SUPPORTING INFORMATION

Dynamic Effects on the Periselectivity, Rate, Isotope Effects, and Mechanism of Cycloadditions of Ketenes with Cyclopentadiene

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Additional Information on Experimental Procedures

General

Cyclopentadiene was cracked by refluxing at atmospheric pressure and stored at –78 °C until used. Diphenylketene was prepared by a literature procedure (Taylor, E. C.; McKillop, A.; Hawks, G. H. *Organic Syntheses, Coll. Vol. 6,* p. 549; *Vol. 6*, p. 36.) starting from diphenylacetyl chloride, purchased from Acros.

Preparation of Samples of 7 for NMR Analysis.

Adapting a literature procedure (Chen, X. –T.; Bhattacharya, S. K.; Zhou, B. Gutteridge, C. E.; Pettus, T. R. R.; Danishefsky, S. J. *J. Am. Chem. Soc.* **1999**, *121*, 6563-6579), a mixture of 0.72 g (10.9 mmol) of cyclopentadiene and 1.41 g (21.6 mmol) of zinc powder in 20 mL of ether was cooled to 0 °C and, while stirring vigorously, a solution of 1.45 mL (2.36 g, 12.9 mmol) of trichloroacetyl chloride in 8 mL of ether was added dropwise over 2 h. After stirring an additional 1 h at 0 °C and allowing to warm to 25 °C slowly, the reaction mixture was filtered through Celite 545. The filtrate was concentrated on a rotary evaporator, and the residue was taken up in ether and washed with saturated aqueous solutions of $NaHCO_3$ and NaCl. The organic layer was dried and the solvent was removed on a rotary evaporator, and the residue was chromatographed on silica gel using 1% ether in hexanes as eluent to afford 0.85 g (44%) of **7** with no observable impurities by ^{1}H or ^{13}C NMR. In an analogous reaction on a larger scale (2.8 g of cyclopentadiene), 4.6 g (61%) of **7** was obtained.

Preparation of Samples of 4 for NMR Analysis.

A mixture of 5.0 mL (4.9 g, 61 mmol) of cyclopentadiene and 2.02 g (8.76 mmol) of diphenylacetyl chloride in 10 mL of dichloromethane was stirred

vigorously at room temperature, while a solution of 1.5 mL (1.1 g, 11 mmol) of triethylamine was added dropwise over 30 min. After stirring an additional 1 h at room temperature, the triethylamine*HCl was filtered away from the reaction mixture and the reaction mixture was allowed to stand overnight. The solvent was removed on a rotary evaporator, and the residue was chromatographed on silica gel using 40% dichloromethane in hexanes as eluent to afford 1.9 g (82%) of **4** with no observable impurities by ^{1}H or ^{13}C NMR. In an analogous reaction using 2.05 g of diphenylacetyl chloride, 1.6 g (69%) of **4** was obtained. The samples were recrystallized from absolute ethanol before NMR analysis.

NMR Integration Results

Integrations for **4**.

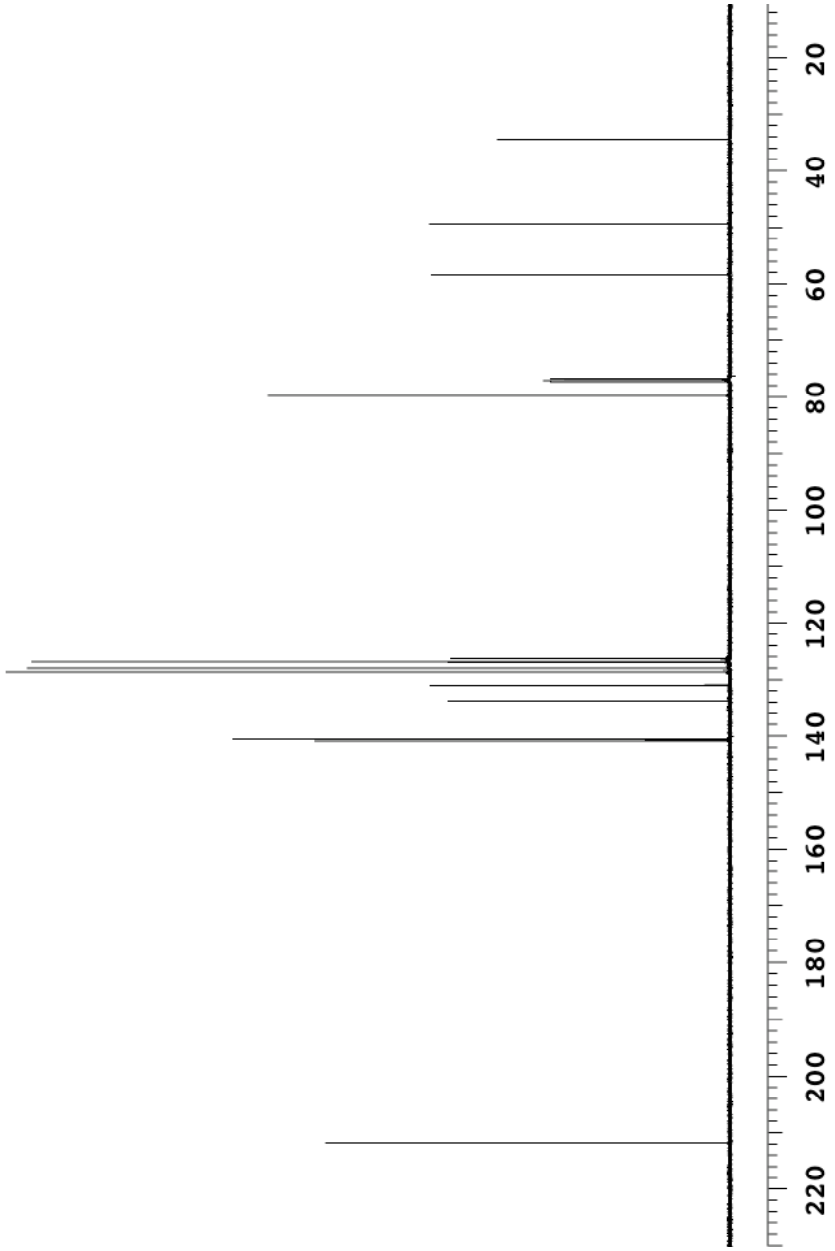
Sample 1							n
C4	1008.42	1005.38	1019.98	1025.67	1033.16	1037.26	6
C3	1013.34	1019.86	1029.39	1041.34	1051.17	1048.73	6
C1	1000.86	999.59	1016.64	1025.73	1036.52	1030.6	6
C2	1000	1001.08	1014.09	1024.38	1025.4	1031.5	6
^{13}C integration Ratio Corrected	C2/(C3*0.9893) C1/(C4*0.9893)						AVE
C2/C3	0.998	0.992	0.996	0.994	0.986	0.994	**0.993**
C1/C4	1.003	1.005	1.008	1.011	1.014	1.004	**1.008**
							95% Confidence
							0.004
							0.004
corrected KIE	(C3*0.9893)/C2 (C4*0.9893)/C1						AVE
3/2	1.002	1.008	1.004	1.006	1.014	1.006	**1.007**
4/1	0.997	0.995	0.993	0.989	0.986	0.996	**0.993**
							95% Confidence
							0.004
							0.004
Sample 2							n
C4	1007.71	1020.6	1027.77	1036.77	1038.43	1056.08	6
C3	1011.54	1028.26	1044.22	1044.25	1048.57	1071.78	6
C1	1002.04	1011.3	1018.33	1029.81	1037.88	1052.67	6
C2	1000	1012.18	1022.95	1028.02	1034.27	1043.86	6
^{13}C integration Ratio Corrected	C2/(C3*0.9893) C1/(C4*0.9893)						AVE
C2/C3	0.999	0.995	0.990	0.995	0.997	0.984	**0.994**
C1/C4	1.005	1.002	1.002	1.004	1.010	1.008	**1.005**
							95% Confidence
							0.005
							0.003
corrected KIE	(C3*0.9893)/C2 (C4*0.9893)/C1						AVE
3/2	1.001	1.005	1.010	1.005	1.003	1.016	**1.007**
4/1	0.995	0.998	0.998	0.996	0.990	0.993	**0.995**

							95% Confidence
							0.005
							0.003
Integrations for **7.**							
Sample 1							
C4	1000	1000	1000	1000	1000	1000	6
C3	996.706	996.772	999.673	993.601	997.263	999.168	6
C2	987.714	985.488	989.353	984.185	985.12	987.938	6
C1	966.558	969.878	972.584	965.399	967.001	969.209	6
^{13}C integration Ratio Corrected	C2/(C3*0.9893) C1/(C4*0.9893)						AVE
C1/C4	0.977	0.980	0.983	0.976	0.977	0.980	**0.979**
C2/C3	1.002	0.999	1.000	1.001	0.999	0.999	**1.000**
							95% Confidence
							0.003
							0.001
corrected KIE	(C3*0.9893)/C2 (C4*0.9893)/C1						AVE
3/2	1.024	1.020	1.017	1.025	1.023	1.021	**1.022**
4/1	0.998	1.001	1.000	0.999	1.001	1.001	**1.000**
							95% Confidence
							0.003
							0.001
Rxn 2							n
C4	1000	1000	1000	1000	1000	1000	12
	1000	1000	1000	1000	1000	1000	
C3	997.478	997.805	999.852	1003.94	994.902	998.586	12
	999.975	1002.44	996.527	1000.38	990.588	989.902	
C2	989.825	990.475	992.592	990.563	986.388	990.934	12
	983.275	987.793	987.5	988.927	975.765	978.574	
C1	968.714	972.596	972.711	974.757	968.05	972.618	12
	970.01	977.903	966.06	969.705	965.733	959.586	
^{13}C integration Ratio Corrected	C2/(C3*0.9893) C1/(C4*0.9893)						AVE
C1/C4	0.979	0.983	0.983	0.985	0.979	0.983	**0.980**
	0.981	0.988	0.977	0.980	0.976	0.970	
C2/C3	1.003	1.003	1.003	0.997	1.002	1.003	**1.000**
	0.994	0.996	1.002	0.999	0.996	0.999	
							95% Confidence
							0.003
							0.002
corrected KIE	(C3*0.9893)/C2 (C4*0.9893)/C1						AVE
4/1	1.021	1.017	1.017	1.015	1.022	1.017	**1.020**
	1.020	1.012	1.024	1.020	1.024	1.031	

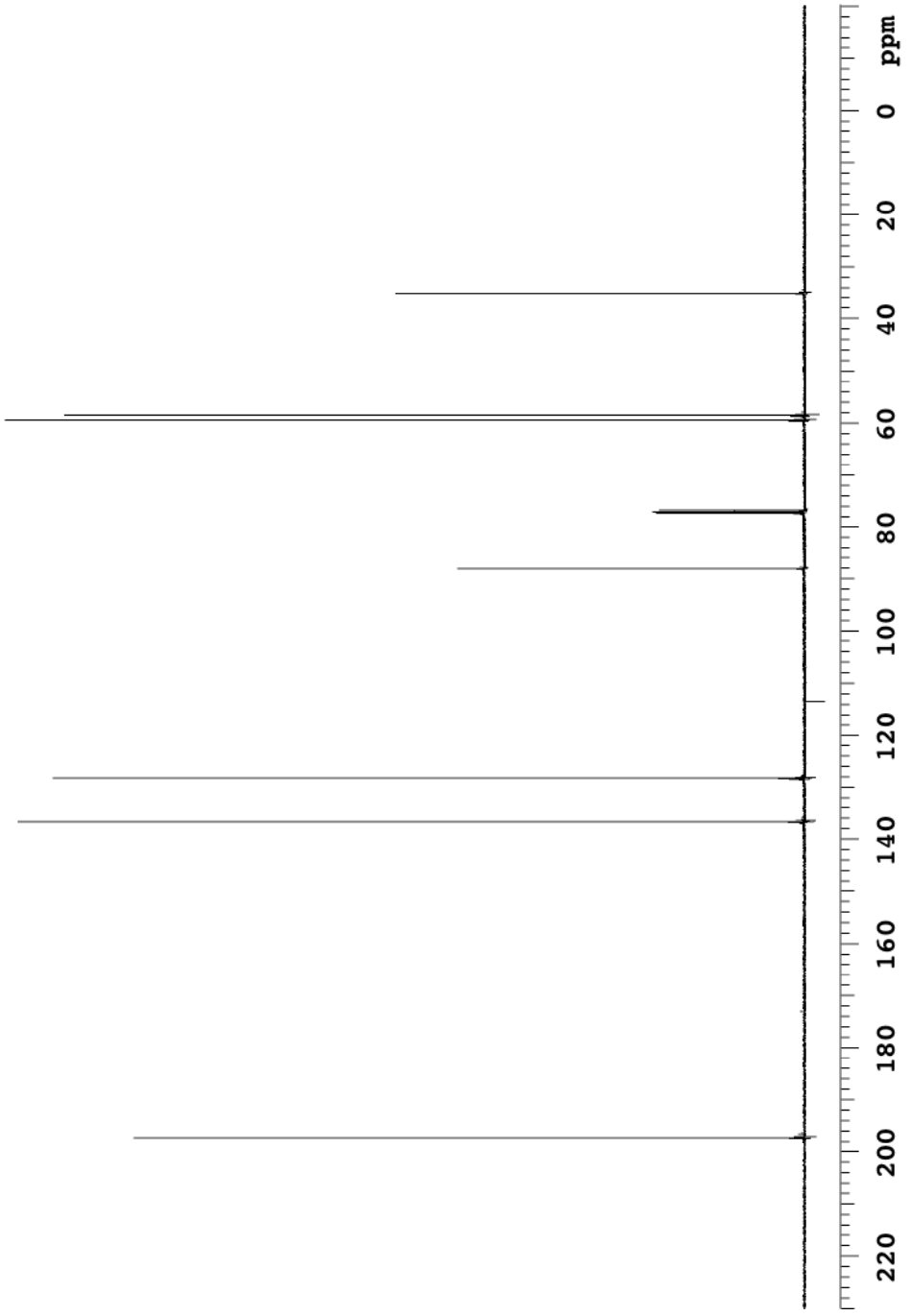
3/2	0.997	0.997	0.997	1.003	0.998	0.997	**1.000**
	1.006	1.004	0.998	1.001	1.004	1.001	
							95% Confidence
							0.003
							0.002

^{13}C NMR Spectra of 4 and 7

Spectrum of 4



Spectrum of 7



Kinetic Simulations

No-Cycloreversion Model

The observed compositions were fit to possible kinetic schemes using Excel spreadsheets. Shown below is the critical part of a spreadsheet that simulates a composition data set without any reversion of **3** to **1** + **2**. Footnotes give the key formulas. The fit produced by this simulation is shown in Figure 2 in the main text.

	A	B	C	D	E	F	G
1		time (h)	ketene	CP	4+2 (pred)	2+2 (pred)	Total Check
2	k total for the cycloaddition	0.000	**0.032**[j]	**0.550**[j]	**0.002**[j]	**0.001**[j]	0.59
3	0.00050[a]	0.024[d]	0.031[e]	0.549[f]	0.003[g]	0.001[h]	0.59[i]
4	Proportion initial 4+2	0.049	0.030	0.548	0.003	0.001	0.59
5	0.828[a]	0.073	0.030	0.548	0.004	0.001	0.59
6	k for 4+2	0.098	0.029	0.547	0.005	0.001	0.59
7	0.000414[b]	0.122	0.028	0.546	0.005	0.001	0.59
8	k 2+2	0.147	0.027	0.546	0.006	0.002	0.59
9	0.000086[c]	0.171	0.027	0.545	0.006	0.002	0.59
10	k rearr	0.196	0.026	0.544	0.007	0.002	0.59
11	0.000029[a]	0.220	0.026	0.544	0.007	0.002	0.59
12	Timestep (s)	0.244	0.025	0.543	0.008	0.002	0.59
13	88	0.269	0.024	0.543	0.008	0.002	0.59

[a]Parameter adjusted for fit. [b]Formula:=A3*A5 [c]Formula:=(1-A5)*A3
[d]Formula:=B2+$A$13/3600 [e]Formula:=C2-$A$13*$A$3*C2*D2 [f]Formula:=D2-$A$13*$A$3*C2*D2 [g]Formula:=E2+$A$13*$A$7*C2*D2-$A$13*$A$11*E2
[h]Formula:=F2+$A$13*$A$9*C2*D2+$A$13*$A$11*E2 [i]Formula:=C3+D3+2*E3+2*F3
[j]Experimental parameter

Cycloreversion Model

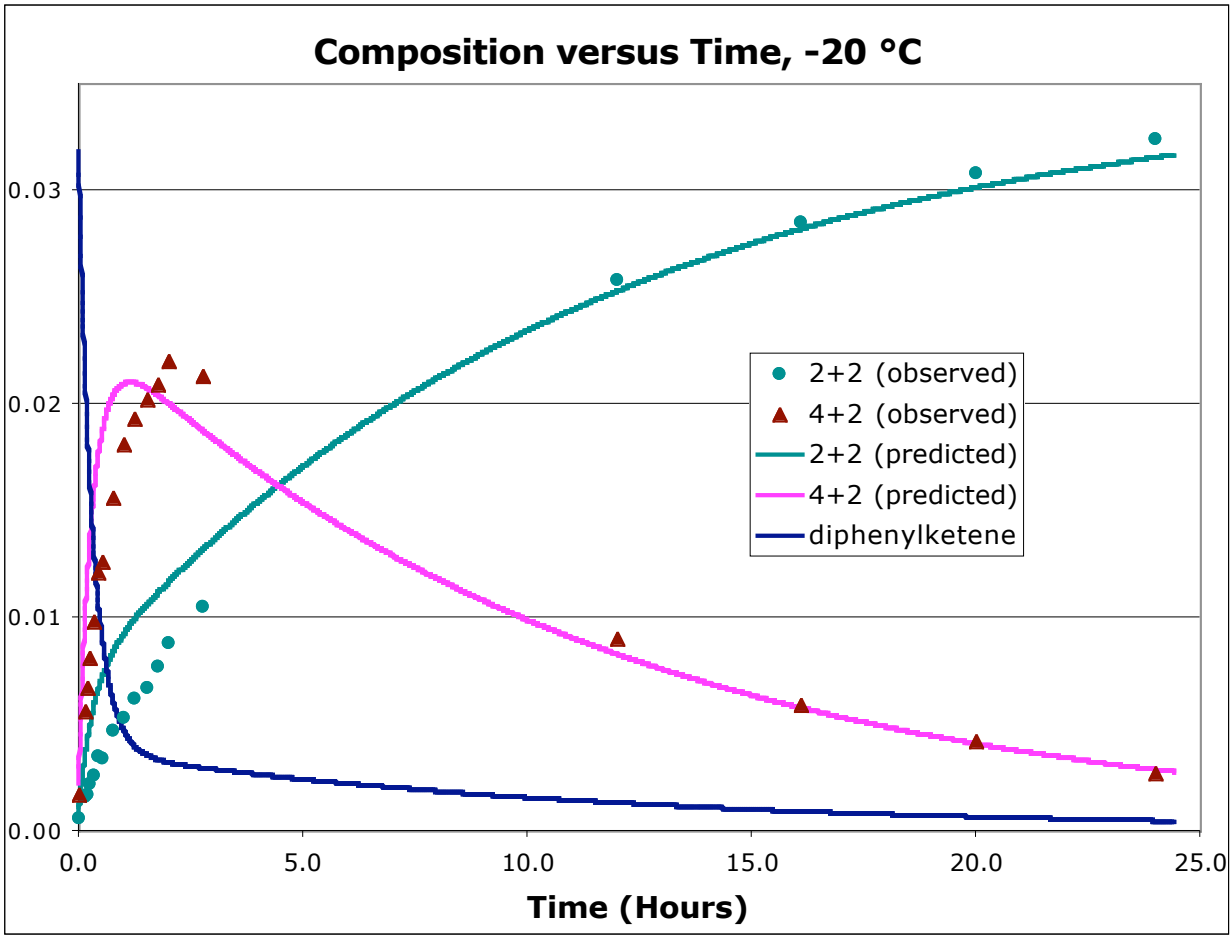
Shown below is the critical part of a spreadsheet that simulates a composition data set. In this spreadsheet, the conversion of **3** to **4** occurs entirely by cycloreversion of **3** to **1** + **2**. Footnotes give the key formulas.

The fit produced by this simulation is shown below the table. To get the 2+2 product at a long-time rate similar to what is observed, the rate of the cycloreversion has to be set very high. To then get the 4+2 product to build up near what is observed, the cycloaddition rate constant has to be raised. This lead to qualitative error in the early points.

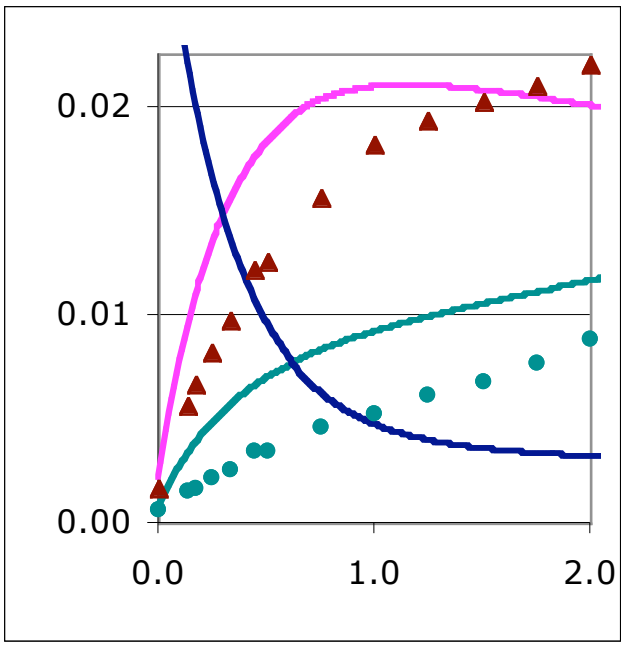
	A	B	C	D	E	F	G
1		time (h)	ketene	CP	4+2 (pred)	2+2 (pred)	Total Check
2	k total for the cycloaddition	0.000	**0.032**[j]	**0.550**[j]	**0.002**[j]	**0.001**[j]	0.59
3	0.0014[a]	0.012[d]	0.031[e]	0.549[f]	0.003[g]	0.001[h]	0.59[i]
4	Proportion initial 4+2	0.024	0.030	0.548	0.004	0.001	0.59
5	0.75[a]	0.037	0.029	0.547	0.005	0.001	0.59

6	k for 4+2	0.049	0.028	0.546	0.006	0.001	0.59
7	0.00105[b]	0.061	0.027	0.545	0.006	0.001	0.59
8	k 2+2	0.073	0.026	0.545	0.007	0.001	0.59
9	0.00035[c]	0.086	0.026	0.544	0.008	0.001	0.59
10	k cycloreversion	0.098	0.025	0.543	0.008	0.002	0.59
11	0.00011[a]	0.110	0.024	0.543	0.009	0.002	0.59
12	Timestep (s)	0.122	0.024	0.542	0.009	0.002	0.59
13	44	0.134	0.023	0.541	0.010	0.002	0.59

[a]Parameter adjusted for fit. [b]Formula:=A3*A5 [c]Formula:=(1-A5)*A3
[d]Formula:=B2+$A$13/3600 [e]Formula:=C2-($A$13*$A$3*C2*D2)+($A$13*$A$11*E2)
[f]Formula:=D2--($A$13*$A$3*C2*D2)+($A$13*$A$11*E2)
[g]Formula:=E2+($A$13*$A$7*C2*D2)-($A$13*$A$11*E2)
[h]Formula:=F2+$A$21*$A$9*C2*D2 [i]Formula:=C3+D3+2*E3+2*F3 [j]Experimental parameter



Expansion of Early Points:



Mixed Model

Shown below is the critical part of a best-fit spreadsheet that simulates a composition data set. In this spreadsheet, the conversion of **3** to **4** occurs partially directly and partially by cycloreversion of **3** to **1** + **2**. Footnotes give the key formulas. The fit produced by this simulation is shown below the table. This is not best-fit – better fits are obtained with higher k's for rearrangement than k for cycloreversion.

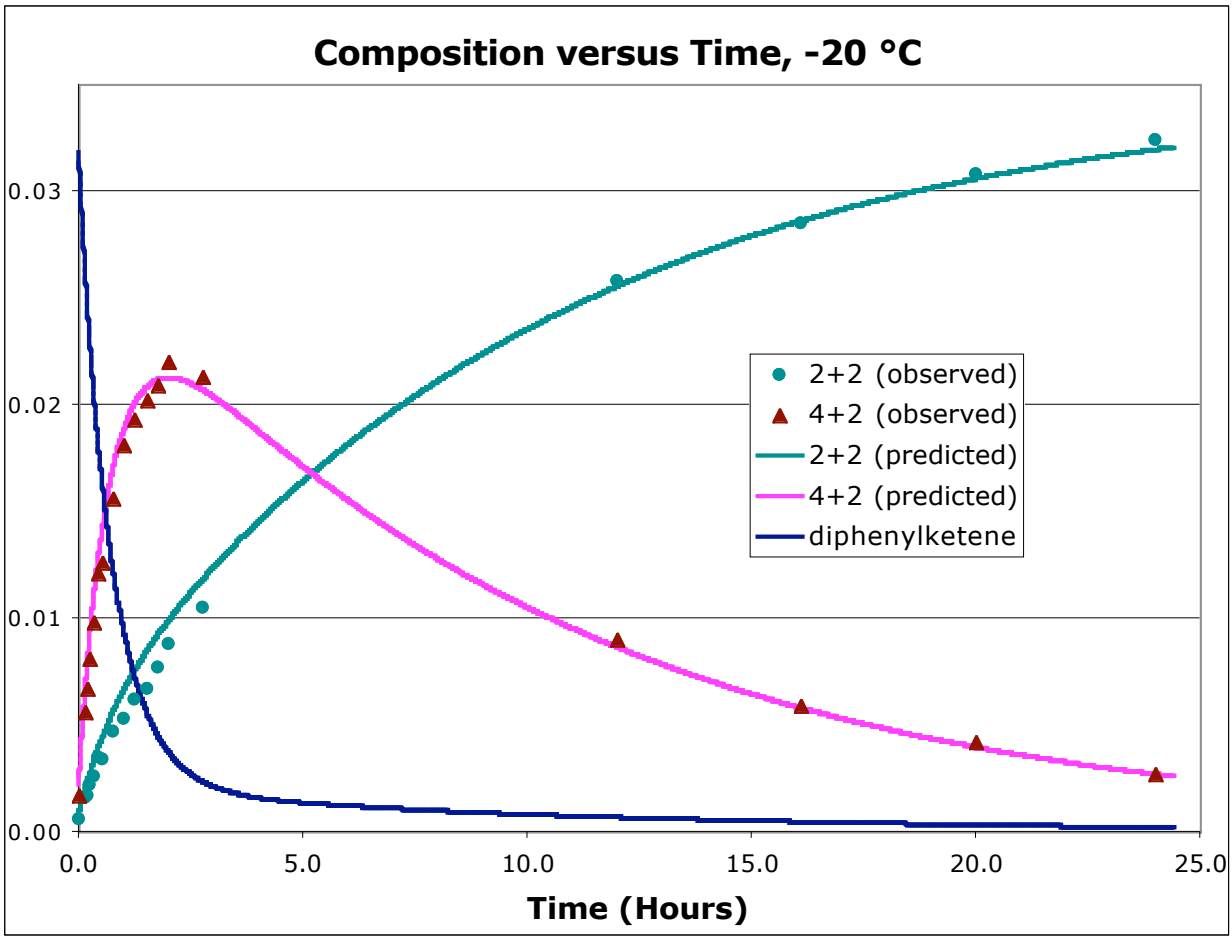
	A	B	C	D	E	F	G
1		time (h)	ketene	CP	4+2 (pred)	2+2 (pred)	Total Check
2	k total for the cycloaddition	0.000	**0.032**[j]	**0.550**[j]	**0.002**[j]	**0.001**[j]	0.59
3	0.00066[a]	0.012[d]	0.031[e]	0.549[f]	0.003[g]	0.001[h]	0.59[i]
4	Proportion initial 4+2	0.024	0.031	0.549	0.003	0.001	0.59
5	0.8[a]	0.037	0.030	0.549	0.003	0.001	0.59
6	k for 4+2	0.049	0.030	0.548	0.004	0.001	0.59
7	0.000528[b]	0.061	0.029	0.548	0.004	0.001	0.59
8	k 2+2	0.073	0.029	0.547	0.004	0.001	0.59
9	0.000132[c]	0.086	0.028	0.547	0.005	0.002	0.59
10	k rearr	0.098	0.028	0.546	0.005	0.002	0.59
11	0.000024	0.110	0.028	0.546	0.006	0.002	0.59
12	k cycloreversion	0.122	0.027	0.545	0.006	0.002	0.59
13	0.00024	0.134	0.027	0.545	0.006	0.002	0.59
14	Timestep (s)	0.147	0.026	0.544	0.007	0.002	0.59
15	88	0.159	0.026	0.544	0.007	0.002	0.59

[a]Parameter adjusted for fit.

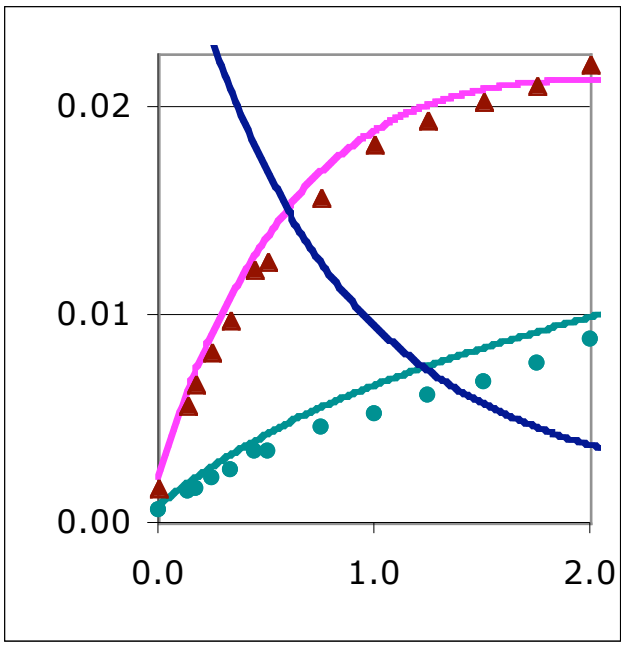
[b]Formula:=A3*A5

[c]Formula:=(1-A5)*A3

[d]Formula:=B2+$A$13/3600
[e]Formula:=C2-($A$15*$A$3*C2*D2)+($A$15*$A$13*E2)
[f]Formula:=D2-($A$15*$A$3*C2*D2)+($A$15*$A$13*E2)
[g]Formula:=E2+($A$15*$A$7*C2*D2)-($A$15*$A$11*E2)-($A$15*$A$13*E2)
[h]Formula:=F2+$A$15*$A$9*C2*D2+$A$15*$A$11*E2
[i]Formula:=C3+D3+2*E3+2*F3
[j]Experimental parameter



Expansion of Early Points:



Theoretical Results

The structures and energies for all stationary points were obtained using Gaussian 98[1] or Gaussian 03.[2] All mPW1K results were obtained with Gaussian 03. Vibrational frequency analyses were carried out on all stationary points. Reaction paths were determined in two ways, either using the IRC algorithm in Gaussian 03 (when it could be successfully applied) or using a home-grown implementation of a damped classical trajectory algorithm (see: Hratchian, H. P.; Schlegel, H. B. *J. Phys. Chem. A.* **2002**, *106*, 165-169).

