Supporting Information for

The Energetic Viability of an Unexpected Skeletal Rearrangement in Cyclooctatin Biosynthesis

Young J. Hong, Dean J. Tantillo*

Department of Chemistry, University of California—Davis, Davis, CA 95616, USA
djtantillo@ucdavis.edu

**djtantillo@ucdavis.edu*

Table of Contents

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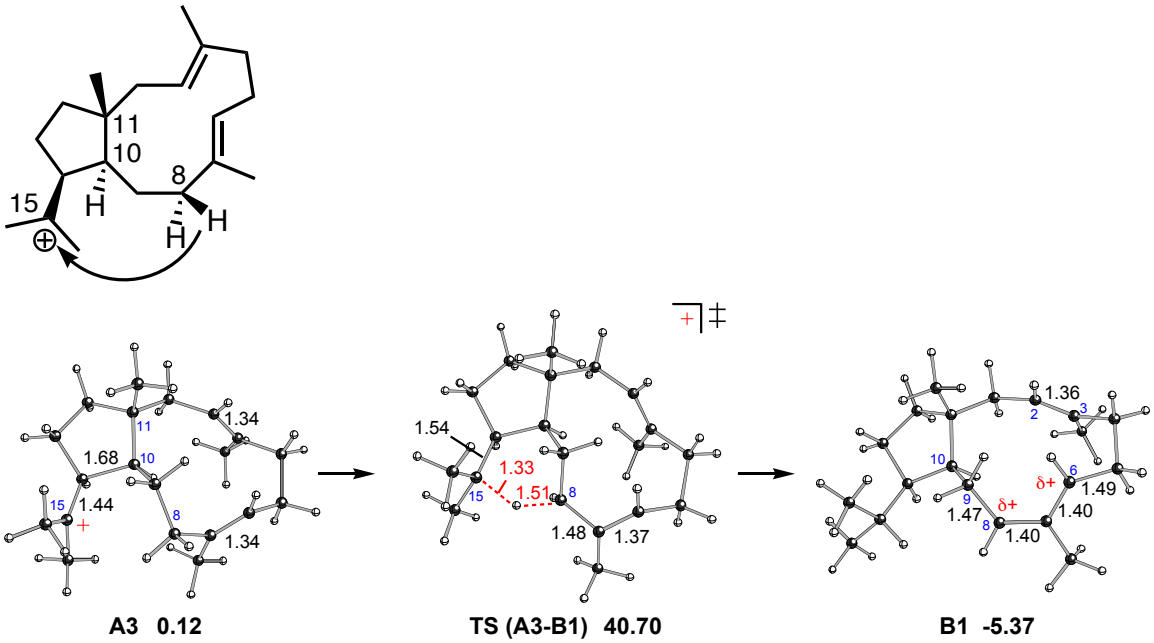

Figure S1. Conversion of **A3** to **B1** via an alternative 1,5-hydride shift (B3LYP/6-31G(d)//B3LYP/6-31G(d)). Computed distances (Å) and energies (kcal/mol) are shown.

Coordinates and Energies

Figure 1
A1
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6977075 hartrees (-490523.128433325 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.487150 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.581778 hartrees (-490450.38151278 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.046425	-2.492870	0.339557
2	6	-0.714863	-1.966957	-0.271884
3	6	-0.778677	-0.371700	-0.192139
4	6	1.175421	2.027461	-0.737833
5	6	2.176201	1.189393	-1.049559
6	6	3.536556	1.050616	-0.419617
7	1	4.323111	1.366359	-1.118809
8	1	3.634451	1.689466	0.463227
9	6	3.811110	-0.437755	-0.033874
10	6	2.655965	-1.055488	0.732421
11	6	0.507001	-2.458611	0.576041
12	1	0.326572	-2.199034	1.625635
13	1	0.510204	-3.557515	0.529547
14	6	1.825890	-1.906333	0.102626
15	6	2.502861	-0.584156	2.157647
16	1	1.660187	-1.042499	2.681781
17	1	3.409704	-0.819911	2.729607
18	1	2.383728	0.506691	2.208628
19	1	3.986871	-1.009972	-0.952381
20	6	-3.039608	-1.331129	0.240026
21	1	-3.927078	-1.460120	0.869461
22	1	-3.376691	-1.191828	-0.793211
23	6	-2.169386	-0.154893	0.706739
24	6	-2.674262	1.192476	0.647685
25	6	-3.679646	1.605520	-0.354478
26	1	-4.660153	1.276650	0.035661
27	1	-3.728026	2.686840	-0.496394
28	1	-3.559367	1.087333	-1.309870
29	6	-2.279137	2.163977	1.692907
30	1	-3.077258	2.125726	2.458051
31	1	-1.347880	1.891420	2.195772
32	1	-2.248897	3.195374	1.332403
33	6	-0.209438	1.866708	-1.374472
34	6	1.303014	3.186507	0.221541
35	1	2.313514	3.303088	0.617695
36	1	0.616688	3.090379	1.075850
37	6	-0.699109	0.409795	-1.510695
38	1	-2.411326	-3.388250	-0.171317
39	1	1.041017	4.128304	-0.280253
40	1	-1.807366	-0.345644	1.724612
41	6	-0.609989	-2.497678	-1.717998
42	1	0.294267	-2.167808	-2.234711
43	1	-0.584846	-3.592193	-1.691206
44	1	-1.471856	-2.204724	-2.328067
45	1	0.029982	-0.010463	0.444250
46	1	-1.907084	-2.761995	1.393946
47	1	2.101169	-2.195293	-0.911546
48	1	-1.646120	0.375803	-2.065355
49	1	0.006283	-0.120548	-2.153323
50	1	-0.235712	2.332483	-2.369726
51	1	4.739950	-0.479193	0.549566
52	1	1.981091	0.431582	-1.808609

53	1	-0.930011	2.450201	-0.778767

TS (A1-B1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6884788 hartrees (-490517.337331788 kcal/mol)
Imaginary Frequencies: 1 (-347.3550 1/cm)
Zero-point correction = 0.485518 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.576426 hartrees (-490447.02307926 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.944497	-2.556020	0.402994
2	6	-0.610297	-2.121563	-0.296081
3	6	-0.655838	-0.556488	-0.261544
4	6	0.842604	2.110803	-0.795068
5	6	1.880540	1.252473	-0.944404
6	6	3.270374	1.280441	-0.377260
7	1	3.985642	1.696845	-1.100971
8	1	3.321198	1.920334	0.510028
9	6	3.716021	-0.182961	-0.035944
10	6	2.642206	-0.964925	0.709614
11	6	0.654929	-2.594594	0.516768
12	1	0.473951	-2.405447	1.580451
13	1	0.744735	-3.683778	0.407917
14	6	1.924312	-1.908651	0.065798
15	6	2.429394	-0.544118	2.144381
16	1	1.661983	-1.127049	2.658585
17	1	3.362833	-0.660376	2.710220
18	1	2.156556	0.518124	2.220189
19	1	3.957173	-0.696471	-0.973835
20	6	-2.865179	-1.317827	0.385766
21	1	-3.672155	-1.377517	1.123865
22	1	-3.327562	-1.192571	-0.600642
23	6	-1.858000	-0.186696	0.674789
24	6	-2.287076	1.262858	0.586582
25	6	-3.518406	1.624924	-0.198374
26	1	-4.384777	1.263777	0.376420
27	1	-3.629869	2.706059	-0.315342
28	1	-3.564763	1.138262	-1.175276
29	6	-2.012678	2.115139	1.800121
30	1	-2.741949	1.821046	2.571159
31	1	-1.016999	1.933436	2.214853
32	1	-2.151991	3.181839	1.607157
33	6	-0.509559	1.694898	-1.269219
34	6	0.959380	3.485854	-0.180274
35	1	1.987390	3.716069	0.106339
36	1	0.328900	3.599447	0.710423
37	6	-0.762065	0.232611	-1.584625
38	1	-2.410214	-3.416691	-0.086474
39	1	0.639557	4.254190	-0.896318
40	1	-1.486259	-0.328913	1.698676
41	6	-0.563286	-2.705292	-1.721458

42	1	0.326591	-2.392038	-2.277625
43	1	-0.546803	-3.799210	-1.671787
44	1	-1.443028	-2.419150	-2.309536
45	1	0.254561	-0.208465	0.217516
46	1	-1.751697	-2.849465	1.442125
47	1	2.234470	-2.148042	-0.952708
48	1	-1.734932	0.108400	-2.070837
49	1	-0.023158	-0.127011	-2.306472
50	1	-1.017541	2.423909	-1.912854
51	1	4.644273	-0.129360	0.546260
52	1	1.689243	0.344949	-1.506140
53	1	-1.262626	1.809665	-0.280747

B1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7089338 hartrees (-490530.173048838 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.489824 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5911667 hartrees (-490456.273015917 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.867418	-2.310288	0.686830
2	6	-0.736995	-1.665917	-0.163087
3	6	-0.946925	-0.128571	0.171562
4	6	1.640386	2.114237	-0.144122
5	6	2.476972	1.219339	-0.811575
6	6	3.925729	0.978083	-0.576411
7	1	4.511841	1.432802	-1.392115
8	1	4.262072	1.441829	0.354715
9	6	4.109992	-0.562929	-0.549807
10	6	2.989731	-1.160740	0.302030
11	6	0.636838	-2.198649	0.343233
12	1	0.677311	-2.064527	1.428809
13	1	0.631120	-3.287492	0.175236
14	6	1.878666	-1.648585	-0.300639
15	6	3.230495	-1.122233	1.788174
16	1	2.350062	-1.374001	2.381970
17	1	4.021396	-1.838883	2.048968
18	1	3.593843	-0.138738	2.114095
19	1	4.060933	-0.954660	-1.571670
20	6	-3.060046	-1.361294	0.563748
21	1	-3.817097	-1.541578	1.332766
22	1	-3.550340	-1.499291	-0.405051
23	6	-2.441151	0.051589	0.678359
24	6	-3.311499	1.202837	0.101118
25	6	-3.914914	0.942173	-1.292265
26	1	-4.719161	0.200671	-1.242435
27	1	-4.353092	1.863734	-1.690392
28	1	-3.188112	0.579015	-2.028845
29	6	-4.441068	1.554588	1.087258
30	1	-5.116164	0.703913	1.235779

31	1	-4.045160	1.844013	2.067391
32	1	-5.042093	2.388409	0.708885
33	6	0.261816	1.963719	-0.309471
34	6	2.191485	3.153739	0.811782
35	1	3.011633	3.720201	0.361103
36	1	2.571462	2.690196	1.729780
37	6	-0.462257	0.868014	-0.974673
38	1	-2.090406	-3.331202	0.358667
39	1	1.413496	3.865371	1.100364
40	1	-2.347579	0.269546	1.749885
41	6	-0.954278	-2.017598	-1.646490
42	1	-0.178936	-1.616550	-2.308236
43	1	-0.946851	-3.105574	-1.774666
44	1	-1.917430	-1.652294	-2.016805
45	1	-0.303407	0.059390	1.038808
46	1	-1.548155	-2.369713	1.736064
47	1	1.898794	-1.708303	-1.389814
48	1	-1.331438	1.267995	-1.499234
49	1	0.150440	0.334198	-1.697728
50	1	-0.366678	2.663040	0.244533
51	1	5.101110	-0.809442	-0.154339
52	1	2.048135	0.639452	-1.620464
53	1	-2.674894	2.099388	0.030645

TS (B1-C1)

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6992195 hartrees (-490524.077228445 kcal/mol)
Imaginary Frequencies: 1 (-186.1571 1/cm)
Zero-point correction = 0.490423 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5862722 hartrees (-490453.201668222 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.664601	-2.131566	-0.781106
2	6	0.698987	-1.163234	-0.047095
3	6	1.257598	0.207271	-0.573953
4	6	-1.803050	1.746125	-0.400499
5	6	-2.194679	0.945174	0.746322
6	6	-3.644412	0.932376	1.280413
7	1	-3.672587	1.296734	2.311687
8	1	-4.263422	1.607699	0.686762
9	6	-4.170252	-0.516617	1.149092
10	6	-3.247948	-1.095917	0.094360
11	6	-0.763548	-1.453187	-0.504561
12	1	-0.916742	-1.053508	-1.513948
13	1	-0.861464	-2.546097	-0.596872
14	6	-1.892643	-1.028789	0.412339
15	6	-3.803154	-1.527852	-1.212703
16	1	-3.050371	-1.672057	-1.988928
17	1	-4.296811	-2.500125	-1.040741
18	1	-4.593952	-0.857896	-1.568233
19	1	-4.069359	-1.078068	2.085921

20	6	3.055517	-1.490220	-0.650997
21	1	3.739015	-1.840558	-1.429369
22	1	3.509599	-1.769499	0.305659
23	6	2.824597	0.046933	-0.727682
24	6	3.779379	0.904054	0.145459
25	6	3.690713	0.698684	1.665789
26	1	3.972749	-0.319023	1.960214
27	1	4.384332	1.378113	2.173173
28	1	2.690715	0.901106	2.063153
29	6	5.231244	0.706627	-0.328636
30	1	5.578409	-0.315947	-0.139437
31	1	5.334568	0.902287	-1.402239
32	1	5.906971	1.386360	0.201373
33	6	-0.482751	2.000885	-0.624950
34	6	-2.853068	2.259836	-1.362424
35	1	-3.510294	3.002461	-0.894724
36	1	-3.495321	1.452893	-1.736450
37	6	0.720253	1.501835	0.112936
38	1	1.620722	-3.146958	-0.370091
39	1	-2.387441	2.736594	-2.228451
40	1	3.046253	0.362722	-1.754888
41	6	0.843094	-1.378532	1.471832
42	1	0.335118	-0.615395	2.073505
43	1	0.429904	-2.353823	1.758053
44	1	1.888328	-1.369386	1.782415
45	1	0.897843	0.252287	-1.610896
46	1	1.375232	-2.199135	-1.839041
47	1	-1.683709	-1.156101	1.472864
48	1	1.486556	2.281458	0.063709
49	1	0.524447	1.331544	1.175225
50	1	-0.249696	2.590331	-1.512106
51	1	-5.221581	-0.555456	0.856079
52	1	-1.440519	0.925875	1.526541
53	1	3.529655	1.957256	-0.053535

