Supporting Information

Computational Studies on the Sterol-like Cyclization of a Monodomain Class II Terpene Cyclase

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The Concerted Pathway for the Concerted Formations of Rings ABC (10 -> 9 -> 11)

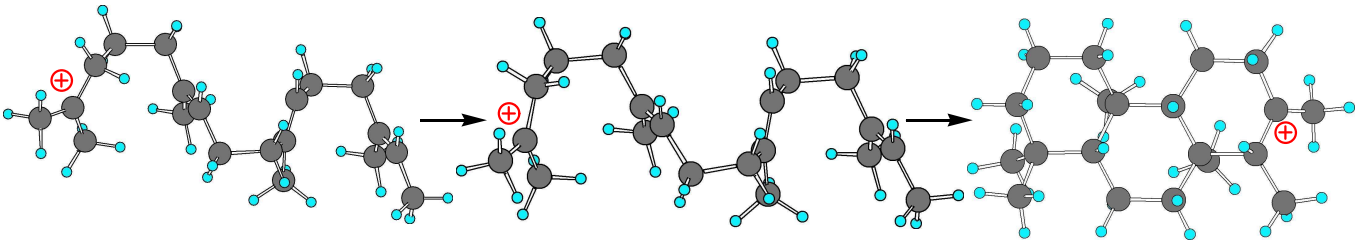


Figure S1. Structures of reactant (10), transition structure (9) and product (11).

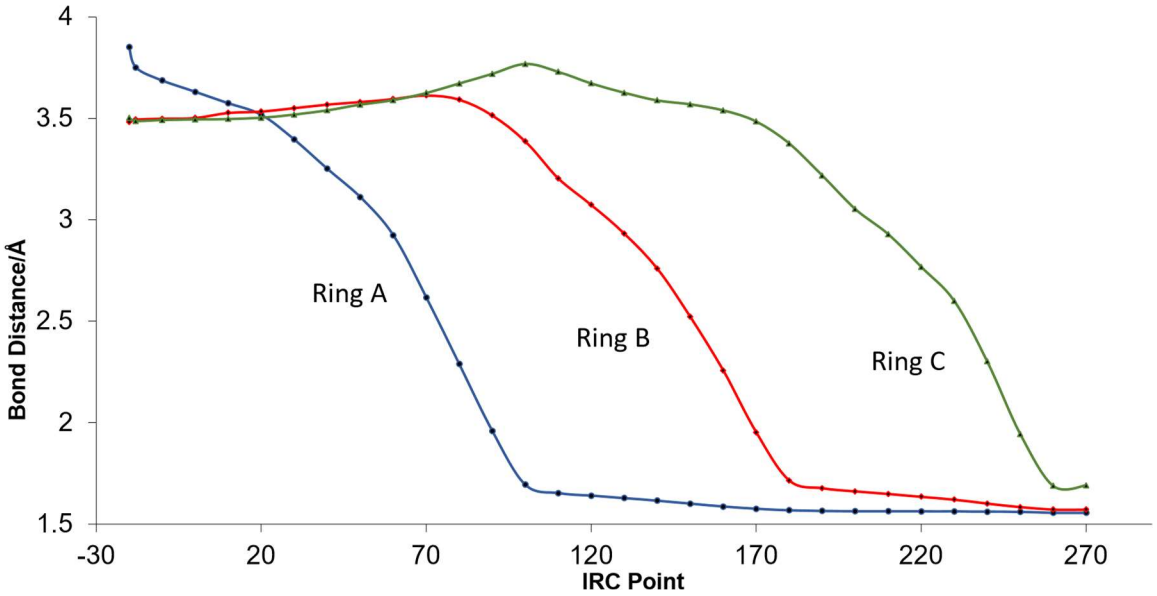


Figure S2. Changes in the bond distances of the three C-C bonds formed in the concerted ring closure of the model ABC 666 ABC system.

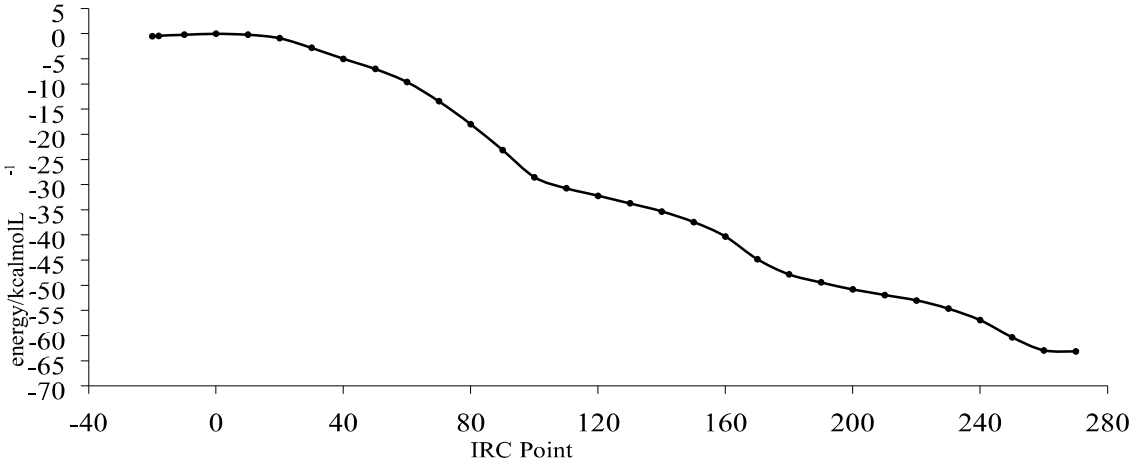


Figure S3. The energy change during the course of the concerted asynchronous cyclizations for rings A-C in the model ABC system

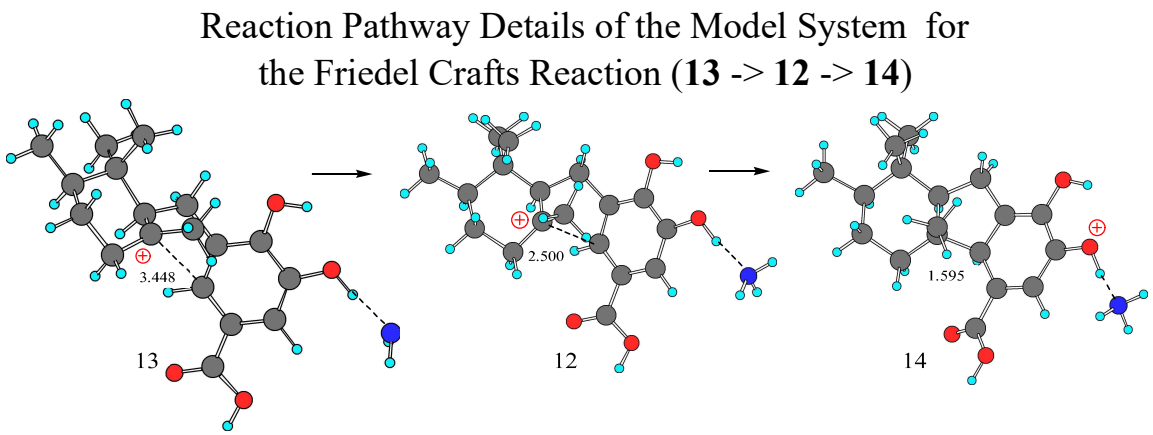


Figure S4. Reaction pathway for the Fridel-Crafts reaction of the CDE model system.

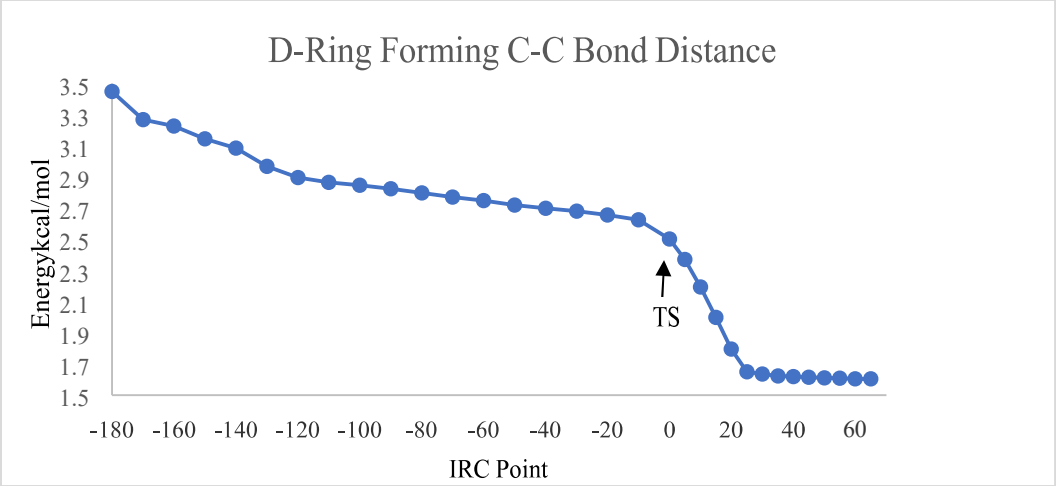


Figure S5 Bond Distances of the forming C-C bond in Ångstroms during the reaction pathway of model CDE. The transition structure (TS) annotated in the figure.

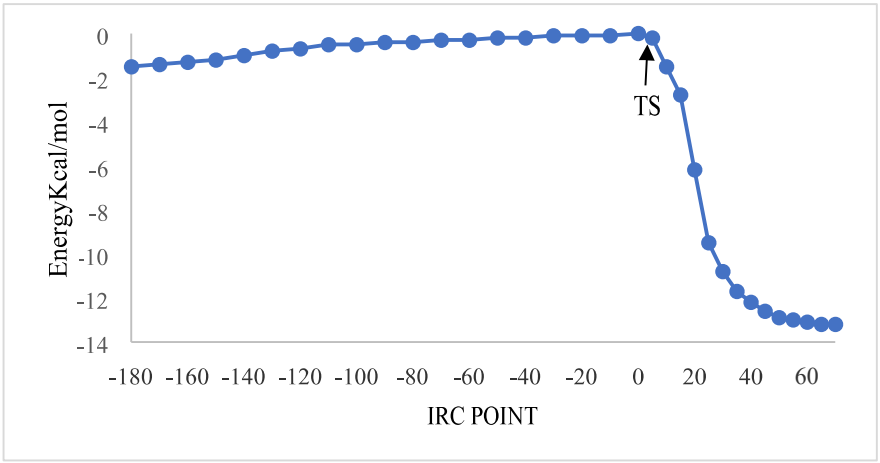


Figure S6. Change in energy along reaction pathway of model system CDE. The transition structure (TS) annotated in the figure.

