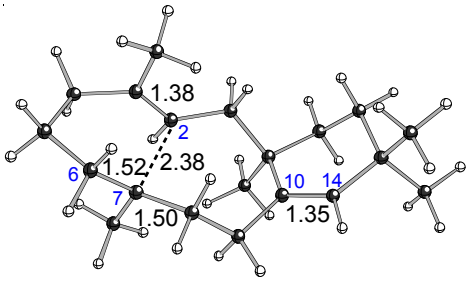
Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.074502	-0.422263	1.397486
2	6	1.017872	0.811908	0.468081
3	6	0.108635	1.998422	0.814251
4	6	-0.769139	2.588883	-0.349802
5	1	-0.952456	3.647203	-0.138421
6	6	-2.079317	1.869556	-0.416112
7	6	-2.199694	0.707089	-1.165517
8	6	-3.474305	-0.111286	-1.312711

9	1	-3.459201	-0.610117	-2.285057
10	6	-3.638376	-1.204798	-0.175472
11	6	-2.306552	-1.855220	0.029601
12	6	0.076254	-1.553477	0.973871
13	1	0.438524	-2.007742	0.049526
14	1	0.128736	-2.336139	1.744298
15	6	-3.164673	2.374876	0.478329
16	1	-3.597924	3.268700	0.004901
17	1	-3.975610	1.664811	0.642343
18	1	-2.768323	2.708753	1.443113
19	6	1.885691	0.953588	-0.551790
20	1	-1.441813	0.569194	-1.938059
21	1	-0.230347	2.522440	-1.297105
22	6	-1.374447	-1.168821	0.791848
23	1	-1.790291	-0.498069	1.547207
24	6	-1.990832	-3.045624	-0.819600
25	1	-0.932166	-3.302320	-0.845076
26	1	-2.532154	-3.908689	-0.406258
27	1	-2.359612	-2.920419	-1.844328
28	1	-4.403635	-1.919342	-0.487788
29	1	-3.981438	-0.717764	0.742384
30	1	-0.545170	1.758405	1.656473
31	6	3.021998	0.039078	-0.954463
32	6	2.995634	-1.259783	-0.118353
33	6	2.504230	-1.026693	1.313565
34	1	2.526111	-1.969710	1.873939
35	6	0.820405	-0.046931	2.875795
36	1	-0.216423	0.234971	3.087067
37	1	1.055208	-0.901303	3.519275
38	1	1.459465	0.785306	3.187542
39	1	1.840993	1.873416	-1.139334
40	1	3.998445	-1.701222	-0.096597
41	1	2.359228	-1.999986	-0.619031
42	6	2.916500	-0.292801	-2.459591
43	1	2.968800	0.614132	-3.072439
44	1	3.740638	-0.947044	-2.764615
45	1	1.976278	-0.806462	-2.690776
46	6	4.346393	0.810070	-0.714677
47	1	5.196306	0.219724	-1.073853
48	1	4.352208	1.764580	-1.252196
49	1	4.503837	1.023959	0.347011
50	1	3.190934	-0.346386	1.831409
51	1	0.737970	2.820697	1.171746
52	1	-4.365510	0.521356	-1.298792

53	1	-1.546292	-0.099570	-0.226947

K



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7774733 hartrees (-490573.182270483 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.487250 (Hartree/Particle)

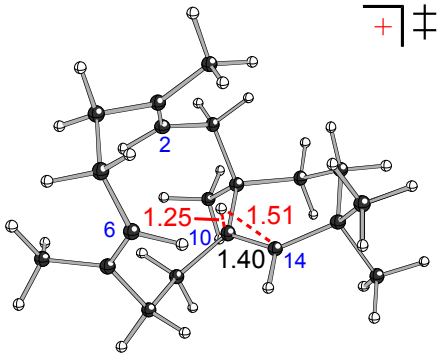
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.6065482 hartrees (-490465.925060982 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.099318	-0.218710	1.201785
2	6	-1.299894	-0.880048	-0.170079
3	6	-0.248807	-1.835702	-0.713191
4	6	0.983589	-1.163943	-1.368490
5	1	1.330705	-1.826234	-2.183288
6	6	2.255371	-0.941165	-0.598243
7	6	3.383795	-0.328567	-1.402159
8	6	4.495269	0.346965	-0.575203
9	1	5.035026	1.045363	-1.219626
10	6	3.873490	1.076747	0.659142
11	6	2.409374	1.298958	0.412310
12	6	-0.013923	0.902164	1.103584
13	1	-0.275440	1.577291	0.287031
14	1	-0.094883	1.501527	2.026797
15	6	2.695676	-1.999598	0.377179
16	1	3.564550	-1.704499	0.966029
17	1	1.908531	-2.350080	1.041215
18	1	3.006101	-2.860500	-0.235566
19	6	-2.383622	-0.635840	-0.929804
20	1	3.814168	-1.162648	-1.977497

21	1	0.688884	-0.240351	-1.878695
22	6	1.448927	0.554947	1.064939
23	1	1.798338	-0.110714	1.849257
24	6	2.058594	2.400052	-0.551078
25	1	1.178131	2.181174	-1.160021
26	1	1.828519	3.306672	0.026015
27	1	2.894813	2.646428	-1.209290
28	1	4.369300	2.040817	0.815655
29	1	4.022548	0.489693	1.568960
30	1	0.069354	-2.560157	0.042500
31	6	-3.528451	0.309816	-0.637343
32	6	-3.149437	1.221952	0.548795
33	6	-2.432808	0.442977	1.652964
34	1	-2.238100	1.091281	2.516091
35	6	-0.728050	-1.247416	2.293499
36	1	0.227647	-1.750026	2.125323
37	1	-0.671155	-0.757439	3.272355
38	1	-1.495218	-2.024608	2.358544
39	1	-2.472757	-1.175564	-1.874625
40	1	-4.049500	1.698564	0.953868
41	1	-2.510658	2.038044	0.185506
42	6	-3.804330	1.168391	-1.891642
43	1	-4.101067	0.544918	-2.742334
44	1	-4.617889	1.875985	-1.697739
45	1	-2.919418	1.744249	-2.185647
46	6	-4.798974	-0.518694	-0.322411
47	1	-5.660774	0.143921	-0.185432
48	1	-5.031988	-1.204042	-1.144354
49	1	-4.681734	-1.119647	0.584334
50	1	-3.095406	-0.351126	2.015458
51	1	-0.725597	-2.430648	-1.497491
52	1	5.233958	-0.380540	-0.228204
53	1	2.972187	0.363168	-2.142455

TS (D-L)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7529657 hartrees (-490557.803506407 kcal/mol)
Imaginary Frequencies: 1 (-463.2480 1/cm)
Zero-point correction = 0.483227 (Hartree/Particle)