C1
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7139843 hartrees (-490533.342288093 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.489877 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6069556 hartrees (-490466.180708556 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.524653	2.129482	-0.705817
2	6	-0.621377	1.058814	-0.034667
3	6	-1.276429	-0.241110	-0.626463
4	6	1.707607	-1.744901	-0.464441
5	6	1.997948	-0.881867	0.739899
6	6	3.392129	-1.013073	1.403839
7	1	3.314122	-0.760459	2.466904
8	1	3.805047	-2.021592	1.342514

9	6	4.274866	0.029021	0.690836
10	6	3.350489	1.021996	0.103686
11	6	0.850409	1.286684	-0.493243
12	1	0.972291	0.939412	-1.526352
13	1	1.023087	2.371275	-0.507861
14	6	1.963228	0.669576	0.376973
15	6	3.802506	2.185393	-0.674809
16	1	3.498993	2.031066	-1.724147
17	1	3.273707	3.096776	-0.365097
18	1	4.882479	2.338389	-0.635766
19	1	5.053725	0.512968	1.298809
20	6	-2.955149	1.580644	-0.582351
21	1	-3.622567	2.014455	-1.332322
22	1	-3.375290	1.846523	0.393418
23	6	-2.830475	0.036526	-0.730050
24	6	-3.823605	-0.790440	0.130712
25	6	-3.696849	-0.652656	1.655951
26	1	-3.910187	0.367963	1.996204
27	1	-4.423709	-1.307585	2.149068
28	1	-2.705379	-0.934157	2.025080
29	6	-5.268115	-0.482556	-0.305423
30	1	-5.548699	0.550922	-0.068942
31	1	-5.402058	-0.627120	-1.383793
32	1	-5.976496	-1.140238	0.209842
33	6	0.436365	-2.078794	-0.755443
34	1	-3.645071	-1.847865	-0.112361
35	6	2.837641	-2.128954	-1.388900
36	1	3.272025	-1.248999	-1.891303
37	1	2.485945	-2.797825	-2.178633
38	6	-0.821716	-1.616272	-0.063472
39	1	-1.402816	3.118803	-0.248348
40	1	3.660458	-2.635739	-0.868591
41	1	-3.098824	-0.219975	-1.762826
42	6	-0.724910	1.216451	1.494579
43	1	-0.243933	0.404890	2.052193
44	1	-0.262828	2.161622	1.810653
45	1	-1.762312	1.246718	1.829252
46	1	-0.943791	-0.238273	-1.673876
47	1	-1.246434	2.226607	-1.764496
48	1	1.891190	1.126733	1.397217
49	1	-1.604125	-2.356554	-0.254738
50	1	-0.706324	-1.579033	1.025284
51	1	0.273284	-2.677976	-1.651450
52	1	4.832433	-0.406416	-0.157976
53	1	1.222600	-1.059101	1.484063

TS (C1-D1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7076182 hartrees (-490529.347496682 kcal/mol)
Imaginary Frequencies: 1 (-526.9280 1/cm)
Zero-point correction = 0.488483 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6033758 hartrees (-490463.934348258 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.515409	2.096129	-0.813398
2	6	-0.610185	1.039152	-0.124165
3	6	-1.296852	-0.275084	-0.648000
4	6	1.677281	-1.821384	-0.459512
5	6	1.964023	-0.847552	0.681761
6	6	3.326972	-0.969921	1.413411
7	1	3.194230	-0.712082	2.470000
8	1	3.735997	-1.980524	1.380439
9	6	4.254130	0.066246	0.746306
10	6	3.322769	1.069259	0.112973
11	6	0.844801	1.233287	-0.643997
12	1	0.917511	0.866117	-1.676894
13	1	1.046558	2.309624	-0.696948
14	6	1.990138	0.577764	0.104575
15	6	3.824608	2.336304	-0.497792
16	1	4.336738	2.061270	-1.430859
17	1	3.035106	3.045763	-0.750392
18	1	4.567325	2.818774	0.143985
19	1	4.981188	0.530412	1.419624
20	6	-2.948892	1.572120	-0.630232
21	1	-3.627558	1.981907	-1.383476
22	1	-3.342484	1.888057	0.341610
23	6	-2.849158	0.021294	-0.710524
24	6	-3.822110	-0.748735	0.223629
25	6	-3.640741	-0.539919	1.735316
26	1	-3.830738	0.498170	2.034313
27	1	-4.357479	-1.161202	2.283590
28	1	-2.640595	-0.816452	2.084227
29	6	-5.276691	-0.440463	-0.177039
30	1	-5.533852	0.607997	0.016262
31	1	-5.451033	-0.637177	-1.241269
32	1	-5.975261	-1.059940	0.395646
33	6	0.404693	-2.154683	-0.728150
34	1	-3.665777	-1.818966	0.026585
35	6	2.829217	-2.333656	-1.291239
36	1	3.370482	-1.521034	-1.798058
37	1	2.469487	-3.011653	-2.069668
38	6	-0.848015	-1.638032	-0.057496
39	1	-1.369324	3.101130	-0.399236
40	1	3.565579	-2.884605	-0.693264
41	1	-3.157556	-0.280287	-1.719525
42	6	-0.657966	1.269921	1.399338
43	1	-0.193637	0.469611	1.984518
44	1	-0.150160	2.210236	1.654991
45	1	-1.683179	1.360013	1.759693
46	1	-0.998020	-0.312680	-1.704923
47	1	-1.265662	2.147101	-1.882246
48	1	2.343519	1.313236	1.079680
49	1	-1.641551	-2.371885	-0.225915
50	1	-0.730839	-1.577874	1.031187
51	1	0.236646	-2.834477	-1.563295
52	1	4.829872	-0.369448	-0.083436
53	1	1.148778	-0.931428	1.398467

D1
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7219341 hartrees (-490538.330867091 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491348 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6140406 hartrees (-490470.626616906 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.572013	2.202745	-0.448879
2	6	-0.672457	1.073518	0.122853
3	6	-1.275256	-0.155276	-0.632589
4	6	1.772414	-1.583931	-0.461175
5	6	1.975564	-0.772478	0.868301
6	6	3.358983	-0.899833	1.533265
7	1	3.274093	-0.541498	2.565299
8	1	3.706002	-1.934705	1.580957
9	6	4.280710	0.024365	0.711357
10	6	3.331619	1.106067	0.147599
11	6	0.796395	1.360917	-0.269641
12	1	0.892543	1.403954	-1.367959
13	1	1.046037	2.391120	0.034955
14	6	1.943705	0.542358	0.214610
15	6	3.778163	1.835118	-1.128636
16	1	3.843396	1.140459	-1.972327
17	1	3.100236	2.648761	-1.401388
18	1	4.770577	2.266308	-0.972071
19	1	5.073283	0.469828	1.317679
20	6	-2.993414	1.612428	-0.433108
21	1	-3.645430	2.117065	-1.151288
22	1	-3.449274	1.756807	0.551751
23	6	-2.831910	0.097942	-0.754487
24	6	-3.825327	-0.846264	-0.024885
25	6	-3.757088	-0.867244	1.510080
26	1	-4.021230	0.103339	1.946726
27	1	-4.475041	-1.595486	1.902681
28	1	-2.769650	-1.150849	1.888693
29	6	-5.262955	-0.536221	-0.481884
30	1	-5.584453	0.459006	-0.152123
31	1	-5.355044	-0.573389	-1.573529
32	1	-5.966530	-1.263302	-0.062648
33	6	0.511750	-1.930518	-0.813646
34	1	-3.602888	-1.866018	-0.372359
35	6	2.958467	-2.068676	-1.266385
36	1	3.480008	-1.265410	-1.797131
37	1	2.613709	-2.779671	-2.022172
38	6	-0.799066	-1.558333	-0.178784
39	1	-1.488267	3.134241	0.122944
40	1	3.694548	-2.585992	-0.642751
41	1	-3.062394	-0.042018	-1.817880
42	6	-0.817720	1.065789	1.658786
43	1	-0.354296	0.205121	2.149009
44	1	-0.360189	1.968928	2.081239

45	1	-1.865900	1.067980	1.959190
46	1	-0.909187	-0.040948	-1.662938
47	1	-1.268993	2.426976	-1.481110
48	1	3.216944	1.877188	0.942496
49	1	-1.536242	-2.306973	-0.480571
50	1	-0.737670	-1.617562	0.914977
51	1	0.433276	-2.583346	-1.683290
52	1	4.769062	-0.511849	-0.105571
53	1	1.135572	-0.992895	1.523990

TS (D1-D2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7155593 hartrees (-490534.330616343 kcal/mol)
Imaginary Frequencies: 1 (-78.8761 1/cm)
Zero-point correction = 0.490560 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6072935 hartrees (-490466.392744185 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.452641	-1.833514	-1.276861
2	6	0.567396	-0.914671	-0.398000
3	6	1.295905	0.451148	-0.585505
4	6	-1.646893	2.047818	-0.367508
5	6	-2.151199	0.853396	0.440001
6	6	-3.566305	0.900792	1.084797
7	1	-3.501407	1.266425	2.112509
8	1	-4.210348	1.596699	0.545239
9	6	-4.127911	-0.542621	1.006920
10	6	-2.983363	-1.437573	0.467148
11	6	-0.922934	-0.908161	-1.036410
12	1	-0.880743	-0.177213	-1.855206
13	1	-1.117469	-1.904359	-1.437127
14	6	-1.991026	-0.505604	-0.130051
15	6	-3.435962	-2.640759	-0.380335
16	1	-3.908940	-2.309036	-1.310020
17	1	-2.613292	-3.318073	-0.624071
18	1	-4.176282	-3.210720	0.187705
19	1	-4.491776	-0.905894	1.970747
20	6	2.889482	-1.422686	-0.900190
21	1	3.596848	-1.681058	-1.692884
22	1	3.213517	-1.967551	-0.007457
23	6	2.841246	0.112032	-0.631949
24	6	3.778741	0.624929	0.493513
25	6	3.503105	0.111548	1.915007
26	1	3.640050	-0.973783	1.996548
27	1	4.208390	0.569842	2.616734
28	1	2.495363	0.357039	2.266397
29	6	5.244400	0.349310	0.108792
30	1	5.459631	-0.725727	0.086731
31	1	5.485665	0.760012	-0.878363
32	1	5.925725	0.804664	0.835221
33	6	-0.343215	2.363358	-0.395901

34	1	3.663135	1.718267	0.519501
35	6	-2.678932	2.841722	-1.132768
36	1	-3.309066	2.197005	-1.760497
37	1	-2.191308	3.572191	-1.783539
38	6	0.813174	1.650209	0.269297
39	1	1.248399	-2.896620	-1.107810
40	1	-3.352052	3.395382	-0.466773
41	1	3.210600	0.615312	-1.533846
42	6	0.522831	-1.470487	1.034176
43	1	0.027358	-0.806915	1.751991
44	1	0.009105	-2.439396	1.053306
45	1	1.529554	-1.636831	1.417497
46	1	1.066542	0.732193	-1.621239
47	1	1.262156	-1.624779	-2.337161
48	1	-2.406945	-1.848777	1.324715
49	1	1.632757	2.366536	0.375306
50	1	0.567560	1.337952	1.292595
51	1	-0.059905	3.206918	-1.024468
52	1	-4.972525	-0.592315	0.311517
53	1	-1.417379	0.741485	1.271177

D2

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7221926 hartrees (-490538.493078426 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491100 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6139367 hartrees (-490470.561418617 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.509718	-1.880574	-1.252548
2	6	0.600424	-0.972558	-0.386560
3	6	1.290642	0.410917	-0.599619
4	6	-1.676871	1.965697	-0.373186
5	6	-2.146607	0.762281	0.424689
6	6	-3.545260	0.746107	1.096241
7	1	-3.606632	1.464033	1.917063
8	1	-4.316506	1.014583	0.367483
9	6	-3.689216	-0.716133	1.552418
10	6	-2.980234	-1.517303	0.436205
11	6	-0.883455	-1.026425	-1.011166
12	1	-0.868582	-0.352311	-1.878116
13	1	-1.065850	-2.052124	-1.343266
14	6	-1.954369	-0.600909	-0.112366
15	6	-3.947900	-1.840093	-0.761998
16	1	-3.435092	-2.374991	-1.564763
17	1	-4.741450	-2.479821	-0.366081
18	1	-4.407884	-0.937786	-1.174177
19	1	-3.171151	-0.872870	2.505974
20	6	2.935445	-1.423448	-0.891622
21	1	3.646570	-1.677825	-1.682288
22	1	3.278441	-1.940970	0.010254

23	6	2.845346	0.113620	-0.653516
24	6	3.776494	0.672443	0.455346
25	6	3.525716	0.174709	1.887107
26	1	3.696555	-0.904339	1.984921
27	1	4.220870	0.666061	2.576505
28	1	2.512979	0.394280	2.241168
29	6	5.246831	0.433049	0.064354
30	1	5.493984	-0.635297	0.058717
31	1	5.469240	0.834002	-0.931218
32	1	5.919365	0.920546	0.778070
33	6	-0.380769	2.308867	-0.412321
34	1	3.630731	1.762352	0.464200
35	6	-2.744437	2.739862	-1.108203
36	1	-3.314424	2.099238	-1.795596
37	1	-2.298715	3.547422	-1.694679
38	6	0.789661	1.610635	0.245280
39	1	1.336323	-2.945929	-1.063893
40	1	-3.469669	3.191449	-0.419784
41	1	3.193486	0.609637	-1.567821
42	6	0.575485	-1.507279	1.056425
43	1	0.066214	-0.844363	1.764714
44	1	0.079432	-2.484674	1.091810
45	1	1.586355	-1.646977	1.439389
46	1	1.044406	0.672165	-1.636853
47	1	1.308481	-1.696806	-2.315727
48	1	-2.543159	-2.471847	0.753722
49	1	1.599092	2.339026	0.345001
50	1	0.552148	1.301551	1.271608
51	1	-0.119781	3.168367	-1.028694
52	1	-4.727999	-1.026890	1.688045
53	1	-1.427647	0.640322	1.274548

TS (D2-E1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7131172 hartrees (-490532.798174172 kcal/mol)
Imaginary Frequencies: 1 (-492.7888 1/cm)
Zero-point correction = 0.488871 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6084825 hartrees (-490467.138853575 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.579525	-1.845436	-1.331505
2	6	0.628424	-1.027862	-0.422528
3	6	1.272525	0.385783	-0.557479
4	6	-1.702215	1.996947	-0.410681
5	6	-2.324155	0.774473	0.133977
6	6	-3.627942	0.796279	0.918117
7	1	-3.656445	1.596871	1.661788
8	1	-4.430179	0.998429	0.195813
9	6	-3.735699	-0.622891	1.509995
10	6	-2.965557	-1.520776	0.513682
11	6	-0.825692	-1.064290	-1.000105