Comment on BPW91 and HF results.

The tables and structures below include structures and pathways determined in BPW91/6-311+G** and HF/6-311+G** calculations. The BPW91 results may be described as resembling the B3LYP results in many ways, including the severe error in the diphenylketene reaction thermodynamics. The BPW91 Claisen transition structure is still far too loose versus high-level calculations or isotope effects. The HF results may be described as roughly resembling the mPW1K results, except for the expected overestimation of activation barriers and presence of an interesting shallow intermediate in the dichloroketene reaction.

Tables of Energies

Potential Energy and Potential Energy + zpe

	Potential E	Erel	E + zpe	Erel	G (298)

mPW1K/6-31G*					
Cyclopentadiene (1)	-194.050307777		-193.954450		-193.980996
diphenylketene (2)	-614.526857967		-614.324131		-614.363761
4+2_prod (3)	-808.608985300	**-20.0**	-808.302749	**-15.2**	-808.346343
2+2_prod (4)	-808.621789989	**-28.0**	-808.316983	**-24.1**	-808.361051
Dichloroketene (5)	-1071.716713780		-1071.700377		-1071.730027
Dichloro 2+2 product (7)	-1265.842698670	**-47.5**	-1265.724480	**-43.7**	-1265.758978
Dichloro 4+2 product (8)	-1265.820221460	**-33.4**	-1265.700386	**-28.6**	-1265.734438
TS 2+2 (10)	-808.538528206	**24.2**	-808.238067	**25.4**	-808.282664
1st_TS (9)	-808.558070111	**12.0**	-808.257180	**13.4**	-808.301799
2nd TS rearrangement (11)	-808.561774659	**9.7**	-808.259142	**12.2**	-808.302256
Dichloro 1st TS (16)	-1265.762969030	**2.5**	-1265.648879	**3.7**	-1265.684413
2nd TS rearrangement (17)	-1265.772099100	**-3.2**	-1265.655971	**-0.7**	-1265.690186
Dichloro 2+2 TS (Similar to 10)	-1265.741809640	**15.8**	-1265.627834	**16.9**	-1265.664257
mPW1K/6-31+G**					
Cyclopentadiene (1)	-194.065760414		-193.970385		-193.996940
diphenylketene (2)	-614.557526647		-614.355495		-614.395272
4+2_product (3)	-808.651513331	**-17.7**	-808.346518	**-13.0**	-808.390383
2+2_product (4)	-808.664448064	**-25.8**	-808.360974	**-22.0**	-808.405385
Dichloroketene (5)	-1071.721742340		-1071.705471		-1071.735130
Dichloro 2+2 product (7)	-1265.860343000	**-45.7**	-1265.742708	**-42.0**	-1265.777245
Dichloro 4+2 product (8)	-1265.837146340	**-31.2**	-1265.717873	**-26.4**	-1265.751940
TS_2+2 (10)	-808.583348892	**25.1**	-808.284112	**26.2**	-808.328798
1st_TS (9)	-808.602438424	**13.1**	-808.302844	**14.5**	-808.347433
2ndTS_rearrangement (11)	-808.605862818	**10.9**	-808.304564	**13.4**	-808.347346
Dichloro 1st TS (16)	-1265.781454000	**3.8**	-1265.668023	**4.9**	-1265.703649
Dichloro 2nd TS rearrangement (17)	-1265.790921280	**-2.1**	-1265.675367	**0.3**	-1265.709641
Dichloro 2+2 TS (similar to 10)	-1265.761164150	**16.5**	-1265.647917	**17.5**	-1265.684532
B3LYP/6-31G*					
Cyclopentadiene (1)	-194.101058102		-194.008164		-194.034761
Diphenylketene (2)	-614.708265406		-614.511947		-614.551798
4+2 Product (3)	-808.819403440	**-6.3**	-808.523103	**-1.9**	-808.567031
2+2 Product (4)	-808.830818866	**-13.5**	-808.535792	**-9.8**	-808.580059
Dichloroketene (5)	-1071.760365880		-1071.744999		-1071.774829
Dichloro 2+2 product (7)	-1265.915221090	**-33.8**	-1265.801424	**-30.3**	-1265.836230
Dichloro 4+2 Product (8)	-1265.892485500	**-19.5**	-1265.777132	**-15.0**	-1265.811431
1st_TS (12)	-808.787217876	**13.9**	-808.495703	**15.3**	-808.540667
Intermediate (13)	-808.789092427	**12.7**	-808.496142	**15.0**	-808.541268
2ndTS giving 4+2 (14)	-808.788846278	**12.8**	-808.495873	**15.2**	-808.540077
2ndTS giving 2+2 (15)	-808.788042815	**13.4**	-808.494911	**15.8**	-808.537909
Another TS that gives 2+2 (Similar to 10)	-808.770273763	**24.5**	-808.479244	**25.6**	-808.524309

Dichloro 1st TS (18)	-1265.854881750	**4.1**	-1265.744640	**5.3**	-1265.780450
Dichloro intermediate (19)	-1265.861418050	**0.0**	-1265.749446	**2.3**	-1265.785253
2nd TS Dichloro 2+2 side (20)	-1265.861232530	**0.1**	-1265.749224	**2.5**	-1265.783310
2nd TS Dichloro 4+2 side (21)	-1265.860844770	**0.4**	-1265.748726	**2.8**	-1265.783246
Dichloro 2+2 TS (Similar to 10)	-1265.835627950	**16.2**	-1265.725699	**17.2**	-1265.762263
B3LYP/6-311+G**					
cyclopentadiene (1)	-194.156236414		-194.064126		-194.090725
diphenylketene (2)	-614.869297097		-614.674116		-614.714171
4+2_product (3)	-809.023654094	**1.2**	-808.729490	**5.5**	-808.773750
2+2_product (4)	-809.037029631	**-7.2**	-808.744159	**-3.7**	-808.788779
Dichloroketene (5)	-1071.865777450		-1071.850429		-1071.880238
Dichloro 2+2 product (7)	-1266.067460330	**-28.5**	-1265.954595	**-25.1**	-1265.989436
Dichloro 4+2 product (8)	-1266.041363820	**-12.1**	-1265.926972	**-7.8**	-1265.961298
1st_TS (12)	-808.996933374	**17.9**	-808.707432	**19.3**	-808.752238
intermediate (13)	-808.997346724	**17.7**	-808.706886	**19.7**	-808.752209
2ndTS giving 4+2 (14)	-808.996569616	**18.2**	-808.705647	**20.5**	-808.749828
2ndTS giving 2+2 (15)	-808.995562396	**18.8**	-808.704693	**21.1**	-808.747885
Another diphenyl TS giving 2+2 directly (Similar to 10)	-808.979959514	**28.6**	-808.691026	**29.6**	-808.736305
Dichloro 1st TS (18)	-1266.010313000	**7.3**	-1265.900988	**8.5**	-1265.936744
Dichloro intermediate (19)	-1266.015030500	**4.4**	-1265.904132	**6.5**	-1265.939927
2ndTS Dichloro 2+2 side (21)	-1266.014687290	**4.6**	-1265.903693	**6.8**	-1265.937815
2ndTS dichloro 4+2 side (20)	-1266.013422600	**5.4**	-1265.902197	**7.8**	-1265.936736
Dichloro alternative 2+2 TS (similar to 10)	-1265.991338390	**19.2**	-1265.882385	**20.2**	-1265.918977
BPW91/6-311+G**					
Cyclopentadiene (1)	-194.124726721		-194.034928		-194.061585
Diphenylketene (2)	-614.791014352		-614.600856		-614.641339
Diphenyl 4+2 product (3)	-808.916083578	**-0.2**	-808.629552	**3.9**	-808.674421
Diphenyl 2+2 product (4)	-808.927937172	**-7.7**	-808.642767	**-4.4**	-808.687877
Dichloroketene (5)	-1071.858726040		-1071.843900		-1071.873817
Dichloro 2+2 product (7)	-1266.030602750	**-29.6**	-1265.920905	**-26.4**	-1265.956006
Dichloro 4+2 product (8)	-1266.005108460	**-13.6**	-1265.893848	**-9.4**	-1265.928390
Diphenyl1stTS (Similar to 12)	-808.894967419	**13.0**	-808.613096	**14.2**	-808.658579
Diphenyl Intermediate (Similar to 13)	-808.897582358	**11.4**	-808.614400	**13.4**	-808.660052
Diphenyl 2nd TS 4+2 side (Similar to 14)	-808.896852932	**11.9**	-808.613239	**14.1**	-808.657779
Diphenyl 2nd TS 2+2 side (Similar to 15)	-808.894947929	**13.0**	-808.611575	**15.2**	-808.655205
Diphenyl 1st TS 2+2 (Similar to 10)	-808.880726010	**22.0**	-808.599118	**23.0**	-808.644631
Dichloro 1st TS (similar to 18)	-1265.977035880	**4.0**	-1265.870947	**4.9**	-1265.907499
Dichloro Intermediate (similar to 19)	-1265.987333580	**-2.4**	-1265.879295	**-0.3**	-1265.915229
Dichloro 2nd TS 4+2 side (similar to 20)	-1265.985259150	**-1.1**	-1265.876743	**1.3**	-1265.911356

Dichloro 2nd TS 2+2 side (similar to 21)	-1265.986706430	**-2.0**	-1265.878631	**0.1**	-1265.912913
Dichloro Alternative TS for 2+2 (similar to 10)	-1265.961418320	**13.8**	-1265.855489	**14.6**	-1265.892874
HF/6-311+G**					
Cyclopentadiene (1)	-192.839556311		-192.741013		-192.767505
Diphenylketene (2)	-610.959930871		-610.751687		-610.791459
Diphenyl 4+2 product (3)	-803.799060173	**0.3**	-803.484376	**5.2**	-803.527731
Diphenyl 2+2 product (4)	-803.818294978	**-11.8**	-803.504847	**-7.6**	-803.548616
Dichloroketene (5)	-1069.584793450		-1069.567725		-1069.597253
Dichloro 2+2 product (7)	-1262.477594600	**-33.4**	-1262.355568	**-29.4**	-1262.389808
Dichloro 4+2 product (8)	-1262.446262840		-1262.322722		-1262.356524
Diphenyl 1st TS (Similar to 9, but later)	-803.738877702	**38.0**	-803.428849	**40.1**	-803.472439
Diphenyl 2nd TS Claisen Rearrangement (Similar to 11)	-803.738361541	**38.4**	-803.427818	**40.7**	-803.470251
Dichloro 1st TS (similar to 18)	-1262.385935040	**24.1**	-1262.268297	**25.4**	-1262.303342
Dichloro intermediate (similar to 19)	-1262.388481330	**22.5**	-1262.269432	**24.7**	-1262.305029
Dichloro 2nd TS 4+2 side (similar to 20)	-1262.388337670	**22.6**	-1262.269213	**24.8**	-1262.303532
Dichloro 2nd TS 2+2 side (similar to 21)	-1262.388306710	**22.6**	-1262.269151	**24.8**	-1262.302991
Dichloro Alternative TS for 2+2 (similar to 10)	-1262.364819370	**37.4**	-1262.247999	**38.1**	-1262.284189

Estimates of Relative Free Energies

	G (298)	Erel	H (298)	S (298)	G(est 253) Estimate – good rel only	Erel
mPW1K/6-31G*						
Cyclopentadiene (1)	-193.980996		-193.94945	66.389	-193.97624	
diphenylketene (2)	-614.363761		-614.31155	109.893	-614.35588	
4+2_prod (3)	-808.346343	**-1.0**	-808.28708	124.722	-808.3374	**-3.3**
2+2_prod (4)	-808.361051	**-10.2**	-808.30076	126.886	-808.35195	**-12.4**
Dichloroketene (5)	-1071.730027		-1071.6945	74.803	-1071.7247	
Dichloro 2+2 product (7)	-1265.758978	**-30.1**	-1265.715	92.457	-1265.7523	**-32.3**
Dichloro 4+2 product (8)	-1265.734438	**-14.7**	-1265.6915	90.359	-1265.728	**-17.0**
TS 2+2 (10)	-808.282664	**39.0**	-808.22136	129.016	-808.27341	**36.8**
1st_TS (9)	-808.301799	**27.0**	-808.24052	128.974	-808.29255	**24.8**
2nd TS rearrangement (11)	-808.302256	**26.7**	-808.24338	123.926	-808.29337	**24.3**
Dichloro 1st TS (16)	-1265.684413	**16.7**	-1265.6387	96.177	-1265.6775	**14.7**
2nd TS rearrangement (17)	-1265.690186	**13.1**	-1265.6469	91.146	-1265.6836	**10.8**
Dichloro 2+2 TS (Similar to 10)	-1265.664257	**29.3**	-1265.6176	98.215	-1265.6572	**27.4**
mPW1K/6-31+G**						
Cyclopentadiene (1)	-193.996940		-193.96537	66.444	-193.99218	
diphenylketene (2)	-614.395272		-614.34287	110.292	-614.38736	

4+2_product (3)	-808.390383	**1.1**	-808.33078	125.443	-808.38139	**-1.2**
2+2_product (4)	-808.405385	**-8.3**	-808.34466	127.799	-808.39622	**-10.5**
Dichloroketene (5)	-1071.735130		-1071.6996	74.842	-1071.7298	
Dichloro 2+2 product (7)	-1265.777245	**-28.3**	-1265.7333	92.592	-1265.7706	**-30.5**
Dichloro 4+2 product (8)	-1265.751940	**-12.5**	-1265.709	90.44	-1265.7455	**-14.8**
TS_2+2 (10)	-808.328798	**39.8**	-808.26734	129.347	-808.31952	**37.7**
1st_TS (9)	-808.347433	**28.1**	-808.28611	129.072	-808.33818	**26.0**
2ndTS_rearrangement (11)	-808.347346	**28.2**	-808.28876	123.304	-808.3385	**25.7**
Dichloro 1st TS (16)	-1265.703649	**17.8**	-1265.6578	96.509	-1265.6967	**15.8**
Dichloro 2nd TS rearrangement (17)	-1265.709641	**14.1**	-1265.6662	91.342	-1265.7031	**11.8**
Dichloro 2+2 TS (similar to 10)	-1265.684532	**29.8**	-1265.6376	98.807	-1265.6774	**27.9**
B3LYP/6-31G*						
Cyclopentadiene (1)	-194.034761		-194.00308	66.686	-194.02998	
Diphenylketene (2)	-614.551798		-614.49906	110.988	-614.54384	
4+2 Product (3)	-808.567031	**12.3**	-808.50699	126.37	-808.55797	**9.9**
2+2 Product (4)	-808.580059	**4.1**	-808.51915	128.19	-808.57087	**1.9**
Dichloroketene (5)	-1071.774829		-1071.7389	75.524	-1071.7694	
Dichloro 2+2 product (7)	-1265.836230	**-16.7**	-1265.7917	93.749	-1265.8295	**-18.9**
Dichloro 4+2 Product (8)	-1265.811431	**-1.2**	-1265.768	91.513	-1265.8049	**-3.4**
1st_TS (12)	-808.540667	**28.8**	-808.47864	130.543	-808.53131	**26.7**
Intermediate (13)	-808.541268	**28.4**	-808.47903	130.989	-808.53187	**26.3**
2ndTS giving 4+2 (14)	-808.540077	**29.2**	-808.47957	127.342	-808.53094	**26.9**
2ndTS giving 2+2 (15)	-808.537909	**30.5**	-808.47875	124.506	-808.52898	**28.1**
Another TS that gives 2+2 (Similar to 10)	-808.524309	**39.1**	-808.46211	130.915	-808.51492	**37.0**
Dichloro 1st TS (18)	-1265.780450	**18.3**	-1265.7342	97.257	-1265.7735	**16.3**
Dichloro intermediate (19)	-1265.785253	**15.3**	-1265.7392	96.892	-1265.7783	**13.2**
2nd TS Dichloro 2+2 side (20)	-1265.783310	**16.5**	-1265.7399	91.355	-1265.7768	**14.2**
2nd TS Dichloro 4+2 side (21)	-1265.783246	**16.5**	-1265.7394	92.378	-1265.7766	**14.3**
Dichloro 2+2 TS (Similar to 10)	-1265.762263	**29.7**	-1265.7152	98.975	-1265.7552	**27.8**
B3LYP/6-311+G**						
cyclopentadiene (1)	-194.090725		-194.05902	66.721	-194.08594	
diphenylketene (2)	-614.714171		-614.66121	111.459	-614.70618	
4+2_product (3)	-808.773750	**19.5**	-808.71329	127.25	-808.76462	**17.3**
2+2_product (4)	-808.788779	**10.1**	-808.72742	129.146	-808.77952	**7.9**
Dichloroketene (5)	-1071.880238		-1071.8444	75.45	-1071.8748	
Dichloro 2+2 product (7)	-1265.989436	**-11.6**	-1265.9448	93.891	-1265.9827	**-13.8**
Dichloro 4+2 product (8)	-1265.961298	**6.1**	-1265.9178	91.64	-1265.9547	**3.8**
1st_TS (12)	-808.752238	**33.0**	-808.69039	130.171	-808.7429	**30.9**
intermediate (13)	-808.752209	**33.1**	-808.68957	131.828	-808.74276	**31.0**
2ndTS giving 4+2 (14)	-808.749828	**34.6**	-808.6893	127.402	-808.74069	**32.3**
2ndTS giving 2+2 (15)	-808.747885	**35.8**	-808.68842	125.16	-808.73891	**33.4**

Another diphenyl TS giving 2+2 directly (Similar to 10)	-808.736305	**43.0**	-808.67383	131.481	-808.72688	**40.9**
Dichloro 1st TS (18)	-1265.936744	**21.5**	-1265.8906	97.104	-1265.9298	**19.4**
Dichloro intermediate (19)	-1265.939927	**19.5**	-1265.8938	96.985	-1265.933	**17.4**
2ndTS Dichloro 2+2 side (21)	-1265.937815	**20.8**	-1265.8943	91.532	-1265.9313	**18.5**
2ndTS dichloro 4+2 side (20)	-1265.936736	**21.5**	-1265.8928	92.461	-1265.9301	**19.2**
Dichloro alternative 2+2 TS (similar to 10)	-1265.918977	**32.6**	-1265.8719	99.096	-1265.9119	**30.7**
BPW91/6-311+G**						
Cyclopentadiene (1)	-194.061585		-194.02971	67.079	-194.05677	
Diphenylketene (2)	-614.641339		-614.58757	113.162	-614.63322	
Diphenyl 4+2 product (3)	-808.674421	**17.9**	-808.61284	129.607	-808.66513	**15.6**
Diphenyl 2+2 product (4)	-808.687877	**9.4**	-808.62551	131.27	-808.67846	**7.2**
Dichloroketene (5)	-1071.873817		-1071.8378	75.882	-1071.8684	
Dichloro 2+2 product (7)	-1265.956006	**-12.9**	-1265.9109	94.954	-1265.9492	**-15.1**
Dichloro 4+2 product (8)	-1265.928390	**4.4**	-1265.8844	92.597	-1265.9217	**2.1**
Diphenyl1stTS (Similar to 12)	-808.658579	**27.8**	-808.59539	133	-808.64904	**25.7**
Diphenyl Intermediate (Similar to 13)	-808.660052	**26.9**	-808.59667	133.391	-808.65049	**24.8**
Diphenyl 2nd TS 4+2 side (Similar to 14)	-808.657779	**28.3**	-808.59645	129.087	-808.64852	**26.0**
Diphenyl 2nd TS 2+2 side (Similar to 15)	-808.655205	**29.9**	-808.59477	127.205	-808.64608	**27.6**
Diphenyl 1st TS 2+2 (Similar to 10)	-808.644631	**36.6**	-808.58141	133.051	-808.63509	**34.5**
Dichloro 1st TS (similar to 18)	-1265.907499	**17.5**	-1265.8601	99.817	-1265.9003	**15.6**
Dichloro Intermediate (similar to 19)	-1265.915229	**12.7**	-1265.8688	97.676	-1265.9082	**10.6**
Dichloro 2nd TS 4+2 side (similar to 20)	-1265.911356	**15.1**	-1265.8672	92.899	-1265.9047	**12.8**
Dichloro 2nd TS 2+2 side (similar to 21)	-1265.912913	**14.1**	-1265.8691	92.3	-1265.9063	**11.8**
Dichloro Alternative TS for 2+2 (similar to 10)	-1265.892874	**26.7**	-1265.8446	101.61	-1265.8856	**24.8**
HF/6-311+G**						
Cyclopentadiene (1)	-192.767505		-192.73616	65.981	-192.76277	
Diphenylketene (2)	-610.791459		-610.73953	109.294	-610.78362	
Diphenyl 4+2 product (3)	-803.527731	**19.6**	-803.46925	123.084	-803.5189	**17.3**
Diphenyl 2+2 product (4)	-803.548616	**6.5**	-803.48921	125.024	-803.53965	**4.2**
Dichloroketene (5)	-1069.597253		-1069.562	74.277	-1069.5919	
Dichloro 2+2 product (7)	-1262.389808	**-15.7**	-1262.3464	91.315	-1262.3833	**-17.9**
Dichloro 4+2 product (8)	-1262.356524		-1262.3141	89.253	-1262.3501	
Diphenyl 1st TS (Similar to 9, but later)	-803.472439	**54.3**	-803.41328	124.508	-803.46351	**52.0**
Diphenyl 2nd TS Claisen Rearrangement (Similar to 11)	-803.470251	**55.7**	-803.41256	121.429	-803.46154	**53.2**
Dichloro 1st TS (similar to 18)	-1262.303342	**38.5**	-1262.2586	94.254	-1262.2966	**36.5**
Dichloro intermediate (similar to 19)	-1262.305029	**37.5**	-1262.2595	95.777	-1262.2982	**35.5**
Dichloro 2nd TS 4+2 side (similar to 20)	-1262.303532	**38.4**	-1262.2601	91.32	-1262.297	**36.2**
Dichloro 2nd TS 2+2 side (similar to 21)	-1262.302991	**38.8**	-1262.2602	90.06	-1262.2965	**36.5**
Dichloro Alternative TS for 2+2 (similar	-1262.284189	**50.6**	-1262.2379	97.335	-1262.2772	**48.6**

to 10)

Cyclopentadiene (1) MPW1K/6-31G(d)

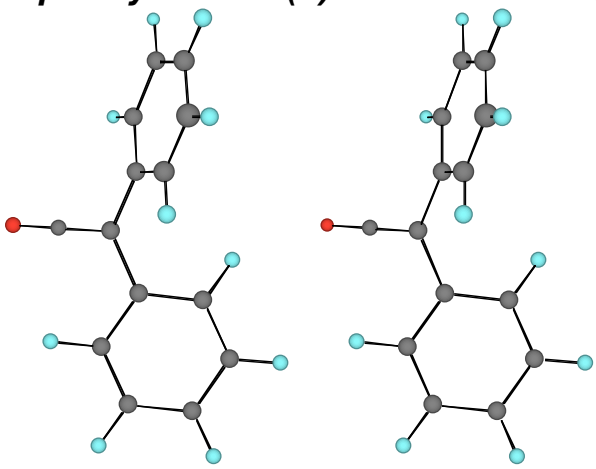
E(RmPW+HF-PW91) = -194.050307777

Zero-point correction=	0.095858 (Hartree/Particle)
Thermal correction to Energy=	0.099912
Thermal correction to Enthalpy=	0.100856
Thermal correction to Gibbs Free Energy=	0.069312
Sum of electronic and zero-point Energies=	-193.954450
Sum of electronic and thermal Energies=	-193.950396
Sum of electronic and thermal Enthalpies=	-193.949452
Sum of electronic and thermal Free Energies=	-193.980996

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	62.695	14.934	66.389

C,0,0.6003919099,0.8506083964,-0.6040098647
C,0,0.6945903468,0.703966072,0.7225490139
C,0,-0.1510700956,-0.4095461893,1.144355466
C,0,-0.7552548618,-0.9344588365,0.0721781566
C,0,-0.3335046789,-0.180688801,-1.1456194429
H,0,1.1050778522,1.5850039238,-1.2103051023
H,0,1.2944446844,1.303482025,1.3893099801
H,0,-0.2597978884,-0.7430230773,2.164544852
H,0,-1.4402259207,-1.7664965693,0.0592733616
H,0,-1.1857776237,0.2711897433,-1.661346368
H,0,0.1553631743,-0.8294398948,-1.8781966969

diphenylketene (2) MPW1K/6-31G(d)



E(RmPW+HF-PW91) = -614.526857967

Zero-point correction=	0.202727 (Hartree/Particle)
Thermal correction to Energy=	0.214367
Thermal correction to Enthalpy=	0.215311
Thermal correction to Gibbs Free Energy=	0.163097
Sum of electronic and zero-point Energies=	-614.324131
Sum of electronic and thermal Energies=	-614.312491
Sum of electronic and thermal Enthalpies=	-614.311547

```
 Sum of electronic and thermal Free Energies=         -614.363761

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  134.517             44.932            109.893

C,0,2.0107521743,0.7815923246,0.037770946
O,0,3.0896866902,1.2008811997,0.0582779763
C,0,0.7804205673,0.3032270398,0.0146704403
C,0,0.1280772595,0.0001187465,1.3054986261
C,0,-1.2368598143,0.2326979191,1.4687354239
C,0,0.8537301403,-0.500166186,2.3847648563
C,0,-1.8541368489,-0.0292418595,2.6786614405
H,0,-1.8107105657,0.624367178,0.642070449
C,0,0.2366893142,-0.7413573535,3.6001348437
H,0,1.9073467942,-0.7130423237,2.2674619849
C,0,-1.1207681068,-0.5118241328,3.7517926314
H,0,-2.9132521769,0.1548917242,2.7861058173
H,0,0.8178664902,-1.1257046361,4.4256154355
H,0,-1.604646416,-0.711048632,4.696449319
C,0,0.1370708948,0.1028662641,-1.3004593401
C,0,-0.705866078,-0.9885477079,-1.5056470786
C,0,0.3687503575,0.9760638986,-2.3613767038
C,0,-1.2979756488,-1.1966374513,-2.7383727681
H,0,-0.8909940642,-1.6757564896,-0.6935069889
C,0,-0.2090253473,0.7529224897,-3.5993014818
H,0,0.9970274482,1.8433044997,-2.2119511252
C,0,-1.0487652487,-0.3314041501,-3.7927134445
H,0,-1.9501647464,-2.0464909249,-2.8782572165
H,0,-0.0136935784,1.439672038,-4.4099441519
H,0,-1.5088343975,-0.4991010787,-4.7552176805
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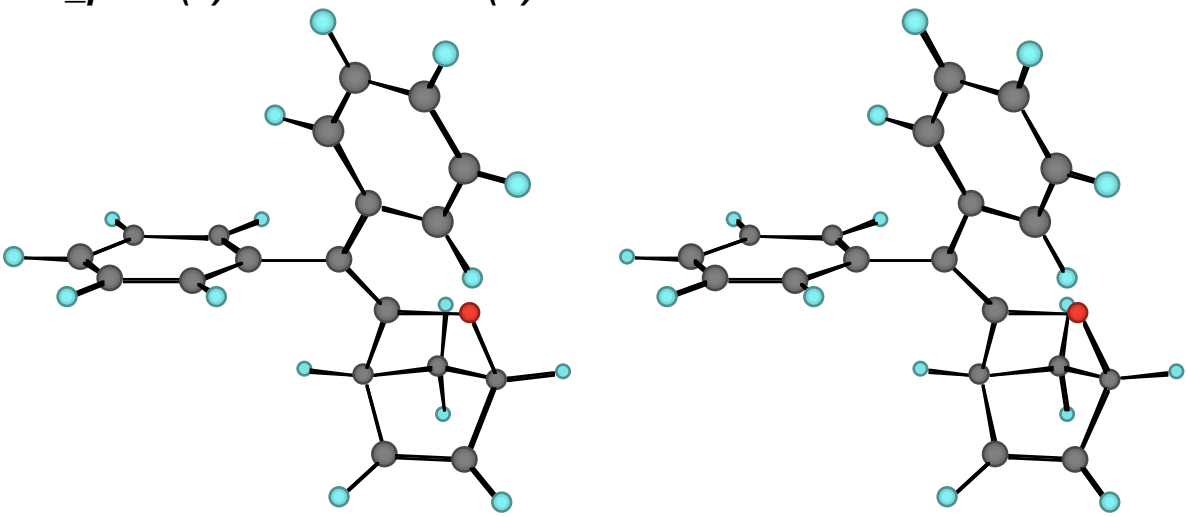
4+2_prod (3) MPW1K/6-31G(d)