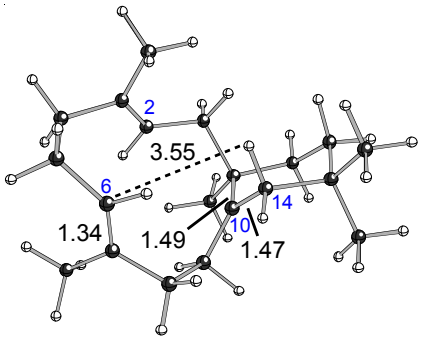
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5812135 hartrees (-490450.027283385 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.263480	-0.553969	1.502453
2	6	-0.714276	-0.995830	0.111369
3	6	0.220493	-2.212318	-0.017542
4	6	1.214362	-2.241867	-1.211503
5	1	1.583777	-3.270346	-1.287645
6	6	2.366071	-1.279482	-0.989303
7	6	2.296363	-0.014208	-1.442378
8	6	3.194534	1.137409	-1.057062
9	1	2.979063	1.994323	-1.703024
10	6	3.034511	1.554979	0.443190
11	6	1.595238	1.724797	0.887838
12	6	-0.423753	0.659908	2.079201
13	1	-0.944990	1.591657	1.852877
14	1	-0.441672	0.562602	3.171483
15	6	3.508495	-1.817735	-0.162300
16	1	3.926331	-2.710596	-0.643699
17	1	4.318751	-1.097567	-0.041471
18	1	3.186062	-2.129372	0.840100
19	6	-1.317030	-0.497343	-1.050771
20	1	1.460202	0.241317	-2.095645
21	1	0.708283	-2.038902	-2.161925

22	6	0.999523	0.738852	1.596413
23	1	1.627195	-0.109864	1.867212
24	6	0.940217	3.019231	0.473344
25	1	-0.121744	3.078410	0.719095
26	1	1.437870	3.860809	0.970964
27	1	1.054333	3.193278	-0.604017
28	1	3.585872	2.491022	0.594642
29	1	3.515877	0.798765	1.069551
30	1	0.787358	-2.313044	0.908046
31	6	-2.485968	0.425643	-1.157354
32	6	-2.958544	0.920949	0.225271
33	6	-2.742612	-0.112744	1.335963
34	1	-3.085553	0.300626	2.290403
35	6	-1.218184	-1.729155	2.502261
36	1	-0.200384	-1.989613	2.803757
37	1	-1.756116	-1.435992	3.408514
38	1	-1.704077	-2.628296	2.110261
39	1	-0.910769	-0.844110	-2.000827
40	1	-4.018358	1.188105	0.162496
41	1	-2.432322	1.850125	0.468549
42	6	-2.179964	1.599164	-2.114012
43	1	-1.887140	1.246959	-3.108478
44	1	-3.077066	2.214872	-2.227578
45	1	-1.382621	2.237810	-1.721881
46	6	-3.570626	-0.489966	-1.820668
47	1	-4.453368	0.128153	-2.009448
48	1	-3.236342	-0.895709	-2.780356
49	1	-3.867590	-1.320276	-1.174528
50	1	-3.360668	-1.000572	1.149594
51	1	-0.441663	-3.086293	-0.065874
52	1	4.250730	0.895164	-1.221988
53	1	-0.071476	-0.021341	-0.345631

L



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7749464 hartrees (-490571.596615464 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.484843 (Hartree/Particle)

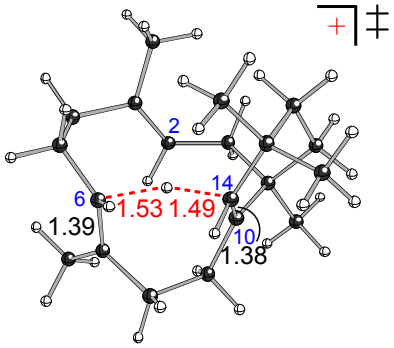
mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.5999907 hartrees (-490461.810164157 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.099799	0.103274	1.524513
2	6	-0.779238	-0.688147	0.299626
3	6	-0.107138	-2.002798	0.358312
4	6	0.921843	-2.402505	-0.749385
5	1	1.070946	-3.482912	-0.644489
6	6	2.236823	-1.658093	-0.593803
7	6	2.467600	-0.566102	-1.341190
8	6	3.587872	0.433697	-1.192003
9	1	3.650326	1.037445	-2.102634
10	6	3.394697	1.371495	0.048959
11	6	1.965168	1.843748	0.223626
12	6	-0.267673	1.468078	1.437203
13	1	-0.723476	2.118479	0.690147
14	1	-0.436486	1.937474	2.415713
15	6	3.178694	-2.192275	0.457052
16	1	3.418774	-3.243852	0.256523
17	1	4.118634	-1.639194	0.494087
18	1	2.738885	-2.159849	1.463324
19	6	-1.266063	-0.181071	-0.993318
20	1	1.712901	-0.307008	-2.084729
21	1	0.500593	-2.240494	-1.744286
22	6	1.201456	1.268607	1.172280
23	1	1.694224	0.557149	1.833199
24	6	1.502280	2.899937	-0.748289
25	1	0.453770	3.182929	-0.629947
26	1	2.099261	3.811038	-0.619609
27	1	1.655217	2.578480	-1.786275
28	1	4.073667	2.226213	-0.057505
29	1	3.703415	0.828182	0.947218
30	1	0.302046	-2.197876	1.348778
31	6	-2.837986	0.063567	-1.014714

32	6	-3.179119	0.973651	0.178837
33	6	-2.638045	0.457565	1.511787
34	1	-2.788611	1.203205	2.299536
35	6	-0.779827	-0.601468	2.855210
36	1	0.289178	-0.772284	3.004018
37	1	-1.123505	0.030489	3.678735
38	1	-1.299340	-1.560526	2.944639
39	1	-0.981025	-0.829831	-1.821443
40	1	-4.269007	1.068237	0.255238
41	1	-2.802632	1.983608	-0.020590
42	6	-3.177663	0.756117	-2.344103
43	1	-2.906797	0.132337	-3.202333
44	1	-4.254668	0.944831	-2.400915
45	1	-2.662307	1.717308	-2.442347
46	6	-3.573354	-1.287929	-0.942551
47	1	-4.653119	-1.129693	-1.027274
48	1	-3.274882	-1.943869	-1.767534
49	1	-3.398635	-1.827307	-0.005127
50	1	-3.188144	-0.436100	1.826203
51	1	-0.983927	-2.681519	0.256852
52	1	4.560018	-0.060364	-1.088536
53	1	-0.798467	0.799203	-1.156926

TS (L-K)



B3LYP/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.7400803 hartrees (-490549.717789053 kcal/mol)
Imaginary Frequencies: 1 (-1244.5122 1/cm)
Zero-point correction = 0.480943 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -781.569628 hartrees (-490442.75726628 kcal/mol)

Coordinates (from last standard orientation):