Reaction Pathway Details of the Conversion of the
Conformer Reactant (**23**) via Transition Structure **22** to the Intermediate **20**

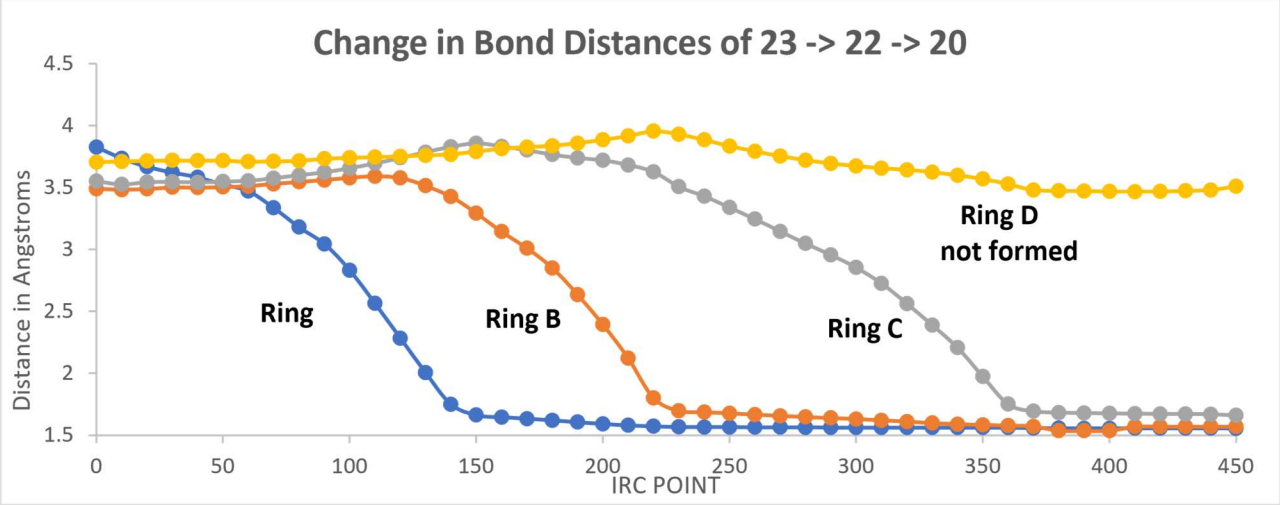


Figure S7. Change C-C bond forming distances in ABC

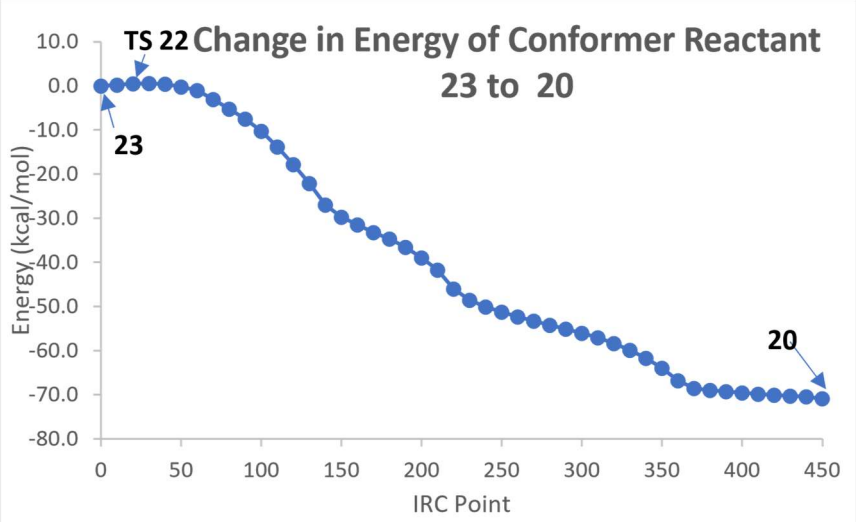


Figure S8. Change in energy along the IRC pathway.

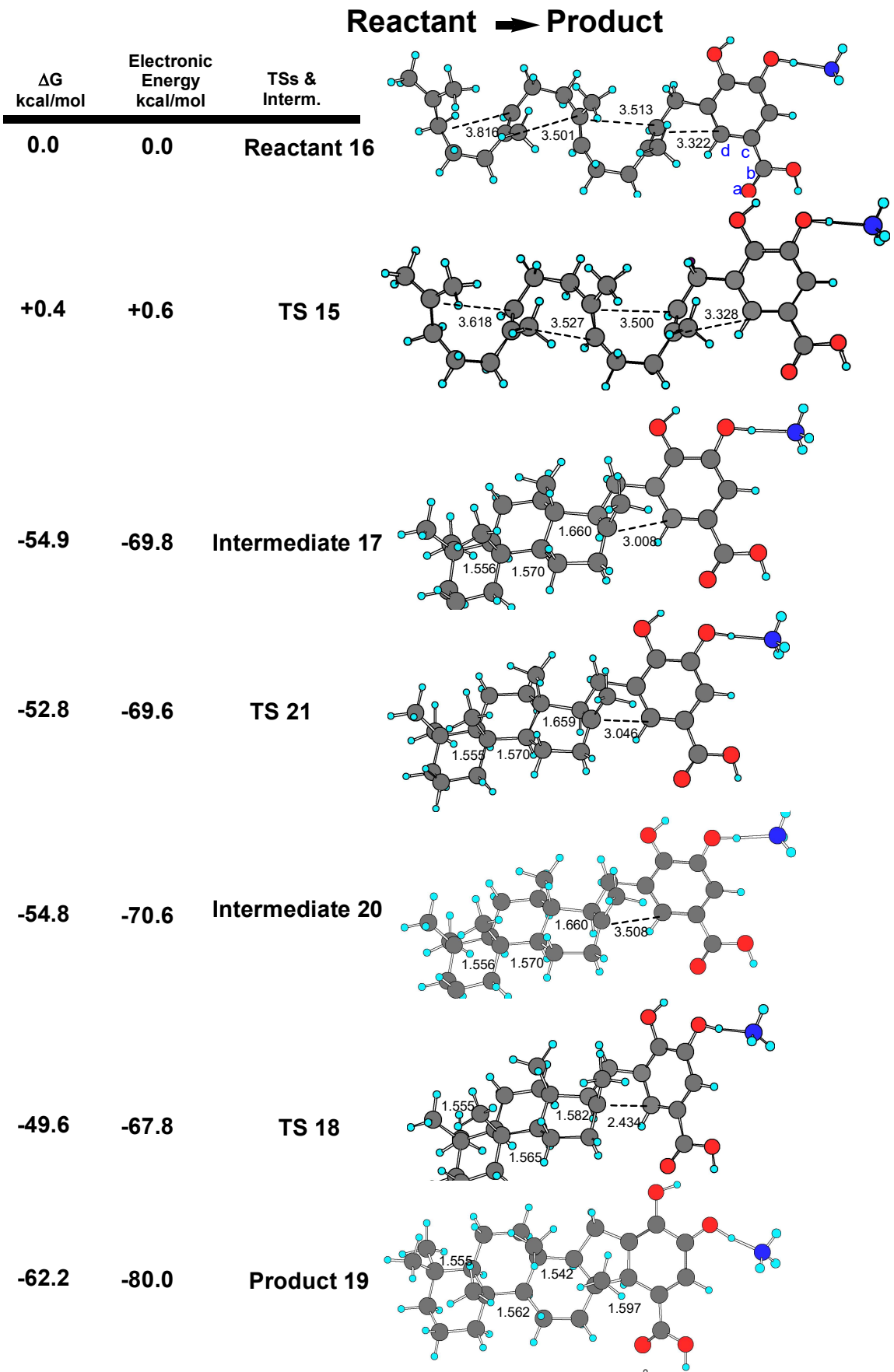


Figure S9. The overall pathway from **16** to **19**. Bond distances in Ångstroms and angles in degrees

Computational Outputs

The letters in the headings refer to the rings present in each structure. The numbers refer to the size of the cycloalkane rings, respectively. For example, ABCDE 66656 is a pentacyclic system with three cyclohexyl rings (ABC), one cylopentyl ring (D) and one six-membered benzene ring (E). This lettering is adopted from the steroid/hopene nomenclature.

TS 9 that Yields Reactant 10 and Product 11 (Figure 2A)

#M062X/6-31G(d) freq(noraman) nopop geom=check guess=read

1	6	0	6.002166	-1.525992	-0.086615
2	6	0	4.855140	0.669782	-0.546854
3	6	0	5.034639	-0.496169	0.320580
4	6	0	1.598601	-0.484863	-0.875090
5	6	0	1.771867	0.623113	-0.137053
6	6	0	2.560420	1.792117	-0.679793
7	6	0	1.209095	0.825960	1.247039
8	6	0	-2.481275	1.739839	-0.177012
9	6	0	-1.912525	-1.012597	1.132998
10	6	0	0.816498	-1.714545	-0.504503
11	6	0	-1.689360	0.612752	-0.777973
12	6	0	-0.650896	-1.622030	-0.992298
13	6	0	-1.445147	-0.585665	-0.234239
14	6	0	3.997257	1.869156	-0.128359
15	6	0	4.257677	-0.711475	1.531340
16	6	0	-4.910990	-0.604633	-0.666008
17	6	0	-3.973712	1.680941	-0.587615
18	6	0	-4.694354	0.510820	0.039526
19	6	0	-5.559874	-1.877712	-0.209006
20	6	0	-5.096801	0.713951	1.477280
21	1	0	6.850009	-1.432349	0.614635
22	1	0	6.373755	-1.407252	-1.104871
23	1	0	5.599702	-2.531232	0.081931
24	1	0	4.424466	0.190931	-1.456366
25	1	0	5.860463	0.954286	-0.897341
26	1	0	1.977537	-0.468477	-1.900415
27	1	0	2.612033	1.736481	-1.773784
28	1	0	2.051589	2.730958	-0.432938
29	1	0	0.868277	-0.099425	1.717652
30	1	0	0.340925	1.492768	1.188977
31	1	0	1.935271	1.308453	1.914436
32	1	0	-2.408401	1.735909	0.917297
33	1	0	-2.063856	2.695607	-0.514844
34	1	0	-2.746530	-1.718803	1.039917
35	1	0	-2.261274	-0.176472	1.742697
36	1	0	-1.117746	-1.529792	1.686274
37	1	0	0.823433	-1.881242	0.579715
38	1	0	1.284196	-2.593987	-0.961814
39	1	0	-1.333422	0.782439	-1.795905
40	1	0	-0.651131	-1.392280	-2.063604
41	1	0	-1.114180	-2.609417	-0.872839
42	1	0	3.990000	1.983174	0.961204
43	1	0	4.477729	2.770532	-0.518467
44	1	0	3.250024	-0.951553	1.123652
45	1	0	4.103079	0.205259	2.107397
46	1	0	4.611412	-1.538481	2.146835
47	1	0	-4.579777	-0.605784	-1.705355
48	1	0	-4.035249	1.621605	-1.680017
49	1	0	-4.454333	2.620740	-0.286910
50	1	0	-4.886254	-2.729776	-0.363187
51	1	0	-5.842937	-1.858957	0.845280