12	1	-0.850220	-0.490391	-1.934238
13	1	-1.063368	-2.104863	-1.243747
14	6	-1.941268	-0.574558	-0.107850
15	6	-3.865474	-2.091608	-0.606113
16	1	-3.294298	-2.670178	-1.337938
17	1	-4.606002	-2.760606	-0.158357
18	1	-4.403537	-1.301293	-1.141256
19	1	-3.250778	-0.649752	2.493303
20	6	2.988516	-1.347701	-0.956762
21	1	3.706134	-1.526916	-1.762042
22	1	3.360865	-1.896767	-0.085481
23	6	2.836855	0.169089	-0.634206
24	6	3.745851	0.709132	0.501559
25	6	3.518736	0.126501	1.904887
26	1	3.735948	-0.947737	1.944040
27	1	4.192638	0.610058	2.620522
28	1	2.497407	0.281258	2.269094
29	6	5.224661	0.555174	0.100406
30	1	5.517900	-0.499810	0.043215
31	1	5.427060	1.012590	-0.874896
32	1	5.876580	1.036957	0.836861
33	6	-0.390814	2.286133	-0.295618
34	1	3.553764	1.790730	0.566987
35	6	-2.683283	2.956750	-1.058668
36	1	-3.262668	2.474996	-1.855726
37	1	-2.143190	3.798278	-1.498902
38	6	0.708200	1.496297	0.371024
39	1	1.456680	-2.926368	-1.199216
40	1	-3.397932	3.362181	-0.332313
41	1	3.159545	0.728859	-1.520817
42	6	0.638569	-1.638728	0.992802
43	1	0.098837	-1.042772	1.740701
44	1	0.180254	-2.634862	0.974912
45	1	1.652737	-1.755864	1.374732
46	1	1.006502	0.698385	-1.575539
47	1	1.363988	-1.619757	-2.384473
48	1	-2.462960	-2.355528	1.013210
49	1	1.502869	2.198340	0.635838
50	1	0.369639	1.073396	1.327014
51	1	-0.077937	3.229919	-0.739826
52	1	-4.770595	-0.943228	1.647980
53	1	-1.467819	0.123210	0.909145

E1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7332163 hartrees (-490545.410560413 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491479 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6235795 hartrees (-490476.612372045 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	1.565953	-1.947358	-1.170348
2	6	0.676221	-1.141096	-0.190037
3	6	1.240430	0.282771	-0.450589
4	6	-1.686564	1.956079	-0.321483
5	6	-2.376156	0.797561	0.112357
6	6	-3.845868	0.858399	0.375866
7	1	-4.145964	1.788525	0.871969
8	1	-4.349726	0.881617	-0.607554
9	6	-4.185164	-0.442258	1.120822
10	6	-3.207551	-1.455913	0.504005
11	6	-0.817189	-1.246511	-0.575726
12	1	-0.961949	-0.879560	-1.599363
13	1	-1.057584	-2.314797	-0.604295
14	6	-1.887502	-0.606698	0.355841
15	6	-3.742034	-2.038166	-0.814489
16	1	-3.049502	-2.755248	-1.263250
17	1	-4.678887	-2.571345	-0.623468
18	1	-3.949834	-1.267063	-1.566423
19	1	-3.993114	-0.315515	2.192810
20	6	2.981889	-1.363085	-0.979727
21	1	3.613136	-1.538781	-1.855082
22	1	3.477920	-1.852713	-0.135466
23	6	2.795698	0.159553	-0.698829
24	6	3.788887	0.790366	0.310250
25	6	3.746683	0.249791	1.747865
26	1	4.038152	-0.805715	1.796432
27	1	4.455720	0.803393	2.372963
28	1	2.759365	0.347306	2.211913
29	6	5.221742	0.698211	-0.246092
30	1	5.563733	-0.342115	-0.298771
31	1	5.291830	1.126071	-1.252791
32	1	5.921213	1.241632	0.397837
33	6	-0.330686	2.174560	-0.142229
34	1	3.545178	1.863540	0.358642
35	6	-2.512335	3.099063	-0.903546
36	1	-3.232102	2.744391	-1.647626
37	1	-1.862939	3.830191	-1.391078
38	6	0.708623	1.371998	0.544190
39	1	1.524314	-3.026035	-0.983858
40	1	-3.074954	3.627964	-0.125307
41	1	2.985707	0.696590	-1.636224
42	6	0.889392	-1.693532	1.234636
43	1	0.448344	-1.077720	2.026688
44	1	0.436435	-2.689261	1.310760
45	1	1.946947	-1.800087	1.478720
46	1	0.844330	0.545698	-1.440978
47	1	1.222684	-1.781809	-2.200495
48	1	-3.009632	-2.284480	1.191828
49	1	1.513999	2.042114	0.851689
50	1	0.318032	0.894769	1.446878
51	1	0.024260	3.125651	-0.541551
52	1	-5.233510	-0.726900	1.003418
53	1	-1.478421	-0.552721	1.384608

TS (E1-E2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7284748 hartrees (-490542.435221748 kcal/mol)

Imaginary Frequencies: 1 (-70.6219 1/cm)
Zero-point correction = 0.492241 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6181204 hartrees (-490473.186732204 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.433077	-1.706432	-1.481388
2	6	0.587794	-1.081885	-0.343422
3	6	1.171166	0.363561	-0.349580
4	6	-1.619523	2.103889	-0.055894
5	6	-2.341849	0.884736	-0.006974
6	6	-3.774443	0.817593	-0.410351
7	1	-4.311321	1.763147	-0.302597
8	1	-3.763811	0.607134	-1.497843
9	6	-4.381484	-0.363185	0.366163
10	6	-3.192465	-1.295911	0.742259
11	6	-0.915946	-1.089760	-0.696692
12	1	-1.069988	-0.584685	-1.658651
13	1	-1.225561	-2.125888	-0.849533
14	6	-1.880512	-0.479869	0.402145
15	6	-3.330186	-2.689531	0.119070
16	1	-2.508873	-3.355927	0.403228
17	1	-4.255801	-3.150496	0.479175
18	1	-3.386151	-2.657012	-0.975279
19	1	-4.882911	0.011730	1.263547
20	6	2.863635	-1.183801	-1.234112
21	1	3.461509	-1.201944	-2.149519
22	1	3.377672	-1.828379	-0.514039
23	6	2.716610	0.261712	-0.671171
24	6	3.761255	0.675604	0.397856
25	6	3.756078	-0.122671	1.710562
26	1	4.017248	-1.174983	1.550133
27	1	4.504211	0.288179	2.397157
28	1	2.790579	-0.090875	2.226799
29	6	5.170181	0.660583	-0.223904
30	1	5.478691	-0.356628	-0.491811
31	1	5.217455	1.274827	-1.130450
32	1	5.908043	1.052300	0.484075
33	6	-0.306232	2.253282	0.372473
34	1	3.549702	1.725692	0.653865
35	6	-2.327488	3.343041	-0.588149
36	1	-2.752157	3.167524	-1.582016
37	1	-1.633722	4.182584	-0.673174
38	6	0.714408	1.281815	0.841391
39	1	1.378246	-2.800289	-1.492364
40	1	-3.145228	3.659193	0.069552
41	1	2.886891	0.960964	-1.499184
42	6	0.824759	-1.889731	0.948888
43	1	0.403273	-1.430992	1.850367
44	1	0.364726	-2.880155	0.849871
45	1	1.886241	-2.043956	1.146133
46	1	0.751902	0.812615	-1.258658
47	1	1.063199	-1.353339	-2.453645

48	1	-3.194578	-1.434386	1.828591
49	1	1.558449	1.841453	1.246211
50	1	0.326525	0.662391	1.658409
51	1	0.060964	3.277518	0.295500
52	1	-5.137531	-0.882384	-0.228251
53	1	-1.290895	-0.393162	1.319385

E2

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7363407 hartrees (-490547.371152657 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491934 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6263001 hartrees (-490478.319575751 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.354901	-1.717892	-1.483046
2	6	0.538045	-1.101249	-0.320340
3	6	1.119298	0.347923	-0.321097
4	6	-1.597408	2.151047	0.097931
5	6	-2.297861	0.923205	-0.002083
6	6	-3.682517	0.874365	-0.572727
7	1	-4.318886	1.500018	0.078554
8	1	-3.737875	1.360076	-1.556379
9	6	-4.118990	-0.597428	-0.523966
10	6	-3.284476	-1.160120	0.639518
11	6	-0.972330	-1.112037	-0.646104
12	1	-1.137002	-0.643060	-1.624132
13	1	-1.299045	-2.150355	-0.750444
14	6	-1.903409	-0.446693	0.449826
15	6	-3.273428	-2.682844	0.770094
16	1	-2.583658	-3.015672	1.553510
17	1	-4.273649	-3.034234	1.043701
18	1	-3.001077	-3.184932	-0.163890
19	1	-5.195399	-0.708938	-0.371672
20	6	2.789447	-1.197267	-1.269639
21	1	3.366054	-1.216452	-2.198618
22	1	3.319651	-1.841006	-0.560738
23	6	2.651939	0.247633	-0.706872
24	6	3.739455	0.668688	0.316162
25	6	3.798599	-0.135595	1.624515
26	1	4.061357	-1.184745	1.446949
27	1	4.572969	0.278217	2.279512
28	1	2.856800	-0.115605	2.183522
29	6	5.120161	0.665191	-0.366325
30	1	5.424955	-0.349512	-0.647505
31	1	5.122972	1.279650	-1.274005
32	1	5.884913	1.062787	0.309147
33	6	-0.293258	2.263172	0.558880
34	1	3.532858	1.716587	0.584517
35	6	-2.311357	3.423227	-0.333753
36	1	-2.556478	3.403062	-1.401826

37	1	-1.688108	4.302653	-0.157096
38	6	0.729098	1.241701	0.910160
39	1	1.298289	-2.811548	-1.501172
40	1	-3.249546	3.567463	0.213433
41	1	2.784473	0.944427	-1.543903
42	6	0.804534	-1.916434	0.961207
43	1	0.374282	-1.478538	1.868905
44	1	0.371821	-2.918044	0.855417
45	1	1.871674	-2.041779	1.150177
46	1	0.659652	0.821401	-1.197004
47	1	0.961288	-1.356708	-2.442945
48	1	-3.702914	-0.754283	1.572815
49	1	1.602460	1.763550	1.302298
50	1	0.362254	0.604457	1.724626
51	1	0.068231	3.291384	0.601757
52	1	-3.865827	-1.105285	-1.462473
53	1	-1.350153	-0.416595	1.390903

TS (E2-F1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7218488 hartrees (-490538.277340488 kcal/mol)
Imaginary Frequencies: 1 (-103.3927 1/cm)
Zero-point correction = 0.489228 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.615271 hartrees (-490471.39870521 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.355452	-2.235100	-1.032375
2	6	-0.288638	-1.090678	-1.161397
3	6	-0.892059	0.098657	-0.331803
4	6	1.266320	2.068452	-0.501520
5	6	1.560342	0.860947	0.278303
6	6	2.015278	0.937981	1.716099
7	1	2.740493	1.764260	1.771429
8	1	1.203932	1.226507	2.395144
9	6	2.706183	-0.403588	2.005216
10	6	3.254313	-0.807410	0.622556
11	6	1.011610	-1.535719	-0.459948
12	1	0.767018	-1.888224	0.549270
13	1	1.460808	-2.380685	-0.991083
14	6	2.082715	-0.413836	-0.352057
15	6	3.768019	-2.242509	0.508347
16	1	4.096392	-2.472083	-0.511210
17	1	4.631603	-2.376323	1.168113
18	1	3.012802	-2.978898	0.800245
19	1	3.492162	-0.310964	2.759118
20	6	-2.628197	-1.566857	-0.495975
21	1	-3.306580	-2.274074	-0.008483
22	1	-3.185982	-1.092467	-1.312259
23	6	-2.084949	-0.502011	0.479330
24	6	-3.111165	0.467581	1.122570
25	6	-4.251910	0.904180	0.185453

26	1	-4.914976	0.063136	-0.046130
27	1	-4.861467	1.673242	0.671349
28	1	-3.901617	1.316022	-0.766884
29	6	-3.703504	-0.159100	2.398394
30	1	-4.237545	-1.089947	2.172482
31	1	-2.924422	-0.389194	3.134592
32	1	-4.418031	0.523105	2.870487
33	6	0.118104	2.265884	-1.178726
34	1	-2.563327	1.369902	1.437181
35	6	2.350687	3.144329	-0.457331
36	1	2.361683	3.663625	0.507533
37	1	2.153467	3.885520	-1.235502
38	6	-1.113647	1.421644	-1.054116
39	1	-1.512098	-2.741143	-1.989580
40	1	3.350984	2.731992	-0.630193
41	1	-1.622812	-1.059514	1.307907
42	6	-0.030730	-0.779087	-2.646997
43	1	0.612847	0.093035	-2.805512
44	1	0.450645	-1.638817	-3.125476
45	1	-0.968290	-0.598915	-3.184043
46	1	-0.078130	0.367146	0.444934
47	1	-1.010533	-2.997613	-0.323910
48	1	4.091183	-0.133233	0.389649
49	1	-1.855369	2.033793	-0.526241
50	1	-1.542468	1.256146	-2.051364
51	1	0.013379	3.188891	-1.745216
52	1	1.987763	-1.144736	2.374144
53	1	2.436573	-0.192044	-1.364637

F1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7263751 hartrees (-490541.117639001 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.489647 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6222857 hartrees (-490475.800499607 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.367592	-1.889943	1.645460
2	6	0.253450	-0.787251	1.506187
3	6	0.888140	0.213020	0.508726
4	6	-1.232956	2.112972	0.194711
5	6	-1.297768	0.754993	-0.428238
6	6	-1.654231	0.609967	-1.917719
7	1	-2.370965	1.404648	-2.161549
8	1	-0.793351	0.765640	-2.576265
9	6	-2.325860	-0.766808	-2.037258
10	6	-3.051999	-0.927793	-0.687668
11	6	-1.001220	-1.417341	0.829014
12	1	-0.669778	-2.015772	-0.028679
13	1	-1.469064	-2.115191	1.530001
14	6	-2.024685	-0.368808	0.350656