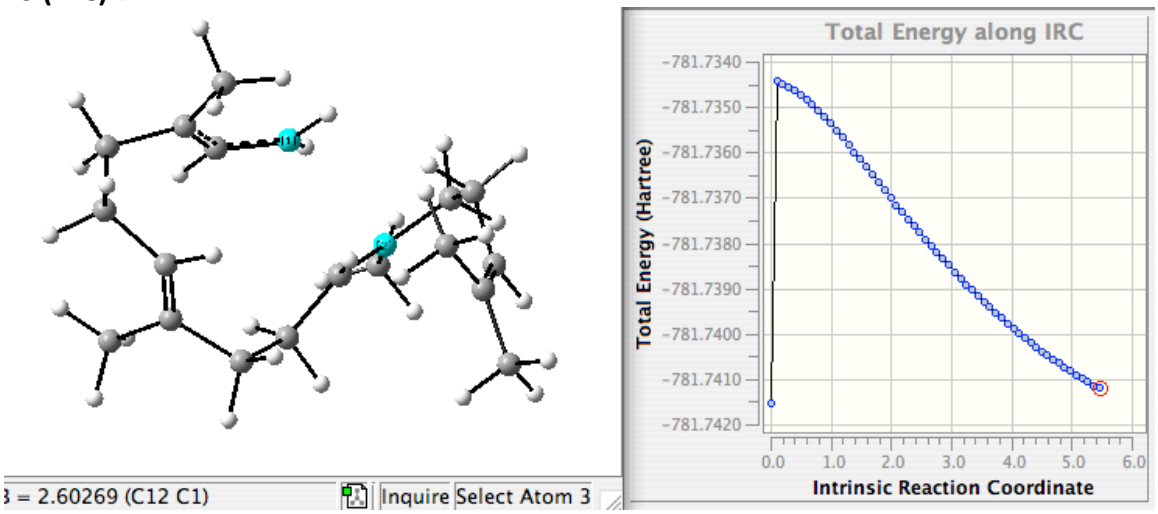
Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.362934	-0.875578	1.324120
2	6	-0.735454	-1.202717	-0.033985
3	6	0.181033	-2.390137	-0.189857
4	6	1.275620	-2.312241	-1.323882
5	1	1.796782	-3.272839	-1.321842
6	6	2.223915	-1.188686	-1.024468
7	6	1.895234	0.103942	-1.401870
8	6	2.619427	1.373986	-0.968846
9	1	2.109984	2.218064	-1.445398
10	6	2.713507	1.646012	0.563667
11	6	1.373355	1.588171	1.277167
12	6	-0.414241	0.012557	2.265901
13	1	-0.977969	0.902117	2.554693
14	1	-0.253287	-0.561391	3.185461
15	6	3.418199	-1.549853	-0.192070
16	1	3.988561	-2.302864	-0.752918
17	1	4.079491	-0.710037	0.008463
18	1	3.149266	-2.025604	0.758776
19	6	-0.961972	-0.404541	-1.140811
20	1	1.362057	0.191991	-2.350273
21	1	0.798885	-2.206622	-2.301425
22	6	0.918265	0.389452	1.689151
23	1	1.603959	-0.448793	1.574226
24	6	0.661415	2.906271	1.444287
25	1	-0.306551	2.821123	1.940383
26	1	1.280833	3.580627	2.048598
27	1	0.509249	3.411132	0.481766
28	1	3.168640	2.634865	0.685798
29	1	3.403033	0.937142	1.028637
30	1	0.653999	-2.628648	0.766171
31	6	-1.998107	0.706733	-1.252276
32	6	-2.509955	1.106101	0.147878
33	6	-2.686193	-0.103555	1.067924
34	1	-3.090732	0.212385	2.035475
35	6	-1.709739	-2.187433	2.071021
36	1	-0.822580	-2.747558	2.379227
37	1	-2.265502	-1.938492	2.980062
38	1	-2.344088	-2.845217	1.467768
39	1	-0.681120	-0.817187	-2.109686
40	1	-3.460952	1.639480	0.042660
41	1	-1.811899	1.816780	0.601477

42	6	-1.405253	1.926547	-1.986046
43	1	-1.048417	1.659713	-2.987746
44	1	-2.170650	2.699451	-2.107997
45	1	-0.573988	2.368590	-1.428256
46	6	-3.156454	0.136880	-2.113342
47	1	-3.917339	0.909002	-2.264947
48	1	-2.801929	-0.176300	-3.101494
49	1	-3.638394	-0.724730	-1.641835
50	1	-3.423949	-0.794784	0.642281
51	1	-0.445068	-3.258278	-0.436232
52	1	3.635725	1.374765	-1.384698
53	1	0.455943	-0.009349	-0.889163