52	1	0	-6.463897	-2.085292	-0.792540
53	1	0	-5.921753	1.433705	1.543280
54	1	0	-4.269244	1.136972	2.060824
55	1	0	-5.414474	-0.205749	1.971131

SCF Done: E(RM062X) = -782.486532150 A.U. after 1 cycles

Frequencies -- -100.5334 19.6544 28.7020

Zero-point correction= 0.507315 (Hartree/Particle)
Thermal correction to Energy= 0.532046
Thermal correction to Enthalpy= 0.532990
Thermal correction to Gibbs Free Energy= 0.451973
Sum of electronic and zero-point Energies= -781.979217
Sum of electronic and thermal Energies= -781.954486
Sum of electronic and thermal Enthalpies= -781.953542
Sum of electronic and thermal Free Energies= -782.034560

Reactant 10 from TS9 (Figure 2A)

#M062X/6-31G(d) freq(noraman) nopop guess=read geom=check

1	6	0	6.371197	-1.240510	0.062183
2	6	0	4.754736	0.576640	-0.622215
3	6	0	5.178193	-0.428047	0.334551
4	6	0	1.542053	-0.515488	-0.932484
5	6	0	1.723067	0.582825	-0.175936
6	6	0	2.492614	1.763466	-0.716854
7	6	0	1.194415	0.752431	1.224642
8	6	0	-2.470782	1.722561	-0.125495
9	6	0	-1.934240	-1.067961	1.118027
10	6	0	0.773048	-1.755311	-0.571566
11	6	0	-1.708965	0.593875	-0.761167
12	6	0	-0.702935	-1.649507	-1.032916
13	6	0	-1.477134	-0.619427	-0.245656
14	6	0	3.935011	1.805252	-0.177887
15	6	0	4.360434	-0.721637	1.513478
16	6	0	-4.955687	-0.553716	-0.648829
17	6	0	-3.967344	1.707862	-0.524144
18	6	0	-4.709235	0.539513	0.081195
19	6	0	-5.631284	-1.822148	-0.218470
20	6	0	-5.096251	0.717520	1.526403
21	1	0	7.151332	-0.816247	0.722404
22	1	0	6.728995	-1.163548	-0.965348
23	1	0	6.247048	-2.280086	0.378264
24	1	0	4.044849	-0.115995	-1.166949
25	1	0	5.545717	0.800651	-1.342587
26	1	0	1.878582	-0.466182	-1.971868
27	1	0	2.526128	1.727534	-1.811900
28	1	0	1.994499	2.698709	-0.437754
29	1	0	0.845653	-0.181542	1.670680
30	1	0	0.338951	1.437837	1.205224
31	1	0	1.943891	1.198946	1.891590
32	1	0	-2.389397	1.689316	0.967724
33	1	0	-2.034187	2.676938	-0.443035
34	1	0	-2.781331	-1.757837	1.020332
35	1	0	-2.261096	-0.239747	1.750281
36	1	0	-1.141393	-1.610628	1.649208
37	1	0	0.801511	-1.944072	0.507883
38	1	0	1.233286	-2.623043	-1.056967
39	1	0	-1.364105	0.779089	-1.780350
40	1	0	-0.721463	-1.404991	-2.100815
41	1	0	-1.167613	-2.636707	-0.919001
42	1	0	3.925864	1.890084	0.913300

43	1	0	4.446980	2.696559	-0.549736
44	1	0	3.353315	-0.969077	1.120108
45	1	0	4.195228	0.178182	2.118577
46	1	0	4.746518	-1.536304	2.124616
47	1	0	-4.631703	-0.537089	-1.690354
48	1	0	-4.039178	1.676343	-1.617099
49	1	0	-4.423384	2.650864	-0.196588
50	1	0	-4.979706	-2.685829	-0.399670
51	1	0	-5.905707	-1.823194	0.838221
52	1	0	-6.544566	-1.992877	-0.799629
53	1	0	-5.892242	1.466432	1.617686
54	1	0	-4.249907	1.091317	2.116621
55	1	0	-5.446840	-0.202966	1.995776

SCF Done: E(RM062X) = -782.487367647 A.U. after 1 cycles

Frequencies -- 22.2311 26.9361 33.9446

Zero-point correction= 0.507463 (Hartree/Particle)
Thermal correction to Energy= 0.533023
Thermal correction to Enthalpy= 0.533967
Thermal correction to Gibbs Free Energy= 0.450566
Sum of electronic and zero-point Energies= -781.979905
Sum of electronic and thermal Energies= -781.954345
Sum of electronic and thermal Enthalpies= -781.953401
Sum of electronic and thermal Free Energies= -782.036802

Product 11 from TS9 (Figure 2A)

#M062X/6-31G(d) freq(noraman) nopop geom=check guess=read

1	6	0	3.663563	-1.785613	-0.911857
2	6	0	3.661693	0.693048	-0.830643
3	6	0	3.105470	-0.571839	-0.151006
4	6	0	1.556555	-0.545599	-0.294828
5	6	0	0.841402	0.748497	0.203133
6	6	0	1.503021	1.963460	-0.488090
7	6	0	0.902710	0.960524	1.731904
8	6	0	-1.474186	1.899345	-0.095071
9	6	0	-1.753213	-0.680915	1.621580
10	6	0	0.855754	-1.799624	0.231957
11	6	0	-0.636863	0.644273	-0.321465
12	6	0	-0.596564	-1.883421	-0.257780
13	6	0	-1.389629	-0.627956	0.135121
14	6	0	3.024876	1.985658	-0.330975
15	6	0	3.600918	-0.668441	1.299523
16	6	0	-2.789045	-0.710174	-0.810374
17	6	0	-2.855077	1.775105	-0.842502
18	6	0	-3.428766	0.504720	-0.386587
19	6	0	-3.555827	-2.019497	-0.670985
20	6	0	-4.528216	0.516897	0.591549
21	1	0	4.748673	-1.684816	-1.018689
22	1	0	3.236100	-1.860903	-1.918745
23	1	0	3.479241	-2.728225	-0.387220
24	1	0	3.490486	0.607607	-1.913933
25	1	0	4.748467	0.727912	-0.688523
26	1	0	1.394311	-0.545262	-1.387765
27	1	0	1.261206	1.938369	-1.561647
28	1	0	1.088439	2.895959	-0.086022
29	1	0	0.999407	0.030417	2.296119
30	1	0	0.016545	1.482697	2.105675
31	1	0	1.758247	1.580953	2.003312
32	1	0	-1.657616	2.097479	0.965076
33	1	0	-0.994521	2.787677	-0.510361

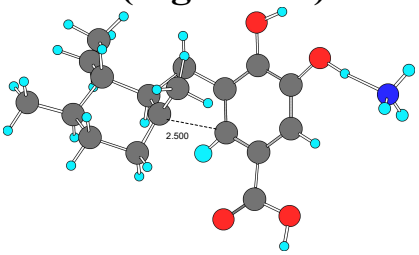
34	1	0	-2.495632	-1.461316	1.813534
35	1	0	-2.143980	0.261685	2.016134
36	1	0	-0.876336	-0.940840	2.214896
37	1	0	0.894508	-1.847180	1.325989
38	1	0	1.366761	-2.697990	-0.125524
39	1	0	-0.524251	0.542536	-1.412682
40	1	0	-0.588933	-1.983259	-1.351334
41	1	0	-1.080084	-2.776727	0.151332
42	1	0	3.297922	2.160418	0.716265
43	1	0	3.425760	2.837874	-0.889210
44	1	0	3.132022	-1.504725	1.830382
45	1	0	3.426078	0.240635	1.878284
46	1	0	4.680738	-0.850988	1.300918
47	1	0	-2.377702	-0.595102	-1.817019
48	1	0	-2.647266	1.748509	-1.916220
49	1	0	-3.488099	2.631237	-0.600158
50	1	0	-2.996456	-2.826538	-1.146243
51	1	0	-3.739349	-2.304450	0.367493
52	1	0	-4.522909	-1.947440	-1.177231
53	1	0	-5.448464	0.567718	-0.019268
54	1	0	-4.519575	1.415945	1.214053
55	1	0	-4.595184	-0.390548	1.192713

SCF Done: E(RM062X) = -782.587175110 A.U. after 1 cycles

Frequencies -- 72.4693 77.5031 102.4451

Zero-point correction= 0.519989 (Hartree/Particle)
Thermal correction to Energy= 0.540305
Thermal correction to Enthalpy= 0.541249
Thermal correction to Gibbs Free Energy= 0.475376
Sum of electronic and zero-point Energies= -782.067186
Sum of electronic and thermal Energies= -782.046870
Sum of electronic and thermal Enthalpies= -782.045926
Sum of electronic and thermal Free Energies= -782.111799

TS 12 (Figure 2B)



#M062X/6-31G(d) freq(noraman) guess=read geom=check nopop

1	6	0	-0.594207	-0.829581	-0.989597
2	6	0	-0.798241	0.562166	-1.033492
3	6	0	5.367436	0.481092	0.629683
4	6	0	3.141681	1.455278	1.183729
5	6	0	3.297167	-1.708545	0.899471
6	6	0	3.928128	0.656035	0.136053
7	6	0	3.868912	-1.298086	-1.493065
8	6	0	3.234057	-0.684962	-0.239583
9	6	0	-1.979128	1.131517	-0.551853
10	6	0	-2.991906	0.327171	-0.037107
11	6	0	1.751437	-0.301649	-0.640755
12	6	0	1.640804	1.739864	0.786000
13	6	0	1.143951	0.385944	0.530711
14	6	0	0.805467	-1.385749	-1.177006