```
E(RmPW+HF-PW91) = -808.608985300

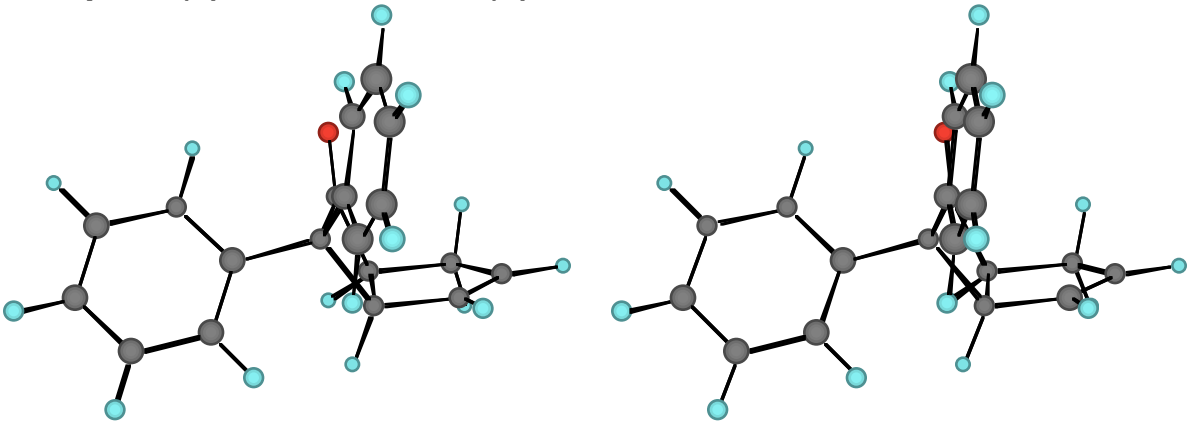
 Zero-point correction=                           0.306236 (Hartree/Particle)
 Thermal correction to Energy=                    0.320958
 Thermal correction to Enthalpy=                  0.321902
 Thermal correction to Gibbs Free Energy=         0.262643
 Sum of electronic and zero-point Energies=           -808.302749
```

```
Sum of electronic and thermal Energies=             -808.288027
Sum of electronic and thermal Enthalpies=           -808.287083
Sum of electronic and thermal Free Energies=        -808.346343

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  201.404             59.909            124.722

C,0,2.2288397183,1.0187230274,0.2832240847
C,0,2.9362352331,1.0275069341,-1.059623082
C,0,3.6437897086,-0.0954701575,-1.1427932222
C,0,3.3676114068,-0.8412359587,0.1403086289
C,0,3.2851152537,0.3004298292,1.1403421773
O,0,1.9796435741,-1.2609124888,0.0912031351
C,0,1.2384533018,-0.124504664,0.1579408183
C,0,-0.0996336006,-0.0977333508,0.0839200604
H,0,1.8225925446,1.9580568878,0.6311177091
H,0,2.7773059948,1.7716944304,-1.82334764
H,0,4.1957585091,-0.4768216467,-1.9861247909
H,0,3.9632718295,-1.7141588618,0.3732445662
H,0,4.2069103111,0.8658148801,1.2354909369
H,0,2.9203196965,-0.0189707388,2.1149230713
C,0,-0.7996382418,1.2031511232,0.2393547552
C,0,-0.707088717,1.9445689328,1.4144334322
C,0,-1.5922373636,1.701075944,-0.7939830564
C,0,-1.3607994581,3.1603791498,1.5448328902
H,0,-0.12541984,1.5524078106,2.236901588
C,0,-2.2483556335,2.9124991939,-0.6654860461
H,0,-1.6881055607,1.1268201378,-1.70423761
C,0,-2.1316208861,3.6496158989,0.5037888887
H,0,-1.2753200096,3.7193737945,2.4656373942
H,0,-2.8515953175,3.2843803903,-1.4811769963
H,0,-2.6448399173,4.5948678478,0.6042121432
C,0,-0.9326051922,-1.2977033706,-0.1375896971
C,0,-2.2296045652,-1.3416702228,0.3779865539
C,0,-0.4842187796,-2.3986915105,-0.8706907463
C,0,-3.0422326883,-2.444247774,0.1815940258
H,0,-2.602159196,-0.4999585736,0.9427558772
C,0,-1.2999814368,-3.4980154468,-1.070228384
H,0,0.5103588024,-2.3892409005,-1.284460206
C,0,-2.5821086109,-3.5300510275,-0.544848299
H,0,-4.039231857,-2.452847395,0.59835968
H,0,-0.9307936968,-4.3350453331,-1.6456747787
H,0,-3.2157175764,-4.3908321197,-0.7021487184
```

2+2_prod (4) MPW1K/6-31G(d)



E(RmPW+HF-PW91) = -808.621789989

Zero-point correction=	0.304807 (Hartree/Particle)
Thermal correction to Energy=	0.320083
Thermal correction to Enthalpy=	0.321027
Thermal correction to Gibbs Free Energy=	0.260739
Sum of electronic and zero-point Energies=	-808.316983
Sum of electronic and thermal Energies=	-808.301707
Sum of electronic and thermal Enthalpies=	-808.300763
Sum of electronic and thermal Free Energies=	-808.361051

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	200.855	61.059	126.886

C,0,-2.1705417418,-1.2823123963,-0.3306824953
C,0,-1.5216904116,-0.0485201909,-1.0041629448
C,0,-2.4817676284,1.0408209252,-0.6348410057
C,0,-3.5797048923,0.5783788149,-0.048413733
C,0,-3.5877831195,-0.9156170602,0.0979196247
C,0,-1.1144571302,-1.1436855528,0.7483908592
O,0,-1.0342275945,-1.569846176,1.8615688778
C,0,-0.2597656181,-0.1773784962,-0.0825460243
H,0,-2.0786015075,-2.2230296927,-0.8693588907
H,0,-1.3269476788,-0.0998416814,-2.0724769411
H,0,-2.2848902581,2.0830847623,-0.8340259565
H,0,-4.4005308888,1.1958310216,0.2862735736
H,0,-4.3457185409,-1.3766404061,-0.5384607073
H,0,-3.7897448053,-1.2400583597,1.1193730071
C,0,0.2579372399,1.0768511032,0.5801849945
C,0,0.5970062036,2.1753138054,-0.2046388251
C,0,0.4260617384,1.1592252409,1.9562136907
C,0,1.0846862713,3.3340092317,0.3721779904
H,0,0.4817068466,2.1211474184,-1.2785654802
C,0,0.9170058776,2.32083965,2.5337972921
H,0,0.1675391874,0.3144305683,2.5753495339
C,0,1.246372444,3.4108153085,1.7473823638
H,0,1.3406817913,4.177683395,-0.2524172492
H,0,1.0397955726,2.3704498845,3.6060983685
H,0,1.6278127543,4.3143779543,2.2000571199
C,0,0.8847779024,-0.9513971267,-0.7224073557
C,0,1.2434699258,-0.7608411701,-2.0519774608

```
C,0,1.6357859952,-1.832940164,0.0494536431
C,0,2.3224150892,-1.4369791284,-2.598190688
H,0,0.6868822029,-0.0744467384,-2.6730171032
C,0,2.7115641587,-2.5119203301,-0.4970641091
H,0,1.3724149207,-1.9884939217,1.0854126908
C,0,3.05883416,-2.3178148396,-1.8239829687
H,0,2.5859577106,-1.2737642725,-3.6331551733
H,0,3.2787687254,-3.1953536029,0.1178916731
H,0,3.8974559387,-2.8476926673,-2.2512065741
```

*Dichloroketene (5) MPW1K/6-31G**

```
E(RmPW+HF-PW91) = -1071.71671378

 Zero-point correction=                           0.016336 (Hartree/Particle)
 Thermal correction to Energy=                    0.021284
 Thermal correction to Enthalpy=                  0.022228
 Thermal correction to Gibbs Free Energy=        -0.013313
 Sum of electronic and zero-point Energies=          -1071.700377
 Sum of electronic and thermal Energies=             -1071.695430
 Sum of electronic and thermal Enthalpies=           -1071.694486
 Sum of electronic and thermal Free Energies=        -1071.730027

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  13.356             15.044             74.803

 C,0,1.2103973572,-0.5266769548,-0.2364618545
 C,0,0.0250118264,-0.0108774896,-0.0048545513
 O,0,2.2534285775,-0.9805336126,-0.4402559479
 Cl,0,-1.2901784142,-1.0320874655,0.3960231269
 Cl,0,-0.2062853342,1.683240146,-0.1036733611
```

*Dichloro 2+2 product (7) MPW1K/6-31G**

```
E(RmPW+HF-PW91) = -1265.84269867

 Zero-point correction=                           0.118219 (Hartree/Particle)
 Thermal correction to Energy=                    0.126706
 Thermal correction to Enthalpy=                  0.127650
 Thermal correction to Gibbs Free Energy=         0.083721
 Sum of electronic and zero-point Energies=          -1265.724480
 Sum of electronic and thermal Energies=             -1265.715993
 Sum of electronic and thermal Enthalpies=           -1265.715049
 Sum of electronic and thermal Free Energies=        -1265.758978

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.509             31.269             92.457

 C,0,-0.6374669443,-0.9054632903,-1.128275205
 C,0,-0.3971676904,0.6124884894,-0.9017327931
 C,0,-1.7215223299,1.0626405266,-0.3682971457
 C,0,-2.6477266996,0.1147737721,-0.4473151078
 C,0,-2.1391597624,-1.1651161679,-1.0411975387
 C,0,0.1176346029,-1.1540650217,0.1708028319
 O,0,0.1736974067,-2.0441664636,0.9496893732
 C,0,0.6639877798,0.2879670167,0.1758651209
```

```
Cl,0,2.2989748865,0.2758324535,-0.5212255301
Cl,0,0.6318041045,1.1627329489,1.6924862171
H,0,-0.1393152829,-1.3470171214,-1.9873897332
H,0,-0.0165187554,1.2183966426,-1.7197358447
H,0,-1.8786593002,2.0577277587,0.0171948913
H,0,-3.6743566067,0.2376478843,-0.135514251
H,0,-2.5794989741,-1.353401022,-2.0217156679
H,0,-2.3559469199,-2.0349862233,-0.4208870332
```

*Dichloro 4+2 product (8) MPW1K/6-31G**

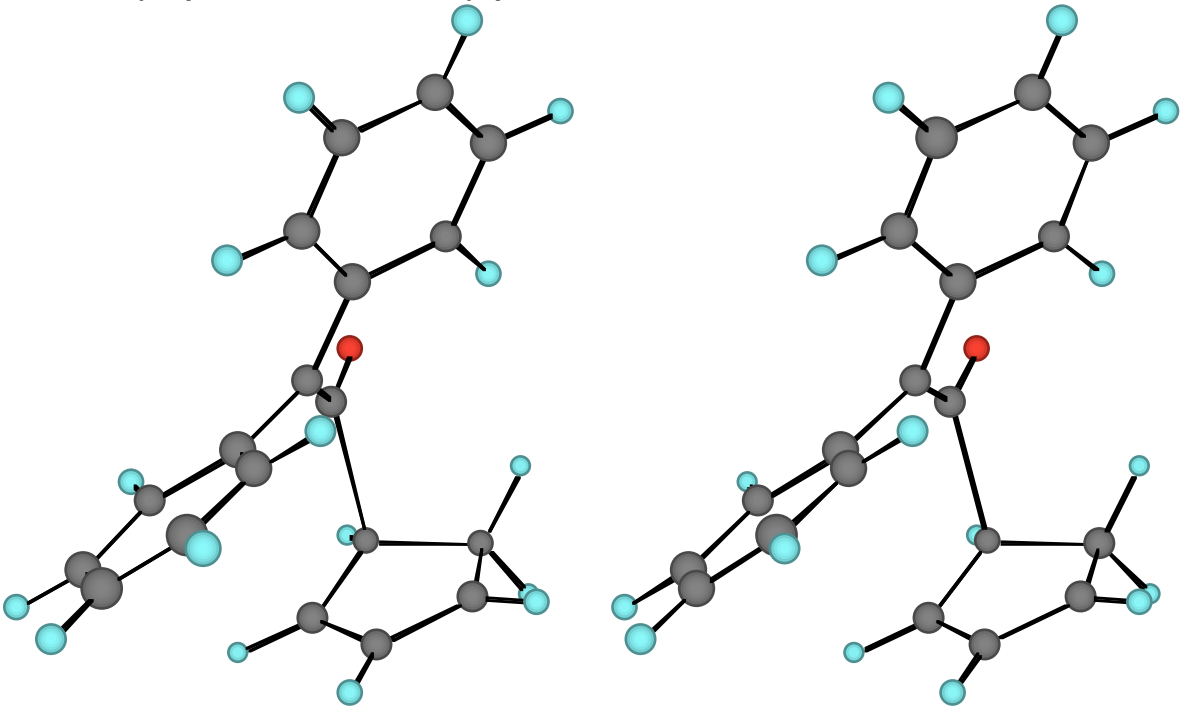
E(RmPW+HF-PW91) = -1265.82022146

Zero-point correction=	0.119835 (Hartree/Particle)
Thermal correction to Energy=	0.127772
Thermal correction to Enthalpy=	0.128716
Thermal correction to Gibbs Free Energy=	0.085784
Sum of electronic and zero-point Energies=	-1265.700386
Sum of electronic and thermal Energies=	-1265.692449
Sum of electronic and thermal Enthalpies=	-1265.691505
Sum of electronic and thermal Free Energies=	-1265.734438

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.178	30.071	90.359

```
C,0,1.3339329209,0.6062914272,0.503670154
C,0,2.049133422,0.8440218928,-0.8132564344
C,0,2.4245175375,-0.3444317823,-1.2779369093
C,0,1.9337319159,-1.3524227111,-0.2682346257
C,0,2.1350918773,-0.597178119,1.0352836149
O,0,0.4789020973,-1.3614736333,-0.3528164879
C,0,0.0898816135,-0.1528290588,0.0986240633
C,0,-1.1819030257,0.2261634024,0.1394081397
Cl,0,-1.650618445,1.7731322802,0.7315582531
Cl,0,-2.4559114395,-0.7936280655,-0.3832988284
H,0,1.1736126805,1.4575898983,1.1515721298
H,0,2.1172723825,1.8016775635,-1.3032082468
H,0,2.8712213537,-0.57653259,-2.2304366889
H,0,2.2662084684,-2.378276583,-0.3510557094
H,0,3.1712078937,-0.3491627425,1.2426540449
H,0,1.6739509118,-1.092768437,1.8872481407
```

TS 2+2 (10) MPW1K/6-31G(d)



E(RmPW+HF-PW91) = -808.538528206

Zero-point correction=	0.300461 (Hartree/Particle)
Thermal correction to Energy=	0.316220
Thermal correction to Enthalpy=	0.317165
Thermal correction to Gibbs Free Energy=	0.255865
Sum of electronic and zero-point Energies=	-808.238067
Sum of electronic and thermal Energies=	-808.222308
Sum of electronic and thermal Enthalpies=	-808.221364
Sum of electronic and thermal Free Energies=	-808.282664

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.431	62.349	129.016

C,0,-2.260224705,-1.1700756517,-0.9462675379
C,0,-2.6835527434,0.1667214536,-0.9770753715
C,0,-2.8386504123,0.6537945857,0.3494856963
C,0,-2.6860006714,-0.3797160803,1.2090608777
C,0,-2.5354322367,-1.6559662104,0.4646955828
C,0,-0.415087283,-1.3773910891,-0.9921042036
O,0,-0.2227189349,-2.4763020215,-1.4174258183
C,0,0.3235901829,-0.3750897848,-0.3786702671
H,0,-2.4900712592,-1.8112114298,-1.78406004
H,0,-2.9015748805,0.7311351071,-1.8669864057
H,0,-3.0167927116,1.6833729795,0.6116227487
H,0,-2.7171059019,-0.313014097,2.2851435485
H,0,-3.4913368577,-2.1930602913,0.4725477656
H,0,-1.7936362233,-2.3341963984,0.8786468869
C,0,0.0417116975,1.0303495986,-0.5777394669
C,0,-0.4285192925,1.5011604751,-1.8088398396
C,0,0.2202717962,1.977648384,0.4470437708
C,0,-0.7292437044,2.846361523,-2.0058861997

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H,0,-0.4913848855,0.8152908445,-2.6410777645
C,0,-0.0722663942,3.3069534682,0.2493311866
H,0,0.5721462632,1.6421692626,1.4111399729
C,0,-0.5571079115,3.7523343396,-0.9813223486
H,0,-1.0793518171,3.1781709991,-2.9730657835
H,0,0.065020594,4.0099999901,1.0585515908
H,0,-0.7812341157,4.7982307019,-1.1314417042
C,0,1.4639024417,-0.8280134488,0.4363301176
C,0,2.5845493752,-0.0075148974,0.6112039941
C,0,1.4934644599,-2.0871133902,1.0445875311
C,0,3.6660115219,-0.4183265018,1.3694642927
H,0,2.6157181208,0.9561578481,0.126083532
C,0,2.5786643408,-2.4981945144,1.7957362385
H,0,0.660939158,-2.7620061779,0.9160546261
C,0,3.6721819779,-1.6653991419,1.9722960995
H,0,4.5166709092,0.2398972167,1.4763068556
H,0,2.5659729023,-3.4785883562,2.2504015796
H,0,4.5181975469,-1.9870707294,2.5615582215
```
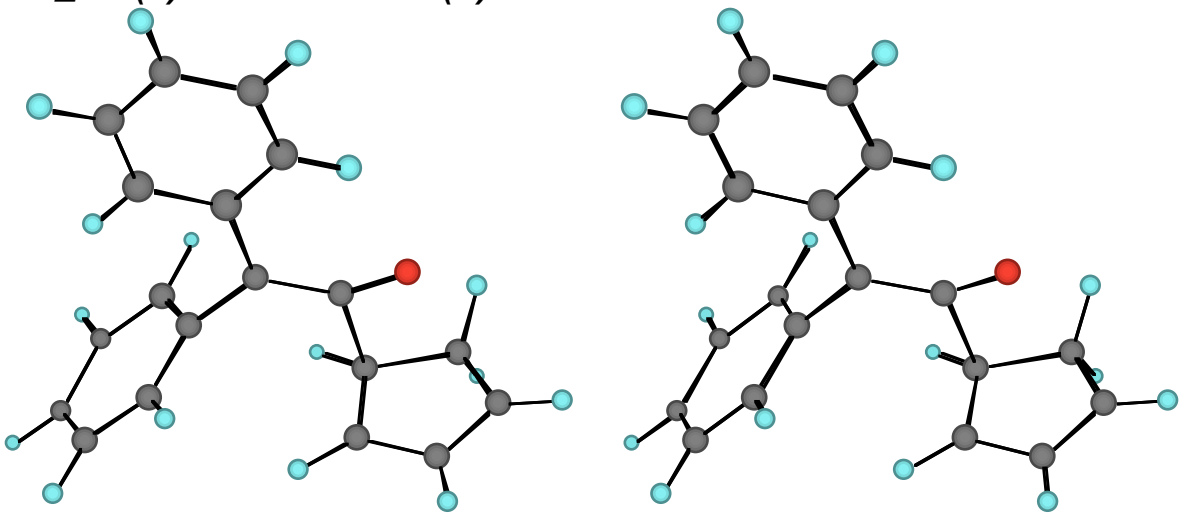
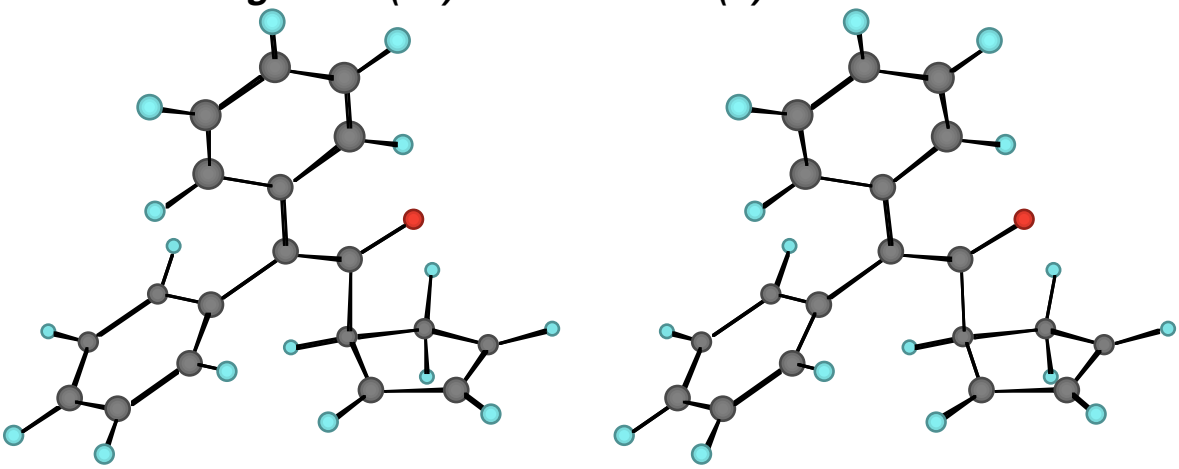

1st_TS (9) MPW1K/6-31G(d)



```
E(RmPW+HF-PW91) = -808.558070111

 Zero-point correction=                           0.300890 (Hartree/Particle)
 Thermal correction to Energy=                    0.316607
 Thermal correction to Enthalpy=                  0.317551
 Thermal correction to Gibbs Free Energy=         0.256271
 Sum of electronic and zero-point Energies=           -808.257180
 Sum of electronic and thermal Energies=              -808.241463
 Sum of electronic and thermal Enthalpies=            -808.240519
 Sum of electronic and thermal Free Energies=         -808.301799

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 198.674             62.309            128.974

 C,0,-2.4098711525,0.3760507549,-0.5020885538
 C,0,-2.5332255987,0.8485496805,0.7968590092
 C,0,-3.5138695931,0.0861421576,1.4947558758
 C,0,-4.0626119257,-0.7973766055,0.6326087549
 C,0,-3.5562155197,-0.5604887905,-0.7432574766
```

```
O,0,-1.581161975,-1.8894359355,0.3882303393
C,0,-1.0471904966,-0.8507016018,0.1153885421
C,0,0.1874028379,-0.2862368728,0.0181634443
H,0,-1.9417082105,0.9401816375,-1.2911669432
H,0,-1.947152807,1.6498230014,1.2148930152
H,0,-3.7219511201,0.1642698026,2.5487101699
H,0,-4.7888340202,-1.5547369092,0.8797428851
H,0,-4.3142358861,-0.0306962292,-1.3303116266
H,0,-3.297937754,-1.4718363214,-1.2736480709
C,0,1.3668827953,-1.164166025,0.1095657038
C,0,1.2726705608,-2.5407027723,0.3546194466
C,0,2.6511084996,-0.625437086,-0.0381670906
C,0,2.4058472706,-3.325858486,0.4538794098
H,0,0.301953759,-2.9946552212,0.4674384827
C,0,3.7807490183,-1.4177716694,0.0615319
H,0,2.767840181,0.4300964822,-0.2284486245
C,0,3.6697686315,-2.7754390241,0.3085121794
H,0,2.2964201924,-4.3841643175,0.644883993
H,0,4.7552135189,-0.9650680308,-0.0560871991
H,0,4.5514635716,-3.394797479,0.3849170826
C,0,0.4163853463,1.1502932732,-0.2789599622
C,0,0.5964857723,2.073349498,0.7488177327
C,0,0.5346593018,1.6002192292,-1.5932612787
C,0,0.8516909996,3.4083745892,0.4749220869
H,0,0.5464856374,1.7284975372,1.7721818357
C,0,0.7850478215,2.9341890034,-1.8722668105
H,0,0.4332901011,0.8870797671,-2.3995173888
C,0,0.9404176724,3.8433849265,-0.8375347627
H,0,0.9864010502,4.1075487309,1.2876770178
H,0,0.8663199181,3.2625904501,-2.8984530668
H,0,1.1389342184,4.8831095081,-1.0531831794
```

2nd TS rearrangement (11) MPW1K/6-31G(d)



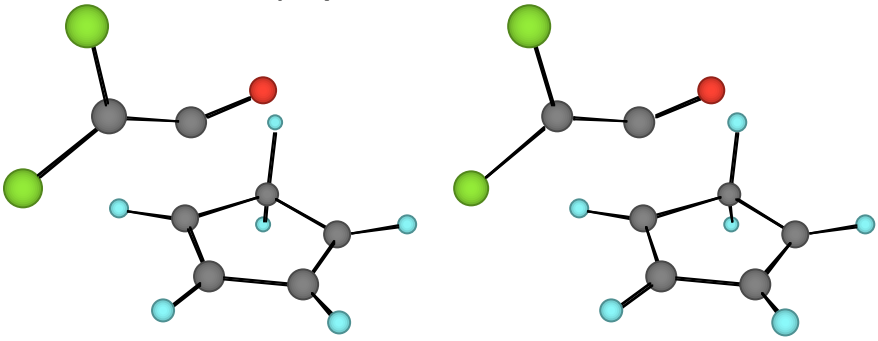
```
E(RmPW+HF-PW91) = -808.561774659

 Zero-point correction=                           0.302633 (Hartree/Particle)
 Thermal correction to Energy=                    0.317456
 Thermal correction to Enthalpy=                  0.318400
 Thermal correction to Gibbs Free Energy=         0.259518
 Sum of electronic and zero-point Energies=          -808.259142
 Sum of electronic and thermal Energies=             -808.244319
 Sum of electronic and thermal Enthalpies=           -808.243375
```

Sum of electronic and thermal Free Energies= -808.302256

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	199.206	60.450	123.926

C,0,2.2257200485,0.8934898767,-2.8194617304
C,0,1.4256017589,1.1738851115,-1.5638498611
C,0,2.3436733691,0.8820460739,-0.4708845726
C,0,3.3708667951,0.0612708978,-0.9452230448
C,0,3.2133343199,-0.0856179641,-2.2959742696
C,0,0.6244606862,-0.1801954414,-1.2721304086
C,0,-0.1748647813,-0.1895217215,-0.1253906287
O,0,0.9465778236,-1.1138210811,-2.01564378
H,0,0.8405154291,2.0802218176,-1.5112900857
H,0,2.2016333494,1.211167193,0.5439100113
H,0,4.0854857314,-0.4614198287,-0.3317269599
H,0,3.7888733243,-0.748619026,-2.9220442975
H,0,2.7415738059,1.8033584909,-3.1407737331
H,0,1.6323034597,0.5103074545,-3.6415688893
C,0,-0.5098690398,1.0847363742,0.5624781491
C,0,-1.2953240677,2.0531964198,-0.0599650565
C,0,-0.0867145015,1.3262371798,1.869874075
C,0,-1.6187349546,3.2358303116,0.5866747644
H,0,-1.6616929407,1.8665078114,-1.0597552172
C,0,-0.4132161064,2.5039033895,2.5211075488
H,0,0.4991901464,0.5718817364,2.3768089235
C,0,-1.176280459,3.4668447566,1.8787480428
H,0,-2.2268512179,3.9729261156,0.0822716681
H,0,-0.0707593319,2.6698533247,3.5323914265
H,0,-1.4306196884,4.3864188018,2.3851121432
C,0,-0.8951237771,-1.3891155491,0.3056301289
C,0,-1.873039656,-1.3091695592,1.3082275392
C,0,-0.6219790866,-2.6598755553,-0.2269675536
C,0,-2.5247660219,-2.4365100076,1.7720479842
H,0,-2.1283486611,-0.3495446406,1.7292873138
C,0,-1.2708060804,-3.7828707444,0.2479221446
H,0,0.0979050303,-2.7420951169,-1.022951708
C,0,-2.2256588544,-3.6837218003,1.249025217
H,0,-3.2743521178,-2.3366295967,2.5440394411
H,0,-1.0345081749,-4.7476036122,-0.178237373
H,0,-2.7366482787,-4.5652145674,1.6083467672

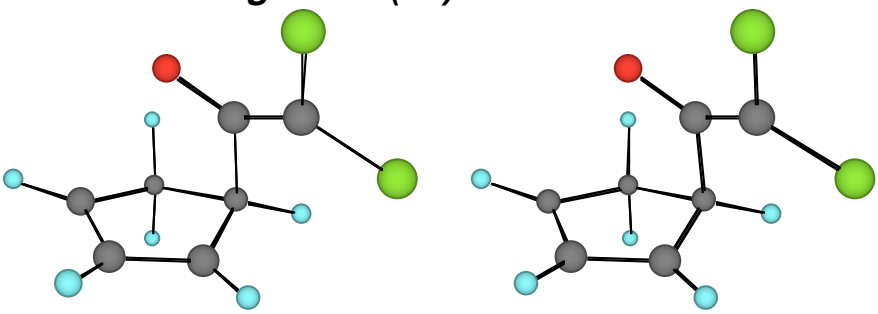
*Dichloro 1st TS (16) MPW1K/6-31G**



key distances OC 2.848 CC 2.154 CC 3.049
E(RmPW+HF-PW91) = -1265.76296903

```
Zero-point correction=                           0.114090 (Hartree/Particle)
Thermal correction to Energy=                    0.123309
Thermal correction to Enthalpy=                  0.124253
Thermal correction to Gibbs Free Energy=         0.078556
Sum of electronic and zero-point Energies=          -1265.648879
Sum of electronic and thermal Energies=             -1265.639660
Sum of electronic and thermal Enthalpies=           -1265.638716
Sum of electronic and thermal Free Energies=        -1265.684413

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   77.378             33.066            96.177

C,0,1.3198145442,0.7568189474,0.7040058887
C,0,1.4887326073,1.0021714142,-0.6338195347
C,0,2.5412787944,0.1683308114,-1.1472623147
C,0,3.0471348055,-0.5590320453,-0.1349057054
C,0,2.3986462645,-0.1746784228,1.1473078747
O,0,0.4495655764,-1.7214227516,-0.0287054035
C,0,-0.1274507003,-0.692613414,0.0362303692
C,0,-1.3038502523,-0.0556964148,-0.0175697006
Cl,0,-1.5954859588,1.6317234928,0.0859844737
Cl,0,-2.7109832946,-1.0493419802,-0.130980439
H,0,0.7244403917,1.3493473379,1.3775934981
H,0,0.9161410871,1.7073175106,-1.2141052786
H,0,2.8272481302,0.1109553005,-2.1841563927
H,0,3.8164397657,-1.3097504608,-0.2128173133
H,0,3.1004695851,0.371330607,1.7861618973
H,0,2.0428773578,-1.030109252,1.7179769629
```