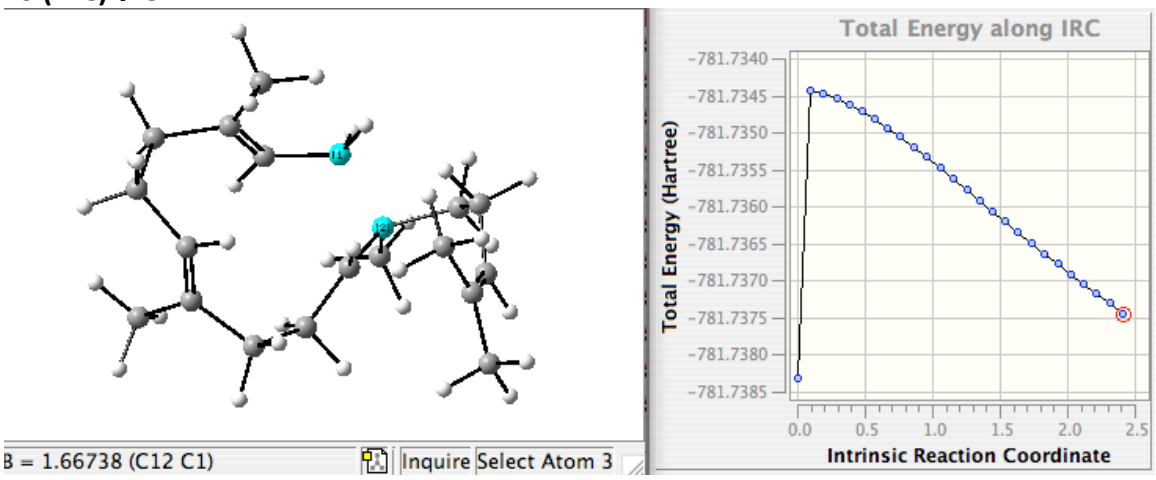
IRC Plots

Figure 1

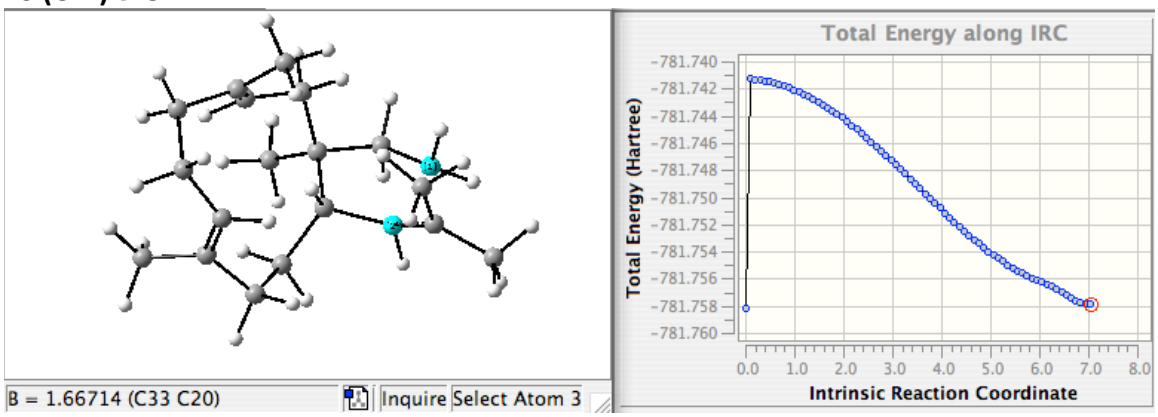
TS (A-C)→A



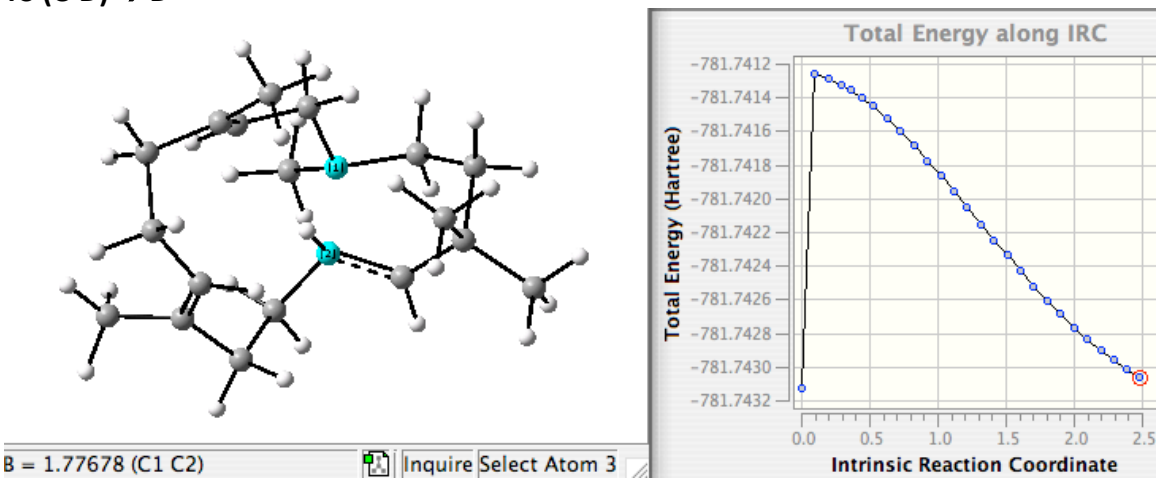
TS (A-C)→C



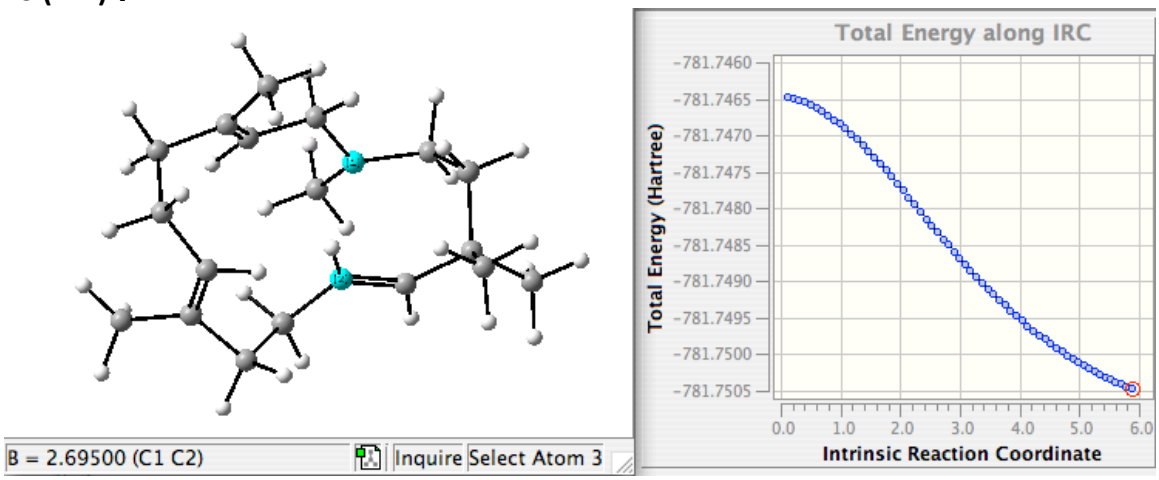