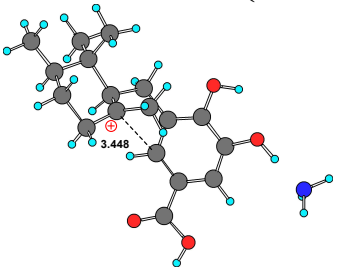
15	6	0	0.478067	-0.341128	1.639917
16	6	0	-2.824670	-1.061576	-0.030191
17	8	0	-3.701352	-1.941041	0.450443
18	6	0	-1.613281	-1.629246	-0.494665
19	7	0	-6.108601	-0.960657	1.040270
20	8	0	-1.110664	3.334223	-0.790023
21	8	0	-3.271462	3.081972	-0.234886
22	6	0	-2.054916	2.617240	-0.552282
23	8	0	-1.421883	-2.957069	-0.360414
24	1	0	-0.088563	1.228616	-1.511028
25	1	0	5.977373	-0.078007	-0.083859
26	1	0	5.839331	1.457625	0.768450
27	1	0	5.399154	-0.041407	1.591194
28	1	0	3.165125	0.942038	2.152404
29	1	0	3.603697	2.435230	1.337289
30	1	0	2.656074	-2.571747	0.693454
31	1	0	3.007897	-1.295888	1.871553
32	1	0	4.318215	-2.087613	0.998276
33	1	0	3.957312	1.258455	-0.784361
34	1	0	4.920694	-1.534449	-1.310530
35	1	0	3.814512	-0.612874	-2.346052
36	1	0	3.369715	-2.232808	-1.766283
37	1	0	-3.900627	0.769332	0.357122
38	1	0	1.886745	0.455699	-1.421631
39	1	0	1.621393	2.362148	-0.112731
40	1	0	1.123498	2.246777	1.603396
41	1	0	1.033262	-1.607904	-2.223686
42	1	0	0.892760	-2.327776	-0.626358
43	1	0	-0.546967	0.042907	1.749799
44	1	0	0.994747	-0.105044	2.579249
45	1	0	0.435486	-1.420685	1.490449
46	1	0	-4.596149	-1.516334	0.700839
47	1	0	-6.700710	-1.776445	1.191598
48	1	0	-6.191587	-0.384216	1.875867
49	1	0	-6.530446	-0.436626	0.275117
50	1	0	-3.220878	4.054472	-0.249623
51	1	0	-2.242510	-3.338266	0.001428

SCF Done: E(RM062X) = -1057.74091304 A.U. after 1 cycles

Frequencies -- -83.1714 29.4614 50.2962

Zero-point correction= 0.447410 (Hartree/Particle)
Thermal correction to Energy= 0.471286
Thermal correction to Enthalpy= 0.472230
Thermal correction to Gibbs Free Energy= 0.395780
Sum of electronic and zero-point Energies= -1057.293503
Sum of electronic and thermal Energies= -1057.269627
Sum of electronic and thermal Enthalpies= -1057.268683
Sum of electronic and thermal Free Energies= -1057.345133

Reactant 13 (Table 2B)



#M062X/6-31G(d) freq(noraman) guess=read geom=check NOPOP

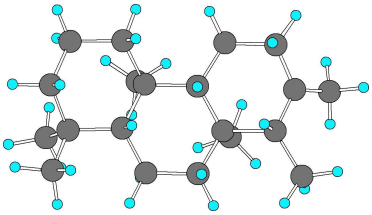
1	6	0	-0.654143	-0.268959	-0.828514
2	6	0	-1.179211	1.023167	-0.754229
3	6	0	5.737934	0.330565	0.110756
4	6	0	3.839240	0.756858	1.660001
5	6	0	3.539442	-1.749485	-0.193264
6	6	0	4.246338	0.680718	0.189328
7	6	0	3.608782	-0.161644	-2.121595
8	6	0	3.347894	-0.290671	-0.618652
9	6	0	-2.477651	1.233484	-0.303842
10	6	0	-3.285951	0.156791	0.081253
11	6	0	1.793683	0.213257	-0.416481
12	6	0	2.316094	1.112113	1.837841
13	6	0	1.631200	0.109134	1.021156
14	6	0	0.764071	-0.525087	-1.286028
15	6	0	0.967409	-1.025884	1.664287
16	6	0	-2.779650	-1.133635	0.013865
17	8	0	-3.427716	-2.257961	0.367089
18	6	0	-1.457801	-1.335693	-0.436005
19	7	0	-6.089509	-1.893891	0.517511
20	8	0	-2.279119	3.603509	-0.490773
21	8	0	-4.247985	2.733145	0.138609
22	6	0	-2.959824	2.638430	-0.239365
23	8	0	-0.964062	-2.599689	-0.442115
24	1	0	-0.595098	1.887682	-1.059058
25	1	0	6.096863	0.297963	-0.920087
26	1	0	6.324695	1.089141	0.635504
27	1	0	5.946821	-0.634996	0.581490
28	1	0	4.053059	-0.186663	2.174814
29	1	0	4.401076	1.537179	2.180785
30	1	0	2.780498	-2.402334	-0.633425
31	1	0	3.520466	-1.894491	0.891829
32	1	0	4.508462	-2.105230	-0.554096
33	1	0	4.110199	1.679299	-0.251413
34	1	0	4.653371	-0.408454	-2.331398
35	1	0	3.417747	0.855739	-2.478565
36	1	0	2.994042	-0.858262	-2.696524
37	1	0	-4.293215	0.334326	0.441598
38	1	0	1.843393	1.271963	-0.695226
39	1	0	2.157496	2.119257	1.441439
40	1	0	2.039257	1.065589	2.892968
41	1	0	0.887947	-0.166257	-2.312267
42	1	0	0.951370	-1.601468	-1.300710
43	1	0	-0.053918	-0.647199	1.871114
44	1	0	1.415297	-1.268498	2.632589
45	1	0	0.839890	-1.899875	1.020607
46	1	0	-4.423669	-2.098273	0.467616
47	1	0	-6.531100	-2.811318	0.482393
48	1	0	-6.443634	-1.432587	1.353355
49	1	0	-6.444002	-1.370716	-0.281384
50	1	0	-4.466352	3.681649	0.149264
51	1	0	-1.700475	-3.188733	-0.191329

SCF Done: E(RM062X) = -1057.74329900 A.U. after 1 cycles

Frequencies -- 22.8165 27.6875 35.9529
Zero-point correction= 0.446923 (Hartree/Particle)
Thermal correction to Energy= 0.471948
Thermal correction to Enthalpy= 0.472892
Thermal correction to Gibbs Free Energy= 0.392175
Sum of electronic and zero-point Energies= -1057.296376

Sum of electronic and thermal Energies= -1057.271351
Sum of electronic and thermal Enthalpies= -1057.270407
Sum of electronic and thermal Free Energies= -1057.351124

Product 14 (Figure 2B)



#M062X/6-31G(d) freq(noraman) guess=read geom=check NOPOP

1	6	0	-0.602481	-1.155326	-0.670453
2	6	0	-0.464268	0.322463	-0.684348
3	6	0	5.276148	0.530004	0.435821
4	6	0	3.048862	1.663685	0.547373
5	6	0	3.223289	-1.428599	1.404249
6	6	0	3.850633	0.531777	-0.118787
7	6	0	3.792247	-1.856250	-0.975131
8	6	0	3.137308	-0.849972	-0.015982
9	6	0	-1.690686	1.075087	-0.356054
10	6	0	-2.856669	0.447270	-0.079897
11	6	0	1.700740	-0.618669	-0.523569
12	6	0	1.609347	1.813237	0.031221
13	6	0	0.866501	0.486631	0.180380
14	6	0	0.743208	-1.815801	-0.655467
15	6	0	0.503419	0.211094	1.647651
16	6	0	-2.932693	-0.991798	-0.114136
17	8	0	-4.004992	-1.642328	0.174631
18	6	0	-1.789536	-1.782582	-0.446191
19	8	0	-0.816487	3.136994	-1.154555
20	8	0	-2.657027	3.171947	0.141137
21	6	0	-1.651181	2.566759	-0.503728
22	8	0	-1.869678	-3.124159	-0.396904
23	1	0	-0.169490	0.654919	-1.696705
24	1	0	5.897680	-0.249561	-0.012559
25	1	0	5.759354	1.490497	0.233366
26	1	0	5.279149	0.384846	1.521545
27	1	0	3.049196	1.516340	1.635401
28	1	0	3.575460	2.609647	0.379661
29	1	0	2.527640	-2.263832	1.543660
30	1	0	3.024686	-0.690359	2.184721
31	1	0	4.229128	-1.820869	1.581592
32	1	0	3.907262	0.764669	-1.194274
33	1	0	4.848903	-2.002370	-0.736802
34	1	0	3.723585	-1.519023	-2.015996
35	1	0	3.308875	-2.837139	-0.900475
36	1	0	-3.756710	1.013559	0.136545
37	1	0	1.838563	-0.232891	-1.547228
38	1	0	1.627268	2.105807	-1.025724
39	1	0	1.099051	2.618970	0.570259
40	1	0	0.915022	-2.418619	-1.554369
41	1	0	0.785594	-2.511755	0.193111
42	1	0	-0.351127	0.829062	1.945735
43	1	0	1.324197	0.466053	2.317009
44	1	0	0.242201	-0.836565	1.830752
45	1	0	-4.874559	-1.063286	0.485938
46	1	0	-2.580078	4.128985	-0.028884
47	1	0	-2.777581	-3.384030	-0.165220
48	7	0	-6.124148	-0.439276	0.923598

49	1	0	-6.778487	-1.183663	1.169064
50	1	0	-6.028034	0.150268	1.750524
51	1	0	-6.577351	0.121583	0.201984

SCF Done: E(RM062X) = -1057.76201626 A.U. after 1 cycles

Frequencies -- 24.7268 47.2974 62.7216

Zero-point correction= 0.447460 (Hartree/Particle)
Thermal correction to Energy= 0.471437
Thermal correction to Enthalpy= 0.472382
Thermal correction to Gibbs Free Energy= 0.395624
Sum of electronic and zero-point Energies= -1057.314556
Sum of electronic and thermal Energies= -1057.290579
Sum of electronic and thermal Enthalpies= -1057.289635
Sum of electronic and thermal Free Energies= -1057.366392