15	6	-3.602985	-2.325930	-0.402500
16	1	-4.089219	-2.373578	0.578222
17	1	-4.353355	-2.593107	-1.153720
18	1	-2.820838	-3.092144	-0.432535
19	1	-3.008076	-0.823184	-2.890241
20	6	2.560165	-1.429249	0.782317
21	1	3.129737	-2.262317	0.360367
22	1	3.256100	-0.830228	1.378864
23	6	1.922706	-0.555419	-0.329708
24	6	2.872997	0.234648	-1.268062
25	6	4.133674	0.789902	-0.581080
26	1	4.809038	-0.019301	-0.282233
27	1	4.683582	1.430128	-1.278222
28	1	3.920347	1.387033	0.312107
29	6	3.278649	-0.646733	-2.463691
30	1	3.822122	-1.539846	-2.133258
31	1	2.405462	-0.976849	-3.038636
32	1	3.935872	-0.095515	-3.143408
33	6	-0.131498	2.495127	0.854736
34	1	2.303000	1.084088	-1.674797
35	6	-2.453694	2.997598	0.060583
36	1	-2.606342	3.320176	-0.975891
37	1	-2.342920	3.893443	0.676143
38	6	1.121074	1.654468	0.895350
39	1	1.652016	-2.021728	2.692873
40	1	-3.365811	2.477534	0.378333
41	1	1.348491	-1.248367	-0.962223
42	6	-0.114456	-0.189713	2.875950
43	1	-0.828787	0.635188	2.805779
44	1	-0.562874	-0.969900	3.499452
45	1	0.771473	0.174022	3.407371
46	1	-0.103647	0.397986	-0.375004
47	1	0.986170	-2.854887	1.297006
48	1	-3.899613	-0.227316	-0.689547
49	1	1.880427	2.113782	0.255282
50	1	1.532596	1.663772	1.914739
51	1	-0.084632	3.470036	1.332034
52	1	-1.577624	-1.558581	-2.173050
53	1	-2.532108	0.054093	1.224089

TS (F1-F2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7250241 hartrees (-490540.269872991 kcal/mol)
Imaginary Frequencies: 1 (-74.2460 1/cm)
Zero-point correction = 0.489087 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6208016 hartrees (-490474.869212016 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.417641	-1.410267	2.020733
2	6	0.269753	-0.422915	1.625768
3	6	0.894069	0.350516	0.453481

4	6	-1.300550	2.105581	-0.152185
5	6	-1.324771	0.663222	-0.552638
6	6	-1.700433	0.282498	-1.996153
7	1	-2.483060	0.976162	-2.330157
8	1	-0.866022	0.402891	-2.695154
9	6	-2.266935	-1.141570	-1.895885
10	6	-2.985082	-1.141524	-0.533045
11	6	-0.939403	-1.243219	1.071944
12	1	-0.565327	-1.982533	0.352850
13	1	-1.381267	-1.810509	1.896599
14	6	-2.007014	-0.355072	0.399720
15	6	-3.438365	-2.513624	-0.031003
16	1	-3.916847	-2.444695	0.952300
17	1	-4.171356	-2.942108	-0.722354
18	1	-2.606231	-3.222119	0.043857
19	1	-2.938161	-1.382828	-2.725092
20	6	2.401257	-1.516354	0.826285
21	1	2.500633	-2.540557	0.459090
22	1	3.398610	-1.193627	1.133147
23	6	1.858911	-0.587762	-0.300281
24	6	2.908340	0.049573	-1.250506
25	6	4.107649	0.707483	-0.543386
26	1	4.774834	-0.042934	-0.106470
27	1	4.698264	1.274894	-1.269860
28	1	3.820634	1.399210	0.256092
29	6	3.407805	-1.002040	-2.257332
30	1	3.927949	-1.823803	-1.751327
31	1	2.583469	-1.430276	-2.839506
32	1	4.114091	-0.551827	-2.961958
33	6	-0.192200	2.624488	0.395474
34	1	2.385270	0.824661	-1.830857
35	6	-2.553511	2.920512	-0.382677
36	1	-2.742028	3.075477	-1.451315
37	1	-2.463458	3.903286	0.086230
38	6	1.094494	1.841262	0.527250
39	1	1.933493	-1.023957	2.904830
40	1	-3.437874	2.423580	0.034999
41	1	1.220172	-1.214679	-0.938819
42	6	-0.168511	0.420413	2.834743
43	1	-0.960687	1.133760	2.596622
44	1	-0.541132	-0.247982	3.617764
45	1	0.671189	0.977493	3.263480
46	1	-0.150903	0.365965	-0.457602
47	1	0.997635	-2.379723	2.303932
48	1	-3.879666	-0.511268	-0.639638
49	1	1.809184	2.183449	-0.227296
50	1	1.551504	2.059517	1.504413
51	1	-0.164491	3.664602	0.708155
52	1	-1.460608	-1.887244	-1.909628
53	1	-2.556675	0.180509	1.180837

F2
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7288344 hartrees (-490542.660874344 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.489188 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6242241 hartrees (-490477.016864991 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.556007	-1.664979	1.380054
2	6	0.417354	-0.600768	1.369164
3	6	0.907825	0.349190	0.264648
4	6	-1.398708	2.112286	0.005433
5	6	-1.441325	0.704404	-0.497669
6	6	-1.989554	0.409135	-1.906479
7	1	-2.771861	1.145677	-2.127715
8	1	-1.229927	0.528737	-2.686882
9	6	-2.598061	-0.999157	-1.811266
10	6	-3.134412	-1.059228	-0.368142
11	6	-0.890224	-1.324784	0.901023
12	1	-0.648057	-1.986287	0.062148
13	1	-1.228159	-1.967697	1.719340
14	6	-2.011993	-0.363835	0.469698
15	6	-3.575426	-2.442715	0.112786
16	1	-3.922942	-2.414672	1.151615
17	1	-4.406416	-2.805787	-0.500814
18	1	-2.769786	-3.181705	0.043260
19	1	-3.380527	-1.166373	-2.557077
20	6	1.984242	-1.819356	-0.086671
21	1	1.332620	-2.520819	-0.616445
22	1	2.997149	-2.218100	-0.175131
23	6	1.868469	-0.393790	-0.693304
24	6	3.247224	0.308866	-0.948448
25	6	4.150407	0.405843	0.290201
26	1	4.444157	-0.584402	0.655655
27	1	5.071520	0.940071	0.036131
28	1	3.682542	0.946813	1.120452
29	6	3.977616	-0.399096	-2.102962
30	1	4.248627	-1.429607	-1.848814
31	1	3.366668	-0.424158	-3.012533
32	1	4.904605	0.133385	-2.338857
33	6	-0.264170	2.592304	0.532746
34	1	3.035719	1.326957	-1.298679
35	6	-2.665605	2.933853	-0.077793
36	1	-2.926640	3.165658	-1.116957
37	1	-2.545829	3.879890	0.455602
38	6	1.038331	1.830928	0.505312
39	1	2.391152	-1.297085	1.986565
40	1	-3.518449	2.400686	0.360376
41	1	1.397700	-0.436085	-1.685332
42	6	0.206838	0.047314	2.745975
43	1	-0.557687	0.829532	2.733999
44	1	-0.108722	-0.718242	3.461786
45	1	1.134956	0.483368	3.131106
46	1	-0.268449	0.415114	-0.545353
47	1	1.214555	-2.600743	1.833242
48	1	-4.008240	-0.393560	-0.319489
49	1	1.706203	2.292593	-0.228652
50	1	1.537481	1.947489	1.478966

51	1	-0.223554	3.600549	0.935774
52	1	-1.832951	-1.770100	-1.973260
53	1	-2.426472	0.120406	1.360157

TS (F2-G1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7288328 hartrees (-490542.659870328 kcal/mol)
Imaginary Frequencies: 1 (-35.9435 1/cm)
Zero-point correction = 0.489099 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6240837 hartrees (-490476.928762587 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.558659	-1.665099	1.376588
2	6	0.421212	-0.598787	1.365284
3	6	0.915327	0.349599	0.263853
4	6	-1.402764	2.110409	0.006430
5	6	-1.445126	0.703824	-0.501605
6	6	-2.010677	0.413575	-1.905228
7	1	-2.800198	1.146260	-2.112977
8	1	-1.261818	0.540144	-2.694796
9	6	-2.611084	-0.997958	-1.808994
10	6	-3.136818	-1.063379	-0.362333
11	6	-0.886902	-1.323721	0.896644
12	1	-0.644276	-1.983044	0.056203
13	1	-1.220205	-1.968971	1.715044
14	6	-2.011449	-0.365396	0.469459
15	6	-3.570152	-2.449494	0.118142
16	1	-3.910906	-2.425291	1.159327
17	1	-4.403967	-2.813840	-0.490855
18	1	-2.762628	-3.185753	0.041388
19	1	-3.397924	-1.167997	-2.549597
20	6	1.988044	-1.818559	-0.089955
21	1	1.336260	-2.518660	-0.621240
22	1	3.000750	-2.217840	-0.177942
23	6	1.873839	-0.391911	-0.693980
24	6	3.253921	0.310585	-0.946826
25	6	4.155440	0.405296	0.293150
26	1	4.447745	-0.585553	0.658096
27	1	5.077379	0.938866	0.040740
28	1	3.687040	0.946116	1.123239
29	6	3.984802	-0.396609	-2.101404
30	1	4.254822	-1.427611	-1.848259
31	1	3.374808	-0.419997	-3.011638
32	1	4.912418	0.135552	-2.335542
33	6	-0.267091	2.589637	0.532422
34	1	3.043298	1.329221	-1.295786
35	6	-2.669420	2.932667	-0.069162
36	1	-2.932361	3.170417	-1.106504
37	1	-2.549132	3.875680	0.469477
38	6	1.037438	1.831613	0.497111
39	1	2.393694	-1.299192	1.984432

40	1	-3.521432	2.396597	0.367118
41	1	1.403810	-0.430349	-1.686548
42	6	0.210038	0.049476	2.741964
43	1	-0.554223	0.831837	2.729465
44	1	-0.105996	-0.716111	3.457493
45	1	1.138215	0.485321	3.127312
46	1	-0.280201	0.415708	-0.559403
47	1	1.214684	-2.600467	1.828579
48	1	-4.012490	-0.400740	-0.306292
49	1	1.700098	2.294020	-0.241107
50	1	1.541989	1.951179	1.468045
51	1	-0.226022	3.596147	0.939702
52	1	-1.843053	-1.764661	-1.977818
53	1	-2.423596	0.118387	1.361276

G1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.733176 hartrees (-490545.38527176 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.490547 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6248734 hartrees (-490477.424307234 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.677258	-1.667428	1.263483
2	6	0.583816	-0.550652	1.201852
3	6	1.139608	0.357233	0.165547
4	6	-1.568837	2.054339	0.052097
5	6	-1.758890	0.715699	-0.615599
6	6	-2.891726	0.583003	-1.659772
7	1	-3.778101	1.143012	-1.342033
8	1	-2.597112	0.971069	-2.640112
9	6	-3.210601	-0.916111	-1.649722
10	6	-3.200966	-1.264677	-0.150788
11	6	-0.735876	-1.274326	0.633965
12	1	-0.475803	-1.783039	-0.299892
13	1	-0.917403	-2.053819	1.381067
14	6	-1.994075	-0.435918	0.431381
15	6	-3.240586	-2.762362	0.164280
16	1	-3.230908	-2.953621	1.243689
17	1	-4.161126	-3.201977	-0.233866
18	1	-2.402090	-3.305573	-0.286458
19	1	-4.166020	-1.154661	-2.127379
20	6	2.206821	-1.786836	-0.174410
21	1	1.592330	-2.467764	-0.770472
22	1	3.225498	-2.178500	-0.206290
23	6	2.117017	-0.342407	-0.725387
24	6	3.512748	0.403936	-0.859643
25	6	4.316592	0.438826	0.448130
26	1	4.600399	-0.565696	0.779580
27	1	5.243014	1.000584	0.291788
28	1	3.777489	0.927084	1.269130

29	6	4.324060	-0.231687	-1.997929
30	1	4.584050	-1.274030	-1.784712
31	1	3.779852	-0.203316	-2.948248
32	1	5.261210	0.318420	-2.131836
33	6	-0.348898	2.490387	0.413788
34	1	3.295391	1.436668	-1.155727
35	6	-2.788460	2.886063	0.360491
36	1	-3.259482	3.252617	-0.559235
37	1	-2.537765	3.752224	0.978341
38	6	0.962362	1.819099	0.087165
39	1	2.476331	-1.351287	1.943564
40	1	-3.547896	2.296535	0.890306
41	1	1.701807	-0.298907	-1.745838
42	6	0.297208	0.089718	2.569826
43	1	-0.457819	0.876238	2.523687
44	1	-0.057312	-0.684554	3.257679
45	1	1.211830	0.515226	2.997231
46	1	-0.819546	0.462482	-1.142556
47	1	1.265590	-2.600854	1.657097
48	1	-4.103170	-0.814635	0.285723
49	1	1.372349	2.202577	-0.856283
50	1	1.706166	2.148174	0.845934
51	1	-0.251884	3.447951	0.918581
52	1	-2.432915	-1.482470	-2.182523
53	1	-2.288405	-0.011546	1.397529

TS (G1-H1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7228319 hartrees (-490538.894245569 kcal/mol)
Imaginary Frequencies: 1 (-56.7345 1/cm)
Zero-point correction = 0.491145 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.613837 hartrees (-490470.49885587 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.584749	-2.182520	-0.237146
2	6	0.631063	-1.342629	0.665145
3	6	1.128104	0.040877	0.480236
4	6	-1.286859	2.114364	0.479466
5	6	-1.594828	0.917480	-0.411705
6	6	-2.766819	1.081984	-1.424077
7	1	-3.519129	1.769325	-1.026466
8	1	-2.430291	1.497001	-2.379322
9	6	-3.390857	-0.313632	-1.542806
10	6	-3.323490	-0.843944	-0.101809
11	6	-0.842666	-1.484492	0.032221
12	1	-0.730126	-1.553144	-1.053999
13	1	-1.151802	-2.472645	0.386709
14	6	-1.892512	-0.420696	0.371381
15	6	-3.716075	-2.312562	0.075445
16	1	-3.583981	-2.647290	1.111378
17	1	-4.772279	-2.449994	-0.178061