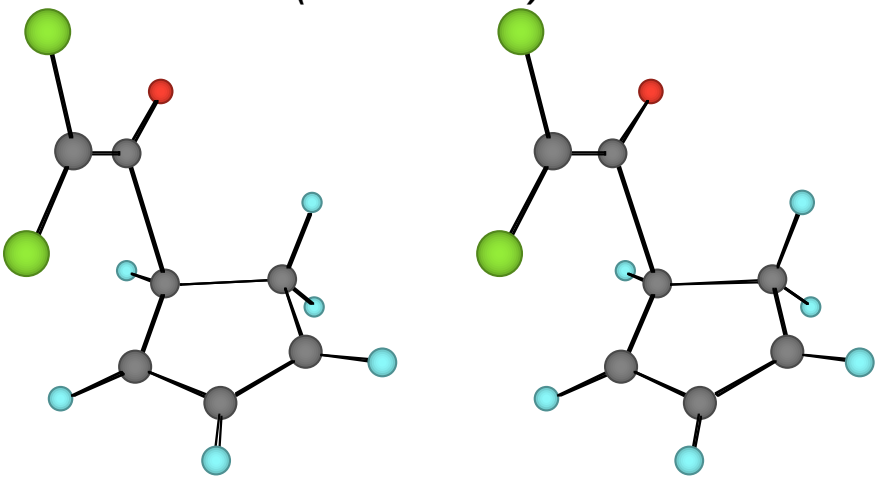
*2nd TS rearrangement (17) MPW1K/6-31G**



```
key distances OC 2.488, CC 2.728
E(RmPW+HF-PW91) = -1265.77209910

 Zero-point correction=                           0.116128 (Hartree/Particle)
 Thermal correction to Energy=                    0.124275
 Thermal correction to Enthalpy=                  0.125219
 Thermal correction to Gibbs Free Energy=         0.081913
 Sum of electronic and zero-point Energies=          -1265.655971
 Sum of electronic and thermal Energies=             -1265.647824
 Sum of electronic and thermal Enthalpies=           -1265.646880
 Sum of electronic and thermal Free Energies=        -1265.690186

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   77.984             30.636            91.146
```

```
C,0,2.3666367549,0.1030711419,-1.1493398868
C,0,1.1123116181,0.7892399167,-0.6468846901
C,0,1.3070840624,0.8968467926,0.7977517362
C,0,2.2659471473,-0.0331701201,1.1957726889
C,0,2.7608248838,-0.6444051835,0.0722629209
C,0,0.0804520729,-0.3936670072,-0.4524328942
C,0,-1.1518172008,-0.0253822355,0.0590334121
O,0,0.530734661,-1.5321750093,-0.5809338619
Cl,0,-2.3415777828,-1.2189050669,0.336658818
Cl,0,-1.740768725,1.595370619,0.031086765
H,0,0.730505813,1.647844529,-1.1831507086
H,0,0.7312196359,1.5396424004,1.4421345366
H,0,2.4781420999,-0.3140798268,2.2134309282
H,0,3.4322068671,-1.4879832153,0.0674174068
H,0,3.1293890718,0.8493486341,-1.3890694287
H,0,2.2039138267,-0.5324866615,-2.0119464736
```

*Dichloro 2+2 TS (Similar to 10) MPW1K/6-31G**



```
key distances 1.908 3.075
E(RmPW+HF-PW91) = -1265.74180964

 Zero-point correction=                           0.113976 (Hartree/Particle)
 Thermal correction to Energy=                    0.123274
 Thermal correction to Enthalpy=                  0.124218
 Thermal correction to Gibbs Free Energy=         0.077553
 Sum of electronic and zero-point Energies=          -1265.627834
 Sum of electronic and thermal Energies=             -1265.618536
 Sum of electronic and thermal Enthalpies=           -1265.617592
 Sum of electronic and thermal Free Energies=        -1265.664257

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  77.356             32.763            98.215

 C,0,0.664933407,1.3186030414,-0.9056468857
 C,0,1.8420224565,0.7433337946,-0.4417646029
 C,0,2.2048697309,1.2816218661,0.8298016213
 C,0,1.3530012522,2.2875343735,1.1184192026
 C,0,0.3729626647,2.4766319568,0.0224062638
 C,0,-0.8794958158,0.2223235119,-0.6783781661
```

O,0,-1.798993337,0.8733459278,-1.0795375581
C,0,-0.6788848066,-0.9874452022,-0.1159427709
Cl,0,0.7956455731,-1.7472621717,0.3209683509
Cl,0,-2.0966764921,-1.9139799488,0.2255805978
H,0,0.5021343205,1.4062102689,-1.9699660832
H,0,2.4318007172,0.0268326787,-0.9891376966
H,0,3.0204896109,0.9320132556,1.4400953799
H,0,1.3586519379,2.8770726823,2.0219347623
H,0,0.5779165929,3.4192008824,-0.4960587093
H,0,-0.6579741932,2.5373988073,0.3647327113

Cyclopentadiene (1) MPW1K/6-31+G(d,p)

E(RmPW+HF-PW91) = -194.065760414

Zero-point correction=	0.095375 (Hartree/Particle)
Thermal correction to Energy=	0.099446
Thermal correction to Enthalpy=	0.100390
Thermal correction to Gibbs Free Energy=	0.068821
Sum of electronic and zero-point Energies=	-193.970385
Sum of electronic and thermal Energies=	-193.966314
Sum of electronic and thermal Enthalpies=	-193.965370
Sum of electronic and thermal Free Energies=	-193.996940

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	62.403	15.041	66.444

C,0,0.60007971,0.8503739738,-0.6051259374
C,0,0.6949467299,0.7041456443,0.724079062
C,0,-0.1505921621,-0.4092216356,1.1458255257
C,0,-0.7555225793,-0.9346372184,0.0710390952
C,0,-0.3337802543,-0.1808039027,-1.1464717412
H,0,1.1048707409,1.584742978,-1.2109986645
H,0,1.2948687976,1.3039522083,1.3899536486
H,0,-0.2598576246,-0.7431979221,2.1654256597
H,0,-1.4403162824,-1.7665593138,0.0585236825
H,0,-1.1859197506,0.2713988503,-1.6609931687
H,0,0.1555654542,-0.8294779684,-1.877987184

diphenylketene (2) MPW1K/6-31+G(d,p)

E(RmPW+HF-PW91) = -614.557526647

Zero-point correction=	0.202031 (Hartree/Particle)
Thermal correction to Energy=	0.213714
Thermal correction to Enthalpy=	0.214658
Thermal correction to Gibbs Free Energy=	0.162254
Sum of electronic and zero-point Energies=	-614.355495
Sum of electronic and thermal Energies=	-614.343813
Sum of electronic and thermal Enthalpies=	-614.342869
Sum of electronic and thermal Free Energies=	-614.395272

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	134.107	45.076	110.292

```
C,0,2.0161898435,0.7841417439,0.0380096255
O,0,3.0951212623,1.2037625436,0.0583497561
C,0,0.7859593374,0.3056774293,0.0148171359
C,0,0.1303396351,0.0033601933,1.3048816774
C,0,-1.2311975688,0.2577286452,1.469442162
C,0,0.8478302543,-0.5187791956,2.379920303
C,0,-1.8536470631,-0.0028129977,2.6781805827
H,0,-1.7986572432,0.6653728319,0.6461000046
C,0,0.2255684821,-0.7606163372,3.5942156778
H,0,1.8971552291,-0.7501001803,2.2612133707
C,0,-1.1284286348,-0.5077997654,3.7481390366
H,0,-2.9091342424,0.1990445977,2.7873068659
H,0,0.7994135633,-1.1622979321,4.4162912262
H,0,-1.6156840449,-0.7060555067,4.6909936847
C,0,0.1410117882,0.1021745962,-1.2997659207
C,0,-0.6848221255,-1.0029104829,-1.5055628786
C,0,0.3521057227,0.9854600419,-2.3572991898
C,0,-1.2797791047,-1.2158458128,-2.7372522326
H,0,-0.8544831891,-1.6972366285,-0.6961168373
C,0,-0.2298972467,0.7589312351,-3.5942977184
H,0,0.9650041103,1.863256302,-2.2072560598
C,0,-1.0515729276,-0.3400521902,-3.7892370015
H,0,-1.9174315648,-2.0762025729,-2.8782976457
H,0,-0.0515461887,1.4531578164,-4.4021930361
H,0,-1.5135688805,-0.5109816956,-4.7499871778
```

4+2_product (3) MPW1K/6-31+G(d,p)

```
E(RmPW+HF-PW91) = -808.651513331

 Zero-point correction=                           0.304995 (Hartree/Particle)
 Thermal correction to Energy=                    0.319788
 Thermal correction to Enthalpy=                  0.320732
 Thermal correction to Gibbs Free Energy=         0.261130
 Sum of electronic and zero-point Energies=          -808.346518
 Sum of electronic and thermal Energies=             -808.331725
 Sum of electronic and thermal Enthalpies=           -808.330781
 Sum of electronic and thermal Free Energies=        -808.390383

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.670             60.176           125.443

 C,0,2.2227710651,1.0244456229,0.2677622391
 C,0,2.9297224184,1.0451147101,-1.0750191383
 C,0,3.648118925,-0.0727203925,-1.1626300453
 C,0,3.3797153336,-0.8254381142,0.1178988135
 C,0,3.2845369991,0.3104772663,1.1231582187
 O,0,1.9926490765,-1.2559986161,0.0631765936
 C,0,1.2420556729,-0.125980549,0.1389179882
 C,0,-0.097533582,-0.1060852635,0.0777010753
 H,0,1.8072470055,1.9581731585,0.6195575218
 H,0,2.7659364711,1.7904352284,-1.836562933
 H,0,4.2021740344,-0.4454927571,-2.0082210601
 H,0,3.9820346218,-1.6949055486,0.3465841345
 H,0,4.2008926633,0.883532641,1.2210545866
 H,0,2.9210547299,-0.016717263,2.0951578164
 C,0,-0.7956482187,1.1967981709,0.2402298608
```

```
C,0,-0.7447468291,1.9048270159,1.4384488954
C,0,-1.5442827958,1.7276431753,-0.8096797187
C,0,-1.3984630013,3.1211365746,1.5776397931
H,0,-0.1953459717,1.4884529322,2.2710965648
C,0,-2.1989474232,2.9406854262,-0.6739776319
H,0,-1.6079853053,1.1790544096,-1.738471709
C,0,-2.1256842969,3.6444312863,0.5203851386
H,0,-1.3461886539,3.6539860851,2.5160306213
H,0,-2.7673902403,3.3384892532,-1.5020403549
H,0,-2.6375351912,4.589473129,0.6269576049
C,0,-0.9350821109,-1.3044293938,-0.1327052667
C,0,-2.2436263951,-1.3258863644,0.3577859957
C,0,-0.4814529646,-2.4285194464,-0.8289267446
C,0,-3.0621279391,-2.4276516606,0.172955573
H,0,-2.6227534817,-0.4677505556,0.8924777573
C,0,-1.3040051962,-3.5260326063,-1.0191386127
H,0,0.5212313587,-2.4394436693,-1.2220401049
C,0,-2.5973657081,-3.5357193992,-0.5181035802
H,0,-4.0669341804,-2.4174889385,0.5698116077
H,0,-0.9303334599,-4.3797445412,-1.5659967054
H,0,-3.2350207311,-4.3946409863,-0.6670252158
```

2+2_product (4) MPW1K/6-31+G(d,p)

```
E(RmPW+HF-PW91) = -808.664448064

 Zero-point correction=                           0.303475 (Hartree/Particle)
 Thermal correction to Energy=                    0.318841
 Thermal correction to Enthalpy=                  0.319785
 Thermal correction to Gibbs Free Energy=         0.259064
 Sum of electronic and zero-point Energies=           -808.360974
 Sum of electronic and thermal Energies=              -808.345607
 Sum of electronic and thermal Enthalpies=            -808.344663
 Sum of electronic and thermal Free Energies=         -808.405385

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 200.076             61.376            127.799

 C,0,-2.1776751003,-1.2782633259,-0.3272726875
 C,0,-1.526148234,-0.0444792708,-0.9998559316
 C,0,-2.4807469505,1.0486114461,-0.62647314
 C,0,-3.5809164685,0.5879917079,-0.0388747859
 C,0,-3.5929252775,-0.9064390408,0.1049186166
 C,0,-1.1136298607,-1.1541905448,0.7437374379
 O,0,-1.0217544906,-1.5968591055,1.8503058257
 C,0,-0.2607967935,-0.1815783735,-0.0835556549
 H,0,-2.091917392,-2.2175663669,-0.869526108
 H,0,-1.3366507562,-0.0921819831,-2.0688427754
 H,0,-2.2822714582,2.0909375843,-0.8235718533
 H,0,-4.3983256937,1.2090597306,0.2970535439
 H,0,-4.3516018379,-1.362398237,-0.5332212771
 H,0,-3.797502122,-1.2308189855,1.1253563264
 C,0,0.2580841509,1.0699230075,0.5848187854
 C,0,0.6385964561,2.1548773252,-0.201274658
 C,0,0.3821728646,1.1668354298,1.9650820375
 C,0,1.1234424211,3.3146784284,0.3778394884
 H,0,0.5579672856,2.0907919272,-1.2776163581
```

```
C,0,0.8720177095,2.3291954637,2.5456664682
H,0,0.0943616202,0.3333939119,2.5868150018
C,0,1.2423041529,3.4059493934,1.7578157432
H,0,1.411513142,4.1468161973,-0.2478884493
H,0,0.9610785302,2.3892997782,3.6205194629
H,0,1.6219090847,4.3091457423,2.2121529136
C,0,0.8841275414,-0.9505379797,-0.7294234878
C,0,1.2180610124,-0.7837783077,-2.0690839863
C,0,1.6620076271,-1.8040078281,0.0491221696
C,0,2.3015496696,-1.4531316539,-2.6184084588
H,0,0.6404538921,-0.1223296178,-2.6973259591
C,0,2.7416266654,-2.4765021121,-0.4999582836
H,0,1.418615457,-1.9417139439,1.0925636758
C,0,3.0661117577,-2.30430148,-1.8369773151
H,0,2.5457824488,-1.307593043,-3.6605019195
H,0,3.3297107317,-3.1367852262,0.1202753588
H,0,3.9073329305,-2.8282983322,-2.2657423322
```

*Dichloroketene (5) MPW1K/6-31+G***

```
E(RmPW+HF-PW91) = -1071.72174234

 Zero-point correction=                           0.016271 (Hartree/Particle)
 Thermal correction to Energy=                    0.021228
 Thermal correction to Enthalpy=                  0.022172
 Thermal correction to Gibbs Free Energy=        -0.013388
 Sum of electronic and zero-point Energies=          -1071.705471
 Sum of electronic and thermal Energies=             -1071.700514
 Sum of electronic and thermal Enthalpies=           -1071.699570
 Sum of electronic and thermal Free Energies=        -1071.735130

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  13.321             15.071             74.842

 C,0,1.2112587129,-0.5270517753,-0.2366302426
 C,0,0.0256013896,-0.0111340188,-0.0049696958
 O,0,2.2545888115,-0.9810384476,-0.4404825313
 Cl,0,-1.2903101578,-1.0308619728,0.3959433139
 Cl,0,-0.207211672,1.6824750519,-0.1033868503
```

*Dichloro 2+2 product (7) MPW1K/6-31+G***

```
E(RmPW+HF-PW91) = -1265.86034300

 Zero-point correction=                           0.117635 (Hartree/Particle)
 Thermal correction to Energy=                    0.126147
 Thermal correction to Enthalpy=                  0.127092
 Thermal correction to Gibbs Free Energy=         0.083098
 Sum of electronic and zero-point Energies=          -1265.742708
 Sum of electronic and thermal Energies=             -1265.734196
 Sum of electronic and thermal Enthalpies=           -1265.733251
 Sum of electronic and thermal Free Energies=        -1265.777245

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.159             31.406             92.592
```

```
C,0,-0.6403275934,-0.9075013505,-1.1249746804
C,0,-0.3981794713,0.6112005268,-0.9005989352
C,0,-1.7233118454,1.0663107525,-0.3724961889
C,0,-2.6518469821,0.1185929192,-0.4514342842
C,0,-2.1428901108,-1.1645504552,-1.0382761855
C,0,0.1237600688,-1.1574833458,0.1670168058
O,0,0.1980732653,-2.0561429918,0.9359865728
C,0,0.6628919205,0.2873395449,0.1778631229
Cl,0,2.2986315201,0.2849616581,-0.5166065213
Cl,0,0.6248183179,1.1585012114,1.6954219125
H,0,-0.1432959571,-1.3503857173,-1.9841404904
H,0,-0.014981032,1.2141581595,-1.7193592323
H,0,-1.8816805242,2.0621444135,0.0101465726
H,0,-3.6787036069,0.2459653335,-0.1426132097
H,0,-2.5805477505,-1.3543759542,-2.0190467878
H,0,-2.3646004143,-2.0306826346,-0.4153390127
```

*Dichloro 4+2 product (8) MPW1K/6-31+G***

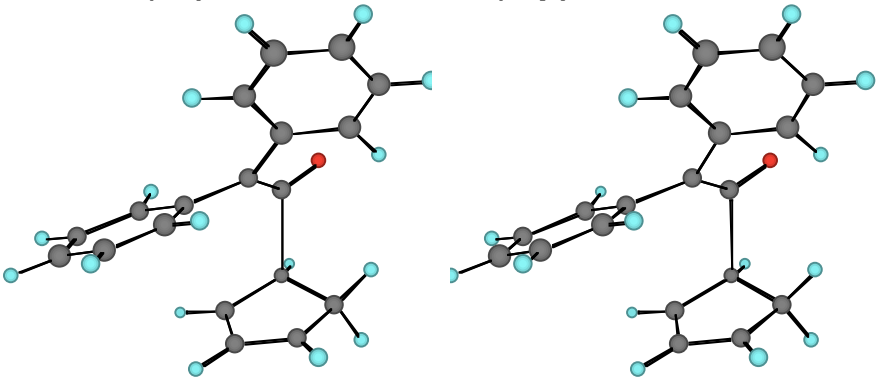
E(RmPW+HF-PW91) = -1265.83714634

Zero-point correction=	0.119273 (Hartree/Particle)
Thermal correction to Energy=	0.127233
Thermal correction to Enthalpy=	0.128177
Thermal correction to Gibbs Free Energy=	0.085206
Sum of electronic and zero-point Energies=	-1265.717873
Sum of electronic and thermal Energies=	-1265.709913
Sum of electronic and thermal Enthalpies=	-1265.708969
Sum of electronic and thermal Free Energies=	-1265.751940

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.840	30.204	90.440

```
C,0,1.3337994121,0.6059368347,0.5034065639
C,0,2.0485760456,0.844125785,-0.8138478398
C,0,2.4250581511,-0.3458288706,-1.2786916306
C,0,1.9363250029,-1.3536468441,-0.2677390682
C,0,2.1348003796,-0.5978065644,1.0360047951
O,0,0.4804367731,-1.361623481,-0.3551914828
C,0,0.0900320093,-0.1524476298,0.0979455379
C,0,-1.1824994429,0.2261397068,0.1390510562
Cl,0,-1.6502131205,1.7719893589,0.7342744354
Cl,0,-2.4575191373,-0.7911270517,-0.3841550887
H,0,1.1722896305,1.4574438816,1.1502981774
H,0,2.116664767,1.8010208009,-1.3052071302
H,0,2.870145579,-0.5774505749,-2.2318859424
H,0,2.2695407634,-2.3792245931,-0.3510486662
H,0,3.1702991972,-0.3490679458,1.2436382303
H,0,1.6724649143,-1.0932274479,1.8869318118
```

TS_2+2 (10) MPW1K/6-31+G(d,p)



key distances 1.867 3.115
E(RmPW+HF-PW91) = -808.583348892

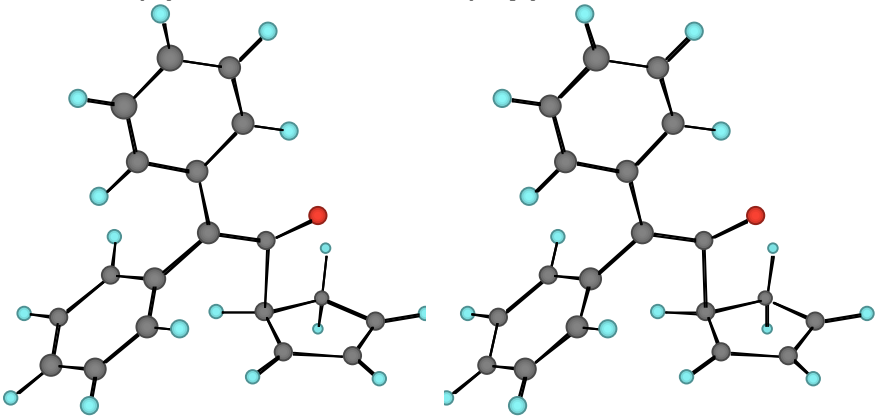
Zero-point correction=	0.299237 (Hartree/Particle)
Thermal correction to Energy=	0.315064
Thermal correction to Enthalpy=	0.316008
Thermal correction to Gibbs Free Energy=	0.254551
Sum of electronic and zero-point Energies=	-808.284112
Sum of electronic and thermal Energies=	-808.268285
Sum of electronic and thermal Enthalpies=	-808.267341
Sum of electronic and thermal Free Energies=	-808.328798

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	197.706	62.616	129.347

C,0,-2.2796121247,-1.1711090492,-0.948431802
C,0,-2.6956670055,0.1674886231,-0.9625884163
C,0,-2.8654179332,0.6339511377,0.3695768189
C,0,-2.7292540701,-0.4162109465,1.2145291753
C,0,-2.5681662481,-1.6786852461,0.4508657792
C,0,-0.4243534733,-1.3785708699,-0.9751615761
O,0,-0.2313456929,-2.4777165638,-1.4032409162
C,0,0.3126805908,-0.3765629782,-0.3646949949
H,0,-2.4914270946,-1.797047021,-1.8022025743
H,0,-2.8915865348,0.7497776868,-1.8463158064
H,0,-3.0462036877,1.6586577396,0.6479458954
H,0,-2.7755001444,-0.3666930191,2.2910432632
H,0,-3.5239472247,-2.2155509824,0.4400301173
H,0,-1.8309542703,-2.3626969293,0.8628775519
C,0,0.0362232413,1.0319537484,-0.5703613406
C,0,-0.3991919049,1.5048084612,-1.8131516084
C,0,0.2031492864,1.9776245926,0.4571936271
C,0,-0.6783077903,2.8536346018,-2.0199423032
H,0,-0.457970752,0.8169800026,-2.6441485665
C,0,-0.069614116,3.3115045238,0.2515247488
H,0,0.5304840209,1.6393262603,1.4290061114
C,0,-0.5191773982,3.760388036,-0.9917587011
H,0,-1.0015663827,3.1885813343,-2.9951108486
H,0,0.0573937957,4.0139779805,1.0626285408
H,0,-0.727089398,4.8083454365,-1.149255749
C,0,1.4633023502,-0.822988643,0.4408392906
C,0,2.5895392533,-0.0037745109,0.5865509258
C,0,1.4975634815,-2.0754317224,1.0633537133

```
C,0,3.6829929929,-0.4099430033,1.3326678214
H,0,2.616269857,0.9548356373,0.0914845855
C,0,2.5932921865,-2.4815036802,1.8038806259
H,0,0.6590977849,-2.7469674753,0.9589201409
C,0,3.6939844773,-1.6502610391,1.9516405541
H,0,4.5376788892,0.2458113449,1.4176349167
H,0,2.5844073738,-3.455767607,2.2709552596
H,0,4.547884535,-1.9677100929,2.5312404638
```

1st_TS (9) MPW1K/6-31+G(d,p)



key distances OC 2.751 CC 1.945 CC 3.054
E(RmPW+HF-PW91) = -808.602438424

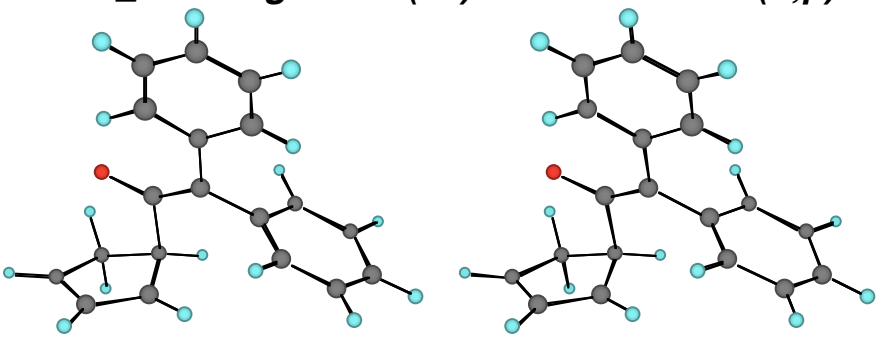
Zero-point correction=	0.299594 (Hartree/Particle)
Thermal correction to Energy=	0.315387
Thermal correction to Enthalpy=	0.316331
Thermal correction to Gibbs Free Energy=	0.255005
Sum of electronic and zero-point Energies=	-808.302844
Sum of electronic and thermal Energies=	-808.287051
Sum of electronic and thermal Enthalpies=	-808.286107
Sum of electronic and thermal Free Energies=	-808.347433

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	197.908	62.636	129.072

```
C,0,-2.4180694319,0.378232305,-0.496521755
C,0,-2.5375249062,0.8401691285,0.8063986189
C,0,-3.5275402044,0.0811772561,1.4974099052
C,0,-4.0841446711,-0.7900532689,0.6264184513
C,0,-3.5648436322,-0.554799473,-0.7443148352
O,0,-1.5747523312,-1.8922918464,0.3945204933
C,0,-1.0443146831,-0.8512933872,0.1227858118
C,0,0.189938987,-0.2866639843,0.0199693412
H,0,-1.9427156533,0.9425176363,-1.2810520326
H,0,-1.9472577808,1.6351129556,1.2305990215
H,0,-3.7381427942,0.1529761702,2.5510453852
H,0,-4.818407319,-1.5416342918,0.8675004711
H,0,-4.3158607783,-0.0234161715,-1.3382278433
H,0,-3.3059982201,-1.4679488769,-1.2719261569
C,0,1.3697053039,-1.1639848706,0.1109472482
C,0,1.2766782975,-2.5423388938,0.3521854952
C,0,2.6542702474,-0.6222690175,-0.0352630014
```

```
C,0,2.4124672865,-3.3267944922,0.4491083349
H,0,0.3068641057,-2.9985104704,0.4639417688
C,0,3.7859067254,-1.4137921679,0.0623218275
H,0,2.7702824344,0.433783489,-0.2228063242
C,0,3.6765069223,-2.7736999162,0.3056992005
H,0,2.3046273771,-4.3854990046,0.6369716366
H,0,4.7595935913,-0.9597343312,-0.0537001827
H,0,4.5588404998,-3.3918150105,0.3804709108
C,0,0.4177642192,1.1500048008,-0.279062453
C,0,0.5995927486,2.0749001976,0.7470728271
C,0,0.5365531001,1.5966489311,-1.5948323236
C,0,0.8553160383,3.41032819,0.4702167629
H,0,0.5528871027,1.7326737417,1.7715316946
C,0,0.7874620448,2.9307872283,-1.8774121248
H,0,0.4368421882,0.8818631856,-2.3998987302
C,0,0.9432237498,3.8432683351,-0.8441049951
H,0,0.9914608492,4.1105628954,1.2815810215
H,0,0.8692020395,3.2562281267,-2.9043037514
H,0,1.1421121568,4.8822133224,-1.0620248549
```

2ndTS_rearrangement (11) MPW1K/6-31+G(d,p)



key distances OC 2.615, CC 2.739
E(RmPW+HF-PW91) = -808.605862818

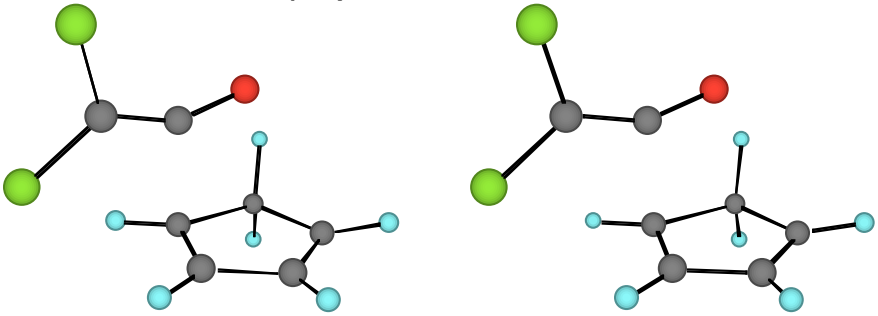
Zero-point correction=	0.301299 (Hartree/Particle)
Thermal correction to Energy=	0.316158
Thermal correction to Enthalpy=	0.317102
Thermal correction to Gibbs Free Energy=	0.258516
Sum of electronic and zero-point Energies=	-808.304564
Sum of electronic and thermal Energies=	-808.289705
Sum of electronic and thermal Enthalpies=	-808.288760
Sum of electronic and thermal Free Energies=	-808.347346

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	198.392	60.835	123.304

```
C,0,2.2400313077,0.8989435452,-2.8233636157
C,0,1.4239661312,1.159652981,-1.5741948676
C,0,2.3288409449,0.8679551807,-0.4720388848
C,0,3.3907921737,0.0818231191,-0.9451057458
C,0,3.2783303467,-0.0261653723,-2.3005699492
C,0,0.6257008968,-0.195682771,-1.2770167847
C,0,-0.1693894662,-0.1990045286,-0.1222947948
O,0,0.9255251676,-1.1335428046,-2.0221252848
H,0,0.8294611383,2.0598640774,-1.5226828382
```

```
H,0,2.1730770269,1.18672726,0.5438647356
H,0,4.11157596,-0.4271604979,-0.3277408968
H,0,3.8982259631,-0.6466711559,-2.9283825326
H,0,2.7103292399,1.8283910959,-3.1573778678
H,0,1.6656036913,0.4785468779,-3.6415345259
C,0,-0.5009740967,1.0776811911,0.5642247916
C,0,-1.3004928055,2.0372482953,-0.0551460806
C,0,-0.0679441128,1.3278333046,1.866987999
C,0,-1.6277314867,3.2210811925,0.5897576618
H,0,-1.6769841535,1.8432421658,-1.0498169034
C,0,-0.3968750686,2.5068477928,2.5167375365
H,0,0.526304473,0.5797053833,2.3736108086
C,0,-1.1739341224,3.4620764355,1.8772127606
H,0,-2.2471258992,3.950315732,0.0880789849
H,0,-0.0471787672,2.6788322896,3.5243127149
H,0,-1.4305468839,4.3816836615,2.3818540843
C,0,-0.8987253369,-1.3920610805,0.3092912779
C,0,-1.8711139808,-1.3029758391,1.3187906484
C,0,-0.6445692326,-2.6656470381,-0.2294957235
C,0,-2.5345075931,-2.4240012129,1.7838076298
H,0,-2.1131749094,-0.3420951514,1.7444785274
C,0,-1.3048962142,-3.7827849767,0.2477613007
H,0,0.0675704429,-2.7550301572,-1.0319153148
C,0,-2.2527539242,-3.6747370531,1.2558132907
H,0,-3.2784607036,-2.316999878,2.5598856721
H,0,-1.0834378094,-4.748809081,-0.1826377361
H,0,-2.7719663109,-4.5506991785,1.6160546645
```