TS15

#M062X/6-31G(d) FREQ(NORAMAN) NOPOP

1	6	0	9.157678	-2.185058	-0.288946
2	6	0	8.367790	0.205632	-0.381931
3	6	0	8.350968	-1.097288	0.284740
4	6	0	5.016994	-0.366722	-0.915216
5	6	0	5.318181	0.563843	0.004241
6	6	0	6.281590	1.681009	-0.321948
7	6	0	4.744656	0.606529	1.397938
8	6	0	1.248423	2.272476	0.097521
9	6	0	1.406105	-0.706742	0.935609
10	6	0	4.058526	-1.515604	-0.770093
11	6	0	1.909415	1.164707	-0.672772
12	6	0	2.638034	-1.128442	-1.250572
13	6	0	1.972737	-0.128844	-0.335363
14	6	0	7.699453	1.440395	0.232500
15	6	0	7.527850	-1.383780	1.449896
16	6	0	-1.448796	0.390272	-0.856060
17	6	0	-0.219567	2.482629	-0.349893
18	6	0	-1.105218	1.324462	0.037850
19	6	0	-2.285979	-0.829688	-0.571309
20	6	0	-1.561560	1.299944	1.473214
21	6	0	-3.764993	-0.574219	-0.345533
22	6	0	-4.351483	0.688784	-0.330673
23	6	0	-6.531792	-0.280983	0.121875
24	6	0	-5.963850	-1.544815	0.105327
25	8	0	-6.623597	-2.710926	0.304953
26	6	0	-4.583490	-1.681064	-0.125311
27	6	0	-5.717518	0.836439	-0.098369
28	8	0	-5.623032	3.223756	-0.213848
29	8	0	-7.609183	2.243200	0.103279
30	6	0	-6.268446	2.209652	-0.081829
31	8	0	-4.040919	-2.923447	-0.129509
32	7	0	-9.333617	-2.287450	0.341520
33	1	0	10.004133	-2.323939	0.406631
34	1	0	9.552777	-1.967743	-1.281878
35	1	0	8.610565	-3.134139	-0.270110
36	1	0	7.875495	-0.052146	-1.348371
37	1	0	9.408060	0.382757	-0.698808
38	1	0	5.426616	-0.229823	-1.919604
39	1	0	6.352236	1.813012	-1.408305
40	1	0	5.910891	2.626509	0.089704

41	1	0	4.268506	-0.329208	1.700804
42	1	0	3.975959	1.386471	1.447390
43	1	0	5.507676	0.866166	2.143812
44	1	0	1.272135	2.076109	1.176124
45	1	0	1.799018	3.206746	-0.063304
46	1	0	0.481527	-1.254361	0.716291
47	1	0	1.164793	0.054016	1.681310
48	1	0	2.098645	-1.424257	1.394652
49	1	0	4.002841	-1.861842	0.269390
50	1	0	4.413229	-2.363721	-1.366952
51	1	0	2.315431	1.450616	-1.644983
52	1	0	2.709294	-0.724448	-2.266586
53	1	0	2.033822	-2.042466	-1.306904
54	1	0	7.681750	1.372042	1.325650
55	1	0	8.323992	2.306557	-0.002162
56	1	0	6.503596	-1.405813	1.015035
57	1	0	7.499548	-0.558936	2.167272
58	1	0	7.744319	-2.342046	1.922065
59	1	0	-1.104913	0.516696	-1.881965
60	1	0	-0.239044	2.624133	-1.436308
61	1	0	-0.595134	3.408327	0.104026
62	1	0	-2.183559	-1.547297	-1.393071
63	1	0	-1.903573	-1.359700	0.313753
64	1	0	-2.350966	2.046331	1.628151
65	1	0	-0.743498	1.557228	2.157602
66	1	0	-1.967498	0.329661	1.770376
67	1	0	-3.751407	1.575636	-0.505053
68	1	0	-7.592024	-0.155961	0.310996
69	1	0	-7.611018	-2.555282	0.346834
70	1	0	-7.851028	3.185017	0.099841
71	1	0	-4.774296	-3.543802	0.029705
72	1	0	-9.831374	-3.174918	0.314797
73	1	0	-9.671837	-1.783856	1.158817
74	1	0	-9.630762	-1.757981	-0.475673

SCF Done: E(RM062X) = -1408.88265681 A.U. after 18 cycles

Frequencies -- -119.0746 5.0853 13.2263

Zero-point correction= 0.652562 (Hartree/Particle)
Thermal correction to Energy= 0.689878
Thermal correction to Enthalpy= 0.690822
Thermal correction to Gibbs Free Energy= 0.577516
Sum of electronic and zero-point Energies= -1408.230095
Sum of electronic and thermal Energies= -1408.192779
Sum of electronic and thermal Enthalpies= -1408.191835
Sum of electronic and thermal Free Energies= -1408.305141

Reactant 16 From TS15

#M062X/6-31G(d) freq(noraman) nopop guess=read geom=check

1	6	0	9.589968	-1.930747	-0.067979
2	6	0	8.301699	0.220102	-0.376700
3	6	0	8.514479	-1.019625	0.347262
4	6	0	5.002249	-0.331720	-0.977934
5	6	0	5.279608	0.555500	-0.004779
6	6	0	6.222791	1.704789	-0.265630
7	6	0	4.700603	0.505361	1.384892
8	6	0	1.235645	2.211581	0.111709
9	6	0	1.391201	-0.805866	0.818246
10	6	0	4.070854	-1.508429	-0.901337
11	6	0	1.898575	1.137107	-0.702867

12	6	0	2.646165	-1.123356	-1.373369
13	6	0	1.963504	-0.169931	-0.421852
14	6	0	7.630692	1.433354	0.298707
15	6	0	7.594364	-1.430988	1.407747
16	6	0	-1.476329	0.371799	-0.888767
17	6	0	-0.231421	2.441786	-0.327518
18	6	0	-1.121558	1.277497	0.029667
19	6	0	-2.325375	-0.846220	-0.632351
20	6	0	-1.571563	1.213353	1.465863
21	6	0	-3.796879	-0.577615	-0.373489
22	6	0	-4.370274	0.691051	-0.337132
23	6	0	-6.551091	-0.260572	0.150214
24	6	0	-5.996335	-1.529814	0.112990
25	8	0	-6.663783	-2.690698	0.317041
26	6	0	-4.622192	-1.677941	-0.146302
27	6	0	-5.729980	0.850384	-0.077189
28	8	0	-5.613154	3.237559	-0.173770
29	8	0	-7.602838	2.274332	0.172862
30	6	0	-6.266342	2.228883	-0.038295
31	8	0	-4.092395	-2.925487	-0.171909
32	7	0	-9.367450	-2.237620	0.422229
33	1	0	10.385884	-1.784043	0.686137
34	1	0	10.011689	-1.693896	-1.045767
35	1	0	9.295851	-2.981276	0.009150
36	1	0	7.546807	-0.220869	-1.093946
37	1	0	9.167518	0.471814	-0.994754
38	1	0	5.395971	-0.117992	-1.975738
39	1	0	6.305804	1.892460	-1.342450
40	1	0	5.838443	2.621712	0.194831
41	1	0	4.227896	-0.450629	1.620613
42	1	0	3.928315	1.277638	1.479909
43	1	0	5.458579	0.718981	2.150261
44	1	0	1.257505	1.970468	1.181193
45	1	0	1.787906	3.150912	-0.009141
46	1	0	0.479578	-1.360489	0.565430
47	1	0	1.126692	-0.078366	1.588911
48	1	0	2.090377	-1.528958	1.258176
49	1	0	4.017114	-1.910831	0.117071
50	1	0	4.448580	-2.313880	-1.541072
51	1	0	2.309629	1.465726	-1.659398
52	1	0	2.715394	-0.678895	-2.372523
53	1	0	2.057937	-2.044403	-1.469014
54	1	0	7.581368	1.293583	1.383304
55	1	0	8.272582	2.302109	0.131207
56	1	0	6.594640	-1.459647	0.925630
57	1	0	7.492304	-0.657587	2.177938
58	1	0	7.834703	-2.397179	1.849468
59	1	0	-1.136180	0.523777	-1.912446
60	1	0	-0.252188	2.614634	-1.409359
61	1	0	-0.602017	3.355543	0.153881
62	1	0	-2.246579	-1.536921	-1.479506
63	1	0	-1.936608	-1.411116	0.228097
64	1	0	-2.367713	1.947720	1.642439
65	1	0	-0.753056	1.461417	2.153063
66	1	0	-1.966760	0.231959	1.740089
67	1	0	-3.764743	1.573429	-0.515329
68	1	0	-7.606101	-0.126174	0.360817
69	1	0	-7.648092	-2.524731	0.384304
70	1	0	-7.835099	3.218512	0.182284
71	1	0	-4.828343	-3.540126	-0.002797
72	1	0	-9.875332	-3.119628	0.408280
73	1	0	-9.680855	-1.729747	1.246764
74	1	0	-9.678243	-1.705646	-0.388245

SCF Done: E(RM062X) = -1408.88353263 A.U. after 1 cycles

Frequencies -- 7.8028 14.2663 17.6488

Zero-point correction= 0.653059 (Hartree/Particle)
Thermal correction to Energy= 0.690922
Thermal correction to Enthalpy= 0.691866
Thermal correction to Gibbs Free Energy= 0.577779
Sum of electronic and zero-point Energies= -1408.230474
Sum of electronic and thermal Energies= -1408.192611
Sum of electronic and thermal Enthalpies= -1408.191667
Sum of electronic and thermal Free Energies= -1408.305753

First Intermediate 17 – Product of TS 15

#M062X/6-31G(d) freq(noraman) guess=read geom=check nopop

1	6	0	5.575021	-1.708903	-2.338507
2	6	0	6.139174	0.545132	-1.474939
3	6	0	5.515894	-0.810165	-1.092181
4	6	0	4.029215	-0.560829	-0.711075
5	6	0	3.770350	0.532787	0.372292
6	6	0	4.479484	1.832836	-0.071384
7	6	0	4.275370	0.157397	1.783219
8	6	0	1.770740	1.969656	1.213133
9	6	0	1.390315	-1.011005	2.026700
10	6	0	3.236002	-1.834673	-0.406239
11	6	0	2.222151	0.795098	0.347163
12	6	0	1.725797	-1.569680	-0.399870
13	6	0	1.347294	-0.461548	0.596553
14	6	0	5.955997	1.625174	-0.413422
15	6	0	6.343004	-1.493594	0.006628
16	6	0	-0.197196	-0.023573	0.190198
17	6	0	0.248899	2.297224	0.962503
18	6	0	-0.446196	1.022672	1.160468
19	6	0	-1.205867	-1.165442	0.131775
20	6	0	-1.199801	0.806133	2.405133
21	6	0	-2.622420	-0.672496	-0.078557
22	6	0	-2.949519	0.628665	-0.459805
23	6	0	-5.315095	0.097501	-0.421787
24	6	0	-5.009125	-1.206750	-0.056467
25	8	0	-5.893103	-2.191573	0.176279
26	6	0	-3.660673	-1.580622	0.115312
27	6	0	-4.277055	1.013801	-0.620237
28	8	0	-3.660082	3.268887	-1.088546
29	8	0	-5.824410	2.696840	-1.210984
30	6	0	-4.525429	2.428446	-0.992803
31	8	0	-3.370270	-2.847180	0.481949
32	7	0	-8.429129	-1.547809	-0.490623
33	1	0	6.587447	-1.692931	-2.755611
34	1	0	4.887489	-1.360083	-3.118035
35	1	0	5.338268	-2.752639	-2.110805
36	1	0	5.675679	0.887287	-2.412108
37	1	0	7.205310	0.402054	-1.688577
38	1	0	3.587721	-0.142882	-1.633595
39	1	0	3.967703	2.232673	-0.960205
40	1	0	4.398788	2.592258	0.715977
41	1	0	4.296012	-0.919140	1.966313
42	1	0	3.663109	0.613023	2.567711
43	1	0	5.292348	0.521039	1.941276
44	1	0	1.924571	1.785234	2.280799
45	1	0	2.310487	2.885177	0.964118
46	1	0	0.565605	-1.709106	2.197817
47	1	0	1.342288	-0.236229	2.798124
48	1	0	2.310614	-1.570687	2.191177