18	1	-3.140309	-2.980452	-0.575725
19	1	-4.412209	-0.284903	-1.935492
20	6	1.978164	-1.229302	-1.378374
21	1	1.236449	-1.251386	-2.183266
22	1	2.936530	-1.494358	-1.829242
23	6	2.002619	0.170840	-0.715359
24	6	3.459579	0.729651	-0.371928
25	6	4.260818	-0.176887	0.569943
26	1	4.466766	-1.153163	0.118711
27	1	5.228064	0.286836	0.788799
28	1	3.753892	-0.342616	1.528637
29	6	4.221049	1.009813	-1.673147
30	1	4.435657	0.093695	-2.232791
31	1	3.669445	1.691453	-2.329425
32	1	5.182188	1.477947	-1.435089
33	6	-0.186293	2.177565	1.238074
34	1	3.297301	1.694550	0.123060
35	6	-2.253903	3.275388	0.528886
36	1	-2.396665	3.720574	-0.462836
37	1	-1.898687	4.059278	1.202744
38	6	0.925526	1.133643	1.455095
39	1	2.463836	-2.484555	0.342479
40	1	-3.242604	2.954956	0.880526
41	1	1.585557	0.968622	-1.349168
42	6	0.575135	-1.819530	2.131832
43	1	-0.216748	-1.327193	2.703337
44	1	0.371052	-2.894572	2.138274
45	1	1.528661	-1.661473	2.646614
46	1	-0.691738	0.738019	-1.015075
47	1	1.096627	-3.097102	-0.585285
48	1	-4.022588	-0.241401	0.495838
49	1	1.860918	1.703691	1.508342
50	1	0.755469	0.694371	2.446012
51	1	-0.026540	3.036279	1.884856
52	1	-2.806834	-0.956232	-2.216665
53	1	-1.900910	-0.246588	1.453360

H1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7324075 hartrees (-490544.903030325 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491565 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6229011 hartrees (-490476.186669261 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.636918	-1.827980	1.043488
2	6	-0.623385	-1.292985	-0.015254
3	6	-1.177806	0.058568	-0.379369
4	6	1.201195	1.938583	0.140367
5	6	2.265764	0.875232	0.152942
6	6	3.496305	1.171944	-0.749129

7	1	3.154604	1.452139	-1.752481
8	1	4.103015	1.999358	-0.371578
9	6	4.271850	-0.175253	-0.778538
10	6	3.330052	-1.264047	-0.175535
11	6	0.818524	-1.239401	0.612204
12	1	0.754581	-0.769148	1.600882
13	1	1.061208	-2.292965	0.790131
14	6	1.927777	-0.580189	-0.222133
15	6	3.787238	-1.711821	1.221416
16	1	3.132673	-2.479681	1.648599
17	1	4.791517	-2.144008	1.159448
18	1	3.839548	-0.879503	1.933744
19	1	4.564302	-0.426071	-1.802433
20	6	-2.350507	-0.590043	1.612392
21	1	-1.784948	-0.170296	2.451739
22	1	-3.350334	-0.819716	1.988544
23	6	-2.372794	0.429245	0.448637
24	6	-3.716329	0.504256	-0.394665
25	6	-4.209035	-0.836739	-0.950905
26	1	-4.447753	-1.547120	-0.151930
27	1	-5.127912	-0.677068	-1.524430
28	1	-3.485670	-1.307066	-1.625263
29	6	-4.803878	1.180411	0.453683
30	1	-5.074146	0.576745	1.327084
31	1	-4.489627	2.168510	0.807438
32	1	-5.710635	1.311729	-0.145920
33	6	-0.004655	1.925540	-0.481636
34	1	-3.501496	1.167648	-1.243598
35	6	1.555642	3.175486	0.932902
36	1	1.709323	2.919583	1.989640
37	1	0.788503	3.951130	0.872015
38	6	-0.634176	0.904643	-1.443772
39	1	-2.355352	-2.493771	0.555319
40	1	2.501038	3.600786	0.575849
41	1	-2.246983	1.455187	0.810954
42	6	-0.584600	-2.209181	-1.271082
43	1	0.164703	-1.901733	-2.004439
44	1	-0.334304	-3.222080	-0.938648
45	1	-1.554570	-2.258715	-1.773365
46	1	2.634996	0.856483	1.189215
47	1	-1.132853	-2.415178	1.816362
48	1	3.310791	-2.151891	-0.818606
49	1	-1.397415	1.415906	-2.035577
50	1	0.071260	0.406518	-2.103933
51	1	-0.672474	2.759807	-0.283475
52	1	5.195713	-0.105609	-0.196051
53	1	1.647112	-0.597530	-1.281309

TS (H1-H2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.73044 hartrees (-490543.6684044 kcal/mol)
Imaginary Frequencies: 1 (-99.6353 1/cm)
Zero-point correction = 0.491760 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6211059 hartrees (-490475.060163309 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.505117	-1.825507	1.275813
2	6	-0.572127	-1.282020	0.147001
3	6	-1.178464	0.038457	-0.254652
4	6	1.192020	1.911592	0.267861
5	6	2.284335	0.883852	0.146959
6	6	3.434272	1.242293	-0.833586
7	1	3.013818	1.527613	-1.805150
8	1	4.040138	2.082613	-0.483819
9	6	4.247483	-0.080048	-0.941129
10	6	3.375798	-1.214015	-0.312194
11	6	0.912221	-1.252901	0.643510
12	1	0.928421	-0.800085	1.642200
13	1	1.169427	-2.308598	0.786630
14	6	1.956531	-0.569122	-0.250409
15	6	3.931840	-1.693461	1.037231
16	1	3.324335	-2.493062	1.475477
17	1	4.941451	-2.094567	0.899280
18	1	4.005735	-0.884438	1.773855
19	1	4.488072	-0.296920	-1.986055
20	6	-2.619648	-0.782084	1.530328
21	1	-2.539757	-0.361116	2.536150
22	1	-3.609367	-1.240082	1.467947
23	6	-2.458964	0.339992	0.471180
24	6	-3.700036	0.584378	-0.474090
25	6	-4.072039	-0.626864	-1.338156
26	1	-4.296712	-1.510793	-0.730219
27	1	-4.968645	-0.403327	-1.925176
28	1	-3.279940	-0.890099	-2.048169
29	6	-4.894916	1.066268	0.362434
30	1	-5.253163	0.291224	1.048617
31	1	-4.644272	1.953644	0.954654
32	1	-5.727762	1.328441	-0.298113
33	6	-0.046008	1.888003	-0.290689
34	1	-3.421744	1.408323	-1.144835
35	6	1.550650	3.106399	1.117748
36	1	1.755711	2.790900	2.149476
37	1	0.764090	3.864445	1.135642
38	6	-0.643494	0.903602	-1.306379
39	1	-1.931197	-2.787065	0.975053
40	1	2.470923	3.574470	0.748461
41	1	-2.321640	1.307779	0.971655
42	6	-0.658672	-2.206256	-1.113151
43	1	-0.021581	-1.865096	-1.933404
44	1	-0.323001	-3.203758	-0.812026
45	1	-1.681911	-2.299894	-1.485305
46	1	2.736287	0.837497	1.149037
47	1	-0.929144	-2.015130	2.185819
48	1	3.339269	-2.081564	-0.981505
49	1	-1.403619	1.418019	-1.896777
50	1	0.088311	0.441239	-1.961265
51	1	-0.737379	2.682127	-0.021452
52	1	5.200921	0.006423	-0.410844
53	1	1.609949	-0.574507	-1.289614

H2
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7379497 hartrees (-490548.380816247 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491753 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6306393 hartrees (-490481.042467143 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.322293	-1.836267	-1.386416
2	6	0.445737	-1.354061	-0.199824
3	6	1.128069	-0.060745	0.225275
4	6	-1.027099	1.820764	-0.395239
5	6	-2.205765	0.914386	-0.185221
6	6	-3.289649	1.448576	0.795166
7	1	-2.819704	1.740362	1.741622
8	1	-3.810852	2.327635	0.406581
9	6	-4.231105	0.224380	0.986580
10	6	-3.489489	-1.028774	0.419204
11	6	-1.061386	-1.361104	-0.576851
12	1	-1.158587	-1.035293	-1.619976
13	1	-1.359537	-2.416155	-0.566558
14	6	-2.015040	-0.537920	0.296999
15	6	-4.116278	-1.537204	-0.887643
16	1	-3.592127	-2.415068	-1.281088
17	1	-5.155226	-1.833518	-0.708710
18	1	-4.132127	-0.773294	-1.674430
19	1	-4.477783	0.096177	2.044587
20	6	2.729534	-1.316112	-1.079287
21	1	3.362046	-1.254448	-1.967537
22	1	3.239631	-1.964366	-0.360086
23	6	2.475353	0.087199	-0.467009
24	6	3.627770	0.730918	0.349999
25	6	4.049880	-0.094898	1.576330
26	1	4.505859	-1.046832	1.283437
27	1	4.798106	0.454221	2.156690
28	1	3.213498	-0.316533	2.250224
29	6	4.834763	1.009041	-0.561416
30	1	5.276262	0.079752	-0.938418
31	1	4.558560	1.627080	-1.423683
32	1	5.614030	1.540414	-0.006064
33	6	0.207077	1.737655	0.184168
34	1	3.266943	1.707217	0.706760
35	6	-1.270371	2.955470	-1.355502
36	1	-1.472433	2.560765	-2.360552
37	1	-0.429562	3.650026	-1.415850
38	6	0.680677	0.805171	1.305374
39	1	1.278311	-2.922265	-1.509394
40	1	-2.165239	3.517510	-1.061688
41	1	2.284340	0.751536	-1.325467
42	6	0.670206	-2.290091	1.034639

43	1	0.034110	-2.003999	1.877187
44	1	0.410342	-3.311181	0.737302
45	1	1.707334	-2.299108	1.383428
46	1	-2.691156	0.852088	-1.170220
47	1	0.952549	-1.387937	-2.317195
48	1	-3.525265	-1.851047	1.143213
49	1	1.466574	1.287728	1.884769
50	1	-0.106278	0.426469	1.948130
51	1	0.959729	2.458327	-0.121704
52	1	-5.177911	0.380009	0.460196
53	1	-1.645501	-0.524567	1.328522

TS (H2-I1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7142699 hartrees (-490533.521504949 kcal/mol)
Imaginary Frequencies: 1 (-371.8705 1/cm)
Zero-point correction = 0.491923 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6156332 hartrees (-490471.625989332 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.379789	-2.227190	-0.849177
2	6	0.434918	-1.352945	0.024552
3	6	1.028548	0.045080	-0.301482
4	6	-0.856908	1.678269	-0.446788
5	6	-2.124534	0.849988	-0.250535
6	6	-3.245540	1.471557	0.605464
7	1	-2.837929	1.791539	1.573869
8	1	-3.703656	2.350222	0.143083
9	6	-4.258192	0.307033	0.790351
10	6	-3.517276	-1.010449	0.393268
11	6	-1.046435	-1.523736	-0.378416
12	1	-1.142082	-1.417863	-1.467182
13	1	-1.320373	-2.561195	-0.149292
14	6	-2.024345	-0.575730	0.326330
15	6	-4.062977	-1.617694	-0.907134
16	1	-3.540777	-2.541010	-1.180466
17	1	-5.122365	-1.866805	-0.785085
18	1	-3.991067	-0.925476	-1.755545
19	1	-4.623426	0.269685	1.820466
20	6	2.780221	-1.626164	-0.655115
21	1	3.468067	-1.915269	-1.453542
22	1	3.222360	-1.969884	0.284395
23	6	2.543989	-0.095018	-0.641579
24	6	3.548059	0.765595	0.171784
25	6	3.611798	0.452956	1.674580
26	1	3.984951	-0.559779	1.862852
27	1	4.302786	1.144317	2.167858
28	1	2.641809	0.550656	2.175145
29	6	4.948135	0.661182	-0.457931
30	1	5.348757	-0.355113	-0.371195
31	1	4.935053	0.929229	-1.520579

32	1	5.646507	1.334859	0.048581
33	6	0.356380	1.121045	-0.982775
34	1	3.229385	1.815088	0.062417
35	6	-1.086780	3.152449	-0.727717
36	1	-1.761153	3.263127	-1.584094
37	1	-0.156346	3.682172	-0.952989
38	6	0.423293	1.329971	0.631219
39	1	1.318597	-3.282613	-0.566431
40	1	-1.562346	3.638614	0.128097
41	1	2.636581	0.249333	-1.680949
42	6	0.645236	-1.742863	1.505340
43	1	0.066741	-1.129418	2.203799
44	1	0.322644	-2.779037	1.649603
45	1	1.691236	-1.674979	1.809160
46	1	-2.501038	0.758251	-1.282243
47	1	1.078681	-2.152659	-1.902327
48	1	-3.626689	-1.762678	1.182786
49	1	1.076857	2.133689	0.946816
50	1	-0.107150	0.798130	1.409674
51	1	1.015300	1.824488	-1.493743
52	1	-5.135479	0.455057	0.152991
53	1	-1.718712	-0.474690	1.378637

I1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7468175 hartrees (-490553.945449425 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.491755 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6414954 hartrees (-490487.854778454 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.408745	-2.421180	-0.249451
2	6	0.463567	-1.383159	0.431375
3	6	1.120202	-0.047081	0.110729
4	6	-0.963535	1.787576	0.077115
5	6	-2.017651	0.798795	-0.355890
6	6	-3.438626	1.411017	-0.075605
7	1	-3.399803	2.122748	0.756831
8	1	-3.792636	1.965074	-0.949333
9	6	-4.350930	0.203916	0.276929
10	6	-3.520882	-1.070339	-0.000977
11	6	-0.974453	-1.561434	-0.130162
12	1	-0.914491	-1.555755	-1.225561
13	1	-1.269331	-2.582053	0.148114
14	6	-2.071231	-0.593839	0.310221
15	6	-3.733918	-1.605320	-1.425868
16	1	-3.131722	-2.497732	-1.626691
17	1	-4.783724	-1.885800	-1.560261
18	1	-3.499159	-0.860193	-2.195935
19	1	-4.630603	0.247291	1.334680
20	6	2.780613	-1.749078	-0.306151