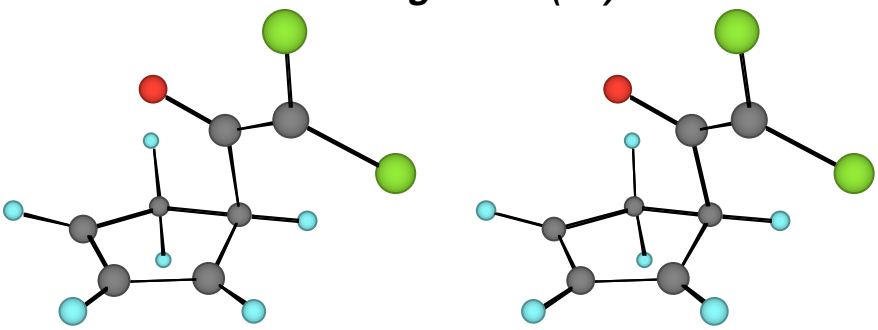
*Dichloro 1st TS (16) MPW1K/6-31+G***



```
key distances CC 2.172, CC 3.052, OC 2.879
E(RmPW+HF-PW91) = -1265.78145400

 Zero-point correction=                           0.113431 (Hartree/Particle)
 Thermal correction to Energy=                    0.122716
 Thermal correction to Enthalpy=                  0.123660
 Thermal correction to Gibbs Free Energy=         0.077805
 Sum of electronic and zero-point Energies=          -1265.668023
 Sum of electronic and thermal Energies=             -1265.658738
 Sum of electronic and thermal Enthalpies=           -1265.657794
 Sum of electronic and thermal Free Energies=        -1265.703649

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  77.005             33.270             96.509

 C,0,1.3291002112,0.7537417309,0.7064255008
 C,0,1.489345294,0.9928270028,-0.6339208147
```

```
C,0,2.5485284518,0.1654759944,-1.1470132739
C,0,3.0639458808,-0.5535642789,-0.1319879165
C,0,2.4097675353,-0.1747073695,1.1485570525
O,0,0.4378679987,-1.7284883178,-0.0324967457
C,0,-0.1378027609,-0.6987392151,0.0319431348
C,0,-1.3107181686,-0.055135874,-0.0180555835
Cl,0,-1.5910869875,1.6334744345,0.0864109835
Cl,0,-2.7224854227,-1.0411549657,-0.1307527794
H,0,0.7286432315,1.3419255609,1.3793327008
H,0,0.9114688179,1.6935674449,-1.2141975779
H,0,2.8335870787,0.1054551827,-2.1837992785
H,0,3.8393376458,-1.2979033249,-0.2102056962
H,0,3.1071682462,0.3700603104,1.7926047588
H,0,2.0545833022,-1.034017545,1.7143609929
```

*Dichloro 2nd TS rearrangement (17) MPW1K/6-31+G***



key distances 2.438 CO, 2.780 CC
E(RmPW+HF-PW91) = -1265.79092128

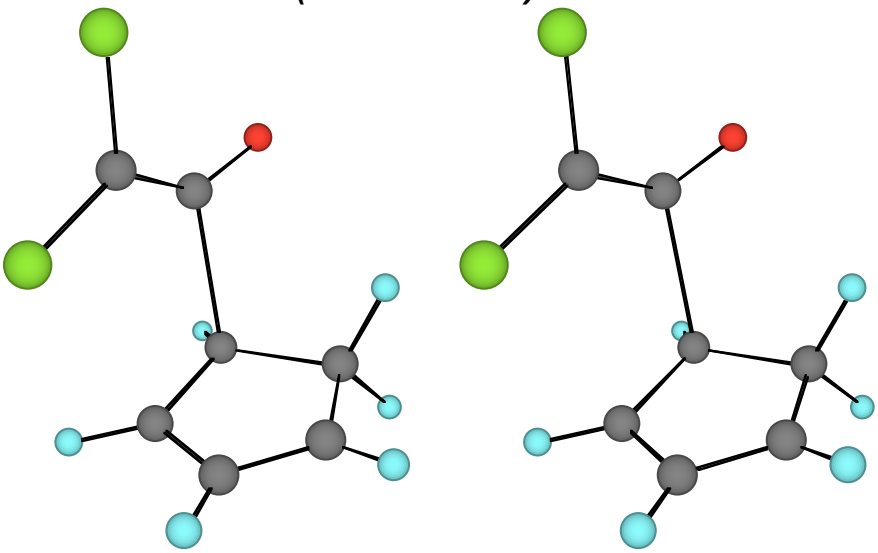
Zero-point correction=	0.115554 (Hartree/Particle)
Thermal correction to Energy=	0.123736
Thermal correction to Enthalpy=	0.124680
Thermal correction to Gibbs Free Energy=	0.081281
Sum of electronic and zero-point Energies=	-1265.675367
Sum of electronic and thermal Energies=	-1265.667185
Sum of electronic and thermal Enthalpies=	-1265.666241
Sum of electronic and thermal Free Energies=	-1265.709641

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.646	30.756	91.342

```
C,0,2.360569492,0.1066097766,-1.1435999401
C,0,1.1134239395,0.7967443891,-0.6278592132
C,0,1.3334503671,0.9148630667,0.8130457169
C,0,2.2855107352,-0.0208754381,1.2035867471
C,0,2.7517397593,-0.6498614303,0.0718724948
C,0,0.085370133,-0.3883529193,-0.4206170186
C,0,-1.1636789239,-0.0318164531,0.0415109759
O,0,0.5570483361,-1.527355966,-0.5247690259
Cl,0,-2.3530543708,-1.2284713592,0.298664935
Cl,0,-1.7510322405,1.588841654,0.0176731766
H,0,0.7228938579,1.6517567968,-1.1631723263
H,0,0.7609970157,1.5566605612,1.4622216136
H,0,2.5066141421,-0.3033871992,2.2185417635
H,0,3.4044527532,-1.5080152769,0.0617131404
```

```
H,0,3.1258697582,0.8521944364,-1.3752454684
H,0,2.1939451635,-0.5205225524,-2.0112929901
```

Dichloro 2+2 TS (similar to 10) mPW1K



```
key distances 1.947, 3.100
E(RmPW+HF-PW91) = -1265.76116415

 Zero-point correction=                           0.113247 (Hartree/Particle)
 Thermal correction to Energy=                    0.122634
 Thermal correction to Enthalpy=                  0.123578
 Thermal correction to Gibbs Free Energy=         0.076632
 Sum of electronic and zero-point Energies=          -1265.647917
 Sum of electronic and thermal Energies=             -1265.638530
 Sum of electronic and thermal Enthalpies=           -1265.637586
 Sum of electronic and thermal Free Energies=        -1265.684532

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  76.954             33.031             98.807

 C,0,-0.3841324967,-0.5375288496,-1.6259990407
 C,0,-1.3358961414,0.4612912817,-1.4875943652
 C,0,-2.5336321994,-0.0568332282,-0.9051296169
 C,0,-2.4012008348,-1.3960644943,-0.7920763914
 C,0,-1.0861023054,-1.8379351576,-1.3136934741
 C,0,1.0002757906,-0.4938165018,-0.2583977659
 O,0,1.7100258625,-1.4203215593,-0.5134557479
 C,0,0.8861778899,0.4731237741,0.6736274733
 Cl,0,-0.2138582284,1.785139292,0.7503412088
 Cl,0,2.0133655179,0.3981252998,1.9810736709
 H,0,0.3584644908,-0.4681912709,-2.4067592989
 H,0,-1.2092671964,1.4796705253,-1.8159200831
 H,0,-3.3850024956,0.5328616361,-0.6099084325
 H,0,-3.1325159205,-2.0668988282,-0.3691303536
 H,0,-1.2264894282,-2.4086837123,-2.2372732723
 H,0,-0.5499584883,-2.4951048816,-0.6318364458
```

Cyclopentadiene (1) B3LYP/6-31G(d)

E(RB+HF-LYP) = -194.101058102

Zero-point correction=	0.092894 (Hartree/Particle)
Thermal correction to Energy=	0.097037
Thermal correction to Enthalpy=	0.097981
Thermal correction to Gibbs Free Energy=	0.066297
Sum of electronic and zero-point Energies=	-194.008164
Sum of electronic and thermal Energies=	-194.004021
Sum of electronic and thermal Enthalpies=	-194.003077
Sum of electronic and thermal Free Energies=	-194.034761

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	60.892	15.532	66.686

C,0,0.6060113819,0.8584337704,-0.6085373113
C,0,0.6994883093,0.7087826711,0.7287459978
C,0,-0.151571919,-0.4119606018,1.1532588261
C,0,-0.761654919,-0.942830538,0.0737003299
C,0,-0.3364714453,-0.1822536595,-1.1556434048
H,0,1.1132278349,1.5965117921,-1.2193869712
H,0,1.3017843824,1.309771887,1.4025751874
H,0,-0.2587531789,-0.7445209875,2.1808302064
H,0,-1.4508669347,-1.7794626404,0.0596005501
H,0,-1.1937654504,0.2708997447,-1.6772984333
H,0,0.1535649003,-0.8342296489,-1.8954671653

Diphenylketene (2) B3LYP/6-31G(d)

E(RB+HF-LYP) = -614.708265406

Zero-point correction=	0.196318 (Hartree/Particle)
Thermal correction to Energy=	0.208257
Thermal correction to Enthalpy=	0.209201
Thermal correction to Gibbs Free Energy=	0.156467
Sum of electronic and zero-point Energies=	-614.511947
Sum of electronic and thermal Energies=	-614.500008
Sum of electronic and thermal Enthalpies=	-614.499064
Sum of electronic and thermal Free Energies=	-614.551798

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	130.683	46.459	110.988

C,0,2.0196603437,0.780829663,0.0403690462
O,0,3.1121886357,1.2032166174,0.0622069309
C,0,0.7792435463,0.3012669959,0.0155752676
C,0,0.1227021878,-0.0026733611,1.3170484719
C,0,-1.2543507251,0.2235965325,1.485948488
C,0,0.8590414616,-0.4946435079,2.4082458255
C,0,-1.8711542118,-0.0378796898,2.7079892337
H,0,-1.8377652513,0.6095068033,0.6556908418
C,0,0.2421149786,-0.7352143899,3.6349921407
H,0,1.9202875438,-0.7000125785,2.2898774925
C,0,-1.1269675397,-0.5129670267,3.7902791375
H,0,-2.9376914131,0.1412154575,2.8169240183

```
H,0,0.8319663566,-1.1129757663,4.4659890561
H,0,-1.6101469817,-0.7116404417,4.7428596197
C,0,0.1347071259,0.1021920583,-1.3119035393
C,0,-0.7253654534,-0.9889746652,-1.5255160384
C,0,0.3862211492,0.9760719958,-2.3833588704
C,0,-1.3147292317,-1.1938204322,-2.7716654931
H,0,-0.9260643574,-1.6780281389,-0.7109289131
C,0,-0.1890120814,0.7557360547,-3.6339338838
H,0,1.028618998,1.8400885123,-2.2309407707
C,0,-1.0463702099,-0.3272771302,-3.8337197809
H,0,-1.9790350554,-2.0420779928,-2.9151937324
H,0,0.021951447,1.4430973944,-4.4489264982
H,0,-1.504078414,-0.4923647716,-4.8051065925
```

4+2 Product (3) B3LYP/6-31G(d)

```
E(RB+HF-LYP) = -808.819403440

 Zero-point correction=                           .296300 (Hartree/Particle)
 Thermal correction to Energy=                    .311471
 Thermal correction to Enthalpy=                  .312415
 Thermal correction to Gibbs Free Energy=         .252373
 Sum of electronic and zero-point Energies=          -808.523103
 Sum of electronic and thermal Energies=             -808.507932
 Sum of electronic and thermal Enthalpies=           -808.506988
 Sum of electronic and thermal Free Energies=        -808.567031

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 195.451             62.370           126.370

 C,0,2.2488217801,1.0273911245,0.2808560593
 C,0,2.9649700438,1.0339792303,-1.0729497055
 C,0,3.6794189323,-0.0975032907,-1.1534827752
 C,0,3.4096440182,-0.8457253029,0.1413350327
 C,0,3.3188506806,0.3058911174,1.1507330353
 O,0,1.9927966753,-1.2773853957,0.096197503
 C,0,1.2442590699,-0.1243958129,0.1626419871
 C,0,-0.1066711749,-0.0985169847,0.0859087236
 H,0,1.844202906,1.9739964232,0.6286416796
 H,0,2.8018523818,1.7786312636,-1.8443101279
 H,0,4.2331341148,-0.4853274154,-2.0008653051
 H,0,4.003178435,-1.7277551905,0.3745845755
 H,0,4.2434200411,0.8788288158,1.2476022689
 H,0,2.9541229881,-0.0139981618,2.1320683923
 C,0,-0.8109341287,1.2132005666,0.2430067701
 C,0,-0.7159130034,1.9630172416,1.4264358699
 C,0,-1.6086507784,1.719354768,-0.7978272481
 C,0,-1.3715793311,3.1892179134,1.5574974037
 H,0,-0.1310199181,1.5699234406,2.2541092677
 C,0,-2.2668756503,2.9412862795,-0.6684211873
 H,0,-1.7062145976,1.1445797562,-1.7148504123
 C,0,-2.1479264192,3.6839858462,0.509241228
 H,0,-1.2832161006,3.7514112873,2.4838154148
 H,0,-2.8722538981,3.31663194,-1.4896903494
 H,0,-2.6621219074,4.6361167648,0.6103569637
 C,0,-0.9440649902,-1.3079358907,-0.1378573117
 C,0,-2.2532360647,-1.3578605009,0.3792296438
```

```
C,0,-0.4905704481,-2.4191504087,-0.8754155108
C,0,-3.069241481,-2.4697557972,0.178634439
H,0,-2.6319178029,-0.5147221402,0.9486556798
C,0,-1.3101700365,-3.5273773099,-1.0791351657
H,0,0.5105324328,-2.4102823718,-1.2883484025
C,0,-2.603280925,-3.5625719078,-0.5533181516
H,0,-4.0728236422,-2.4801595588,0.5968240024
H,0,-0.93535023,-4.3684309765,-1.657576298
H,0,-3.238999164,-4.4295459984,-0.713276193
```

2+2 Product (4) B3LYP/6-31G(d)

E(RB+HF-LYP) = -808.830818866

Zero-point correction=	0.295026 (Hartree/Particle)
Thermal correction to Energy=	0.310723
Thermal correction to Enthalpy=	0.311667
Thermal correction to Gibbs Free Energy=	0.250760
Sum of electronic and zero-point Energies=	-808.535792
Sum of electronic and thermal Energies=	-808.520096
Sum of electronic and thermal Enthalpies=	-808.519152
Sum of electronic and thermal Free Energies=	-808.580059

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	194.981	63.357	128.190

```
C,0,-2.211265789,-1.2907418365,-0.3045212849
C,0,-1.5423919545,-0.0696357304,-1.0184209269
C,0,-2.5035050115,1.0484939134,-0.6963493146
C,0,-3.6107018232,0.6191170073,-0.0806585342
C,0,-3.6297481589,-0.8781645456,0.1394788824
C,0,-1.1212712577,-1.1704326831,0.763394924
O,0,-1.0199255291,-1.6169336173,1.8804193101
C,0,-0.261063105,-0.1931163956,-0.0833122128
H,0,-2.1610687325,-2.246628256,-0.8350844576
H,0,-1.3371673973,-0.1625190851,-2.0881042056
H,0,-2.2998740047,2.0846307132,-0.9475507889
H,0,-4.4325522118,1.2597652637,0.2281356587
H,0,-4.4100008776,-1.366184425,-0.4610887543
H,0,-3.8189510433,-1.1533156672,1.1851878801
C,0,0.2525884599,1.0765419818,0.5882986068
C,0,0.5941610331,2.1874022519,-0.1978348725
C,0,0.4196020819,1.1598941834,1.9760583407
C,0,1.0804964872,3.3552316547,0.3870200809
H,0,0.483698532,2.1365365281,-1.2783906909
C,0,0.908870488,2.3303829053,2.5615190536
H,0,0.1633139047,0.3092943999,2.5979914022
C,0,1.2395676155,3.4314288378,1.7727096176
H,0,1.3371716169,4.2053113942,-0.2400275985
H,0,1.0297502856,2.3774660605,3.6407981397
H,0,1.6198944578,4.3406373681,2.2306842252
C,0,0.9017718398,-0.9630155449,-0.7308575796
C,0,1.2671470151,-0.757650622,-2.0683192544
C,0,1.6624574132,-1.8552154272,0.039429551
C,0,2.3597595043,-1.4270464253,-2.6217855291
H,0,0.7050799954,-0.0653720343,-2.6885131425
C,0,2.7519086767,-2.5274319658,-0.5146801219
```

```
H,0,1.3956868281,-2.0257814118,1.0780453749
C,0,3.105130001,-2.3173587879,-1.8483646535
H,0,2.6260711471,-1.2511521934,-3.6608618875
H,0,3.3241336183,-3.2178809202,0.0994060728
H,0,3.9531370197,-2.8414354234,-2.280810345
```

*Dichloroketene (5) B3LYP/6-31G**

```
E(RB+HF-LYP) = -1071.76036588

 Zero-point correction=                           0.015367 (Hartree/Particle)
 Thermal correction to Energy=                    0.020476
 Thermal correction to Enthalpy=                  0.021420
 Thermal correction to Gibbs Free Energy=        -0.014464
 Sum of electronic and zero-point Energies=          -1071.744999
 Sum of electronic and thermal Energies=             -1071.739890
 Sum of electronic and thermal Enthalpies=           -1071.738946
 Sum of electronic and thermal Free Energies=        -1071.774829

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  12.849             15.525            75.524

 O,0,-2.2692216631,-0.8142460661,0.7414229189
 C,0,-1.2164770048,-0.4364993103,0.3974462256
 C,0,-0.0276786011,-0.0099346254,0.0090149994
 Cl,0,0.2062343955,1.666458159,-0.3879199203
 Cl,0,1.3007483657,-1.1257186212,-0.1044418857
```

*Dichloro 2+2 product (7) B3LYP/6-31G**

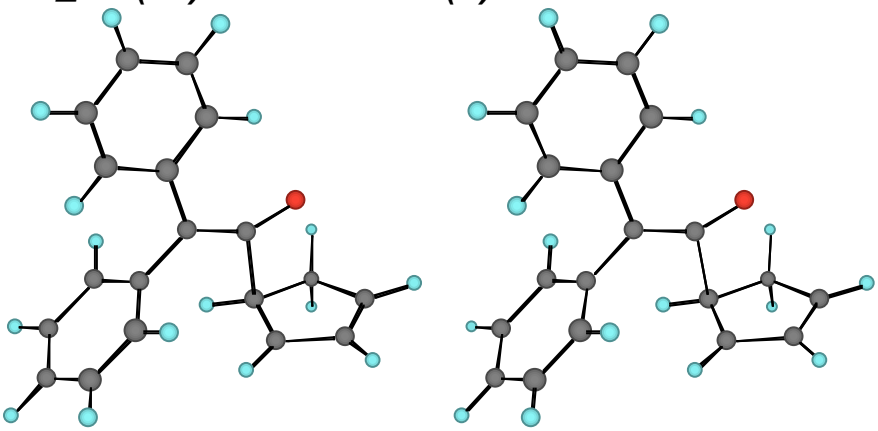
```
E(RB+HF-LYP) = -1265.91522109

 Zero-point correction=                           0.113797 (Hartree/Particle)
 Thermal correction to Energy=                    0.122590
 Thermal correction to Enthalpy=                  0.123534
 Thermal correction to Gibbs Free Energy=         0.078991
 Sum of electronic and zero-point Energies=          -1265.801424
 Sum of electronic and thermal Energies=             -1265.792631
 Sum of electronic and thermal Enthalpies=           -1265.791687
 Sum of electronic and thermal Free Energies=        -1265.836230

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  76.927             32.607            93.749

 C,0,-0.6513981568,-0.9154480862,-1.1432616893
 C,0,-0.4071184016,0.6189740052,-0.9133949822
 C,0,-1.7457712323,1.0843185081,-0.3970921472
 C,0,-2.6814595401,0.1313034209,-0.4675408041
 C,0,-2.1696237493,-1.1722740904,-1.0377441877
 C,0,0.1386445984,-1.1833693769,0.1507519356
 O,0,0.230408655,-2.1023147443,0.910671957
 C,0,0.6617387193,0.2859772721,0.1792970175
 Cl,0,2.3390854647,0.3159292611,-0.5123224429
 Cl,0,0.6074065704,1.1500804215,1.7387488771
 H,0,-0.1713830936,-1.3560092076,-2.0209367774
 H,0,-0.0094076285,1.2220436923,-1.7334373307
```

```
H,0,-1.9030437433,2.0923712116,-0.0281887323
H,0,-3.7169547848,0.262439582,-0.1660080266
H,0,-2.6160900053,-1.3874324091,-2.0178986633
H,0,-2.3868280058,-2.033949438,-0.3942463631
```

*Dichloro 4+2 Product (8) B3LYP/6-31G**

```
E(RB+HF-LYP) = -1265.89248550

 Zero-point correction=                           0.115353 (Hartree/Particle)
 Thermal correction to Energy=                    0.123591
 Thermal correction to Enthalpy=                  0.124535
 Thermal correction to Gibbs Free Energy=         0.081055
 Sum of electronic and zero-point Energies=          -1265.777132
 Sum of electronic and thermal Energies=             -1265.768894
 Sum of electronic and thermal Enthalpies=           -1265.767950
 Sum of electronic and thermal Free Energies=        -1265.811431

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  77.555             31.489             91.513

 C,0,1.3487685896,0.6106634422,0.5025372792
 C,0,2.0751894191,0.849903168,-0.823391835
 C,0,2.4562317152,-0.3480467693,-1.2900685272
 C,0,1.9678723099,-1.365271199,-0.2740537411
 C,0,2.1596605047,-0.6051144531,1.0443216173
 O,0,0.480551691,-1.3784794002,-0.3614978506
 C,0,0.0895055867,-0.1541177826,0.0981307264
 C,0,-1.1924000898,0.2285192332,0.1403479099
 Cl,0,-1.6694366457,1.7981062623,0.7447859127
 Cl,0,-2.4893059943,-0.8046870143,-0.3848315129
 H,0,1.1895190349,1.4679704401,1.1527736906
 H,0,2.1404449783,1.8125294457,-1.3179589348
 H,0,2.9057048224,-0.5832693003,-2.2477113157
 H,0,2.2946340477,-2.3992325624,-0.3605071872
 H,0,3.1998628161,-0.3523994138,1.2594959517
 H,0,1.6950774405,-1.1051044609,1.8997252269
```

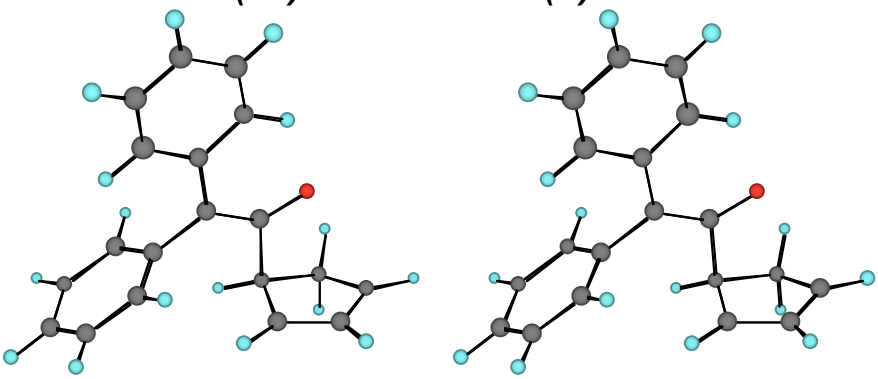
1st_TS (12) B3LYP/6-31G(d)



```
E(RB+HF-LYP) = -808.787217876

 Zero-point correction=                           0.291515 (Hartree/Particle)
```

```
Thermal correction to Energy=                  0.307632
Thermal correction to Enthalpy=                0.308576
Thermal correction to Gibbs Free Energy=       0.246551
Sum of electronic and zero-point Energies=          -808.495703
Sum of electronic and thermal Energies=             -808.479586
Sum of electronic and thermal Enthalpies=           -808.478642
Sum of electronic and thermal Free Energies=        -808.540667

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  193.042             64.361           130.543

C,0,2.4224001946,-0.4459040534,0.3370244007
C,0,2.6554784443,-0.2540329039,-1.0385338914
C,0,3.2577900442,-1.4247596738,-1.5931668029
C,0,3.5171545678,-2.305297632,-0.5837782172
C,0,3.2123336269,-1.6779255537,0.7421325939
O,0,0.7720634111,-2.3768078842,-0.073251471
C,0,0.6823778767,-1.1672793746,0.0229399132
C,0,-0.2944332654,-0.1941013023,0.0340384595
H,0,2.2733765203,0.3843416619,1.0166631182
H,0,2.369610304,0.6297755457,-1.594793412
H,0,3.4236887769,-1.596344196,-2.6504808796
H,0,3.919289293,-3.3057177357,-0.6990937089
H,0,4.1470979699,-1.3487324256,1.224657294
H,0,2.6961358147,-2.3469771127,1.433300513
C,0,-1.7095691195,-0.6063464924,0.1723196
C,0,-2.1124344505,-1.9598112203,0.2477789633
C,0,-2.7306538326,0.3706340149,0.216335136
C,0,-3.4569503778,-2.306389027,0.346348024
H,0,-1.3619189702,-2.7403432253,0.2297276444
C,0,-4.0736103339,0.0153775163,0.3165513817
H,0,-2.4690005791,1.4215091619,0.1615771184
C,0,-4.4511524223,-1.3261556563,0.3825806067
H,0,-3.7286575682,-3.3580595872,0.4010228329
H,0,-4.8288712948,0.7974313216,0.3431060556
H,0,-5.498890836,-1.6032009132,0.4635256649
C,0,0.0152551226,1.2699291556,0.0484413394
C,0,0.1240985746,1.9989464108,-1.1470546354
C,0,0.1448158611,1.9700320886,1.2606377402
C,0,0.3826180632,3.3716975476,-1.1351373662
H,0,-0.0086799959,1.4778669279,-2.0918276029
C,0,0.4081947231,3.3407004753,1.2774157771
H,0,0.0338054473,1.426429819,2.195643951
C,0,0.5310695913,4.045576722,0.0780958627
H,0,0.4631743607,3.9143959362,-2.07364645
H,0,0.5116764444,3.859333921,2.2271954504
H,0,0.7329596943,5.1134077264,0.0896208667
```

Intermediate (13) B3LYP/6-31G(d)



E(RB+HF-LYP) = -808.789092427

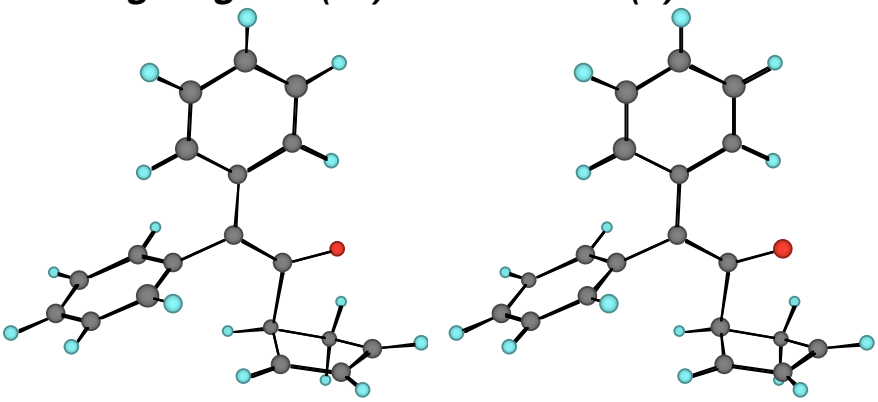
Zero-point correction=	0.292950 (Hartree/Particle)
Thermal correction to Energy=	0.309117
Thermal correction to Enthalpy=	0.310062
Thermal correction to Gibbs Free Energy=	0.247825
Sum of electronic and zero-point Energies=	-808.496142
Sum of electronic and thermal Energies=	-808.479975
Sum of electronic and thermal Enthalpies=	-808.479031
Sum of electronic and thermal Free Energies=	-808.541268

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	193.974	64.931	130.989

1	6	0	-2.337371	-0.396465	-0.499095
2	6	0	-2.513296	-0.343401	0.950947
3	6	0	-3.037914	-1.571054	1.397524
4	6	0	-3.344475	-2.346916	0.301601
5	6	0	-3.252730	-1.535761	-0.955325
6	8	0	-0.836645	-2.293690	-0.507083
7	6	0	-0.833646	-1.053349	-0.402899
8	6	0	0.223860	-0.167662	-0.116155
9	1	0	-2.360891	0.537964	-1.052680
10	1	0	-2.198238	0.483173	1.574109
11	1	0	-3.106539	-1.882787	2.433573
12	1	0	-3.686257	-3.375740	0.334381
13	1	0	-4.244152	-1.128410	-1.210013
14	1	0	-2.873550	-2.095842	-1.810485
15	6	0	1.619969	-0.625814	-0.067809
16	6	0	1.981320	-1.994638	-0.147963
17	6	0	2.674145	0.306544	0.098356
18	6	0	3.308191	-2.395372	-0.029985
19	1	0	1.204373	-2.729884	-0.309021
20	6	0	3.999171	-0.103144	0.207486
21	1	0	2.449150	1.365730	0.149505
22	6	0	4.329201	-1.458438	0.147890
23	1	0	3.548376	-3.454223	-0.091147
24	1	0	4.778915	0.643679	0.336319
25	1	0	5.364892	-1.778319	0.227623
26	6	0	-0.016561	1.311692	-0.078154
27	6	0	-0.014439	2.016655	1.137648
28	6	0	-0.203668	2.045081	-1.262361
29	6	0	-0.214557	3.397805	1.171726