49	1	0	3.552305	-2.278226	0.544533
50	1	0	3.426441	-2.594255	-1.169845
51	1	0	2.018916	1.088859	-0.694876
52	1	0	1.422540	-1.265886	-1.411029
53	1	0	1.183483	-2.490223	-0.158820
54	1	0	6.524677	1.368952	0.487930
55	1	0	6.373778	2.572061	-0.770489
56	1	0	5.863411	-2.414569	0.356705
57	1	0	6.524882	-0.856145	0.874064
58	1	0	7.320398	-1.774306	-0.400561
59	1	0	-0.064524	0.419921	-0.801586
60	1	0	0.146231	2.642197	-0.071095
61	1	0	-0.088198	3.072396	1.653691
62	1	0	-0.927799	-1.834290	-0.689615
63	1	0	-1.175808	-1.786698	1.033700
64	1	0	-2.171766	1.300326	2.234204
65	1	0	-0.731987	1.326001	3.247982
66	1	0	-1.398779	-0.241301	2.631997
67	1	0	-2.192459	1.381646	-0.662603
68	1	0	-6.346995	0.406683	-0.546296
69	1	0	-6.836670	-1.914027	-0.057080
70	1	0	-5.880481	3.640045	-1.444606
71	1	0	-4.217553	-3.323399	0.557460
72	1	0	-8.975896	-2.405402	-0.432938
73	1	0	-8.889461	-0.868754	0.112507
74	1	0	-8.523317	-1.207220	-1.445745

SCF Done: E(RM062X) = -1408.99474617 A.U. after 1 cycles
Frequencies -- 16.6714 21.9944 29.4300

Zero-point correction= 0.665141 (Hartree/Particle)
Thermal correction to Energy= 0.698128
Thermal correction to Enthalpy= 0.699072
Thermal correction to Gibbs Free Energy= 0.601539
Sum of electronic and zero-point Energies= -1408.329606
Sum of electronic and thermal Energies= -1408.296618
Sum of electronic and thermal Enthalpies= -1408.295674
Sum of electronic and thermal Free Energies= -1408.393207

TS 18 Connecting 20 and 19

#M062X/6-31G(d) FREQ(NORAMAN) NOPOP GEOM=CHECK GUESS=READ

1	6	0	6.067790	-0.862416	-2.017486
2	6	0	6.101033	1.161102	-0.587610
3	6	0	5.628729	-0.303391	-0.654082
4	6	0	4.075494	-0.309167	-0.572109
5	6	0	3.446775	0.456115	0.636830
6	6	0	4.022948	1.890733	0.650427
7	6	0	3.724055	-0.194270	2.010798
8	6	0	1.119870	1.442527	1.283442
9	6	0	1.102708	-1.715406	1.357185
10	6	0	3.445224	-1.695339	-0.748406
11	6	0	1.915260	0.543136	0.327296
12	6	0	1.938490	-1.599630	-1.005689
13	6	0	1.208351	-0.829118	0.107317
14	6	0	5.551670	1.926976	0.611384
15	6	0	6.319713	-1.142817	0.430874
16	6	0	-0.349804	1.714722	0.772117
17	6	0	-2.553434	-0.937317	-0.902182
18	6	0	-2.679025	0.458443	-1.056578

19	6	0	-3.861395	1.117229	-0.704373
20	6	0	-4.944246	0.403620	-0.203391
21	6	0	-0.226225	-0.461870	-0.447965
22	6	0	-0.896493	0.362589	0.598672
23	6	0	-1.172274	-1.564635	-0.940710
24	6	0	-1.657013	-0.227370	1.732635
25	6	0	-4.850035	-0.988659	-0.085655
26	8	0	-5.800956	-1.784653	0.394951
27	6	0	-3.643193	-1.647719	-0.424290
28	7	0	-8.184442	-0.664062	0.782344
29	8	0	-2.874315	3.250478	-1.074562
30	8	0	-5.072055	3.143077	-0.626950
31	6	0	-3.864141	2.599653	-0.832362
32	8	0	-3.531276	-2.969530	-0.185009
33	1	0	7.130448	-0.650872	-2.176735
34	1	0	5.508518	-0.399013	-2.838940
35	1	0	5.942124	-1.947469	-2.083242
36	1	0	5.780758	1.669368	-1.509263
37	1	0	7.197711	1.186224	-0.582828
38	1	0	3.764542	0.276307	-1.456133
39	1	0	3.635062	2.438967	-0.221904
40	1	0	3.676921	2.424149	1.544379
41	1	0	3.894614	-1.271332	1.952902
42	1	0	2.898540	-0.028975	2.710080
43	1	0	4.611438	0.238919	2.476355
44	1	0	1.071691	1.026325	2.295688
45	1	0	1.578739	2.430000	1.368448
46	1	0	0.352648	-2.499273	1.208134
47	1	0	0.833759	-1.164400	2.262782
48	1	0	2.046017	-2.222001	1.560432
49	1	0	3.644876	-2.331349	0.121891
50	1	0	3.898669	-2.205948	-1.602542
51	1	0	1.869765	1.044612	-0.653712
52	1	0	1.780763	-1.079682	-1.961616
53	1	0	1.501707	-2.600758	-1.109007
54	1	0	5.965927	1.518789	1.540701
55	1	0	5.882450	2.969966	0.569977
56	1	0	5.931317	-2.167316	0.453533
57	1	0	6.219824	-0.722094	1.433188
58	1	0	7.390700	-1.207822	0.210091
59	1	0	-0.297548	2.257223	-0.176042
60	1	0	-0.900151	2.308175	1.505944
61	1	0	-1.920233	1.048482	-1.557829
62	1	0	-5.853885	0.915871	0.091447
63	1	0	-0.014745	0.202334	-1.292891
64	1	0	-0.885212	-1.898782	-1.942437
65	1	0	-1.165614	-2.451444	-0.299272
66	1	0	-2.657239	0.227511	1.769057
67	1	0	-1.160089	0.051437	2.670905
68	1	0	-1.764408	-1.310771	1.671746
69	1	0	-6.685591	-1.300384	0.564597
70	1	0	-8.820284	-1.446629	0.931627
71	1	0	-8.288577	-0.048965	1.587396
72	1	0	-8.537441	-0.156367	-0.027349
73	1	0	-4.973926	4.107446	-0.722433
74	1	0	-4.389679	-3.283327	0.152514

SCF Done: E(RM062X) = -1408.99161573 A.U. after 1 cycles

Frequencies -- -123.8479 24.2744 33.8005

Zero-point correction= 0.666090 (Hartree/Particle)
Thermal correction to Energy= 0.697541
Thermal correction to Enthalpy= 0.698485

Thermal correction to Gibbs Free Energy= 0.606782
Sum of electronic and zero-point Energies= -1408.325525
Sum of electronic and thermal Energies= -1408.294075
Sum of electronic and thermal Enthalpies= -1408.293131
Sum of electronic and thermal Free Energies= -1408.384833

Final Product 19

#M062X/6-31G(d) freq(noraman) guess=read geom=check NOPOP

1	6	0	6.020231	-1.443266	-1.703608
2	6	0	6.041739	0.914005	-0.944707
3	6	0	5.583116	-0.505967	-0.565470
4	6	0	4.031009	-0.500250	-0.467958
5	6	0	3.391459	0.590009	0.451970
6	6	0	3.958717	1.963480	0.027292
7	6	0	3.674156	0.401576	1.957021
8	6	0	1.039281	1.706659	0.767224
9	6	0	1.080234	-1.292330	1.810608
10	6	0	3.416898	-1.881344	-0.210137
11	6	0	1.860412	0.565152	0.142551
12	6	0	1.910701	-1.877871	-0.475975
13	6	0	1.157861	-0.815211	0.346647
14	6	0	5.487411	1.999244	-0.027961
15	6	0	6.292736	-0.979359	0.711620
16	6	0	-0.371664	1.819791	0.156617
17	6	0	-2.520101	-1.193871	-0.578419
18	6	0	-2.384274	0.282941	-0.653453
19	6	0	-3.634594	1.042906	-0.462019
20	6	0	-4.818560	0.422448	-0.254098
21	6	0	-0.239394	-0.637803	-0.280976
22	6	0	-1.124634	0.498048	0.303815
23	6	0	-1.179856	-1.846955	-0.416452
24	6	0	-1.605162	0.300996	1.748961
25	6	0	-4.889101	-1.016600	-0.227836
26	8	0	-5.981774	-1.658918	-0.000426
27	6	0	-3.721409	-1.815933	-0.424817
28	7	0	-8.154784	-0.421931	0.513553
29	8	0	-2.705687	3.070296	-1.288601
30	8	0	-4.637858	3.156177	-0.137132
31	6	0	-3.585629	2.526180	-0.675900
32	8	0	-3.803030	-3.154243	-0.316749
33	1	0	7.076961	-1.272142	-1.935891
34	1	0	5.443226	-1.259564	-2.617770
35	1	0	5.915955	-2.499340	-1.436755
36	1	0	5.711865	1.118242	-1.974370
37	1	0	7.138468	0.947913	-0.955108
38	1	0	3.707189	-0.213752	-1.485225
39	1	0	3.564621	2.216915	-0.968944
40	1	0	3.609720	2.741998	0.715847
41	1	0	3.708437	-0.644928	2.267177
42	1	0	2.909066	0.901942	2.559969
43	1	0	4.628063	0.849689	2.240541
44	1	0	0.968430	1.593887	1.855757
45	1	0	1.541059	2.662801	0.597673
46	1	0	0.210429	-1.939829	1.968956
47	1	0	1.018655	-0.475881	2.532253
48	1	0	1.957402	-1.884171	2.078172
49	1	0	3.625439	-2.213828	0.813818
50	1	0	3.876683	-2.626379	-0.866021
51	1	0	1.810733	0.739136	-0.946642
52	1	0	1.751609	-1.677578	-1.546321