TS (C-D)→C



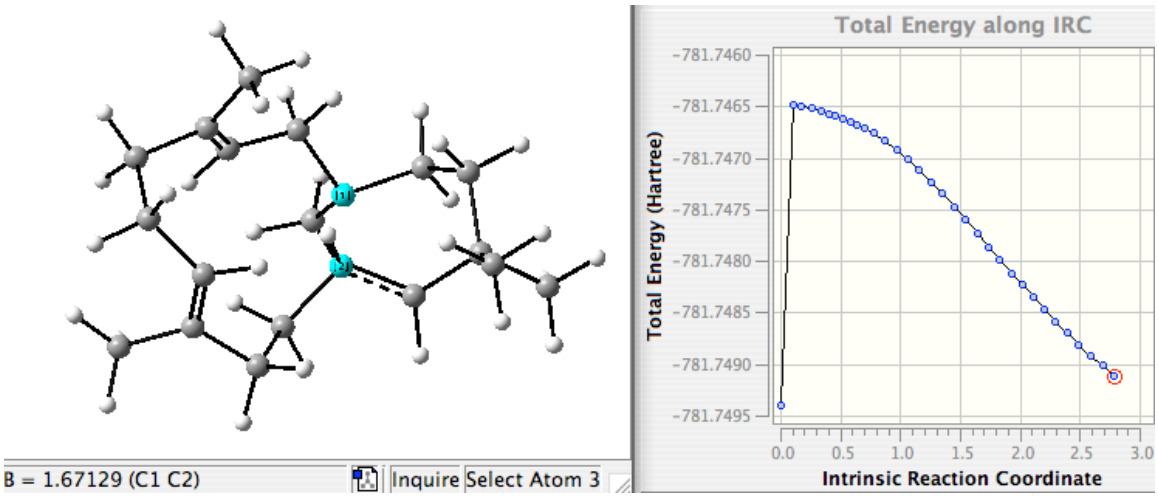
TS (C-D) →D



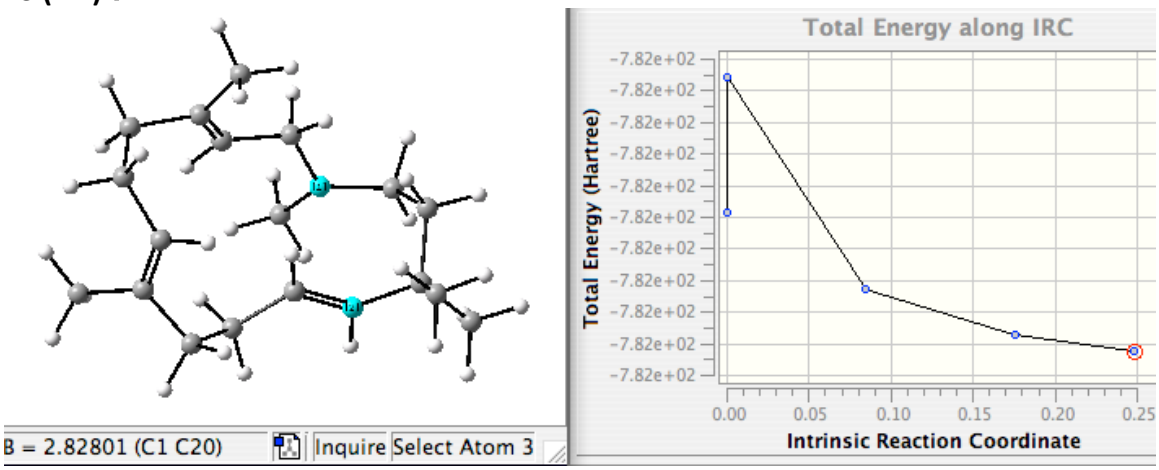
TS (D-E)→D



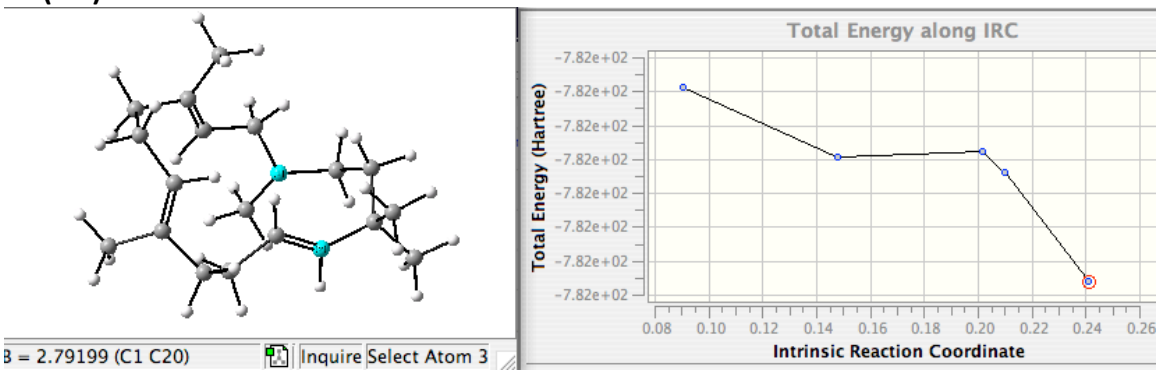
TS (D-E)→E



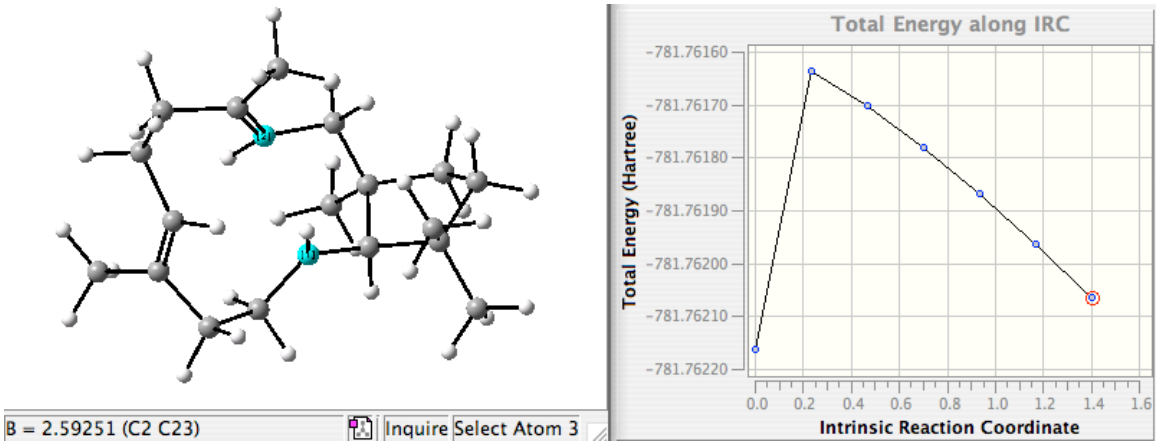