21	1	3.432408	-2.183168	-1.067403
22	1	3.301510	-1.828641	0.654205
23	6	2.434750	-0.274683	-0.612453
24	6	3.571392	0.768374	-0.448918
25	6	4.069087	0.898357	1.000126
26	1	4.554260	-0.021978	1.343198
27	1	4.811507	1.699628	1.071166
28	1	3.260652	1.134737	1.702132
29	6	4.733771	0.446796	-1.403194
30	1	5.227477	-0.493446	-1.134546
31	1	4.395468	0.367774	-2.442962
32	1	5.488777	1.238047	-1.357916
33	6	0.695305	1.242757	0.385869
34	1	3.173409	1.744365	-0.761064
35	6	-0.887425	3.061101	-0.733884
36	1	-0.760181	2.852372	-1.800747
37	1	-0.088998	3.728736	-0.400439
38	6	-0.373281	1.740390	1.397697
39	1	1.412224	-3.372610	0.289731
40	1	-1.836953	3.598246	-0.615828
41	1	2.128293	-0.247656	-1.678452
42	6	0.512280	-1.608098	1.970857
43	1	-0.092454	-0.894812	2.534158
44	1	0.129434	-2.611903	2.182946
45	1	1.535869	-1.551850	2.353705
46	1	-1.915536	0.657810	-1.439005
47	1	1.056335	-2.627924	-1.267379
48	1	-3.793331	-1.867064	0.701521
49	1	-0.059876	2.673384	1.862311
50	1	-0.735963	0.999673	2.099750
51	1	1.366123	2.034080	0.075992
52	1	-5.281444	0.218734	-0.298366
53	1	-2.034229	-0.469322	1.401246

Figure 3
A2
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6972092 hartrees (-490522.815745092 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.487436 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5796813 hartrees (-490449.065812563 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	2.026313	-2.401498	-0.717019
2	6	0.902321	-1.746299	0.108617
3	6	0.938384	-0.259814	-0.328150
4	6	-1.767987	2.317893	0.014622
5	6	-2.712314	1.611801	-0.628902
6	6	-2.499354	0.484848	-1.604032
7	1	-2.938245	0.762131	-2.573473
8	1	-1.431314	0.338397	-1.791920

9	6	-3.134938	-0.878860	-1.202291
10	6	-2.814299	-1.388420	0.194400
11	6	-0.491451	-2.364280	-0.309210
12	1	-0.677848	-2.132103	-1.364055
13	1	-0.338693	-3.452888	-0.259117
14	6	-1.676381	-2.016872	0.548204
15	6	-3.902411	-1.170613	1.218032
16	1	-3.621724	-1.541784	2.208266
17	1	-4.144124	-0.103365	1.307340
18	1	-4.828731	-1.676086	0.914335
19	1	-4.223809	-0.785950	-1.289234
20	6	3.218880	-1.440537	-0.623090
21	1	3.969168	-1.619069	-1.400031
22	1	3.726555	-1.549103	0.338273
23	6	2.630745	-0.025997	-0.796544
24	6	3.134703	1.089158	-0.061782
25	6	3.611446	1.013301	1.337219
26	1	4.543568	1.583430	1.447627
27	1	2.879448	1.539154	1.973078
28	1	3.743919	0.003352	1.720861
29	6	3.167717	2.430505	-0.698686
30	1	4.178508	2.540445	-1.131358
31	1	2.459587	2.527597	-1.524839
32	1	3.046176	3.248913	0.017049
33	6	-0.274772	2.044264	-0.161824
34	1	-0.041916	1.979861	-1.232522
35	6	-2.123420	3.433156	0.966794
36	1	-3.205824	3.555032	1.065031
37	1	-1.705547	4.391617	0.628962
38	6	0.200411	0.742120	0.551264
39	1	2.278171	-3.404272	-0.357996
40	1	-1.712873	3.249366	1.969876
41	1	2.538849	0.235509	-1.852888
42	6	1.147830	-1.955553	1.613997
43	1	0.430283	-1.411125	2.232252
44	1	1.053421	-3.018846	1.860138
45	1	2.151688	-1.644546	1.921247
46	1	0.528050	-0.189479	-1.338381
47	1	1.710964	-2.502050	-1.763971
48	1	-3.754478	1.877211	-0.446933
49	1	0.746509	0.964999	1.475413
50	1	-0.691427	0.196001	0.881366
51	1	0.287953	2.906015	0.214333
52	1	-2.836531	-1.616040	-1.957842
53	1	-1.608278	-2.362142	1.579410

TS (A2-B2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6800767 hartrees (-490512.064930017 kcal/mol)
Imaginary Frequencies: 1 (-173.8137 1/cm)
Zero-point correction = 0.487256 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5657702 hartrees (-490440.336458202 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.684249	-2.692814	0.537737
2	6	-0.423853	-2.196004	-0.235337
3	6	-0.512677	-0.642494	-0.082215
4	6	0.834413	2.447960	-0.467109
5	6	1.704040	2.116747	0.542538
6	6	1.667851	1.102141	1.643162
7	1	1.980648	1.637465	2.549471
8	1	0.645459	0.776414	1.833722
9	6	2.625582	-0.155416	1.553121
10	6	2.802633	-0.875885	0.223909
11	6	0.919824	-2.638359	0.438152
12	1	0.855287	-2.409717	1.509834
13	1	1.025752	-3.727760	0.355253
14	6	2.118687	-1.963296	-0.185874
15	6	3.921802	-0.320972	-0.630480
16	1	4.024681	-0.861907	-1.575583
17	1	3.758515	0.740909	-0.867842
18	1	4.884032	-0.372809	-0.103932
19	1	3.617650	0.175846	1.880179
20	6	-2.718133	-1.560129	0.388921
21	1	-3.556343	-1.650610	1.087798
22	1	-3.133776	-1.553646	-0.625292
23	6	-1.856891	-0.304283	0.646320
24	6	-2.419611	1.089781	0.330881
25	6	-3.477670	1.180843	-0.761217
26	1	-4.403475	0.718331	-0.396292
27	1	-3.709249	2.222588	-1.004502
28	1	-3.196398	0.658013	-1.679596
29	6	-2.763456	1.929855	1.557093
30	1	-3.618543	1.469958	2.070750
31	1	-1.934692	1.971945	2.270892
32	1	-3.050313	2.950095	1.285356
33	6	-0.263275	1.683647	-1.048269
34	1	-1.447335	1.667629	-0.115427
35	6	1.032613	3.793226	-1.168446
36	1	1.903568	4.322969	-0.776322
37	1	0.157650	4.437220	-1.014645
38	6	-0.291923	0.209864	-1.340885
39	1	-2.052852	-3.652616	0.162326
40	1	1.167092	3.675401	-2.249301
41	1	-1.621463	-0.299881	1.719823
42	6	-0.492596	-2.699607	-1.689544
43	1	0.312275	-2.301068	-2.315704
44	1	-0.408559	-3.791659	-1.707299
45	1	-1.444764	-2.440892	-2.167103
46	1	0.287733	-0.367619	0.585144
47	1	-1.448085	-2.832732	1.600787
48	1	2.542955	2.807034	0.633928
49	1	-1.043438	0.011898	-2.109246
50	1	0.684980	-0.051763	-1.763077
51	1	-0.817043	2.279600	-1.777251
52	1	2.266130	-0.843727	2.325264
53	1	2.433245	-2.393737	-1.136860

B2
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6943024 hartrees (-490520.991699024 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.488949 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5757521 hartrees (-490446.600200271 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.790334	-2.202761	-1.133635
2	6	0.700097	-1.707954	-0.148597
3	6	0.819379	-0.160885	-0.410020
4	6	-1.617618	2.566453	-0.031970
5	6	-2.648968	1.805085	-0.578271
6	6	-2.540193	0.550155	-1.350242
7	1	-2.907381	0.837053	-2.352078
8	1	-1.504676	0.249856	-1.476458
9	6	-3.408903	-0.684466	-0.932443
10	6	-2.969721	-1.391883	0.337739
11	6	-0.702242	-2.285319	-0.536604
12	1	-0.977989	-1.926155	-1.535553
13	1	-0.564236	-3.371947	-0.640423
14	6	-1.815465	-2.073729	0.463188
15	6	-3.942589	-1.291848	1.488878
16	1	-3.579245	-1.811153	2.379972
17	1	-4.130480	-0.242502	1.762627
18	1	-4.917953	-1.718801	1.220744
19	1	-4.455645	-0.374052	-0.845875
20	6	2.964573	-1.218386	-0.978986
21	1	3.601564	-1.202076	-1.867529
22	1	3.603506	-1.525954	-0.145695
23	6	2.327936	0.176757	-0.697367
24	6	3.124060	1.084058	0.285183
25	6	3.421533	0.515282	1.683310
26	1	4.077497	-0.360527	1.634303
27	1	3.943360	1.268919	2.283152
28	1	2.524798	0.223814	2.239930
29	6	4.443116	1.520752	-0.379674
30	1	5.105189	0.662869	-0.544607
31	1	4.267717	1.999487	-1.349944
32	1	4.981082	2.233278	0.254494
33	6	-0.346295	2.052589	0.274481
34	1	2.528817	2.001280	0.427459
35	6	-1.840544	4.058159	0.206870
36	1	-1.196052	4.647750	-0.455543
37	1	-1.609340	4.341151	1.237825
38	6	0.009644	0.676964	0.655885
39	1	2.078021	-3.240875	-0.934582
40	1	-2.874997	4.342957	0.001466
41	1	2.329397	0.739272	-1.639733
42	6	1.059127	-2.130776	1.286875
43	1	0.435223	-1.638468	2.041189
44	1	0.911178	-3.210739	1.403065

45	1	2.101903	-1.920260	1.531668
46	1	0.313431	-0.004924	-1.368364
47	1	1.397515	-2.168054	-2.158841
48	1	-3.630945	2.280138	-0.607641
49	1	0.636024	0.756092	1.553973
50	1	-0.885835	0.115782	0.916617
51	1	0.446843	2.796561	0.370389
52	1	-3.361153	-1.368160	-1.787049
53	1	-1.650705	-2.561107	1.423447

TS (B2-C2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6722557 hartrees (-490507.157174307 kcal/mol)
Imaginary Frequencies: 1 (-112.8786 1/cm)
Zero-point correction = 0.489432 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5592282 hartrees (-490436.231287782 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.591403	-2.081956	-1.084419
2	6	0.701025	-1.419785	-0.003124
3	6	1.017044	0.088027	-0.240125
4	6	-1.683780	2.084504	0.068794
5	6	-2.613430	0.962572	-0.180276
6	6	-2.881411	0.349723	-1.546973
7	1	-3.473970	1.040564	-2.160767
8	1	-1.952815	0.161752	-2.089305
9	6	-3.624190	-0.946621	-1.144566
10	6	-3.190245	-1.052093	0.315481
11	6	-0.788120	-1.720619	-0.288897
12	1	-1.012121	-1.514189	-1.339421
13	1	-0.940075	-2.809496	-0.175935
14	6	-1.840409	-1.135497	0.616659
15	6	-4.235377	-1.100915	1.388809
16	1	-3.823513	-0.928739	2.386993
17	1	-5.057291	-0.400904	1.202008
18	1	-4.678717	-2.107678	1.377728
19	1	-4.708966	-0.833978	-1.212399
20	6	2.915265	-1.302328	-1.026178
21	1	3.481990	-1.394296	-1.957004
22	1	3.552364	-1.709432	-0.234530
23	6	2.524659	0.172784	-0.721437
24	6	3.554643	0.963918	0.128310
25	6	3.881410	0.388609	1.517298
26	1	4.376232	-0.586916	1.447945
27	1	4.572337	1.056878	2.042987
28	1	2.998152	0.269465	2.153783
29	6	4.855697	1.150973	-0.673960
30	1	5.356893	0.192034	-0.851759
31	1	4.664489	1.615019	-1.648514
32	1	5.557758	1.792037	-0.130091
33	6	-0.394079	2.140050	0.446360

34	1	3.133467	1.969863	0.278403
35	6	-2.474589	3.382745	-0.145701
36	1	-2.982031	3.412920	-1.116954
37	1	-1.790609	4.234447	-0.102414
38	6	0.531143	1.039678	0.889845
39	1	1.719100	-3.158582	-0.924603
40	1	-3.237658	3.517856	0.631353
41	1	2.495137	0.709144	-1.678181
42	6	1.093668	-1.959602	1.386021
43	1	0.559736	-1.475182	2.211624
44	1	0.879841	-3.033417	1.446613
45	1	2.159424	-1.828130	1.582455
46	1	0.435260	0.353079	-1.132707
47	1	1.125990	-1.954926	-2.072061
48	1	-3.550085	1.146264	0.351731
49	1	1.380618	1.506657	1.389691
50	1	0.030431	0.460906	1.673169
51	1	0.018024	3.145835	0.507597
52	1	-3.344843	-1.820573	-1.740433
53	1	-1.586520	-1.053279	1.671481

TS (C1-C2)

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7012348 hartrees (-490525.341849348 kcal/mol)
Imaginary Frequencies: 1 (-44.3619 1/cm)
Zero-point correction = 0.489591 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5941588 hartrees (-490458.150588588 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.497898	-1.613329	-1.541339
2	6	0.617650	-0.956404	-0.443899
3	6	1.245982	0.468381	-0.422335
4	6	-1.687753	2.076708	-0.137339
5	6	-2.400030	0.907463	0.549097
6	6	-3.930046	0.842384	0.285234
7	1	-4.491244	1.560922	0.885822
8	1	-4.158083	1.045442	-0.764980
9	6	-4.314246	-0.608588	0.602434
10	6	-3.115187	-1.400203	0.279771
11	6	-0.872213	-0.933774	-0.879404
12	1	-1.029690	-0.220592	-1.694743
13	1	-1.125507	-1.926713	-1.266403
14	6	-1.911681	-0.575544	0.264546
15	6	-3.168667	-2.849002	0.041825
16	1	-2.216809	-3.358834	0.205570
17	1	-3.980390	-3.324370	0.602479
18	1	-3.426795	-2.975566	-1.026485
19	1	-4.454656	-0.759219	1.693596
20	6	2.932035	-1.147151	-1.207323
21	1	3.577152	-1.173324	-2.090025
22	1	3.385653	-1.827030	-0.477730