53	1	0	1.486137	-2.870613	-0.272019
54	1	0	5.908326	1.890673	0.978570
55	1	0	5.810510	2.984218	-0.381641
56	1	0	5.904458	-1.945754	1.051725
57	1	0	6.209173	-0.273775	1.540075
58	1	0	7.360484	-1.113625	0.505083
59	1	0	-0.283787	2.075837	-0.906297
60	1	0	-0.917913	2.641177	0.633568
61	1	0	-2.010093	0.567493	-1.654121
62	1	0	-5.734679	0.992998	-0.140147
63	1	0	-0.036635	-0.311048	-1.313300
64	1	0	-0.934097	-2.498978	-1.262426
65	1	0	-1.207919	-2.495078	0.469833
66	1	0	-2.424309	0.996670	1.964293
67	1	0	-0.812216	0.511428	2.465557
68	1	0	-1.964557	-0.715104	1.943186
69	1	0	-6.870681	-1.069738	0.210815
70	1	0	-8.824470	-1.150541	0.764592
71	1	0	-8.121066	0.227745	1.299172
72	1	0	-8.554190	0.081180	-0.278935
73	1	0	-4.549369	4.104313	-0.346483
74	1	0	-4.726342	-3.407633	-0.147061

SCF Done: E(RM062X) = -1409.01106547 A.U. after 1 cycles
Frequencies -- 21.7011 35.0903 46.9362
Zero-point correction= 0.665961 (Hartree/Particle)
Thermal correction to Energy= 0.697638
Thermal correction to Enthalpy= 0.698582
Thermal correction to Gibbs Free Energy= 0.606122
Sum of electronic and zero-point Energies= -1408.345104
Sum of electronic and thermal Energies= -1408.313428
Sum of electronic and thermal Enthalpies= -1408.312483
Sum of electronic and thermal Free Energies= -1408.404943

Second Intermediate 20 from TS 18

#M062X/6-31G(d) FREQ(NORAMAN) NOPOP GEOM=CHECK GUESS=READ

1	6	0	5.712960	1.059194	-2.501078
2	6	0	6.196561	1.442864	-0.099675
3	6	0	5.581470	0.444048	-1.097899
4	6	0	4.074116	0.288708	-0.747762
5	6	0	3.744870	-0.079274	0.732407
6	6	0	4.451318	0.940555	1.655751
7	6	0	4.192677	-1.498882	1.145742
8	6	0	1.681585	-0.015095	2.318585
9	6	0	1.322074	-2.213686	0.145073
10	6	0	3.288054	-0.591622	-1.723194
11	6	0	2.195290	0.123464	0.885946
12	6	0	1.775114	-0.411384	-1.549121
13	6	0	1.332883	-0.700657	-0.105856
14	6	0	5.945844	1.080052	1.360269
15	6	0	6.368718	-0.874836	-1.098298
16	6	0	0.165833	0.398280	2.406757
17	6	0	-2.607781	-0.226813	-0.757327
18	6	0	-2.996612	1.105860	-0.602876
19	6	0	-4.312210	1.428763	-0.291700
20	6	0	-5.275953	0.425407	-0.129702
21	6	0	-0.207420	-0.089282	-0.000353

22	6	0	-0.516217	-0.393859	1.377772
23	6	0	-1.176869	-0.601326	-1.073464
24	6	0	-1.350531	-1.531193	1.773704
25	6	0	-4.907210	-0.903371	-0.280293
26	8	0	-5.715939	-1.969872	-0.138612
27	6	0	-3.567287	-1.221289	-0.587922
28	7	0	-8.319081	-1.276119	-0.232302
29	8	0	-3.837012	3.765101	-0.194947
30	8	0	-5.951027	3.082488	0.108780
31	6	0	-4.643494	2.868809	-0.129471
32	8	0	-3.220144	-2.529864	-0.684744
33	1	0	6.743238	1.393839	-2.661717
34	1	0	5.057401	1.929862	-2.620836
35	1	0	5.481538	0.341120	-3.293753
36	1	0	5.767310	2.436478	-0.296149
37	1	0	7.273450	1.524781	-0.290336
38	1	0	3.670215	1.309702	-0.871305
39	1	0	3.975808	1.925334	1.531277
40	1	0	4.319279	0.649285	2.705198
41	1	0	4.233056	-2.202268	0.311523
42	1	0	3.533154	-1.927384	1.906408
43	1	0	5.191476	-1.476657	1.585332
44	1	0	1.795650	-1.031272	2.707269
45	1	0	2.210108	0.651897	3.002337
46	1	0	0.504229	-2.694876	-0.399486
47	1	0	1.223531	-2.483468	1.201254
48	1	0	2.245589	-2.664894	-0.217707
49	1	0	3.563318	-1.647176	-1.616110
50	1	0	3.529826	-0.322491	-2.755389
51	1	0	2.035095	1.176717	0.604926
52	1	0	1.518336	0.625358	-1.805886
53	1	0	1.235159	-1.063753	-2.243865
54	1	0	6.473351	0.153020	1.613375
55	1	0	6.366782	1.850981	2.013818
56	1	0	5.892403	-1.627276	-1.737199
57	1	0	6.493684	-1.307146	-0.103668
58	1	0	7.370580	-0.695988	-1.503276
59	1	0	0.098475	1.466379	2.177675
60	1	0	-0.219474	0.201859	3.409492
61	1	0	-2.286785	1.917854	-0.737793
62	1	0	-6.297783	0.686529	0.122100
63	1	0	-0.044028	0.987425	-0.111979
64	1	0	-0.879675	-0.149727	-2.024941
65	1	0	-1.103737	-1.683990	-1.201476
66	1	0	-2.342505	-1.072778	1.958097
67	1	0	-1.024236	-1.969728	2.721382
68	1	0	-1.505518	-2.277384	0.991399
69	1	0	-6.690674	-1.696364	-0.129169
70	1	0	-8.870179	-2.122386	-0.365949
71	1	0	-8.698275	-0.808754	0.589041
72	1	0	-8.513195	-0.674006	-1.030587
73	1	0	-6.062810	4.045157	0.199407
74	1	0	-4.043319	-3.044412	-0.586525

SCF Done: E(RM062X) = -1408.99596857 A.U. after 1 cycles
Frequencies -- 17.3515 21.0692 24.8153

Zero-point correction= 0.665420 (Hartree/Particle)
Thermal correction to Energy= 0.698102
Thermal correction to Enthalpy= 0.699046
Thermal correction to Gibbs Free Energy= 0.602911
Sum of electronic and zero-point Energies= -1408.330548
Sum of electronic and thermal Energies= -1408.297867
Sum of electronic and thermal Enthalpies= -1408.296923

Sum of electronic and thermal Free Energies= -1408.393058

TS 21 of Interconversion of Conformers 17 and 20

#M062X/6-31G(d) freq(noraman) nopop guess=read geom=check

1	6	0	5.691161	-1.316597	-2.451317
2	6	0	6.198412	0.783049	-1.233322
3	6	0	5.572755	-0.616283	-1.087174
4	6	0	4.069119	-0.429539	-0.737359
5	6	0	3.755450	0.479808	0.492367
6	6	0	4.469465	1.836143	0.282371
7	6	0	4.211251	-0.108282	1.845812
8	6	0	1.707949	1.749095	1.475441
9	6	0	1.330627	-1.330068	1.769118
10	6	0	3.272576	-1.735496	-0.680380
11	6	0	2.206866	0.735482	0.446818
12	6	0	1.762278	-1.474838	-0.699960
13	6	0	1.335400	-0.547638	0.449391
14	6	0	5.960161	1.687929	-0.028586
15	6	0	6.359225	-1.456989	-0.070330
16	6	0	-0.194748	-0.055274	0.058825
17	6	0	0.189379	2.100379	1.234113
18	6	0	-0.496028	0.806038	1.183007
19	6	0	-1.187847	-1.179590	-0.227704
20	6	0	-1.295046	0.369820	2.337774
21	6	0	-2.612776	-0.671410	-0.307954
22	6	0	-2.939912	0.647572	-0.628577
23	6	0	-5.304455	0.169717	-0.378084
24	6	0	-4.998680	-1.148374	-0.068054
25	8	0	-5.881503	-2.115128	0.234122
26	6	0	-3.649018	-1.558598	-0.029957
27	6	0	-4.266509	1.066171	-0.656069
28	8	0	-3.646958	3.320842	-1.126197
29	8	0	-5.825272	2.794929	-1.055154
30	6	0	-4.517078	2.495381	-0.970088
31	8	0	-3.363022	-2.837277	0.299172
32	7	0	-8.448749	-1.412076	-0.208491
33	1	0	6.720076	-1.236983	-2.817458
34	1	0	5.034340	-0.854960	-3.198132
35	1	0	5.452050	-2.382964	-2.393566
36	1	0	5.769731	1.260817	-2.126652
37	1	0	7.274011	0.678813	-1.420817
38	1	0	3.667824	0.130644	-1.601314
39	1	0	3.987184	2.367074	-0.552362
40	1	0	4.350954	2.463847	1.174229
41	1	0	4.241995	-1.200003	1.856147
42	1	0	3.562663	0.210945	2.667182
43	1	0	5.215326	0.235860	2.099100
44	1	0	1.828819	1.393181	2.503085
45	1	0	2.242048	2.698056	1.398659
46	1	0	0.509688	-2.053092	1.788380
47	1	0	1.242323	-0.697540	2.657726
48	1	0	2.251471	-1.903929	1.873728
49	1	0	3.547905	-2.331535	0.197124
50	1	0	3.506990	-2.356131	-1.549753
51	1	0	2.042661	1.195190	-0.540755
52	1	0	1.502390	-1.006567	-1.659101
53	1	0	1.214251	-2.421344	-0.639083
54	1	0	6.495613	1.299407	0.845907
55	1	0	6.382767	2.679815	-0.219154
56	1	0	5.873558	-2.421991	0.114052
57	1	0	6.498284	-0.959471	0.891344
58	1	0	7.355548	-1.668820	-0.473227

59	1	0	-0.026092	0.551383	-0.836140
60	1	0	0.112913	2.617555	0.272488
61	1	0	-0.178913	2.741437	2.037728
62	1	0	-0.906594	-1.656760	-1.172821
63	1	0	-1.136254	-1.969374	0.528208
64	1	0	-2.272090	0.866999	2.205901
65	1	0	-0.876952	0.747574	3.276785
66	1	0	-1.478146	-0.704656	2.373513
67	1	0	-2.181254	1.384415	-0.878550
68	1	0	-6.335263	0.505963	-0.396188
69	1	0	-6.836131	-1.814178	0.088827
70	1	0	-5.882140	3.744440	-1.261270
71	1	0	-4.214059	-3.290834	0.442719
72	1	0	-8.607626	-1.042762	-1.144241
73	1	0	-9.003619	-2.263259	-0.134522
74	1	0	-8.852850	-0.744319	0.445433