TS (E-F)→E



TS (E-F)→F



TS (F-G)→F



TS (F-G)→G

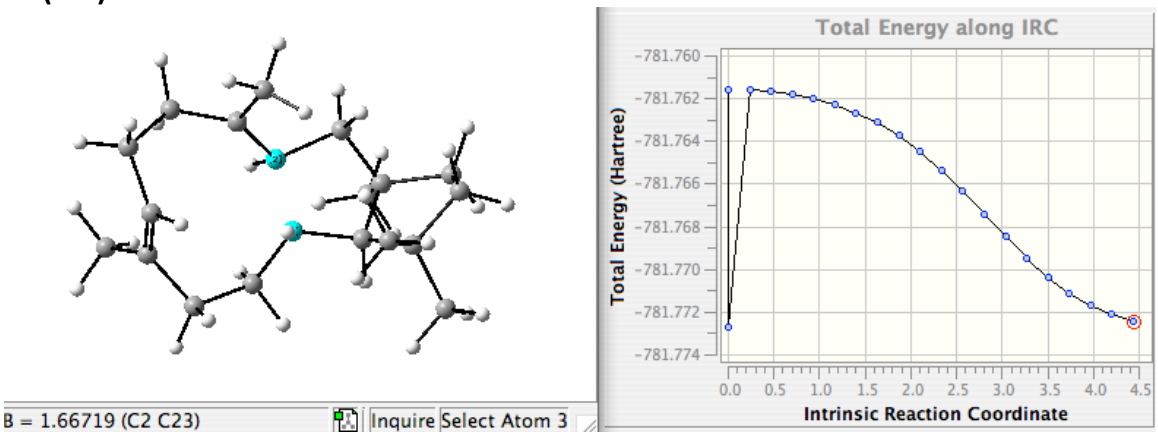
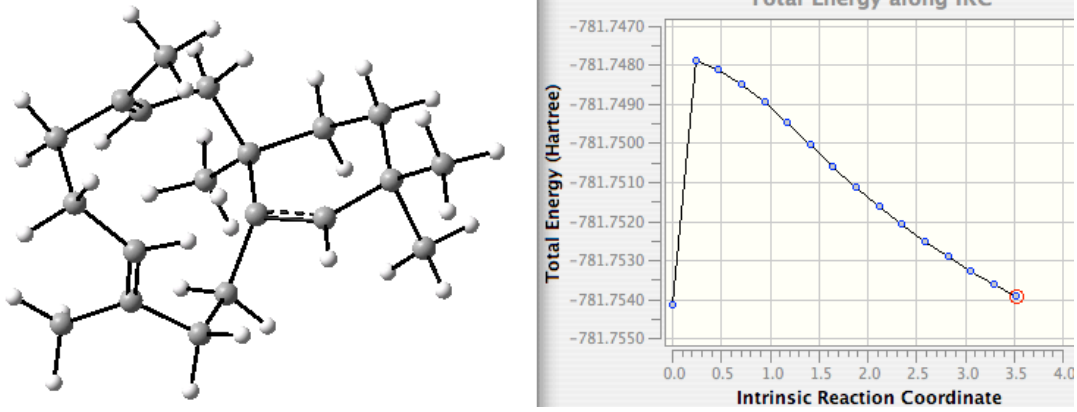
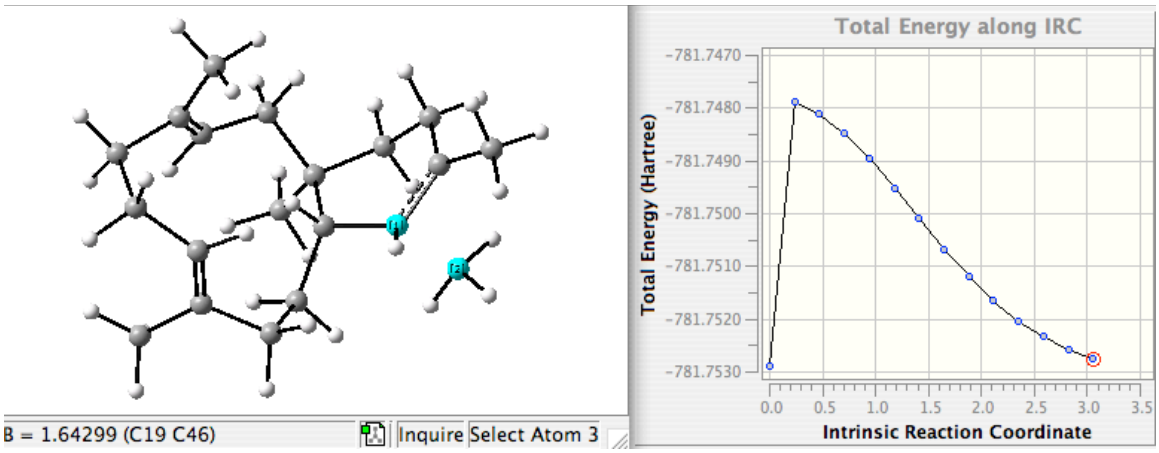


Figure 3