30	1	0	0.155940	1.469587	2.061652
31	6	0	-0.413699	3.424981	-1.231509
32	1	0	-0.179504	1.521585	-2.214988
33	6	0	-0.421453	4.106502	-0.013291
34	1	0	-0.209667	3.919826	2.125281
35	1	0	-0.561588	3.968460	-2.161319
36	1	0	-0.580386	5.181244	0.012085

2ndTS giving 4+2 (14) B3LYP/6-31G(d)



E(RB+HF-LYP) = -808.788846278

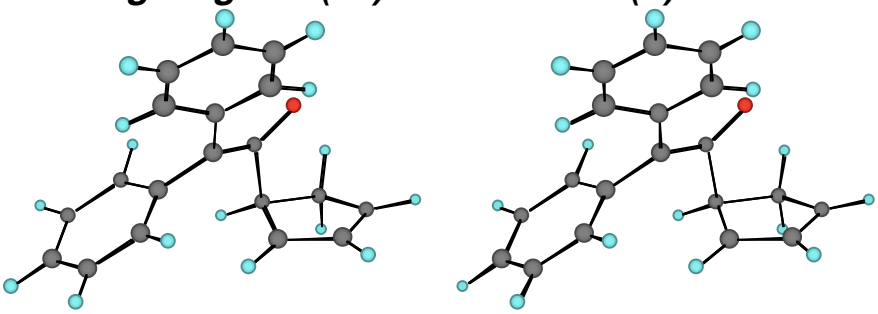
Zero-point correction=	0.292974	(Hartree/Particle)
Thermal correction to Energy=	0.308330	
Thermal correction to Enthalpy=	0.309274	
Thermal correction to Gibbs Free Energy=	0.248770	
Sum of electronic and zero-point Energies=	-808.495873	
Sum of electronic and thermal Energies=	-808.480517	
Sum of electronic and thermal Enthalpies=	-808.479572	
Sum of electronic and thermal Free Energies=	-808.540077	

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	193.480	62.706	127.342

C,0,2.2017798447,0.8509082351,-2.8154630916
C,0,1.5069773679,1.1632795146,-1.4845783439
C,0,2.5807017524,1.036966393,-0.4900940728
C,0,3.5780325729,0.2076546527,-1.0047909369
C,0,3.2506859808,-0.0978868026,-2.32105102
C,0,0.7672833207,-0.2390893653,-1.1051409212
C,0,-0.1640154797,-0.2246802668,-0.0648768564
O,0,1.2132447868,-1.201919961,-1.7808769793
H,0,0.856600889,2.031894971,-1.4243553627
H,0,2.5195789475,1.41894615,0.5213438155
H,0,4.3926336912,-0.2291573042,-0.4386748848
H,0,3.7757721048,-0.8066482466,-2.9513642831
H,0,2.6753353573,1.7649199261,-3.2056296344
H,0,1.5480790887,0.4314439397,-3.579702408
C,0,-0.5319536311,1.0748014999,0.5881646829
C,0,-1.465398944,1.9429586168,-0.0032734845
C,0,0.0181472306,1.4446841586,1.8266598472
C,0,-1.8137868274,3.1501633716,0.6050659423
H,0,-1.9189500853,1.6613350165,-0.9503149604
C,0,-0.3346468702,2.6472259662,2.4428708944

```
H,0,0.7206045322,0.7711236341,2.3111798736
C,0,-1.2480763333,3.5070685573,1.8306736379
H,0,-2.5330592416,3.8085933655,0.1244639395
H,0,0.1048179462,2.9115765425,3.4014472415
H,0,-1.5214479071,4.4447069324,2.307345006
C,0,-0.9427977714,-1.417705994,0.3035458979
C,0,-1.8928951947,-1.352461123,1.3513038576
C,0,-0.7718758839,-2.6725016994,-0.3310376157
C,0,-2.6064917206,-2.4756444879,1.7584318805
H,0,-2.0655089809,-0.4099538418,1.8588655773
C,0,-1.4849117903,-3.7921402305,0.0868810434
H,0,-0.0764887066,-2.7509123723,-1.156290294
C,0,-2.4075034002,-3.707441645,1.1322725237
H,0,-3.3247750139,-2.3852275965,2.5698410491
H,0,-1.3260694396,-4.7405735528,-0.4210309155
H,0,-2.9686068152,-4.5836639833,1.4465088857
```

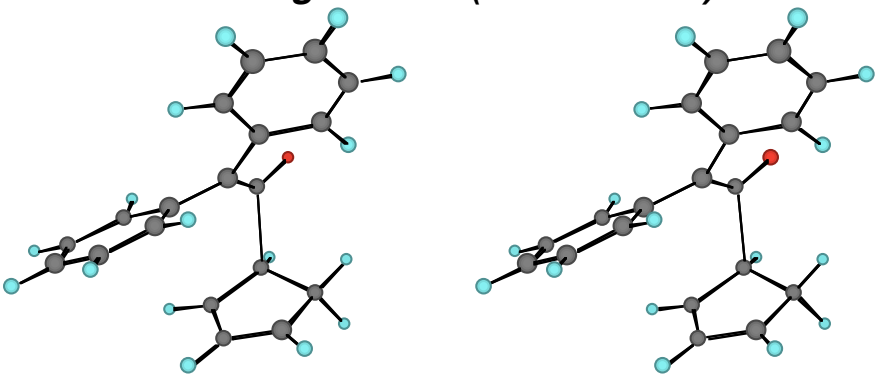
2ndTS giving 2+2 (15) B3LYP/6-31G(d)



```
E(RB+HF-LYP) = -808.788042815

 Zero-point correction=                           .293131 (Hartree/Particle)
 Thermal correction to Energy=                    .308346
 Thermal correction to Enthalpy=                  .309290
 Thermal correction to Gibbs Free Energy=         .250133
 Sum of electronic and zero-point Energies=          -808.494911
 Sum of electronic and thermal Energies=             -808.479697
 Sum of electronic and thermal Enthalpies=           -808.478753
 Sum of electronic and thermal Free Energies=        -808.537909

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 193.490             62.780            124.506

 C,0,-0.3350196762,1.1730561307,-0.9592019136
 C,0,-0.5204150899,1.2838746783,0.5134773962
 C,0,-1.9001299674,1.1128126593,0.8046442056
 C,0,-2.6144210578,1.0746866658,-0.3609555565
 C,0,-1.7379443181,1.3800789316,-1.5461432627
 O,0,-0.9850988547,-1.1415033894,-1.2135577223
 C,0,-0.0886432554,-0.3868243738,-0.8194714243
 C,0,0.9949179868,-0.7335296151,0.0727532982
 H,0,0.4738450596,1.7457678094,-1.4052501837
 H,0,0.2510684689,1.5513594848,1.2207181081
 H,0,-2.3104469086,0.9930338953,1.801484112
 H,0,-3.6837507826,0.9044601086,-0.4342973868
 H,0,-1.8769568634,2.424809949,-1.8641882297
 H,0,-1.9366541758,0.7284896371,-2.3998682334
```

```
C,0,2.2000862921,0.141496386,0.1300384574
C,0,2.8417279905,0.5626551256,-1.0487390653
C,0,2.7503000077,0.5544734426,1.3592941106
C,0,3.9718615939,1.3802943677,-1.0032772479
H,0,2.456282775,0.2273164879,-2.007920325
C,0,3.879559923,1.3697138969,1.4060583642
H,0,2.2789301806,0.2297117384,2.2834068473
C,0,4.4944845753,1.7902035195,0.2238169309
H,0,4.4497831869,1.6877577808,-1.9299077404
H,0,4.2793595929,1.6794624593,2.3682472358
H,0,5.3755002811,2.4251404207,0.2603445851
C,0,1.0863105536,-2.0744724055,0.6763742237
C,0,2.3214215622,-2.5896199355,1.1322664399
C,0,-0.0633920288,-2.8784405585,0.8738619573
C,0,2.4033636293,-3.8264595423,1.7675761525
H,0,3.2294668517,-2.0179146096,0.9776050835
C,0,0.0232169552,-4.1059041863,1.5193507567
H,0,-1.0154026735,-2.5302495365,0.4963447977
C,0,1.2546852267,-4.5912886691,1.9713438057
H,0,3.3710830527,-4.1944351108,2.0990717285
H,0,-0.8784701864,-4.6958600065,1.6639323117
H,0,1.3172114729,-5.5572558125,2.4656335854
```

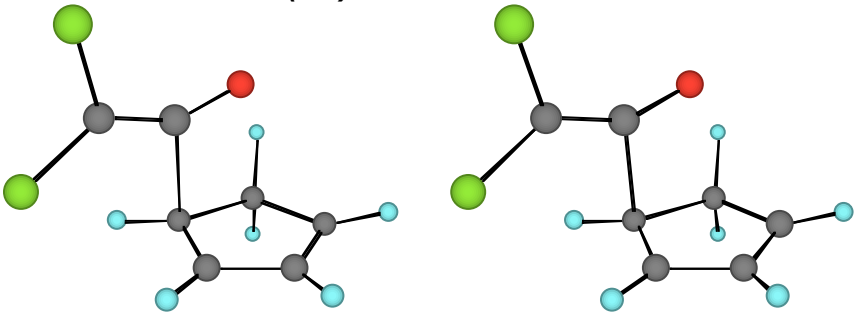
Another TS that gives 2+2 (Similar to 10) B3LYP/6-31G(d)



```
key distances 1.85/2.97
E(RB+HF-LYP) = -808.770273763

 Zero-point correction=                           0.291029 (Hartree/Particle)
 Thermal correction to Energy=                    0.307222
 Thermal correction to Enthalpy=                  0.308166
 Thermal correction to Gibbs Free Energy=         0.245964
 Sum of electronic and zero-point Energies=           -808.479244
 Sum of electronic and thermal Energies=              -808.463052
 Sum of electronic and thermal Enthalpies=            -808.462108
 Sum of electronic and thermal Free Energies=         -808.524309

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 192.785             64.474            130.915

 C,0,-2.2611051943,-1.1980776388,-0.9129352907
 C,0,-2.7435416722,0.1381727956,-0.9875609879
 C,0,-2.9657662988,0.6493783051,0.3260034677
 C,0,-2.8054783879,-0.3613214763,1.2298849088
 C,0,-2.5669336145,-1.6599934004,0.5195192076
```

```
C,0,-0.4217759181,-1.3790486912,-0.9974749924
O,0,-0.1958032278,-2.4823102651,-1.4400500407
C,0,0.3462709025,-0.3697178817,-0.3881631603
H,0,-2.4958930188,-1.8715139985,-1.7322749303
H,0,-2.9443775354,0.6793388166,-1.9024812599
H,0,-3.2048768779,1.6811276881,0.5570134926
H,0,-2.8873450125,-0.2677621037,2.3075975717
H,0,-3.497794615,-2.2530859146,0.5135719991
H,0,-1.8015770465,-2.2917283264,0.9794425704
C,0,0.054952413,1.0452398937,-0.5789756577
C,0,-0.4204327928,1.5231744825,-1.8208366071
C,0,0.2347910337,2.001904626,0.4523426832
C,0,-0.7112429767,2.8785678783,-2.0224444633
H,0,-0.4930897658,0.8324551845,-2.6555476083
C,0,-0.0522228964,3.3428355106,0.2504034564
H,0,0.5813615108,1.6663348835,1.4246681891
C,0,-0.5316425316,3.792941473,-0.9914661172
H,0,-1.0622276609,3.2123748297,-2.9958533054
H,0,0.0849529787,4.0496525334,1.065070201
H,0,-0.7498136322,4.8463738917,-1.1446821102
C,0,1.4899569684,-0.831347519,0.431678914
C,0,2.6139893007,-0.0006137979,0.6393113629
C,0,1.529393861,-2.1172912247,1.0129674355
C,0,3.702355884,-0.4271779462,1.396477018
H,0,2.6435920521,0.9804296974,0.1774000429
C,0,2.6205487221,-2.5410887788,1.766236196
H,0,0.69951652,-2.7998189005,0.8629781443
C,0,3.7151106357,-1.6988862463,1.9716390445
H,0,4.5530077832,0.2381017104,1.5244004942
H,0,2.611963336,-3.5385783373,2.198942606
H,0,4.5656621802,-2.0311217149,2.5605157208
```

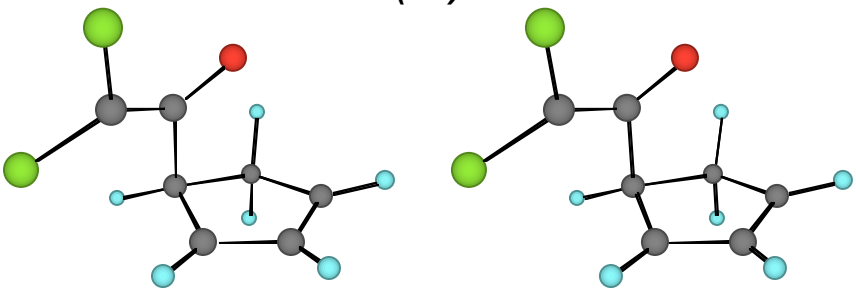
*Dichloro 1st TS (18) B3LYP/6-31G**



```
key distances OC 2.896 CC 2.071 CC 3.089
E(RB+HF-LYP) = -1265.85488175

 Zero-point correction=                           0.110242 (Hartree/Particle)
 Thermal correction to Energy=                    0.119697
 Thermal correction to Enthalpy=                  0.120642
 Thermal correction to Gibbs Free Energy=         0.074432
 Sum of electronic and zero-point Energies=          -1265.744640
 Sum of electronic and thermal Energies=             -1265.735184
 Sum of electronic and thermal Enthalpies=           -1265.734240
 Sum of electronic and thermal Free Energies=        -1265.780450

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
```

```
Total                    75.111             33.989             97.257

C,0,-1.3017655448,0.7261971462,-0.6826644612
C,0,-1.5233911672,1.0153873164,0.660434567
C,0,-2.5867177014,0.1879991549,1.1656232514
C,0,-3.0806773959,-0.5622894533,0.1450236547
C,0,-2.4119054264,-0.1876900095,-1.1438866919
O,0,-0.4386831821,-1.7378406175,-0.0030948267
C,0,0.1053768458,-0.6678536878,-0.0762748984
C,0,1.3062949865,-0.0514271972,0.0322346989
Cl,0,1.6325486025,1.6575947269,-0.0933452215
Cl,0,2.7250901996,-1.0752341411,0.1294269305
H,0,-0.7294227578,1.3504724597,-1.356703325
H,0,-0.9580600428,1.7321942271,1.2442060158
H,0,-2.8951094471,0.1451114486,2.2035661653
H,0,-3.8548369901,-1.3172274521,0.2232838892
H,0,-3.101704316,0.3837051683,-1.7855937119
H,0,-2.0745482053,-1.0536004899,-1.720330195
```

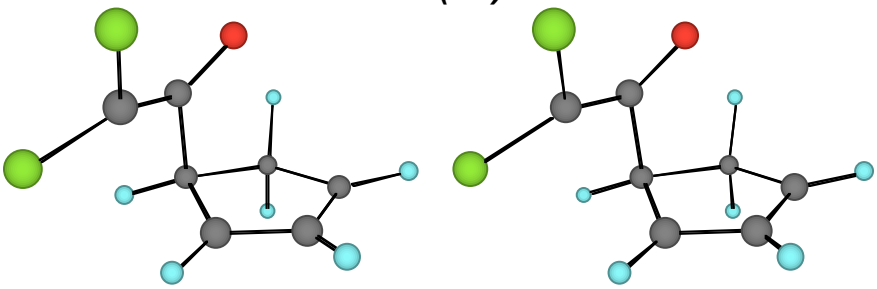
*Dichloro intermediate (19) B3LYP/6-31G**



```
key distances OC 2.770 CC 2.758
E(RB+HF-LYP) = -1265.86141805

 Zero-point correction=                           0.111972 (Hartree/Particle)
 Thermal correction to Energy=                    0.121258
 Thermal correction to Enthalpy=                  0.122202
 Thermal correction to Gibbs Free Energy=         0.076165
 Sum of electronic and zero-point Energies=          -1265.749446
 Sum of electronic and thermal Energies=             -1265.740160
 Sum of electronic and thermal Enthalpies=           -1265.739216
 Sum of electronic and thermal Free Energies=        -1265.785253

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  76.091             33.993             96.892

 C,0,-1.1247714577,0.5872376083,-0.8006859915
 C,0,-1.3736737551,0.9767116205,0.5973564138
 C,0,-2.3884543425,0.1536697189,1.1288145978
 C,0,-2.905848807,-0.6263317667,0.1222957887
 C,0,-2.3761018478,-0.1954992082,-1.2128553651
 O,0,-0.3927964466,-1.6910418857,-0.3489987972
 C,0,-0.0326715325,-0.5106276572,-0.3834314587
 C,0,1.1699535595,0.0186903354,0.1292973823
 Cl,0,1.7127888693,1.6526116149,-0.2044470281
 Cl,0,2.432284588,-1.0712982456,0.6055217442
 H,0,-0.7433572812,1.3433456965,-1.4846600283
 H,0,-0.8182298998,1.7352554275,1.1328166397
```

```
H,0,-2.6613779377,0.1001662712,2.1763916905
H,0,-3.648523941,-1.4062373296,0.2520401082
H,0,-3.0950652821,0.4795513605,-1.7024956089
H,0,-2.1679137623,-1.0291775262,-1.8851208014
```

*2nd TS Dichloro 2+2 side (20) B3LYP/6-31G**



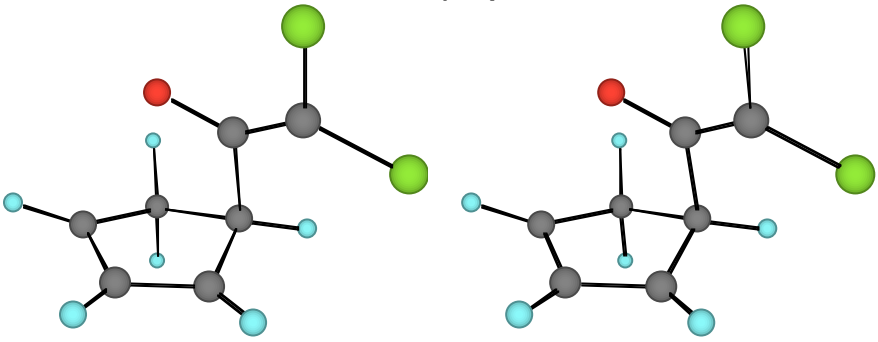
key distances OC 2.907 CC 2.551
E(RB+HF-LYP) = -1265.86123253

Zero-point correction=	0.112008 (Hartree/Particle)
Thermal correction to Energy=	0.120384
Thermal correction to Enthalpy=	0.121328
Thermal correction to Gibbs Free Energy=	0.077923
Sum of electronic and zero-point Energies=	-1265.749224
Sum of electronic and thermal Energies=	-1265.740848
Sum of electronic and thermal Enthalpies=	-1265.739904
Sum of electronic and thermal Free Energies=	-1265.783310

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.542	31.928	91.355

```
C,0,-1.143996788,0.5909189578,-0.8174079084
C,0,-1.2325300209,0.9046410216,0.6312692265
C,0,-2.2274148851,0.0751433892,1.2119011567
C,0,-2.8827266456,-0.6094323242,0.2256575983
C,0,-2.448261628,-0.1505694703,-1.1381748609
O,0,-0.3186520905,-1.6948039006,-0.610069108
C,0,-0.0320420389,-0.5026358472,-0.5507225202
C,0,1.1124231652,0.0397786604,0.1180493148
Cl,0,1.7147295956,1.6537116707,-0.2351430471
Cl,0,2.3295032462,-1.0533387554,0.6992349186
H,0,-0.8379463312,1.3888256071,-1.4923449917
H,0,-0.6779702012,1.683098775,1.1359640603
H,0,-2.4040012098,-0.0234939588,2.2768863146
H,0,-3.6572796865,-1.3517275097,0.3881465707
H,0,-3.1906058032,0.5432125412,-1.5605578988
H,0,-2.3076453079,-0.9748901324,-1.8405350482
```

*2nd TS Dichloro 4+2 side (21) B3LYP/6-31G**



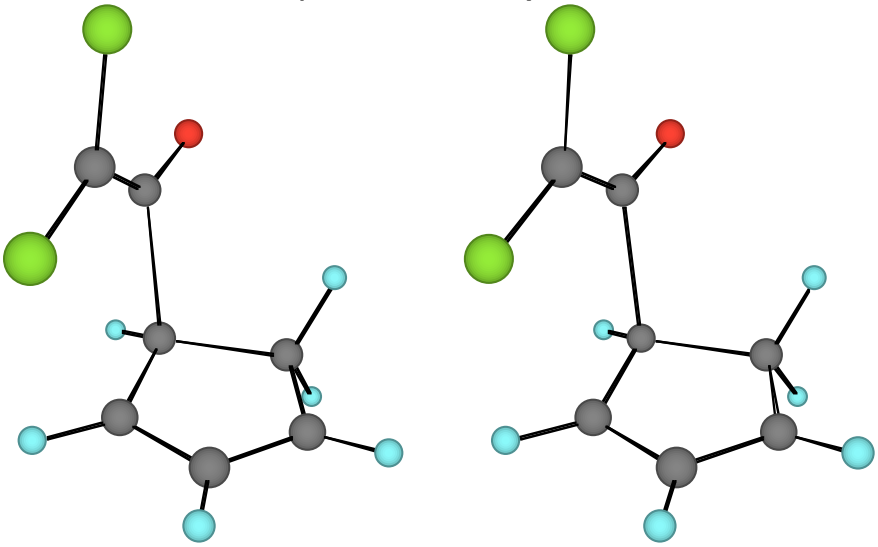
key distances OC 2.391 CC 2.947
E(RB+HF-LYP) = -1265.86084477

Zero-point correction=	0.112119 (Hartree/Particle)
Thermal correction to Energy=	0.120546
Thermal correction to Enthalpy=	0.121491
Thermal correction to Gibbs Free Energy=	0.077599
Sum of electronic and zero-point Energies=	-1265.748726
Sum of electronic and thermal Energies=	-1265.740298
Sum of electronic and thermal Enthalpies=	-1265.739354
Sum of electronic and thermal Free Energies=	-1265.783246

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.644	31.759	92.378

C,0,2.376878288,0.1157490426,-1.1203291
C,0,1.1375487737,0.8245155709,-0.5587893054
C,0,1.4368927711,0.9731128765,0.8792666452
C,0,2.3729767425,0.0074886531,1.2441359431
C,0,2.7703964035,-0.6691878951,0.0938379201
C,0,0.0932575563,-0.3763536068,-0.3599386328
C,0,-1.1942886738,-0.0424594255,0.0257674905
O,0,0.5983085543,-1.5217287886,-0.4264927655
Cl,0,-2.3984211899,-1.2795929418,0.2068663067
Cl,0,-1.8229681181,1.5918873464,-0.0444724241
H,0,0.738082185,1.6845768419,-1.0918559154
H,0,0.8957712899,1.6315269331,1.5481549255
H,0,2.6390990251,-0.2625163983,2.2593036098
H,0,3.4049064322,-1.5477908551,0.0700752804
H,0,3.1531990543,0.8586374873,-1.3576107326
H,0,2.1841206479,-0.4967998729,-2.0005268123

*Dichloro 2+2 TS (Similar to 10) B3LYP/6-31G**



key distances: 1.846 3.112
E(RB+HF-LYP) = -1265.83562795

Zero-point correction=	0.109929 (Hartree/Particle)
Thermal correction to Energy=	0.119447
Thermal correction to Enthalpy=	0.120391
Thermal correction to Gibbs Free Energy=	0.073365
Sum of electronic and zero-point Energies=	-1265.725699
Sum of electronic and thermal Energies=	-1265.716181
Sum of electronic and thermal Enthalpies=	-1265.715237
Sum of electronic and thermal Free Energies=	-1265.762263

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.954	33.729	98.975

C,0,0.7063077878,0.1649202152,-1.5412068003
C,0,-0.5865373012,0.6412358169,-1.8685519297
C,0,-1.4421738109,-0.4340350669,-2.2602980129
C,0,-0.6967248516,-1.5738274201,-2.3389311284
C,0,0.7346435176,-1.2916316541,-2.0169058841
C,0,1.1053268143,0.0353651966,0.2569756859
O,0,2.2244364642,-0.4332614689,0.357426497
C,0,0.1426620167,0.4155469591,1.1486423152
Cl,0,-1.3875654735,1.1783769794,0.809808881
Cl,0,0.3761188106,-0.0321729989,2.8258360787
H,0,1.5480798397,0.8136520615,-1.7742452104
H,0,-0.8756806245,1.6848333657,-1.872647181
H,0,-2.5024195785,-0.3424987689,-2.4651082808
H,0,-1.0724113525,-2.5580582169,-2.599602
H,0,1.3442483083,-1.3722140513,-2.9320422698
H,0,1.1762594208,-1.990533493,-1.3000519133

cyclopentadiene (1) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -194.156236414

Zero-point correction=	0.092110 (Hartree/Particle)

```
 Thermal correction to Energy=                    0.096268
 Thermal correction to Enthalpy=                  0.097212
 Thermal correction to Gibbs Free Energy=         0.065511
 Sum of electronic and zero-point Energies=           -194.064126
 Sum of electronic and thermal Energies=              -194.059968
 Sum of electronic and thermal Enthalpies=            -194.059024
 Sum of electronic and thermal Free Energies=         -194.090725

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   60.409            15.649            66.721

 C,0,0.2858330672,-0.1518990532,-1.1722038957
 C,0,-0.6449040011,0.8600922539,-0.5609186524
 C,0,-0.6753512112,0.6809537452,0.7743970734
 C,0,0.2098695453,-0.4335675707,1.134609047
 C,0,0.7772008926,-0.9305400967,0.0178428559
 H,0,-1.1900637841,1.6019616733,-1.1283589879
 H,0,-1.2548986835,1.2580750368,1.4836761406
 H,0,0.3705508445,-0.7875764804,2.1449921489
 H,0,1.4757725637,-1.753829279,-0.0433881411
 H,0,1.1102823315,0.3257711605,-1.7189127499
 H,0,-0.2275330284,-0.7946377818,-1.9003669801
```

diphenylketene (2) B3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) = -614.869297097

 Zero-point correction=                           0.195181 (Hartree/Particle)
 Thermal correction to Energy=                    0.207140
 Thermal correction to Enthalpy=                  0.208084
 Thermal correction to Gibbs Free Energy=         0.155126
 Sum of electronic and zero-point Energies=           -614.674116
 Sum of electronic and thermal Energies=              -614.662158
 Sum of electronic and thermal Enthalpies=            -614.661213
 Sum of electronic and thermal Free Energies=         -614.714171

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  129.982            46.514           111.459

 C,0,2.0232594223,0.7820146923,0.0404007989
 O,0,3.1076256085,1.2011303494,0.062070106
 C,0,0.7885298295,0.3047650359,0.0157586998
 C,0,0.1265664487,0.0029408839,1.3148621186
 C,0,-1.2397537188,0.272673369,1.4875184773
 C,0,0.8450499446,-0.5306154548,2.3950684835
 C,0,-1.8637399863,0.0154417973,2.7044243986
 H,0,-1.8099823679,0.6899190695,0.6660849676
 C,0,0.2210242368,-0.769543883,3.6170433093
 H,0,1.8958685057,-0.771937382,2.2739436648
 C,0,-1.1369335168,-0.5017063998,3.7769222028
 H,0,-2.9207431277,0.2295753059,2.8180282995
 H,0,0.7955278441,-1.1801066783,4.4399085015
 H,0,-1.625081203,-0.6970116052,4.7247581518
 C,0,0.1412697647,0.1005558784,-1.309503851
 C,0,-0.6813979947,-1.0155690225,-1.5260302448
 C,0,0.3510942009,0.9932232884,-2.3710378269
```

```
C,0,-1.2734697524,-1.2283064481,-2.7672286979
H,0,-0.850850032,-1.7189640593,-0.7194755238
C,0,-0.2285415109,0.7669822363,-3.6170591417
H,0,0.9614848617,1.8767980447,-2.2166225326
C,0,-1.0467653112,-0.3422587841,-3.8205309935
H,0,-1.9069141534,-2.0960672929,-2.9147208366
H,0,-0.0513618727,1.4683077573,-4.4248171285
H,0,-1.5061056612,-0.5131390908,-4.7872948086
```

4+2_product (3) B3LYP/6-311+G(d,p)

```
E(RB+HF-LYP) = -809.023654094

 Zero-point correction=                           0.294164 (Hartree/Particle)
 Thermal correction to Energy=                    0.309421
 Thermal correction to Enthalpy=                  0.310365
 Thermal correction to Gibbs Free Energy=         0.249904
 Sum of electronic and zero-point Energies=           -808.729490
 Sum of electronic and thermal Energies=              -808.714233
 Sum of electronic and thermal Enthalpies=            -808.713289
 Sum of electronic and thermal Free Energies=         -808.773750

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 194.164             62.695            127.250