23	6	2.799147	0.292155	-0.618635
24	6	3.769472	0.644762	0.539740
25	6	3.609248	-0.146262	1.846377
26	1	3.821036	-1.213936	1.711031
27	1	4.320344	0.223606	2.593296
28	1	2.607189	-0.048397	2.276960
29	6	5.224980	0.558162	0.045380
30	1	5.505967	-0.474352	-0.194898
31	1	5.380899	1.165077	-0.854070
32	1	5.918054	0.916257	0.814327
33	6	-0.374127	2.310596	0.004363
34	1	3.583360	1.701587	0.782594
35	6	-2.531361	3.043295	-0.943703
36	1	-2.961041	2.577546	-1.841203
37	1	-1.924466	3.887854	-1.279350
38	6	0.681950	1.446989	0.646722
39	1	1.399337	-2.705240	-1.563657
40	1	-3.369333	3.451918	-0.364965
41	1	3.073738	0.998696	-1.411939
42	6	0.774564	-1.769596	0.854311
43	1	0.414536	-1.246077	1.750035
44	1	0.237678	-2.725576	0.779317
45	1	1.817801	-2.011779	1.056075
46	1	0.925901	0.889178	-1.384173
47	1	1.195887	-1.239189	-2.528654
48	1	-2.269991	1.044594	1.631628
49	1	1.477748	2.092829	1.030382
50	1	0.294061	0.906530	1.519453
51	1	0.021218	3.190918	-0.502142
52	1	-5.231105	-1.000127	0.144463
53	1	-1.404130	-0.968880	1.173428

C2

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7080507 hartrees (-490529.618894757 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.490678 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.6006559 hartrees (-490462.227583809 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.328038	-1.669936	-1.491607
2	6	0.547972	-1.031307	-0.309830
3	6	1.122015	0.414848	-0.338019
4	6	-1.699219	2.180943	0.152466
5	6	-2.542345	0.931736	0.355687
6	6	-3.584798	0.644170	-0.765721
7	1	-4.417539	1.348753	-0.753077
8	1	-3.124120	0.706091	-1.756682
9	6	-4.047424	-0.796155	-0.474753
10	6	-2.972039	-1.411417	0.343586
11	6	-0.970137	-1.025162	-0.654052

12	1	-1.177411	-0.392547	-1.519571
13	1	-1.245636	-2.050566	-0.938458
14	6	-1.903208	-0.467492	0.570745
15	6	-3.050993	-2.776984	0.896372
16	1	-2.091946	-3.149565	1.261074
17	1	-3.727908	-2.708679	1.766342
18	1	-3.514299	-3.487936	0.204648
19	1	-4.942306	-0.814870	0.175401
20	6	2.771273	-1.161460	-1.296125
21	1	3.331628	-1.183218	-2.234957
22	1	3.306095	-1.819142	-0.602875
23	6	2.650685	0.280610	-0.714695
24	6	3.734702	0.673721	0.323235
25	6	3.751261	-0.122221	1.636837
26	1	3.985029	-1.181372	1.473506
27	1	4.528803	0.272614	2.300044
28	1	2.801866	-0.061056	2.179296
29	6	5.125537	0.635590	-0.336563
30	1	5.411937	-0.386159	-0.613378
31	1	5.157844	1.249657	-1.243977
32	1	5.889394	1.015081	0.350558
33	6	-0.387146	2.338396	0.391663
34	1	3.543658	1.724455	0.586374
35	6	-2.526585	3.381101	-0.267731
36	1	-2.948106	3.262657	-1.274222
37	1	-1.923770	4.292378	-0.267896
38	6	0.681247	1.352312	0.819113
39	1	1.254477	-2.763523	-1.501334
40	1	-3.373188	3.543174	0.414049
41	1	2.807256	0.983497	-1.542220
42	6	0.819208	-1.847966	0.965189
43	1	0.480758	-1.360014	1.885326
44	1	0.330000	-2.828758	0.901823
45	1	1.885448	-2.033831	1.095085
46	1	0.678134	0.848785	-1.242632
47	1	0.924008	-1.305300	-2.445413
48	1	-3.127258	1.111357	1.274774
49	1	1.537037	1.934972	1.168723
50	1	0.363004	0.773037	1.693171
51	1	-0.006596	3.343496	0.213759
52	1	-4.326320	-1.407347	-1.343199
53	1	-1.358241	-0.616080	1.501150

TS (C2-E2)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.674092 hartrees (-490508.30947092 kcal/mol)
Imaginary Frequencies: 1 (-866.7943 1/cm)
Zero-point correction = 0.488076 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.5709262 hartrees (-490443.571899762 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z

1	6	1.511228	-2.099582	-1.002081
2	6	0.617984	-1.350908	0.017809
3	6	1.033649	0.140798	-0.241098
4	6	-1.685067	2.014712	0.090668
5	6	-2.231041	0.694173	-0.261667
6	6	-2.883637	0.337781	-1.617212
7	1	-3.495830	1.150949	-2.011388
8	1	-2.126325	0.091990	-2.366598
9	6	-3.745871	-0.853816	-1.125504
10	6	-3.326043	-0.814437	0.339788
11	6	-0.877667	-1.607560	-0.296468
12	1	-1.028232	-1.566582	-1.380877
13	1	-1.134108	-2.630410	0.010476
14	6	-1.824571	-0.634243	0.402296
15	6	-4.156597	-1.274423	1.492549
16	1	-3.786293	-0.898160	2.450501
17	1	-5.213939	-1.025760	1.373405
18	1	-4.066016	-2.372184	1.518983
19	1	-4.818290	-0.694922	-1.262912
20	6	2.873952	-1.404090	-0.914417
21	1	3.484693	-1.584254	-1.803696
22	1	3.440147	-1.795731	-0.062888
23	6	2.552343	0.102263	-0.724524
24	6	3.633204	0.897984	0.054711
25	6	3.926291	0.417453	1.486601
26	1	4.361884	-0.588117	1.495409
27	1	4.655897	1.082815	1.961205
28	1	3.037930	0.401207	2.126846
29	6	4.941176	0.932010	-0.758247
30	1	5.381660	-0.067492	-0.851006
31	1	4.776084	1.321280	-1.769621
32	1	5.682682	1.573331	-0.269874
33	6	-0.423103	2.170331	0.562744
34	1	3.284930	1.940108	0.117928
35	6	-2.573192	3.211623	-0.183034
36	1	-2.825502	3.303495	-1.246120
37	1	-2.079792	4.138767	0.117993
38	6	0.668888	1.174449	0.873810
39	1	1.560935	-3.176097	-0.803449
40	1	-3.519045	3.145121	0.370866
41	1	2.543183	0.559802	-1.721941
42	6	0.936547	-1.851027	1.441705
43	1	0.301921	-1.398038	2.213191
44	1	0.783349	-2.934817	1.499250
45	1	1.972035	-1.650146	1.726283
46	1	0.472363	0.447354	-1.133666
47	1	1.095607	-1.976525	-2.012153
48	1	-3.377825	0.628346	0.377284
49	1	1.549307	1.767733	1.119682
50	1	0.419853	0.657650	1.809152
51	1	-0.129382	3.209861	0.708858
52	1	-3.486008	-1.820983	-1.570355
53	1	-1.528703	-0.460559	1.438651

Figure 5
TS (G1-J1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)

HF = -781.6844695 hartrees (-490514.821455945 kcal/mol)
Imaginary Frequencies: 1 (-1087.5970 1/cm)
Zero-point correction = 0.487837 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.579469 hartrees (-490448.93259219 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.668352	-1.733172	1.010166
2	6	0.575489	-0.621084	0.884700
3	6	1.223252	0.328890	-0.119227
4	6	-1.592397	2.017687	0.099929
5	6	-2.007598	0.733019	-0.550244
6	6	-3.379805	0.740611	-1.265905
7	1	-4.145324	1.226760	-0.651339
8	1	-3.339698	1.268094	-2.224787
9	6	-3.699503	-0.751537	-1.386445
10	6	-3.340422	-1.302736	0.003346
11	6	-0.751312	-1.308429	0.388554
12	1	-0.593107	-1.709795	-0.620683
13	1	-0.873850	-2.173548	1.047676
14	6	-2.047802	-0.502806	0.436869
15	6	-3.268294	-2.830175	0.076084
16	1	-3.043540	-3.183092	1.088774
17	1	-4.235310	-3.258243	-0.208709
18	1	-2.515427	-3.242390	-0.604657
19	1	-4.743576	-0.940671	-1.654505
20	6	2.385683	-1.780613	-0.341804
21	1	1.824782	-2.391335	-1.058083
22	1	3.383380	-2.220128	-0.267716
23	6	2.418027	-0.307698	-0.815601
24	6	3.787170	0.434461	-0.609313
25	6	4.276734	0.454986	0.845020
26	1	4.501256	-0.552677	1.211847
27	1	5.200871	1.037615	0.918952
28	1	3.545811	0.911733	1.522762
29	6	4.855404	-0.145859	-1.548409
30	1	5.099245	-1.184035	-1.297601
31	1	4.532003	-0.118623	-2.595182
32	1	5.780542	0.434414	-1.468315
33	6	-0.278941	2.462168	0.081428
34	1	3.627909	1.476685	-0.921365
35	6	-2.630529	2.900502	0.723497
36	1	-3.304694	3.306112	-0.041700
37	1	-2.189857	3.734315	1.274568
38	6	0.940051	1.667260	-0.347760
39	1	2.373633	-1.453075	1.799371
40	1	-3.260529	2.321839	1.410708
41	1	2.228186	-0.244715	-1.896965
42	6	0.357613	0.051763	2.258555
43	1	-0.362427	0.872734	2.244472
44	1	-0.012071	-0.698213	2.967001
45	1	1.301417	0.441456	2.651372
46	1	-1.254578	0.470734	-1.308116

47	1	1.230913	-2.693270	1.298775
48	1	-4.135709	-0.979716	0.688560
49	1	0.022904	2.105289	-1.130884
50	1	1.742361	2.270936	-0.770089
51	1	-0.060946	3.493180	0.351955
52	1	-3.074771	-1.217665	-2.161181
53	1	-2.196841	-0.154127	1.464446

J1

B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.7306704 hartrees (-490543.812982704 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.490832 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.622065 hartrees (-490475.66200815 kcal/mol)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	1.705085	-1.857375	0.759295
2	6	0.633611	-0.729217	0.868204
3	6	1.237932	0.384742	-0.011131
4	6	-1.707653	1.913669	0.159772
5	6	-1.919057	0.832639	-0.756644
6	6	-3.202006	0.709608	-1.598074
7	1	-4.019977	1.310541	-1.187376
8	1	-3.015061	1.066290	-2.615737
9	6	-3.557783	-0.778992	-1.520181
10	6	-3.328340	-1.114201	-0.042595
11	6	-0.700563	-1.285036	0.272466
12	1	-0.534685	-1.612311	-0.760960
13	1	-0.926563	-2.189013	0.850834
14	6	-1.969230	-0.427857	0.351088
15	6	-3.415790	-2.603841	0.308819
16	1	-3.226006	-2.785413	1.372084
17	1	-4.425585	-2.965828	0.089279
18	1	-2.712791	-3.205094	-0.276143
19	1	-4.583660	-0.982808	-1.841274
20	6	2.376972	-1.682069	-0.607950
21	1	1.788557	-2.172965	-1.392424
22	1	3.370893	-2.136945	-0.637896
23	6	2.408614	-0.152616	-0.847946
24	6	3.771812	0.546581	-0.550347
25	6	4.300948	0.330768	0.874819
26	1	4.552291	-0.719921	1.061689
27	1	5.216496	0.911907	1.028840
28	1	3.578448	0.651326	1.634585
29	6	4.827667	0.149228	-1.593521
30	1	5.081149	-0.915535	-1.531058
31	1	4.481787	0.351452	-2.614037
32	1	5.753038	0.713606	-1.435974
33	6	-0.329581	2.329555	0.550457
34	1	3.588896	1.624403	-0.669782
35	6	-2.837871	2.651689	0.781264

36	1	-3.181707	3.396298	0.044150
37	1	-2.544391	3.190096	1.685321
38	6	0.840584	1.662735	-0.121809
39	1	2.442925	-1.720149	1.556900
40	1	-3.700082	2.009932	0.984495
41	1	2.200552	0.059412	-1.904890
42	6	0.457924	-0.352691	2.353558
43	1	-0.335619	0.375793	2.547712
44	1	0.214949	-1.248266	2.937424
45	1	1.387516	0.060703	2.756149
46	1	-1.018885	0.644225	-1.344415
47	1	1.267245	-2.851544	0.900835
48	1	-4.108770	-0.594574	0.531398
49	1	-0.312101	3.420676	0.376764
50	1	1.400720	2.310707	-0.793821
51	1	-0.280280	2.271198	1.650552
52	1	-2.890199	-1.371763	-2.158974
53	1	-2.068749	-0.060341	1.378499

Figure S1
A3
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6981019 hartrees (-490523.375923269 kcal/mol)
Imaginary Frequencies: none found
Zero-point correction = 0.487735 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-1.864139	-2.491155	0.629898
2	6	-0.696134	-1.915708	-0.207519
3	6	-0.813676	-0.335153	-0.075489
4	6	1.180642	2.053255	-0.439657
5	6	2.276803	1.535219	-1.014124
6	6	3.630891	1.275351	-0.418618
7	1	4.416791	1.715474	-1.046362
8	1	3.733311	1.728690	0.571979
9	6	3.897365	-0.261813	-0.331644
10	6	2.833979	-0.999619	0.460241
11	6	0.674908	-2.382632	0.392680
12	1	0.637134	-2.238530	1.477473
13	1	0.730539	-3.469695	0.230066
14	6	1.889702	-1.706445	-0.186148
15	6	2.922379	-0.831364	1.957981
16	1	2.120395	-1.331502	2.506040
17	1	3.872531	-1.242697	2.323527
18	1	2.917197	0.228025	2.245519
19	1	3.946342	-0.664688	-1.350372
20	6	-2.999290	-1.476240	0.484603
21	1	-3.817577	-1.626639	1.196611
22	1	-3.421622	-1.509940	-0.523994
23	6	-2.268104	-0.142457	0.752709
24	6	-2.936647	1.090720	0.424652
25	6	-3.767870	1.262803	-0.784991
26	1	-4.787732	1.530143	-0.462408