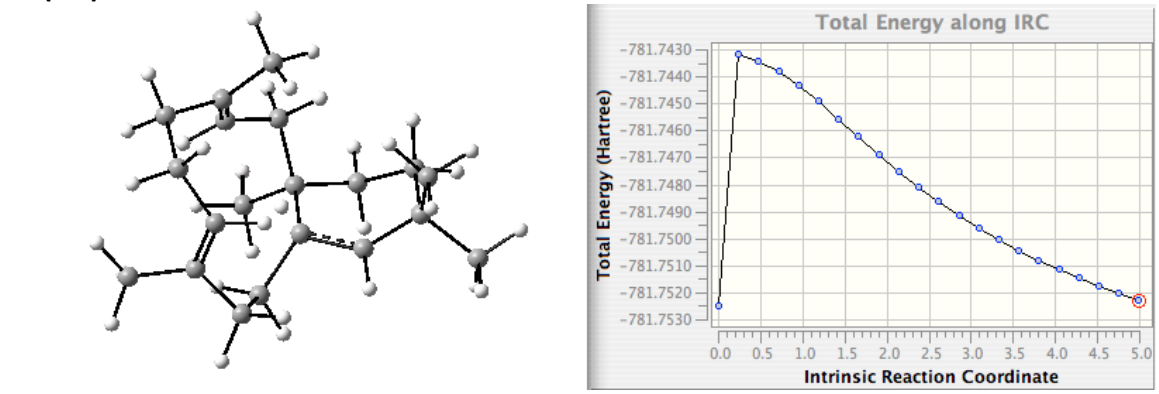
TS (D-H)→D



TS (D-H)→H



TS (D-I) → D



TS (D-I) → I

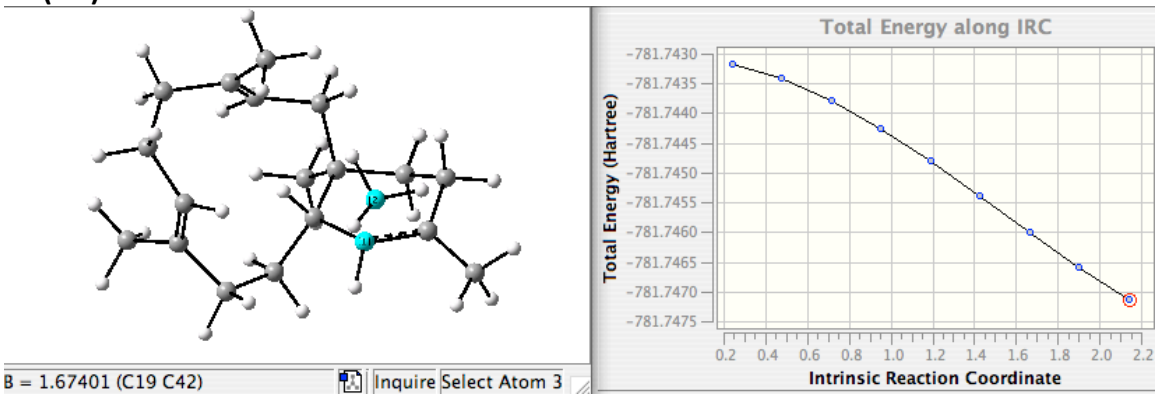
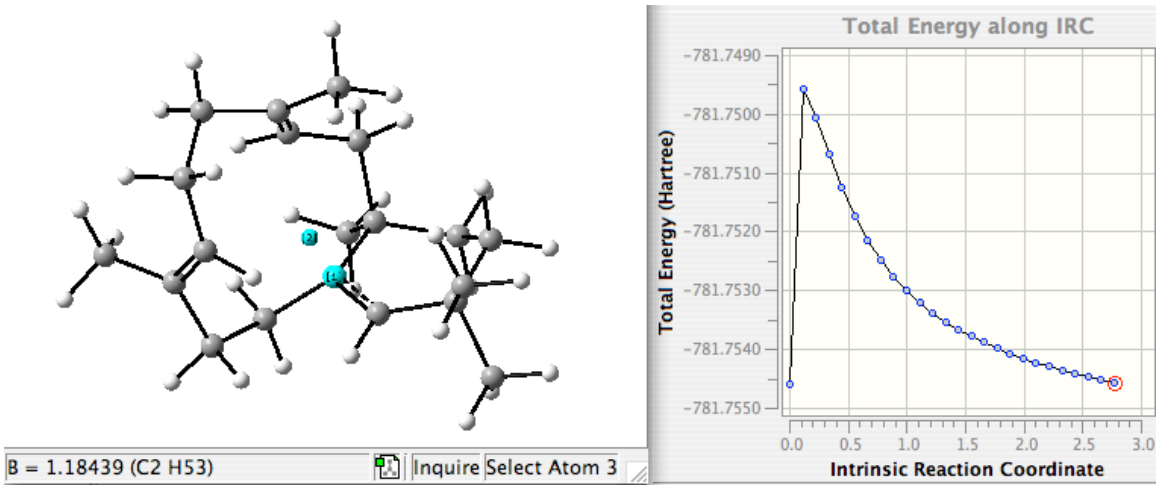
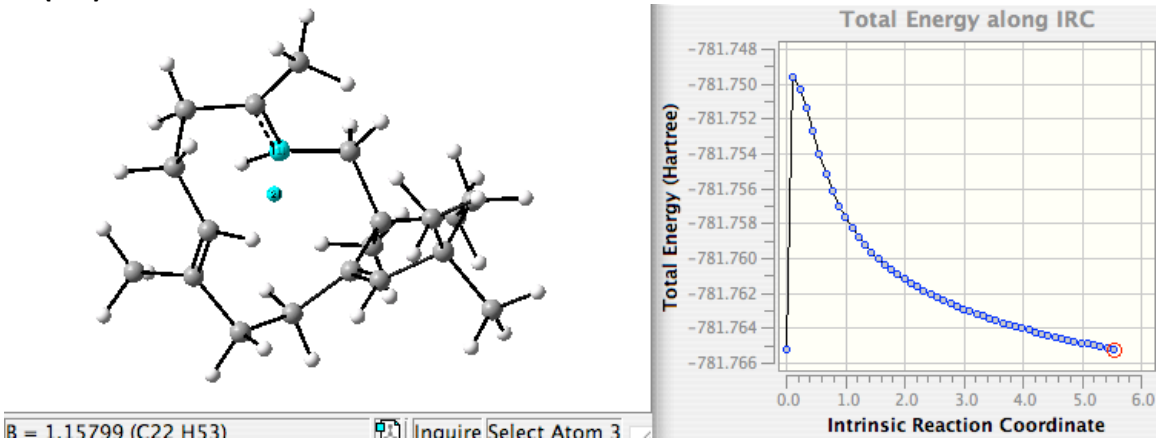