 C                      2.23655   1.03251   0.26239
 C                      2.95463   1.05467  -1.08929
 C                      3.68179  -0.06525  -1.17481
 C                      3.42124  -0.82501   0.11411
 C                      3.31192   0.31607   1.13098
 O                      2.00522  -1.27067   0.05669
 C                      1.24544  -0.12787   0.13541
 C                     -0.10294  -0.10845   0.0751
 H                      1.82099   1.96979   0.6141
 H                      2.78678   1.80026  -1.85504
 H                      4.23993  -0.43946  -2.02206
 H                      4.02147  -1.70079   0.34064
 H                      4.22721   0.89763   1.23371
 H                      2.9468   -0.01529   2.10518
 C                     -0.80539   1.20481   0.23985
 C                     -0.77493   1.90467   1.45309
 C                     -1.53379   1.75644  -0.82415
 C                     -1.42974   3.12844   1.59395
 H                     -0.24157   1.47752   2.29558
 C                     -2.18851   2.97766  -0.68682
 H                     -1.58154   1.22015  -1.76554
 C                     -2.13679   3.6706    0.52313
 H                     -1.39383   3.65232   2.54304
 H                     -2.73907   3.39017  -1.52534
 H                     -2.6483    4.62054   0.63078
 C                     -0.94631  -1.3144   -0.13145
 C                     -2.2601   -1.34172   0.37079
 C                     -0.49497  -2.44639  -0.83496
 C                     -3.0814   -2.45105   0.19065
 H                     -2.64132  -0.48357   0.91093
 C                     -1.32131  -3.5503   -1.02164
 H                      0.50838  -2.45879  -1.23576
```

C	-2.61782	-3.56345	-0.50853
H	-4.08709	-2.44364	0.59702
H	-0.94856	-4.40648	-1.57385
H	-3.25737	-4.42693	-0.65371

2+2_product (4) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -809.037029631

Zero-point correction=	0.292871 (Hartree/Particle)
Thermal correction to Energy=	0.308668
Thermal correction to Enthalpy=	0.309612
Thermal correction to Gibbs Free Energy=	0.248251
Sum of electronic and zero-point Energies=	-808.744159
Sum of electronic and thermal Energies=	-808.728361
Sum of electronic and thermal Enthalpies=	-808.727417
Sum of electronic and thermal Free Energies=	-808.788779

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	193.692	63.722	129.146

C	-2.21613	-1.28291	-0.30831
C	-1.54679	-0.05598	-1.01212
C	-2.50281	1.06134	-0.6757
C	-3.60888	0.62936	-0.06586
C	-3.63161	-0.86909	0.13965
C	-1.12101	-1.18515	0.75382
O	-1.01019	-1.65344	1.85364
C	-0.26194	-0.19493	-0.08468
H	-2.1691	-2.23068	-0.84799
H	-1.35101	-0.13519	-2.08135
H	-2.30011	2.09737	-0.91764
H	-4.42676	1.26871	0.24734
H	-4.41	-1.34505	-0.46768
H	-3.82587	-1.15164	1.17946
C	0.25548	1.06709	0.59591
C	0.64997	2.15885	-0.18847
C	0.3666	1.16706	1.98554
C	1.13361	3.3237	0.39923
H	0.58401	2.09736	-1.26961
C	0.85525	2.33444	2.57459
H	0.07345	0.33306	2.60991
C	1.23848	3.41614	1.78728
H	1.43187	4.15808	-0.22618
H	0.93367	2.39394	3.65465
H	1.61743	4.32178	2.24736
C	0.89933	-0.95892	-0.7397
C	1.22001	-0.80341	-2.09239
C	1.70541	-1.79539	0.04371
C	2.31522	-1.46422	-2.64785
H	0.62312	-0.15884	-2.7263
C	2.79622	-2.45928	-0.51163
H	1.47601	-1.92857	1.09446
C	3.10669	-2.29665	-1.86071
H	2.54687	-1.32657	-3.69833
H	3.40382	-3.10506	0.11256
H	3.95565	-2.81349	-2.29359

*Dichloroketene (5) B3LYP/6-311+G***

E(RB+HF-LYP) = -1071.86577745

Zero-point correction=	0.015348 (Hartree/Particle)
Thermal correction to Energy=	0.020444
Thermal correction to Enthalpy=	0.021388
Thermal correction to Gibbs Free Energy=	-0.014461
Sum of electronic and zero-point Energies=	-1071.850429
Sum of electronic and thermal Energies=	-1071.845334
Sum of electronic and thermal Enthalpies=	-1071.844390
Sum of electronic and thermal Free Energies=	-1071.880238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	12.829	15.502	75.450

C,0,1.2191733704,-0.530495457,-0.238176233
C,0,0.031956844,-0.0138994385,-0.0062107089
O,0,2.2673583232,-0.9865951669,-0.4429765691
Cl,0,-1.3039310837,-1.0487457937,0.4007556398
Cl,0,-0.2046364383,1.7051652472,-0.1060418631

*Dichloro 2+2 product (7) B3LYP/6-311+G***

E(RB+HF-LYP) = -1266.06746033

Zero-point correction=	0.112865 (Hartree/Particle)
Thermal correction to Energy=	0.121691
Thermal correction to Enthalpy=	0.122635
Thermal correction to Gibbs Free Energy=	0.078024
Sum of electronic and zero-point Energies=	-1265.954595
Sum of electronic and thermal Energies=	-1265.945770
Sum of electronic and thermal Enthalpies=	-1265.944825
Sum of electronic and thermal Free Energies=	-1265.989436

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.362	32.800	93.891

C,0,-0.654010508,-0.9183470763,-1.1389179576
C,0,-0.4081856958,0.616923146,-0.9113618511
C,0,-1.7473081631,1.0871424147,-0.4034490162
C,0,-2.682627932,0.1381025027,-0.4732043773
C,0,-2.1719772128,-1.1696949513,-1.0317142759
C,0,0.1479864839,-1.1899503091,0.1447482882
O,0,0.2652948709,-2.1140265094,0.8847554164
C,0,0.6583251301,0.2840768161,0.1817680739
Cl,0,2.336047775,0.3295180234,-0.5025790955
Cl,0,0.5960165448,1.1415291899,1.7422049369
H,0,-0.1781897632,-1.3588374795,-2.0156307243
H,0,-0.0083704222,1.214549007,-1.7304396378
H,0,-1.9056226006,2.0951205185,-0.0421414624
H,0,-3.716541346,0.2745880578,-0.1774510419
H,0,-2.6160536375,-1.3875482565,-2.0091464735
H,0,-2.3958872487,-2.0229776549,-0.3840865979

*Dichloro 4+2 product (8) B3LYP/6-311+G***

E(RB+HF-LYP) = -1266.04136382

Zero-point correction=	0.114392 (Hartree/Particle)
Thermal correction to Energy=	0.122663
Thermal correction to Enthalpy=	0.123607
Thermal correction to Gibbs Free Energy=	0.080066
Sum of electronic and zero-point Energies=	-1265.926972
Sum of electronic and thermal Energies=	-1265.918701
Sum of electronic and thermal Enthalpies=	-1265.917757
Sum of electronic and thermal Free Energies=	-1265.961298

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	76.972	31.694	91.640

C,0,1.3462101815,0.6080830145,0.5030762892
C,0,2.0699803074,0.8466159262,-0.8239276442
C,0,2.4535461752,-0.3483559259,-1.288221698
C,0,1.9705934025,-1.3666487684,-0.2718293808
C,0,2.1582263688,-0.6068237831,1.0454950749
O,0,0.481433556,-1.3785397439,-0.3635342177
C,0,0.0884093427,-0.1558889324,0.0977661218
C,0,-1.1892298028,0.228084495,0.1398366866
Cl,0,-1.6664443495,1.7961985444,0.7460567954
Cl,0,-2.4890548082,-0.7981670963,-0.3865759155
H,0,1.1864364511,1.4635073623,1.1506146616
H,0,2.132857145,1.8058660953,-1.3196206984
H,0,2.8999970022,-0.5819722448,-2.2446634483
H,0,2.2979112459,-2.3973650341,-0.3595378922
H,0,3.1953298196,-0.3526532638,1.2597037636
H,0,1.6930697183,-1.1059957365,1.8974296998

1st_TS (12) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -808.996933374

Zero-point correction=	0.289501 (Hartree/Particle)
Thermal correction to Energy=	0.305599
Thermal correction to Enthalpy=	0.306543
Thermal correction to Gibbs Free Energy=	0.244695
Sum of electronic and zero-point Energies=	-808.707432
Sum of electronic and thermal Energies=	-808.691334
Sum of electronic and thermal Enthalpies=	-808.690390
Sum of electronic and thermal Free Energies=	-808.752238

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.766	64.483	130.171

C	2.39279	-0.46087	0.32305
C	2.62612	-0.2816	-1.06207
C	3.23157	-1.4504	-1.60191
C	3.5091	-2.313	-0.58201
C	3.21519	-1.67074	0.73564
O	0.76676	-2.36958	-0.02763
C	0.70917	-1.15685	0.05113

C	-0.28168	-0.19277	0.04085
H	2.2768	0.38599	0.9854
H	2.3341	0.5926	-1.62559
H	3.3896	-1.63855	-2.65488
H	3.91443	-3.3106	-0.68945
H	4.15157	-1.3146	1.19011
H	2.7284	-2.33612	1.44746
C	-1.69353	-0.60299	0.16963
C	-2.09828	-1.95489	0.25414
C	-2.71497	0.37382	0.1934
C	-3.44276	-2.29855	0.33861
H	-1.35013	-2.7345	0.25425
C	-4.05705	0.02083	0.28014
H	-2.45459	1.42237	0.13333
C	-4.43502	-1.31866	0.35271
H	-3.71629	-3.34668	0.40007
H	-4.81139	0.80051	0.2908
H	-5.48133	-1.59372	0.42324
C	0.01944	1.27321	0.05623
C	0.10809	2.00656	-1.13472
C	0.15738	1.96732	1.26771
C	0.3577	3.37891	-1.11986
H	-0.0364	1.49242	-2.07898
C	0.41319	3.33727	1.28778
H	0.05739	1.42225	2.2005
C	0.51792	4.04751	0.09233
H	0.42168	3.92531	-2.05465
H	0.52315	3.85127	2.23653
H	0.71266	5.11406	0.10622

intermediate (13) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -808.997346724

Zero-point correction=	0.290461 (Hartree/Particle)
Thermal correction to Energy=	0.306829
Thermal correction to Enthalpy=	0.307773
Thermal correction to Gibbs Free Energy=	0.245137
Sum of electronic and zero-point Energies=	-808.706886
Sum of electronic and thermal Energies=	-808.690518
Sum of electronic and thermal Enthalpies=	-808.689574
Sum of electronic and thermal Free Energies=	-808.752209

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.538	65.603	131.828

C,0,2.348609125,-0.4702339976,0.3122869279
C,0,2.5182559069,-0.3362326343,-1.1202327449
C,0,3.0541659594,-1.5312816086,-1.6420224845
C,0,3.3794625109,-2.3627445362,-0.600391327
C,0,3.2469921814,-1.6433646405,0.703427476
O,0,0.7927762407,-2.3469135278,0.1987503705
C,0,0.7989783752,-1.1121614429,0.1961799519
C,0,-0.2402229718,-0.1799552493,0.0835722166
H,0,2.3592771104,0.4246722979,0.9228563234
H,0,2.2005174545,0.5211121033,-1.6948268823
H,0,3.1277110468,-1.7757924609,-2.6928114143

```
H,0,3.739215765,-3.3790923334,-0.696018443
H,0,4.2289836614,-1.2546319183,1.0099815093
H,0,2.8548148451,-2.2632040485,1.5074747457
C,0,-1.6462408214,-0.5983209656,0.160863647
C,0,-2.0427443859,-1.953466689,0.2687379818
C,0,-2.6795333744,0.3676142323,0.1007445999
C,0,-3.3862104288,-2.3092180248,0.2802880808
H,0,-1.2838379201,-2.7177218108,0.3463650289
C,0,-4.0197293127,0.0021673095,0.1184554739
H,0,-2.4273088583,1.4172822046,0.0290825177
C,0,-4.3866825609,-1.3403271923,0.204940749
H,0,-3.6537129223,-3.357618261,0.3600115841
H,0,-4.7819765168,0.7722657757,0.0657084546
H,0,-5.4326612981,-1.6252905738,0.2228075048
C,0,0.0373184871,1.2928373323,0.093453927
C,0,0.0579436347,2.03689338,-1.0943183812
C,0,0.2259040052,1.979371184,1.302205196
C,0,0.2867512816,3.4124876065,-1.0795660348
H,0,-0.1227471414,1.5286633218,-2.0356208035
C,0,0.4635269814,3.3528260691,1.3212205204
H,0,0.1797644233,1.4264112758,2.2345458134
C,0,0.4972579883,4.0743897911,0.1288395671
H,0,0.2974289008,3.966645529,-2.011907125
H,0,0.6126546623,3.8603700017,2.2681106792
H,0,0.6768513748,5.1435575768,0.1421254848
```

2ndTS giving 4+2 (14) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -808.996569616

Zero-point correction=	0.290922 (Hartree/Particle)
Thermal correction to Energy=	0.306331
Thermal correction to Enthalpy=	0.307275
Thermal correction to Gibbs Free Energy=	0.246742
Sum of electronic and zero-point Energies=	-808.705647
Sum of electronic and thermal Energies=	-808.690239
Sum of electronic and thermal Enthalpies=	-808.689295
Sum of electronic and thermal Free Energies=	-808.749828

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.225	62.984	127.402

C	2.18559	0.83709	-2.78727
C	1.54872	1.16099	-1.43001
C	2.66782	1.05276	-0.48892
C	3.63404	0.21359	-1.03196
C	3.23726	-0.11921	-2.32445
C	0.81872	-0.25105	-1.03186
C	-0.15662	-0.22671	-0.04516
O	1.29482	-1.21494	-1.68356
H	0.89303	2.02036	-1.34606
H	2.65565	1.44957	0.51639
H	4.4697	-0.21874	-0.4995
H	3.72221	-0.84679	-2.96141
H	2.65828	1.74218	-3.19173
H	1.50217	0.42682	-3.52659
C	-0.54043	1.07377	0.59493

C	-1.53959	1.88221	0.03307
C	0.05914	1.50199	1.78688
C	-1.9027	3.09178	0.62261
H	-2.0324	1.55382	-0.87586
C	-0.30575	2.70879	2.38426
H	0.80794	0.87136	2.25407
C	-1.28407	3.51089	1.80004
H	-2.67269	3.70415	0.16584
H	0.17189	3.01944	3.30725
H	-1.56805	4.44992	2.26182
C	-0.95006	-1.41639	0.29933
C	-1.89106	-1.3595	1.35321
C	-0.80642	-2.65605	-0.36583
C	-2.62321	-2.47728	1.73568
H	-2.0415	-0.42941	1.88578
C	-1.5399	-3.77036	0.02606
H	-0.11604	-2.73151	-1.19307
C	-2.45268	-3.69466	1.07772
H	-3.33176	-2.39535	2.55311
H	-1.40295	-4.70653	-0.50498
H	-3.02683	-4.56566	1.37324

2ndTS giving 2+2 (15) B3LYP/6-311+G(d,p)

E(RB+HF-LYP) = -808.995562396

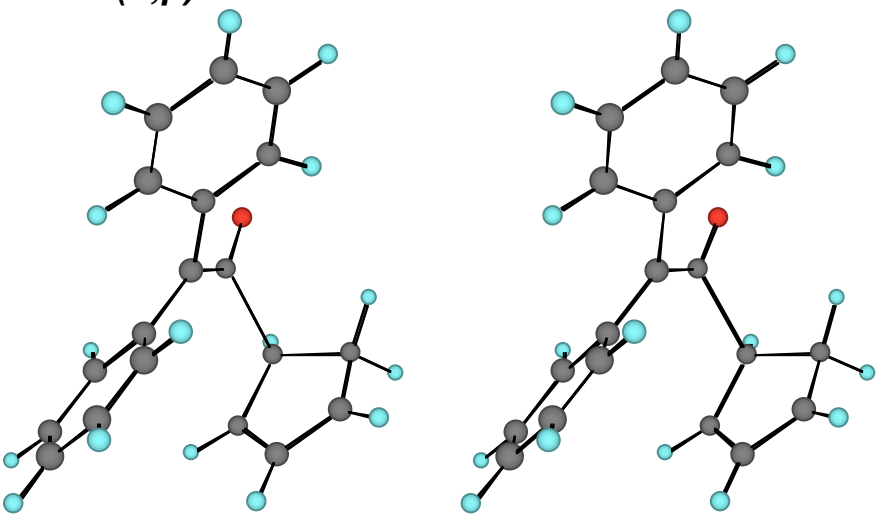
Zero-point correction=	0.290869 (Hartree/Particle)
Thermal correction to Energy=	0.306200
Thermal correction to Enthalpy=	0.307144
Thermal correction to Gibbs Free Energy=	0.247677
Sum of electronic and zero-point Energies=	-808.704693
Sum of electronic and thermal Energies=	-808.689362
Sum of electronic and thermal Enthalpies=	-808.688418
Sum of electronic and thermal Free Energies=	-808.747885

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	192.144	63.162	125.160

C	-1.31425	1.66116	-1.23742
C	-1.5131	1.79351	0.23066
C	-2.89633	1.64371	0.51083
C	-3.60195	1.60878	-0.65711
C	-2.71023	1.86731	-1.8387
O	-1.92552	-0.66756	-1.48503
C	-1.05599	0.1042	-1.0812
C	0.02444	-0.22448	-0.18117
H	-0.50395	2.22679	-1.68298
H	-0.74785	2.05672	0.94282
H	-3.31682	1.54613	1.50302
H	-4.6717	1.45918	-0.73521
H	-2.83363	2.9024	-2.18495
H	-2.91299	1.19847	-2.67562
C	1.22532	0.65202	-0.11577
C	1.8711	1.08067	-1.28659
C	1.77247	1.04927	1.11713
C	3.00258	1.89268	-1.22967
H	1.49225	0.7545	-2.24895

C	2.90073	1.86126	1.17538
H	1.30064	0.71674	2.03549
C	3.52027	2.29059	0.00092
H	3.48533	2.20478	-2.14935
H	3.29756	2.16039	2.13936
H	4.40044	2.92181	0.04624
C	0.12236	-1.56406	0.42206
C	1.36999	-2.11196	0.78694
C	-1.03109	-2.33228	0.70037
C	1.46241	-3.35304	1.40956
H	2.27799	-1.56449	0.56985
C	-0.93448	-3.56215	1.3352
H	-1.99821	-1.957	0.39889
C	0.31128	-4.08375	1.69334
H	2.43769	-3.75026	1.66895
H	-1.83723	-4.12544	1.54525
H	0.38138	-5.05073	2.17891

Another diphenyl TS giving 2+2 directly (Similar to 10) B3LYP/6-311+G(d,p)



key distances 1.819 3.171
E(RB+HF-LYP) = -808.979959514

Zero-point correction=	0.288934 (Hartree/Particle)
Thermal correction to Energy=	0.305182
Thermal correction to Enthalpy=	0.306126
Thermal correction to Gibbs Free Energy=	0.243655
Sum of electronic and zero-point Energies=	-808.691026
Sum of electronic and thermal Energies=	-808.674778
Sum of electronic and thermal Enthalpies=	-808.673834
Sum of electronic and thermal Free Energies=	-808.736305

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	191.504	64.691	131.481

C	0	-2.25313	-1.19327	-0.92742
C	0	-2.73596	0.14719	-0.98958
C	0	-2.99863	0.63001	0.32238

C	0	-2.86963	-0.39902	1.20953
C	0	-2.6104	-1.68177	0.48368
C	0	-0.4449	-1.38383	-0.96552
O	0	-0.20165	-2.48858	-1.38757
C	0	0.32905	-0.37419	-0.36451
H	0	-2.4801	-1.84309	-1.76565
H	0	-2.91594	0.70144	-1.89803
H	0	-3.24948	1.65291	0.5682
H	0	-2.99	-0.32581	2.28294
H	0	-3.54234	-2.26699	0.43563
H	0	-1.86584	-2.32438	0.95584
C	0	0.04833	1.04086	-0.56112
C	0	-0.40257	1.52213	-1.80786
C	0	0.22815	1.99493	0.47004
C	0	-0.67108	2.88003	-2.01478
H	0	-0.47134	0.83488	-2.64268
C	0	-0.03972	3.33629	0.26433
H	0	0.55966	1.65717	1.44446
C	0	-0.49486	3.79079	-0.98378
H	0	-1.00104	3.21817	-2.99124
H	0	0.09439	4.04111	1.07793
H	0	-0.69608	4.84448	-1.14067
C	0	1.48746	-0.82479	0.43844
C	0	2.626	-0.00447	0.58355
C	0	1.52806	-2.09017	1.05752
C	0	3.73069	-0.42091	1.31932
H	0	2.65396	0.9596	0.09194
C	0	2.63374	-2.50347	1.79153
H	0	0.68664	-2.76393	0.95729
C	0	3.7437	-1.67141	1.93481
H	0	4.5926	0.23314	1.39885
H	0	2.62686	-3.48392	2.25565
H	0	4.60558	-1.99568	2.50664

*Dichloro 1st TS (18) B3LYP/6-311+G***

E(RB+HF-LYP) = -1266.01031300

Zero-point correction=	0.109325 (Hartree/Particle)
Thermal correction to Energy=	0.118762
Thermal correction to Enthalpy=	0.119706
Thermal correction to Gibbs Free Energy=	0.073569
Sum of electronic and zero-point Energies=	-1265.900988
Sum of electronic and thermal Energies=	-1265.891551
Sum of electronic and thermal Enthalpies=	-1265.890607
Sum of electronic and thermal Free Energies=	-1265.936744

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.524	34.046	97.104

C,0,-1.2782758451,0.6926999196,-0.6774922699
C,0,-1.5094690428,0.9938290558,0.6652992614
C,0,-2.5819145263,0.1830160888,1.1653599889
C,0,-3.081593513,-0.5611795607,0.1445302342
C,0,-2.4058819717,-0.1982471289,-1.140537088
O,0,-0.4218245253,-1.7351234311,-0.013621801
C,0,0.0930236246,-0.6540397981,-0.0894965425

```
C,0,1.2953422759,-0.0425313781,0.0381294607
Cl,0,1.6277059042,1.663803606,-0.1065728606
Cl,0,2.7122667907,-1.0635836552,0.1448372494
H,0,-0.719599561,1.3275088519,-1.3498618282
H,0,-0.9422692802,1.7074135412,1.2467984208
H,0,-2.8944508633,0.1426527876,2.1993850558
H,0,-3.8611629939,-1.3070870399,0.2238908488
H,0,-3.0841935895,0.39139415,-1.7743143439
H,0,-2.0906493328,-1.0659171971,-1.7221766246
```

*Dichloro intermediate (19) B3LYP/6-311+G***

```
E(RB+HF-LYP) = -1266.01503050

 Zero-point correction=                           0.110898 (Hartree/Particle)
 Thermal correction to Energy=                    0.120240
 Thermal correction to Enthalpy=                  0.121184
 Thermal correction to Gibbs Free Energy=         0.075104
 Sum of electronic and zero-point Energies=          -1265.904132
 Sum of electronic and thermal Energies=             -1265.894790
 Sum of electronic and thermal Enthalpies=           -1265.893846
 Sum of electronic and thermal Free Energies=        -1265.939927

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  75.452             34.261             96.985

 C,0,-1.1266404498,0.5711967497,-0.7794288239
 C,0,-1.3720861117,0.9585257614,0.6165232493
 C,0,-2.4116234949,0.162270245,1.1404959139
 C,0,-2.9535856815,-0.5907218887,0.1319239299
 C,0,-2.384241071,-0.1965966475,-1.1948992102
 O,0,-0.3684405195,-1.7056662064,-0.3432953428
 C,0,-0.024185242,-0.5261540547,-0.3680691943
 C,0,1.1812263585,0.0124135167,0.1214615581
 Cl,0,1.6954611753,1.6554623031,-0.1993972249
 Cl,0,2.4644525493,-1.0635240553,0.5617366361
 H,0,-0.7398712266,1.3240776502,-1.4596033109
 H,0,-0.8049924444,1.7022551086,1.1560574186
 H,0,-2.6925512828,0.1170170397,2.1836701707
 H,0,-3.7242072792,-1.340788928,0.2564606397
 H,0,-3.0784751493,0.480517892,-1.7117016678
 H,0,-2.1840976252,-1.0463014166,-1.8463350347
```

*2ndTS Dichloro 2+2 side (21) B3LYP/6-311+G***

```
E(RB+HF-LYP) = -1266.01468729

 Zero-point correction=                           0.110994 (Hartree/Particle)
 Thermal correction to Energy=                    0.119418
 Thermal correction to Enthalpy=                  0.120362
 Thermal correction to Gibbs Free Energy=         0.076872
 Sum of electronic and zero-point Energies=          -1265.903693
 Sum of electronic and thermal Energies=             -1265.895269
 Sum of electronic and thermal Enthalpies=           -1265.894325
 Sum of electronic and thermal Free Energies=        -1265.937815

                    E (Thermal)             CV                S
```

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	74.936	32.136	91.532

C,0,-1.1417738837,0.5742135658,-0.8214741734
C,0,-1.2184048206,0.8812960054,0.6304957426
C,0,-2.2229156485,0.062979271,1.2108608796
C,0,-2.9002407195,-0.5973112703,0.2283268933
C,0,-2.4525601482,-0.1567475363,-1.1352649253
O,0,-0.2793057082,-1.7019540563,-0.6520427613
C,0,-0.0205929922,-0.5107281174,-0.5694652408
C,0,1.1074937606,0.0431273857,0.1195750868
Cl,0,1.7026504866,1.6570316426,-0.2357867526
Cl,0,2.3228011326,-1.0332981518,0.7254844151
H,0,-0.8419185353,1.3745804859,-1.4918420186
H,0,-0.667179068,1.6602208202,1.1331098994
H,0,-2.3973444872,-0.0354746077,2.27358485
H,0,-3.6907580991,-1.3187372247,0.3929390943
H,0,-3.1844642044,0.5388371453,-1.566281201
H,0,-2.3226007524,-0.9882393366,-1.8283543721

*2ndTS dichloro 4+2 side (20) B3LYP/6-311+G***

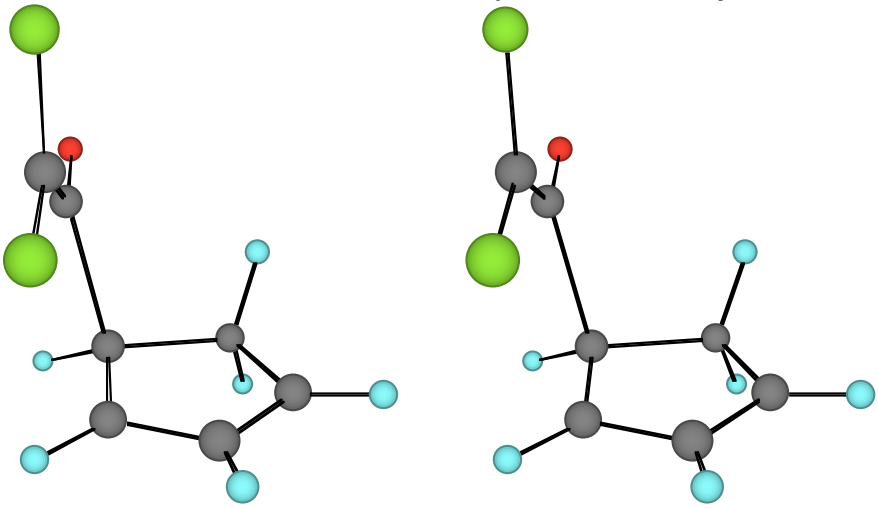
E(RB+HF-LYP) = -1266.01342260

Zero-point correction=	0.111226 (Hartree/Particle)
Thermal correction to Energy=	0.119674
Thermal correction to Enthalpy=	0.120618
Thermal correction to Gibbs Free Energy=	0.076687
Sum of electronic and zero-point Energies=	-1265.902197
Sum of electronic and thermal Energies=	-1265.893749
Sum of electronic and thermal Enthalpies=	-1265.892805
Sum of electronic and thermal Free Energies=	-1265.936736

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	75.096	31.887	92.461

C,0,2.3633662244,0.1256471148,-1.108538549
C,0,1.1368759879,0.8413240722,-0.5277287989
C,0,1.4702872574,0.996072669,0.9021925666
C,0,2.3915947419,0.0200423544,1.252321532
C,0,2.7446105558,-0.6761002577,0.0950285697
C,0,0.0978545581,-0.3656443765,-0.3187818373
C,0,-1.2014704567,-0.0497991396,-0.0002755789
O,0,0.6298719652,-1.5030603935,-0.3467466079
Cl,0,-2.3940237241,-1.2967849312,0.1782208554
Cl,0,-1.845275756,1.5762179636,-0.09054857
H,0,0.7286848634,1.6968235565,-1.055218488
H,0,0.9498239275,1.6615780906,1.577302624
H,0,2.6706560698,-0.2540443681,2.2599465646
H,0,3.3516724772,-1.5708056962,0.0637277321
H,0,3.1467477057,0.8613681558,-1.3320617494
H,0,2.162817182,-0.4700527597,-1.9954600952

*Dichloro alternative 2+2 TS (similar to 10) B3LYP/6-311+G***



key distances 1.833 3.095
E(RB+HF-LYP) = -1265.99133839

Zero-point correction=	0.108954 (Hartree/Particle)
Thermal correction to Energy=	0.118501
Thermal correction to Enthalpy=	0.119445
Thermal correction to Gibbs Free Energy=	0.072361
Sum of electronic and zero-point Energies=	-1265.882385
Sum of electronic and thermal Energies=	-1265.872838
Sum of electronic and thermal Enthalpies=	-1265.871893
Sum of electronic and thermal Free Energies=	-1265.918977

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	74.360	33.888	99.096

C,0,-0.3538215519,-0.5224110099,-1.5766208318
C,0,-1.3477456012,0.480358426,-1.4742593714
C,0,-2.5480355193,-0.0480008508,-0.9158554245
C,0,-2.4077495604,-1.3970843274,-0.7853109604
C,0,-1.0758667113,-1.8409288118,-1.286687916
C,0,0.9870986323,-0.4756855008,-0.3283587312
O,0,1.7457291597,-1.3961466242,-0.5510276032
C,0,0.911997983,0.4811660692,0.6404861941
Cl,0,-0.1827206086,1.8351273554,0.7273782524
Cl,0,1.9633380907,0.3131969399,2.0294153999
H,0,0.3176577281,-0.46034224,-2.4278473794
H,0,-1.2314683791,1.4961446713,-1.8237951909
H,0,-3.4194387698,0.5343823123,-0.6503099492
H,0,-3.1516693032,-2.0706658619,-0.3782229531
H,0,-1.2002294321,-2.4123768332,-2.2186202008
H,0,-0.5464483443,-2.5039660427,-0.5988333434

*MP2/6-311+G** Single Point Energies of Selected B3LYP/6-311+G** Structures*

1 MP2=-193.5407574
2 MP2=-613.0664258

3 MP2=-806.6354869
4 MP2=-806.6534785
5 MP2=-1070.3191294
7 MP2=-1263.9340279
8 MP2=-1263.904964

*Cyclopentadiene (1) BPW91/6-311+G***

E(RB-PW91) = -194.124726721

Zero-point correction=	0.089799 (Hartree/Particle)
Thermal correction to Energy=	0.094069
Thermal correction to Enthalpy=	0.095013
Thermal correction to Gibbs Free Energy=	0.063141
Sum of electronic and zero-point Energies=	-194.034928
Sum of electronic and thermal Energies=	-194.030658
Sum of electronic and thermal Enthalpies=	-194.029714
Sum of electronic and thermal Free Energies=	-194.061585

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	59.029	16.286	67.079

C,0,0.286107462,-0.1520561786,-1.1733662859
C,0,-0.6462520581,0.8623395552,-0.5655369773
C,0,-0.6766851618,0.681783033,0.7793302264
C,0,0.208814538,-0.4330459106,1.1397317785
C,0,0.7803983285,-0.9337443106,0.0150720495
H,0,-1.1940788268,1.6083194681,-1.1383362816
H,0,-1.2600185936,1.2626881998,1.493196144
H,0,0.3702079822,-0.7896019126,2.1566645326
H,0,1.4833867737,-1.7622643899,-0.0486922208
H,0,1.1147075053,0.3273914338,-1.7261900036
H,0,-0.228503492,-0.7981899299,-1.9080269182

*Diphenylketene (2) BPW91/6-311+G***

E(RB-PW91) = -614.791014352

Zero-point correction=	0.190158 (Hartree/Particle)
Thermal correction to Energy=	0.202498
Thermal correction to Enthalpy=	0.203442
Thermal correction to Gibbs Free Energy=	0.149675
Sum of electronic and zero-point Energies=	-614.600856
Sum of electronic and thermal Energies=	-614.588517
Sum of electronic and thermal Enthalpies=	-614.587572
Sum of electronic and thermal Free Energies=	-614.641339

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	127.069	48.119	113.162

C,0,2.0334594686,0.786037937,0.0406200854
O,0,3.1277858934,1.2090397549,0.0624639302
C,0,0.7904724794,0.3055610175,0.0158037996
C,0,0.129699988,0.001579188,1.3158751972