27	1	-3.417501	2.136861	-1.351842
28	1	-3.817928	0.389773	-1.432642
29	6	-2.861539	2.232494	1.366270
30	1	-3.632889	2.043502	2.135558
31	1	-1.907685	2.266084	1.901482
32	1	-3.089694	3.197090	0.907025
33	6	-0.158453	1.943738	-1.171543
34	6	1.149856	2.713198	0.917765
35	1	2.138705	2.794997	1.373045
36	1	0.508067	2.168664	1.628355
37	6	-0.612939	0.476860	-1.362621
38	1	-2.162627	-3.491171	0.301403
39	1	0.740629	3.730034	0.841934
40	1	-1.954642	-0.110038	1.801264
41	6	-0.841217	-2.415891	-1.660938
42	1	-0.033674	-2.075555	-2.313349
43	1	-0.819015	-3.510524	-1.666320
44	1	-1.786993	-2.105607	-2.119327
45	1	-0.074728	0.013184	0.648776
46	1	-1.580260	-2.571037	1.686876
47	1	1.993064	-1.789441	-1.268540
48	1	-1.492165	0.422978	-2.016907
49	1	0.183741	-0.024647	-1.916971
50	1	-0.090590	2.399037	-2.167758
51	1	4.887833	-0.412232	0.117323
52	1	2.163234	1.131444	-2.023522
53	1	-0.921286	2.527000	-0.634984

TS (A3-B1)
B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.6313964 hartrees (-490481.517554964 kcal/mol)
Imaginary Frequencies: 1 (-1113.9943 1/cm)
Zero-point correction = 0.485696 (Hartree/Particle)

Coordinates (from last standard orientation):

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-2.409511	-2.192238	0.715144
2	6	-1.100572	-1.991996	-0.097419
3	6	-0.836330	-0.491570	0.162111
4	6	1.575571	2.158883	-0.389711
5	6	2.436032	1.312539	-1.040368
6	6	3.728971	0.740401	-0.539386
7	1	4.548834	0.923087	-1.247817
8	1	4.023135	1.181354	0.417170
9	6	3.581431	-0.833781	-0.420466
10	6	2.419124	-1.386428	0.415089
11	6	0.185554	-2.747047	0.431666
12	1	0.188818	-2.688788	1.525971
13	1	0.107337	-3.811144	0.173709
14	6	1.487505	-2.190833	-0.146056
15	6	2.446439	-0.995179	1.874266
16	1	1.655303	-1.469712	2.459256
17	1	3.405474	-1.283783	2.324711
18	1	2.360327	0.091869	2.010587

19	1	3.523231	-1.241651	-1.436496
20	6	-3.220055	-0.887301	0.478862
21	1	-4.056574	-0.775330	1.175568
22	1	-3.633942	-0.879449	-0.534715
23	6	-2.143750	0.228126	0.661717
24	6	-2.376461	1.617925	0.046312
25	6	-3.082181	1.727649	-1.280379
26	1	-4.156083	1.573501	-1.090369
27	1	-2.974188	2.722919	-1.720206
28	1	-2.779657	0.970732	-2.006913
29	6	-2.699861	2.715149	1.030872
30	1	-3.693707	2.502827	1.455009
31	1	-1.997999	2.738113	1.870675
32	1	-2.743121	3.701538	0.561352
33	6	0.227100	1.576548	-0.255330
34	6	2.002306	3.230430	0.573953
35	1	3.080797	3.211199	0.752028
36	1	1.481342	3.163246	1.537150
37	6	-0.160788	0.278668	-0.940655
38	1	-2.974662	-3.080673	0.414970
39	1	1.769462	4.216378	0.150910
40	1	-2.040108	0.389364	1.740456
41	6	-1.350694	-2.353589	-1.574483
42	1	-0.485857	-2.144399	-2.212025
43	1	-1.566144	-3.424085	-1.662164
44	1	-2.206227	-1.815444	-1.997716
45	1	-0.138104	-0.472548	1.001970
46	1	-2.186398	-2.293257	1.785494
47	1	1.639228	-2.438132	-1.198724
48	1	-0.797052	0.453634	-1.812037
49	1	0.685624	-0.292987	-1.286191
50	1	-0.994100	2.098156	-0.332487
51	1	4.532687	-1.185927	0.002196
52	1	2.046550	0.760563	-1.888708
53	1	0.116810	1.500714	0.832977

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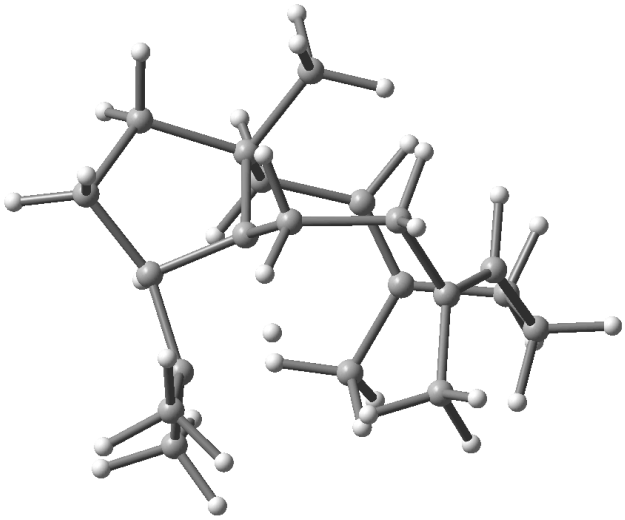
transition state structure for 1,3-hydride shift from A1



B3LYP/6-31G(d)//B3LYP/6-31G(d)
HF = -781.5987959 hartrees
Imaginary Frequencies: 1 (-1434.25 1/cm)
Zero-point correction = 0.484276 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31G(d)
HF = -781.4861761 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.351376	0.920884	0.053517
2	6	0	2.232054	0.091301	0.660504
3	6	0	1.164123	0.121860	-0.398032
4	6	0	0.866206	1.646253	-0.517605
5	6	0	2.419758	2.122234	-0.382071
6	1	0	4.123483	1.239577	0.757075
7	1	0	3.834688	0.445553	-0.805161
8	1	0	1.850753	0.736474	1.461363
9	1	0	0.582907	-0.932364	0.442206
10	1	0	2.744024	2.544188	-1.335682
11	1	0	2.468688	2.916411	0.368458
12	6	0	0.340243	2.123817	-1.883411
13	1	0	-0.672367	1.785369	-2.094620
14	1	0	0.326164	3.219674	-1.878879
15	1	0	0.987983	1.814479	-2.708080
16	6	0	-0.028777	2.259924	0.618914
17	1	0	0.115653	3.347284	0.561925
18	1	0	0.341822	1.958978	1.604191
19	6	0	1.211202	-0.725975	-1.668079
20	1	0	1.835232	-0.174723	-2.386222
21	1	0	1.736280	-1.659780	-1.485301
22	6	0	-0.156933	-1.054103	-2.354710
23	1	0	-0.489336	-0.194221	-2.938199
24	1	0	0.059692	-1.850369	-3.079745
25	6	0	-1.268339	-1.478717	-1.406620
26	6	0	-2.302541	-0.645515	-1.197371
27	1	0	-2.323053	0.266442	-1.794809
28	6	0	-1.483210	1.912614	0.440304
29	6	0	-2.265217	1.091444	1.161150
30	1	0	-1.928565	2.329217	-0.460505
31	6	0	-1.911061	0.493956	2.497597
32	1	0	-1.849227	-0.602208	2.452942
33	1	0	-0.974394	0.881865	2.908261
34	1	0	-2.698314	0.724366	3.226835
35	6	0	-3.582511	0.632058	0.564236
36	6	0	-3.423582	-0.725384	-0.196133
37	1	0	-4.354266	0.513967	1.334181
38	1	0	-3.950300	1.383302	-0.144439
39	1	0	-4.375983	-0.939384	-0.700775
40	1	0	-3.265378	-1.538370	0.520367
41	6	0	1.817197	-1.283481	1.155129
42	6	0	2.465997	-2.546851	0.662342
43	1	0	1.793698	-3.408604	0.686811
44	1	0	2.949388	-2.469964	-0.309902
45	1	0	3.264940	-2.751743	1.392989

46	6	0	1.296899	-1.381880	2.568836
47	1	0	0.732076	-2.303841	2.729775
48	1	0	2.175143	-1.405111	3.231899
49	1	0	0.687412	-0.525863	2.860064
50	6	0	-1.144689	-2.851344	-0.791915
51	1	0	-1.927312	-3.059810	-0.059058
52	1	0	-1.216200	-3.619446	-1.574246
53	1	0	-0.174506	-3.009920	-0.303214

Scheme 2, eq 1 reactant
B3LYP/6-31+G(d,p)
HF = -506.5567499 hartrees
Imaginary Frequencies: 0
Zero-point correction = 0.292334 (Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -506.4594646 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.049037	-0.005567	0.118686
2	6	0	-0.064869	0.222252	1.298102
3	1	0	-0.564314	0.466042	2.239741
4	6	0	-0.218805	-0.311611	-1.150048
5	1	0	-0.903556	-0.512897	-1.981909
6	6	0	0.685475	0.886810	-1.513381
7	1	0	0.085827	1.779047	-1.717633
8	1	0	1.244809	0.668917	-2.430006
9	6	0	0.904458	1.499121	0.925702
10	1	0	1.572130	1.728238	1.761055
11	1	0	0.194403	2.326280	0.822879
12	6	0	1.663977	1.170859	-0.356487
13	1	0	2.299677	2.032275	-0.606208
14	6	0	2.570955	-0.030673	-0.091354
15	1	0	3.134942	-0.360354	-0.969902
16	1	0	3.284708	0.160503	0.715359
17	6	0	0.962826	-0.770977	1.446441
18	1	0	1.376977	-0.976137	2.436008
19	6	0	0.662214	-1.554066	-0.915254
20	1	0	0.058235	-2.441792	-0.704848
21	1	0	1.260067	-1.780875	-1.803888
22	6	0	1.618486	-1.306139	0.275191
23	1	0	2.274838	-2.149198	0.504252
24	6	0	-2.146919	1.089167	-0.064072
25	1	0	-2.284263	1.690688	0.841772
26	1	0	-2.039314	1.768655	-0.913793
27	6	0	-2.193176	-1.033869	0.410168
28	1	0	-2.343580	-1.195047	1.482903
29	1	0	-2.107649	-2.011980	-0.073982
30	6	0	-3.216855	-0.030828	-0.178589
31	1	0	-4.140571	0.115968	0.383997
32	1	0	-3.475747	-0.255196	-1.216417

Scheme 2, eq 1 TS
B3LYP/6-31+G(d,p)
HF = -506.5199175 hartrees
Imaginary Frequencies: 1 (-310.79 cm -1)
Zero-point correction = 0.293726(Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -506.4259492 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.813981	-0.510427	0.050184
2	6	0	0.081132	-0.934666	-1.100033
3	1	0	-0.473701	-1.513054	-1.842257
4	6	0	-0.073325	0.122127	1.253253
5	1	0	-0.720399	0.079577	2.133958
6	6	0	1.259270	-0.623589	1.528855
7	1	0	1.073400	-1.653726	1.854512
8	1	0	1.763385	-0.118260	2.359509
9	6	0	1.454425	-1.525666	-0.777547
10	1	0	2.038922	-1.591316	-1.702073
11	1	0	1.326390	-2.547605	-0.404438
12	6	0	2.139927	-0.631594	0.259910
13	1	0	3.128756	-1.034770	0.500082
14	6	0	2.293409	0.780029	-0.350115
15	1	0	2.892016	1.431250	0.295182
16	1	0	2.819536	0.715537	-1.309098
17	6	0	-0.012496	0.533438	-1.336878
18	1	0	-0.445311	0.892148	-2.264014
19	6	0	0.267111	1.575341	0.878808
20	1	0	-0.619848	2.211998	0.866538
21	1	0	0.976661	2.020147	1.582052
22	6	0	0.896026	1.444521	-0.529086
23	1	0	0.978359	2.414855	-1.027064
24	6	0	-2.157430	-1.199881	0.330973
25	1	0	-2.446088	-1.859234	-0.492254
26	1	0	-2.119795	-1.790611	1.251817
27	6	0	-2.139607	0.792037	-0.700348
28	1	0	-2.395456	0.452822	-1.703120
29	1	0	-2.015799	1.871238	-0.655065
30	6	0	-2.990966	0.084282	0.353039
31	1	0	-4.043692	-0.003105	0.067670
32	1	0	-2.938310	0.586390	1.321973

Scheme 2, eq 2 TS
B3LYP/6-31+G(d,p)
HF = -429.0868813 hartrees
Imaginary Frequencies: 1 (-497.11 cm -1)
Zero-point correction = 0.254769(Hartree/Particle)

mPW1PW91/6-31+G(d,p)//B3LYP/6-31+G(d,p)
HF = -428.9973519 hartrees

Coordinates (from last standard orientation):

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.679097	-1.346592	0.096983
2	6	0	-1.310223	-0.441362	-1.059239
3	6	0	0.381948	-0.540560	1.173466
4	6	0	-0.857946	-1.397853	1.151169
5	1	0	-2.588554	-1.938952	0.057747
6	1	0	-1.047603	-2.027943	2.013902
7	6	0	-1.633876	1.038795	-0.741544
8	1	0	-1.204194	1.671046	-1.527849
9	6	0	0.201554	0.944477	1.085595
10	1	0	1.075624	-0.818536	1.967480
11	1	0	-1.863855	-0.727004	-1.958090
12	6	0	1.095619	-0.339979	-0.160786
13	6	0	0.198044	-0.630404	-1.355713
14	1	0	0.505576	-0.054438	-2.233647
15	1	0	0.373730	-1.687141	-1.593473
16	6	0	-1.123304	1.508220	0.639566
17	1	0	-1.820379	1.175774	1.421939
18	1	0	-1.097383	2.600945	0.684531
19	1	0	-2.714731	1.201685	-0.772333
20	6	0	2.512706	-0.876400	-0.219370
21	1	0	3.015054	-0.607808	-1.152454
22	1	0	3.124527	-0.549688	0.624308
23	1	0	2.432276	-1.969084	-0.166857
24	1	0	0.754199	1.520903	1.822435
25	6	0	1.531778	1.537062	-0.263599
26	1	0	0.927655	2.444036	-0.292153
27	1	0	2.430741	1.688608	0.328393
28	1	0	1.794106	1.345170	-1.303045