Figure 4

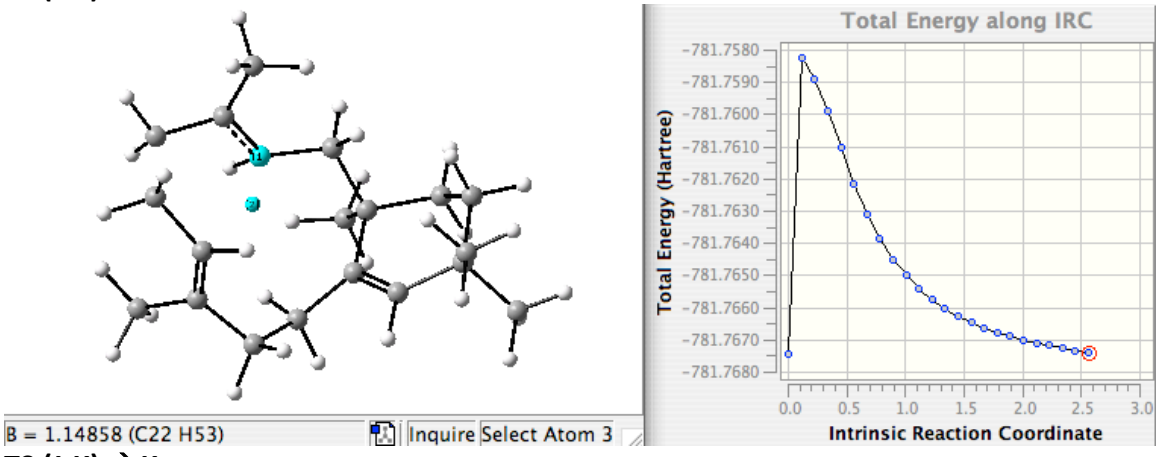
TS (D-J) → D



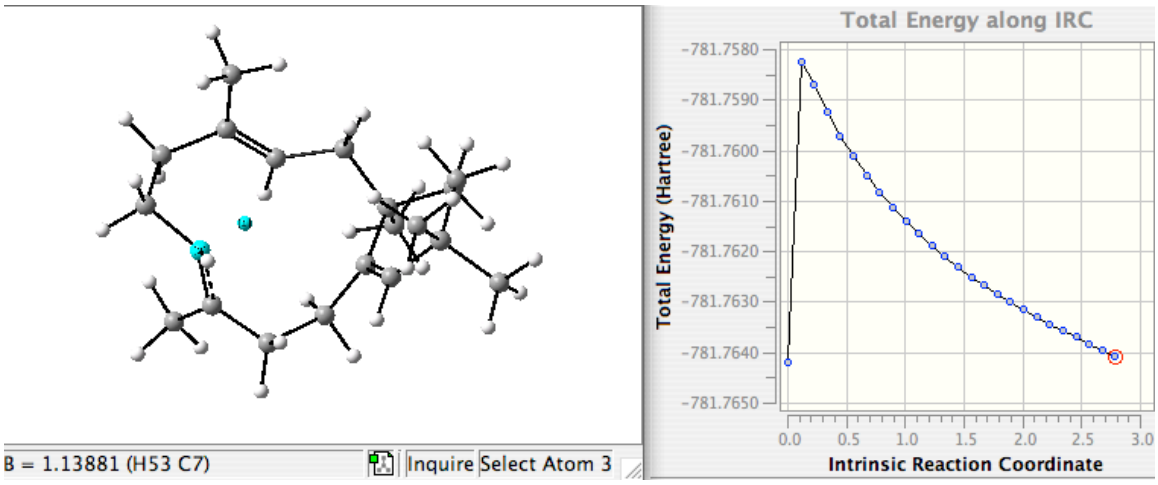
TS (D-J) →J



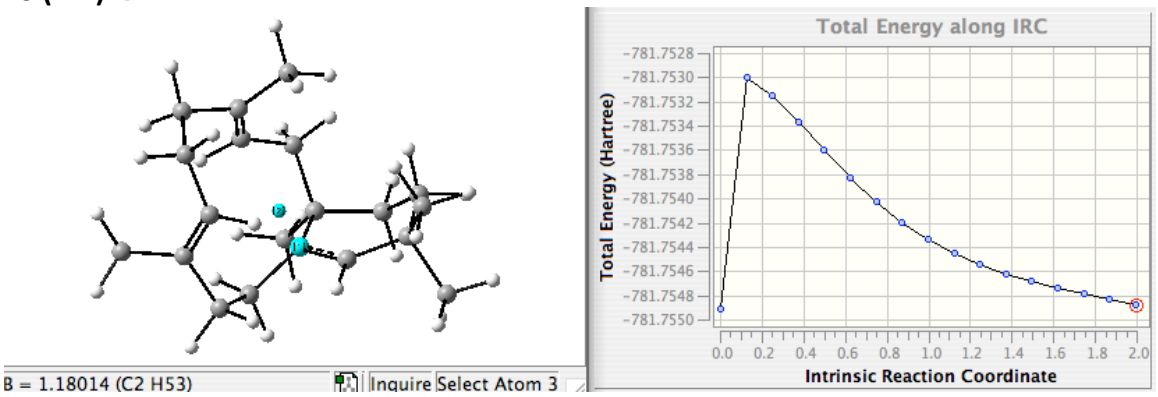
TS (J-K) →J



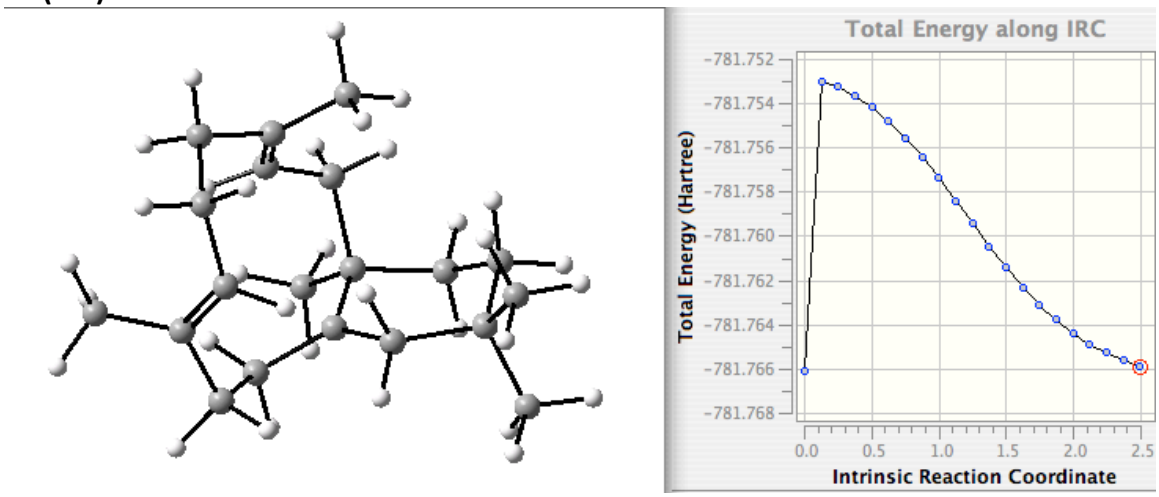
TS (J-K) →K



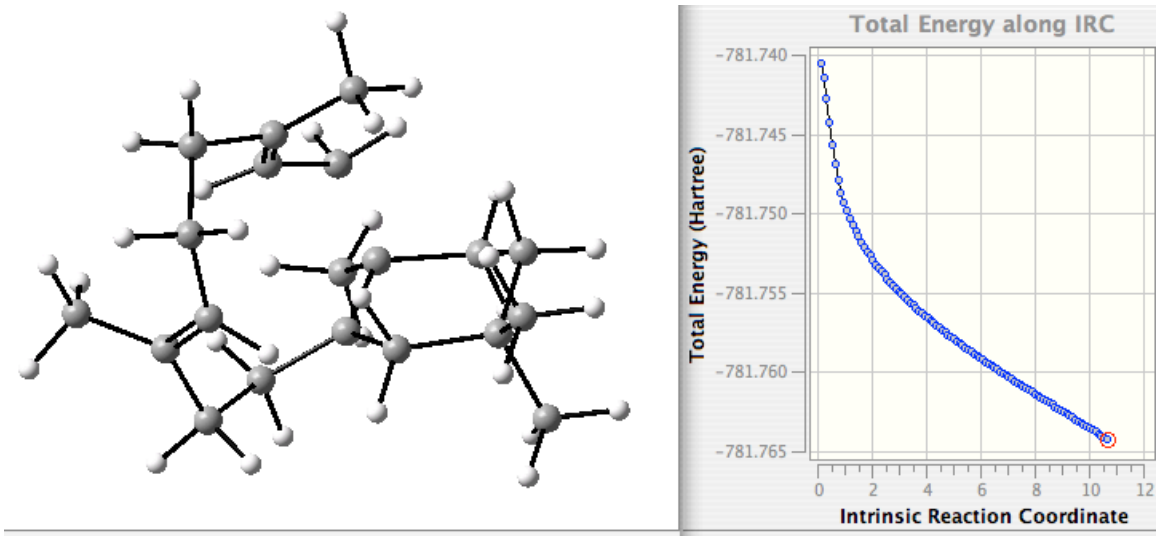
TS (D-L) → D



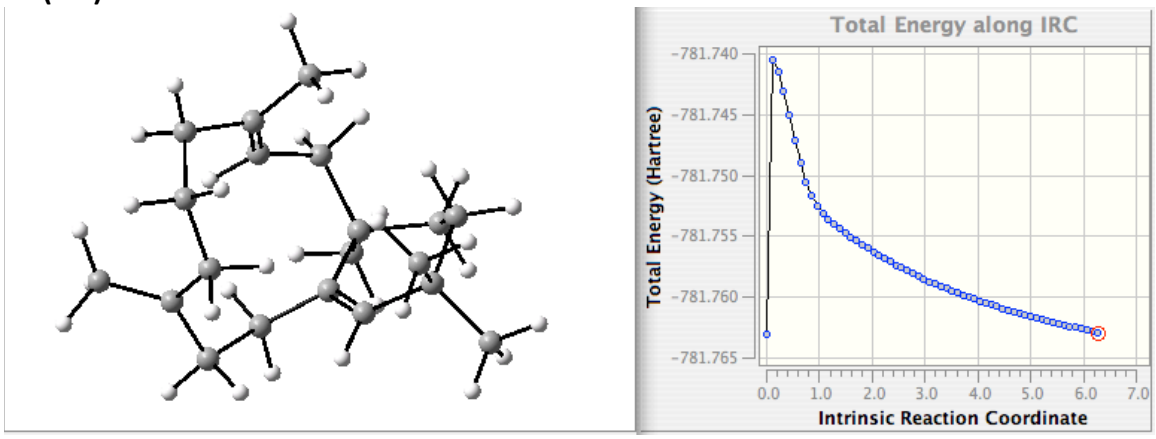
TS (D-L) → L



TS (L-K) → L


Total Energy along IRC
-781.740
-781.745
-781.750
-781.755
-781.760
-781.765
Total Energy (Hartree)
0
2
4
6
8
10
12
Intrinsic Reaction Coordinate

TS (L-K) → K


Total Energy along IRC
-781.740
-781.745
-781.750
-781.755
-781.760
-781.765
Total Energy (Hartree)
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0
Intrinsic Reaction Coordinate