SCF Done: E(RM062X) = -1408.99447418 A.U. after 1 cycles

Frequencies -- -16.6869 21.0899 28.4463

Zero-point correction= 0.665128 (Hartree/Particle)
Thermal correction to Energy= 0.697128
Thermal correction to Enthalpy= 0.698073
Thermal correction to Gibbs Free Energy= 0.604595
Sum of electronic and zero-point Energies= -1408.329346
Sum of electronic and thermal Energies= -1408.297346
Sum of electronic and thermal Enthalpies= -1408.296402
Sum of electronic and thermal Free Energies= -1408.389880

TS 22 – Conformer of TS 15 that Gave Directly Product 19

#M062X/6-31G(d) FREQ(NORAMAN) NOPOP GEOM=CHECK GUESS=READ

1	6	0	-9.248823	1.204670	-1.410821
2	6	0	-8.314210	-0.485719	0.206236
3	6	0	-8.347063	0.889686	-0.292561
4	6	0	-5.040278	-0.470075	-0.859662
5	6	0	-5.229807	-0.432712	0.468789
6	6	0	-6.135715	-1.437314	1.141811
7	6	0	-4.578013	0.558073	1.399524
8	6	0	-1.116686	-1.500567	1.475404
9	6	0	-1.367969	1.127712	-0.145183
10	6	0	-4.148762	0.419329	-1.680636
11	6	0	-1.855564	-1.320931	0.179573
12	6	0	-2.734112	-0.192885	-1.838929
13	6	0	-1.965917	-0.197519	-0.539495
14	6	0	-7.532472	-0.872828	1.465913
15	6	0	-7.488518	1.944764	0.225694
16	6	0	1.500072	-0.928819	-0.683677
17	6	0	0.342896	-1.963542	1.248297
18	6	0	1.192524	-0.889789	0.616540
19	6	0	2.344304	0.104261	-1.399222
20	6	0	1.662399	0.212592	1.531812
21	6	0	3.765411	0.173755	-0.877358
22	6	0	4.594763	-0.949858	-0.884130
23	6	0	6.403374	0.318063	0.116460
24	6	0	5.593683	1.440016	0.133643
25	8	0	5.945611	2.658441	0.611146
26	6	0	4.277564	1.362570	-0.366286
27	6	0	5.895501	-0.882979	-0.399611
28	8	0	6.340815	-3.188467	-0.853149
29	8	0	7.965905	-1.938072	0.044411
30	6	0	6.714389	-2.116002	-0.439670

31	8	0	3.509550	2.482226	-0.319659
32	7	0	8.660722	2.751998	0.965101
33	1	0	-10.066148	1.803991	-0.972174
34	1	0	-9.679096	0.326602	-1.893587
35	1	0	-8.762624	1.867266	-2.135510
36	1	0	-7.895848	-1.016264	-0.680291
37	1	0	-9.357024	-0.841717	0.210556
38	1	0	-5.495658	-1.300021	-1.406759
39	1	0	-6.258375	-2.320808	0.503842
40	1	0	-5.682330	-1.781699	2.078223
41	1	0	-4.119568	1.403306	0.880776
42	1	0	-3.779188	0.055598	1.957489
43	1	0	-5.286983	0.947369	2.142489
44	1	0	-1.111566	-0.573047	2.060634
45	1	0	-1.632038	-2.252597	2.084644
46	1	0	-0.482714	1.336353	-0.757985
47	1	0	-1.052612	1.160078	0.900069
48	1	0	-2.071950	1.953376	-0.314207
49	1	0	-4.058543	1.417723	-1.235063
50	1	0	-4.587633	0.555928	-2.675565
51	1	0	-2.292868	-2.229697	-0.238334
52	1	0	-2.834227	-1.213069	-2.225743
53	1	0	-2.191323	0.388438	-2.594576
54	1	0	-7.456880	-0.024393	2.154450
55	1	0	-8.110585	-1.635775	1.994207
56	1	0	-6.488117	1.651987	-0.164007
57	1	0	-7.376834	1.908315	1.313012
58	1	0	-7.743860	2.941085	-0.135104
59	1	0	1.141335	-1.770727	-1.274355
60	1	0	0.335447	-2.859122	0.617112
61	1	0	0.770863	-2.253342	2.216732
62	1	0	2.370818	-0.130633	-2.468618
63	1	0	1.891594	1.098851	-1.310424
64	1	0	2.599853	-0.077700	2.023661
65	1	0	0.931140	0.406777	2.325746
66	1	0	1.852076	1.150701	1.001231
67	1	0	4.228145	-1.899036	-1.263963
68	1	0	7.413401	0.360720	0.507863
69	1	0	6.930561	2.695450	0.786711
70	1	0	8.401351	-2.804589	-0.028743
71	1	0	4.068901	3.179634	0.066881
72	1	0	8.984988	3.707393	1.099697
73	1	0	9.015195	2.207192	1.748412
74	1	0	9.120979	2.399384	0.128159

SCF Done: E(RM062X) = -1408.88215572 A.U. after 1 cycles

Frequencies -- -118.5394 9.2243 11.0298

Zero-point correction= 0.653315 (Hartree/Particle)
Thermal correction to Energy= 0.690240
Thermal correction to Enthalpy= 0.691184
Thermal correction to Gibbs Free Energy= 0.579683
Sum of electronic and zero-point Energies= -1408.228841
Sum of electronic and thermal Energies= -1408.191916
Sum of electronic and thermal Enthalpies= -1408.190972
Sum of electronic and thermal Free Energies= -1408.302473

Conformer 23 from TS 22

#M062X/6-31G(d) FREQ(NORAMAN) nopop geom=check guess=read

1	6	0	-9.611791	1.287839	-1.062029
2	6	0	-8.235738	-0.464876	0.129291

3	6	0	-8.482270	0.926001	-0.194357
4	6	0	-5.013936	-0.530439	-0.896739
5	6	0	-5.198242	-0.475545	0.435588
6	6	0	-6.105239	-1.469730	1.119753
7	6	0	-4.550834	0.532579	1.348728
8	6	0	-1.097312	-1.513413	1.439984
9	6	0	-1.355620	1.094027	-0.213518
10	6	0	-4.135607	0.355224	-1.734730
11	6	0	-1.833667	-1.352760	0.140206
12	6	0	-2.718225	-0.251879	-1.890608
13	6	0	-1.947765	-0.238289	-0.592335
14	6	0	-7.490294	-0.863782	1.418963
15	6	0	-7.543057	1.965214	0.233831
16	6	0	1.529977	-0.950552	-0.712132
17	6	0	0.365395	-1.971015	1.223252
18	6	0	1.212538	-0.899008	0.585290
19	6	0	2.376120	0.078668	-1.430903
20	6	0	1.669965	0.216350	1.491208
21	6	0	3.788735	0.166990	-0.889106
22	6	0	4.623802	-0.951854	-0.858609
23	6	0	6.408965	0.346771	0.144941
24	6	0	5.593379	1.464426	0.124866
25	8	0	5.930782	2.694509	0.582618
26	6	0	4.286100	1.369116	-0.394856
27	6	0	5.916015	-0.867718	-0.354066
28	8	0	6.379453	-3.180191	-0.749809
29	8	0	7.984423	-1.902168	0.144801
30	6	0	6.741416	-2.097049	-0.354384
31	8	0	3.511055	2.484679	-0.383421
32	7	0	8.641184	2.814877	0.960954
33	1	0	-10.366612	1.714234	-0.374959
34	1	0	-10.066310	0.435432	-1.568447
35	1	0	-9.356363	2.091356	-1.758695
36	1	0	-7.511299	-0.619101	-0.728350
37	1	0	-9.099383	-1.091596	-0.106303
38	1	0	-5.449486	-1.383539	-1.424852
39	1	0	-6.236825	-2.360278	0.494405
40	1	0	-5.662635	-1.799616	2.066155
41	1	0	-4.094092	1.368569	0.814645
42	1	0	-3.752751	0.040477	1.917015
43	1	0	-5.262824	0.933539	2.082592
44	1	0	-1.098804	-0.578863	2.013969
45	1	0	-1.610747	-2.260777	2.056572
46	1	0	-0.471360	1.299044	-0.828919
47	1	0	-1.040037	1.139875	0.831205
48	1	0	-2.062937	1.914725	-0.392378
49	1	0	-4.052008	1.359284	-1.302491
50	1	0	-4.581467	0.473816	-2.728465
51	1	0	-2.266036	-2.268469	-0.267711
52	1	0	-2.813032	-1.276619	-2.266688
53	1	0	-2.181484	0.324785	-2.653926
54	1	0	-7.385162	-0.002674	2.086296
55	1	0	-8.110822	-1.590087	1.950228
56	1	0	-6.554877	1.649843	-0.158704
57	1	0	-7.411908	1.961063	1.322650
58	1	0	-7.798952	2.961869	-0.123289
59	1	0	1.179842	-1.800378	-1.296559
60	1	0	0.365366	-2.872551	0.600567
61	1	0	0.790725	-2.249270	2.196236
62	1	0	2.419693	-0.171091	-2.496364
63	1	0	1.914732	1.070993	-1.363008
64	1	0	2.608879	-0.060236	1.988133
65	1	0	0.934790	0.411851	2.281154
66	1	0	1.852573	1.150726	0.951501
67	1	0	4.268209	-1.910740	-1.224335
68	1	0	7.411807	0.403700	0.552694
69	1	0	6.913529	2.742515	0.767784

70	1	0	8.424820	-2.767919	0.096927
71	1	0	4.060991	3.193515	-0.004199
72	1	0	8.957943	3.775160	1.077355
73	1	0	8.992193	2.289735	1.759121
74	1	0	9.111271	2.447147	0.136069

SCF Done: E(RM062X) = -1408.88304807 A.U. after 1 cycles

Frequencies -- 11.7933 15.4169 20.9796

Zero-point correction= 0.653622 (Hartree/Particle)
Thermal correction to Energy= 0.691218
Thermal correction to Enthalpy= 0.692162
Thermal correction to Gibbs Free Energy= 0.579484
Sum of electronic and zero-point Energies= -1408.229426
Sum of electronic and thermal Energies= -1408.191830
Sum of electronic and thermal Enthalpies= -1408.190886
Sum of electronic and thermal Free Energies= -1408.303564