```
C,0,-1.2459069554,0.2637780239,1.4841265298
C,0,0.8528410405,-0.525997641,2.4052692487
C,0,-1.8740559543,0.0019310708,2.7046935617
H,0,-1.8183712879,0.6801141919,0.6544235232
C,0,0.2235168187,-0.7671746896,3.6304855666
H,0,1.9124274427,-0.7615996523,2.2859368438
C,0,-1.1435339254,-0.5091414606,3.7856721832
H,0,-2.9400085358,0.2094878229,2.8148341418
H,0,0.802051008,-1.1740861394,4.4616722694
H,0,-1.6365340413,-0.7076602182,4.7383750196
C,0,0.1426962857,0.1037206235,-1.3104226259
C,0,-0.692113938,-1.013101083,-1.5229109791
C,0,0.3603657952,0.9951465366,-2.3809473028
C,0,-1.2901955622,-1.2252568633,-2.7679833041
H,0,-0.864171329,-1.7173697189,-0.7081344648
C,0,-0.224522272,0.7669674639,-3.6304334803
H,0,0.9811308932,1.8804267918,-2.2279748605
C,0,-1.056262705,-0.3411929349,-3.8296244734
H,0,-1.9348461696,-2.0941904672,-2.9123627882
H,0,-0.0415850297,1.4683651783,-4.4463532377
H,0,-1.5211434801,-0.512948961,-4.8014719277
```

*Diphenyl 4+2 product (3) BPW91/6-311+G***

E(RB-PW91) = -808.916083578

Zero-point correction=	0.286531 (Hartree/Particle)
Thermal correction to Energy=	0.302299
Thermal correction to Enthalpy=	0.303243
Thermal correction to Gibbs Free Energy=	0.241663
Sum of electronic and zero-point Energies=	-808.629552
Sum of electronic and thermal Energies=	-808.613784
Sum of electronic and thermal Enthalpies=	-808.612840
Sum of electronic and thermal Free Energies=	-808.674421

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	189.696	65.079	129.607

```
C,0,-2.4514198272,0.3535784706,-0.1417008036
C,0,-3.0957589182,-0.0757089729,1.1797538416
C,0,-3.4719103749,-1.3629821215,1.0440098993
C,0,-3.0513745244,-1.7665779657,-0.3576149313
C,0,-3.3036267227,-0.4771210752,-1.1496399891
O,0,-1.5475756497,-1.7901552848,-0.3522718338
C,0,-1.1613794481,-0.4763788898,-0.2006353075
C,0,0.1342763788,-0.0676476879,-0.0920800537
H,0,-2.331652188,1.4247470366,-0.3110515574
H,0,-3.1106109539,0.5363478357,2.0799687182
H,0,-3.8617501636,-2.0360977539,1.8050335189
H,0,-3.3762576969,-2.7304533152,-0.7569372516
H,0,-4.3566961049,-0.1721711995,-1.1622612502
H,0,-2.8889458542,-0.5090618676,-2.1664456727
C,0,0.4027415815,1.4051050595,-0.0070766291
C,0,0.1231620163,2.2677417269,-1.0846649688
C,0,0.9653543562,1.959999442,1.160091599
C,0,0.3716817422,3.6432686265,-0.9913050445
H,0,-0.280818587,1.8480671299,-2.008210861
```

```
C,0,1.2148449395,3.3327578863,1.2552229054
H,0,1.2024241075,1.3027179734,1.9986604945
C,0,0.9157359854,4.1811269493,0.1804786235
H,0,0.1486239126,4.2932879155,-1.8396692828
H,0,1.642119506,3.7429507276,2.172302923
H,0,1.1119362921,5.252118891,0.2545604787
C,0,1.305181793,-0.9796196238,-0.0706905278
C,0,2.5710017467,-0.5027800868,-0.4848547724
C,0,1.2263947283,-2.3221366265,0.3687592164
C,0,3.6995644244,-1.3270230863,-0.4717169843
H,0,2.6667589031,0.5286464029,-0.8258338065
C,0,2.3588506403,-3.1400169134,0.3899905086
H,0,0.2699395177,-2.7225444639,0.697646
C,0,3.6023829904,-2.6524935009,-0.0325927143
H,0,4.6599056437,-0.9295019276,-0.806103752
H,0,2.2682381122,-4.1696631388,0.7422049786
H,0,4.4831697055,-3.2966976303,-0.018092211
```

*Diphenyl 2+2 product (4) BPW91/6-311+G***

```
E(RB-PW91) = -808.927937172

 Zero-point correction=                           0.285170 (Hartree/Particle)
 Thermal correction to Energy=                    0.301487
 Thermal correction to Enthalpy=                  0.302431
 Thermal correction to Gibbs Free Energy=         0.240060
 Sum of electronic and zero-point Energies=           -808.642767
 Sum of electronic and thermal Energies=              -808.626451
 Sum of electronic and thermal Enthalpies=            -808.625506
 Sum of electronic and thermal Free Energies=         -808.687877

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 189.186             66.041            131.270

 C,0,-2.2221330212,-1.280010878,-0.3287015579
 C,0,-1.5525911186,-0.0385455789,-1.0135207256
 C,0,-2.5072162734,1.0735940591,-0.6518870393
 C,0,-3.6209913372,0.6252087862,-0.0481144243
 C,0,-3.6438601123,-0.8790342736,0.120499875
 C,0,-1.1271825891,-1.1920390365,0.7427685779
 O,0,-1.0189268612,-1.6737513712,1.8477480069
 C,0,-0.2632174177,-0.189083866,-0.0891121444
 H,0,-2.1668531917,-2.2257638283,-0.8852555105
 H,0,-1.3578809628,-0.0973176904,-2.0921496334
 H,0,-2.3025333451,2.1210929342,-0.8732270538
 H,0,-4.4448093536,1.2613572374,0.2801224221
 H,0,-4.4239125591,-1.3444901762,-0.5057271555
 H,0,-3.8460190701,-1.1902806517,1.1579589475
 C,0,0.2603380218,1.068549888,0.5987415203
 C,0,0.6810354429,2.1585371515,-0.1862929171
 C,0,0.3487060323,1.1719022422,1.9963427993
 C,0,1.1662269725,3.3261451229,0.4095168705
 H,0,0.6347239761,2.091164207,-1.2751906747
 C,0,0.8397240213,2.3414635371,2.5925613294
 H,0,0.0346569782,0.335665124,2.6202521048
 C,0,1.2479749206,3.4222216376,1.8049515793
 H,0,1.4856707071,4.1609995613,-0.2171438841
```

```
H,0,0.9003374352,2.4042901477,3.6806980762
H,0,1.6297509484,4.3316455856,2.2718822578
C,0,0.8980516472,-0.9549024134,-0.7461370069
C,0,1.1887935644,-0.8453299012,-2.1165185102
C,0,1.7373752627,-1.7526802384,0.0549068571
C,0,2.2885474084,-1.5119349411,-2.6717839364
H,0,0.5640441335,-0.2301451866,-2.7651544783
C,0,2.8315022193,-2.4226926979,-0.5006806515
H,0,1.5282828566,-1.8493916801,1.1211166896
C,0,3.1130793361,-2.3050949927,-1.8673696316
H,0,2.4980548194,-1.4091195789,-3.7381231816
H,0,3.4659448562,-3.0395912485,0.1381888641
H,0,3.9669787809,-2.8277454276,-2.3012570262
```

*Dichloroketene (5) BPW91/6-311+G***

E(RB-PW91) = -1071.85872604

```
 Zero-point correction=                           0.014826 (Hartree/Particle)
 Thermal correction to Energy=                    0.020019
 Thermal correction to Enthalpy=                  0.020963
 Thermal correction to Gibbs Free Energy=        -0.015091
 Sum of electronic and zero-point Energies=          -1071.843900
 Sum of electronic and thermal Energies=             -1071.838707
 Sum of electronic and thermal Enthalpies=           -1071.837763
 Sum of electronic and thermal Free Energies=        -1071.873817

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  12.562             15.766            75.882

 C,0,1.2209785127,-0.5312814801,-0.2385305788
 C,0,0.0259977729,-0.0113062491,-0.0050455784
 O,0,2.2799073081,-0.9920560865,-0.4454320662
 Cl,0,-1.3074022163,-1.0509147185,0.4017672612
 Cl,0,-0.2056046178,1.7092661931,-0.1061841158
```

*Dichloro 2+2 product (7) BPW91/6-311+G***

E(RB-PW91) = -1266.03060275

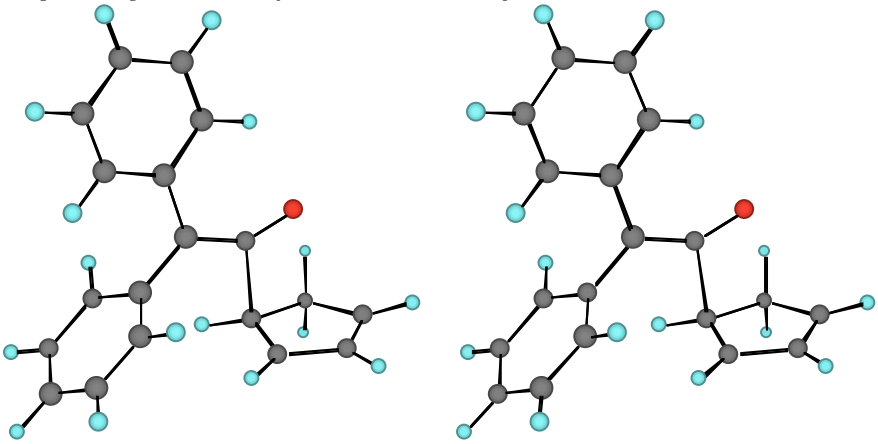
```
 Zero-point correction=                           0.109698 (Hartree/Particle)
 Thermal correction to Energy=                    0.118768
 Thermal correction to Enthalpy=                  0.119713
 Thermal correction to Gibbs Free Energy=         0.074597
 Sum of electronic and zero-point Energies=         -1265.920905
 Sum of electronic and thermal Energies=            -1265.911834
 Sum of electronic and thermal Enthalpies=          -1265.910890
 Sum of electronic and thermal Free Energies=       -1265.956006

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  74.528             33.815            94.954

 C,0,-0.6551080206,-0.9181013112,-1.1401989059
 C,0,-0.4095998161,0.6199882541,-0.9132485414
 C,0,-1.7484623263,1.0888405326,-0.3995266198
 C,0,-2.6886664551,0.1319198043,-0.4697656335
```

```
C,0,-2.1759026035,-1.1723234732,-1.0366773382
C,0,0.1445668529,-1.1931828909,0.1517806709
O,0,0.2577277913,-2.1263046993,0.8969625682
C,0,0.6591308374,0.2884351909,0.1845827552
Cl,0,2.3405998835,0.3161968035,-0.5087724854
Cl,0,0.6019044719,1.1620170937,1.7405164957
H,0,-0.1726159619,-1.3618931843,-2.02039432
H,0,-0.0070175285,1.2228747663,-1.736965218
H,0,-1.9082696364,2.1027730843,-0.0347830843
H,0,-3.729118008,0.2669907644,-0.170496239
H,0,-2.6219622248,-1.3868656333,-2.0220957289
H,0,-2.4011638251,-2.0365350957,-0.3922924546
```

*Dichloro 4+2 product (8) BPW91/6-311+G***

```
E(RB-PW91) = -1266.00510846

 Zero-point correction=                           0.111261 (Hartree/Particle)
 Thermal correction to Energy=                    0.119770
 Thermal correction to Enthalpy=                  0.120714
 Thermal correction to Gibbs Free Energy=         0.076718
 Sum of electronic and zero-point Energies=          -1265.893848
 Sum of electronic and thermal Energies=             -1265.885339
 Sum of electronic and thermal Enthalpies=           -1265.884395
 Sum of electronic and thermal Free Energies=        -1265.928390

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  75.157             32.738            92.597

 C,0,1.350153317,0.6037700555,0.5122296676
 C,0,2.0663788392,0.8474538585,-0.8186323727
 C,0,2.4578752108,-0.3546715414,-1.2870580412
 C,0,1.9847324843,-1.3724729205,-0.2666007144
 C,0,2.1662596051,-0.6121856132,1.0532184652
 O,0,0.4784489613,-1.3933697046,-0.3610568664
 C,0,0.0911949925,-0.1623504753,0.1016222314
 C,0,-1.1956640094,0.233456015,0.1344066189
 Cl,0,-1.6652948604,1.8024202289,0.745571284
 Cl,0,-2.4973893436,-0.7881096502,-0.3984032299
 H,0,1.1865619271,1.4624530666,1.1665009081
 H,0,2.1111634806,1.8110283529,-1.3229269869
 H,0,2.8935716647,-0.5892692731,-2.2559287826
 H,0,2.3116270032,-2.4109142256,-0.3545018038
 H,0,3.2091541738,-0.3511181768,1.2679275518
 H,0,1.7003788913,-1.1164982164,1.9104119977
```

*Diphenyl1stTS (Similar to 12) BPW91/6-311+G***



key distances OC 2.886 CC 2.008 CC 3.191
E(RB-PW91) = -808.894967419

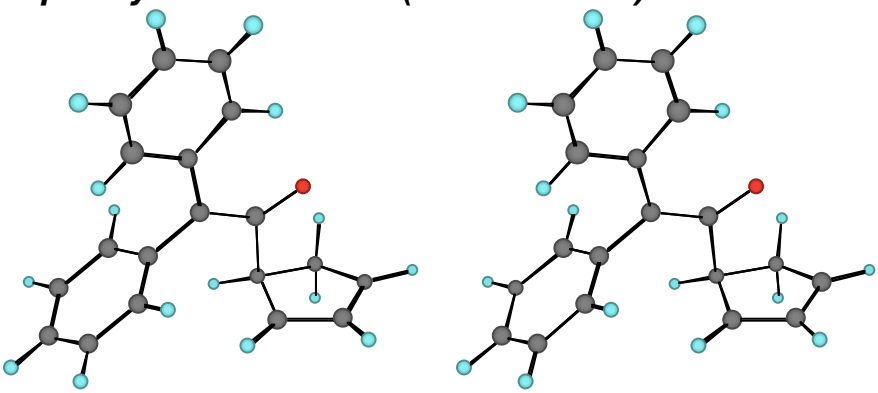
Zero-point correction=	0.281871 (Hartree/Particle)
Thermal correction to Energy=	0.298637
Thermal correction to Enthalpy=	0.299581
Thermal correction to Gibbs Free Energy=	0.236388
Sum of electronic and zero-point Energies=	-808.613096
Sum of electronic and thermal Energies=	-808.596331
Sum of electronic and thermal Enthalpies=	-808.595386
Sum of electronic and thermal Free Energies=	-808.658579

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.397	67.114	133.000

C,0,2.4627365444,-0.4353235968,0.3351770798
C,0,2.6910509675,-0.2449924589,-1.0377193605
C,0,3.335586923,-1.40577755,-1.58443707
C,0,3.6111743906,-2.2803090012,-0.5687034232
C,0,3.235323068,-1.6709284978,0.7477016835
O,0,0.7581687522,-2.3952299299,-0.147133484
C,0,0.6411289121,-1.1938985753,-0.0365475223
C,0,-0.3196698817,-0.2045988209,0.0186214736
H,0,2.247412275,0.3793254332,1.0225272572
H,0,2.3940243872,0.6367407536,-1.6007474341
H,0,3.5297718437,-1.5708281408,-2.6425371123
H,0,4.0540989839,-3.2692070914,-0.6756261009
H,0,4.145510454,-1.3473293434,1.2890536685
H,0,2.6929066302,-2.3572709149,1.4110379937
C,0,-1.7344413564,-0.6091467511,0.1753140486
C,0,-2.1504986778,-1.9635096702,0.2506817648
C,0,-2.7485164625,0.3819151899,0.2396594478
C,0,-3.5003600711,-2.2982503226,0.370571634
H,0,-1.4065704635,-2.7578059303,0.2150993377
C,0,-4.0966622168,0.0374217345,0.3607665181
H,0,-2.4740825629,1.4349122655,0.1833142504
C,0,-4.4872341067,-1.3050916888,0.4277661483
H,0,-3.7832657699,-3.3515972884,0.424798452
H,0,-4.8475578076,0.829212653,0.4019888247
H,0,-5.5403251001,-1.5734037745,0.5252528793
C,0,0.0024391886,1.2567410015,0.0370792622

```
C,0,0.1257983892,1.988428077,-1.1596835669
C,0,0.1240048173,1.9537821222,1.2565057238
C,0,0.3978418336,3.3626929662,-1.1412641913
H,0,-0.0095056126,1.4691641752,-2.1105467959
C,0,0.3998939527,3.3259579801,1.2787683429
H,0,-0.0042721035,1.4067917593,2.1929291395
C,0,0.5424612868,4.0339440044,0.0785539927
H,0,0.490897636,3.910069423,-2.0812704816
H,0,0.4983555332,3.8444225684,2.2344394426
H,0,0.7549066555,5.1043060388,0.0944826364
```

*Diphenyl Intermediate (Similar to 13) BPW91/6-311+G***



key distances OC 2.691 CC 3.011
E(RB-PW91) = -808.897582358

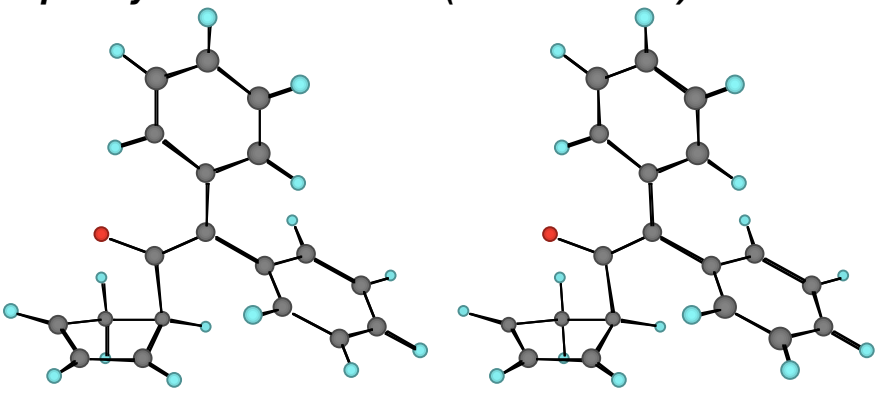
Zero-point correction=	0.283182 (Hartree/Particle)
Thermal correction to Energy=	0.299965
Thermal correction to Enthalpy=	0.300909
Thermal correction to Gibbs Free Energy=	0.237531
Sum of electronic and zero-point Energies=	-808.614400
Sum of electronic and thermal Energies=	-808.597618
Sum of electronic and thermal Enthalpies=	-808.596673
Sum of electronic and thermal Free Energies=	-808.660052

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	188.231	67.669	133.391

```
C,0,-2.3833369664,-0.3688462918,-0.1009775462
C,0,-2.3995000556,-0.2860682141,1.3588381043
C,0,-2.9214016301,-1.4890177618,1.883399343
C,0,-3.3858674202,-2.2684007979,0.8408825098
C,0,-3.3766099844,-1.4856884882,-0.4368084288
O,0,-0.915079299,-2.3121779176,-0.2233420127
C,0,-0.8805558622,-1.0677063512,-0.1678087539
C,0,0.2216724529,-0.1822402934,-0.1184860352
H,0,-2.423075733,0.5597237367,-0.6729216355
H,0,-1.9802437521,0.5375675875,1.9310519937
H,0,-2.8946843356,-1.781883714,2.9314291232
H,0,-3.7746516545,-3.2818767847,0.9319861786
H,0,-4.3753556881,-1.039548979,-0.6063212778
H,0,-3.1096054673,-2.0783801304,-1.3185840754
C,0,1.5935489864,-0.654796437,-0.3285048869
C,0,1.9218139152,-2.0256206748,-0.5266932726
```

```
C,0,2.6760414587,0.2695679386,-0.3076693568
C,0,3.2491247578,-2.4379331111,-0.6466641179
H,0,1.1171494373,-2.7550788459,-0.5879562191
C,0,3.9987144503,-0.1522694255,-0.4370859843
H,0,2.4710053169,1.3312619751,-0.1740441876
C,0,4.2994003409,-1.5108510509,-0.6034329351
H,0,3.4651583202,-3.4984189875,-0.7919407642
H,0,4.8020064162,0.5867741113,-0.4099377735
H,0,5.334315391,-1.8400173052,-0.7108257317
C,0,0.0060035426,1.3010081715,-0.0670609157
C,0,0.1387795773,2.0165418424,1.1392303871
C,0,-0.2810555764,2.0288951221,-1.2399590454
C,0,-0.0366363739,3.4054302818,1.1787630373
H,0,0.3977454477,1.4721904055,2.0497291858
C,0,-0.4668698719,3.4160264715,-1.201864832
H,0,-0.3526715122,1.4952051348,-2.1900103069
C,0,-0.3476153881,4.1091227034,0.0090090147
H,0,0.0716368626,3.9384449493,2.1253652304
H,0,-0.6949926438,3.9574869344,-2.1220151001
H,0,-0.4870041312,5.1910514499,0.0390937498
```

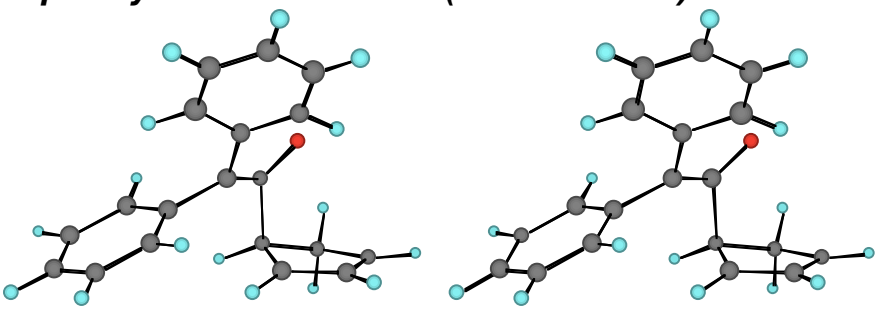
*Diphenyl 2nd TS 4+2 side (Similar to 14) BPW91/6-311+G***



```
key distances: OC 2.280 CC 3.140
E(RB-PW91) = -808.896852932

 Zero-point correction=                           0.283614 (Hartree/Particle)
 Thermal correction to Energy=                    0.299463
 Thermal correction to Enthalpy=                  0.300407
 Thermal correction to Gibbs Free Energy=         0.239074
 Sum of electronic and zero-point Energies=           -808.613239
 Sum of electronic and thermal Energies=              -808.597390
 Sum of electronic and thermal Enthalpies=            -808.596446
 Sum of electronic and thermal Free Energies=         -808.657779

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 187.916             65.125            129.087

 C,0,2.189354148,0.852573526,-2.7874324909
 C,0,1.5571992165,1.1671871594,-1.4225061618
 C,0,2.6861933146,1.0352230656,-0.47927201
 C,0,3.6324330203,0.1752312188,-1.0368642474
 C,0,3.2115362731,-0.1470894019,-2.3349623335
 C,0,0.8258968368,-0.2324402255,-1.0394774821
```

```
C,0,-0.1585099728,-0.2214966715,-0.0451702144
O,0,1.2945143142,-1.2076697053,-1.70379195
H,0,0.906871065,2.0385698619,-1.3238718647
H,0,2.6823168833,1.4243679072,0.536536948
H,0,4.4687289738,-0.2814632882,-0.5114297763
H,0,3.6843112284,-0.87906635,-2.9878910723
H,0,2.6913297295,1.7572580498,-3.1759681848
H,0,1.4902536239,0.4752349604,-3.5402222512
C,0,-0.5478108977,1.0796640179,0.5931742624
C,0,-1.5402570817,1.8975659055,0.0161810383
C,0,0.0397995175,1.5028389564,1.8010242516
C,0,-1.9066990964,3.1127317624,0.6067653159
H,0,-2.0242078263,1.570638644,-0.9063715383
C,0,-0.3302836367,2.7146292084,2.398787024
H,0,0.7836062645,0.8618823419,2.2783962427
C,0,-1.300302819,3.5267080968,1.7995304354
H,0,-2.67186905,3.7345690363,0.1379506864
H,0,0.1385354639,3.0229108644,3.3353411863
H,0,-1.5879330598,4.472095664,2.2627282091
C,0,-0.9462809813,-1.4127330196,0.2969359928
C,0,-1.8862531756,-1.3597088714,1.3620412741
C,0,-0.801720493,-2.657200461,-0.3740547811
C,0,-2.6094479748,-2.4868555706,1.7531620386
H,0,-2.0370943018,-0.4217538341,1.8961567075
C,0,-1.5244682189,-3.7813322521,0.028646902
H,0,-0.1173341162,-2.7249118194,-1.2172445509
C,0,-2.4331344843,-3.7100437894,1.0930376662
H,0,-3.3176925587,-2.4086850008,2.5805611255
H,0,-1.3861782883,-4.7228913895,-0.5069697952
H,0,-3.0032195118,-4.5901139316,1.395354647
```

*Diphenyl 2nd TS 2+2 side (Similar to 15) BPW91/6-311+G***



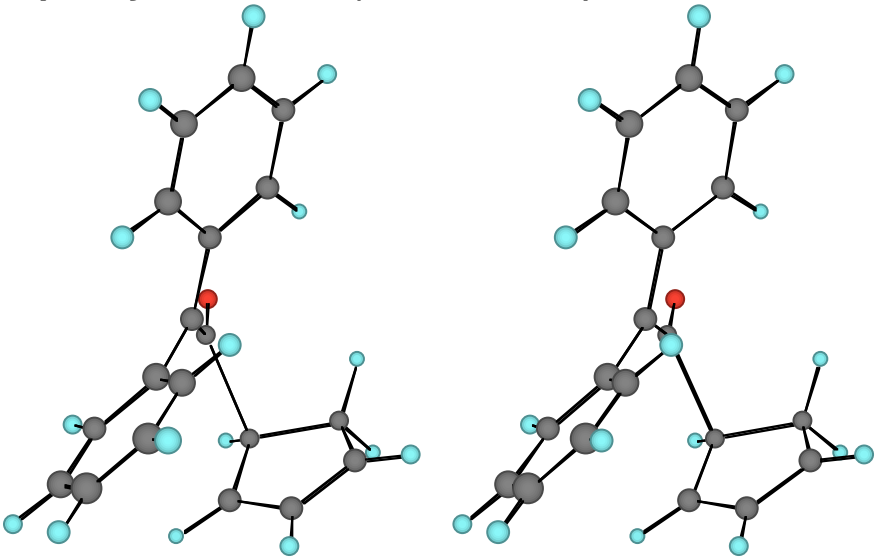
key distances CC 2.463 OC 3.026
E(RB-PW91) = -808.894947929

Zero-point correction=	0.283373 (Hartree/Particle)
Thermal correction to Energy=	0.299237
Thermal correction to Enthalpy=	0.300182
Thermal correction to Gibbs Free Energy=	0.239743
Sum of electronic and zero-point Energies=	-808.611575
Sum of electronic and thermal Energies=	-808.595710
Sum of electronic and thermal Enthalpies=	-808.594766
Sum of electronic and thermal Free Energies=	-808.655205

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.774	65.466	127.205

C,0,-1.3293765344,1.6658697684,-1.2351798724
C,0,-1.4932324386,1.6757767522,0.2551310195
C,0,-2.871965491,1.4456911406,0.5465060183
C,0,-3.6071260297,1.4777250279,-0.6106110045
C,0,-2.7498785886,1.8522557505,-1.7922196841
O,0,-1.7858282503,-0.6937335612,-1.6724496339
C,0,-0.9952831981,0.1205983704,-1.1847570488
C,0,0.0464008955,-0.1906454866,-0.2043416675
H,0,-0.5500921019,2.3035387511,-1.6570895622
H,0,-0.7355403055,1.9813314047,0.970255936
H,0,-3.2709745159,1.2623974907,1.5433525779
H,0,-4.6810318086,1.3026690802,-0.6771560078
H,0,-2.9278533231,2.9055716475,-2.0760502161
H,0,-2.9411772769,1.2247592787,-2.6728931649
C,0,1.2526799152,0.6737049363,-0.1298351015
C,0,1.881288341,1.142040175,-1.3043238858
C,0,1.8228296291,1.0356562217,1.1123942775
C,0,3.0173712042,1.9563989363,-1.2404349157
H,0,1.4853044139,0.8393078896,-2.2755370561
C,0,2.9555657337,1.8506597893,1.1754915678
H,0,1.3612569659,0.6753831754,2.0338597065
C,0,3.5575234488,2.3184630184,-0.0010768314
H,0,3.4887212674,2.2982960473,-2.1637692282
H,0,3.3708439967,2.1237696288,2.1473946917
H,0,4.4441623281,2.9523822041,0.0493596024
C,0,0.1032874743,-1.5209079411,0.4294246863
C,0,1.3353484045,-2.0986044877,0.821321629
C,0,-1.0813513078,-2.2506843962,0.7060122349
C,0,1.3829732904,-3.3356886109,1.4702745922
H,0,2.2659155521,-1.5763919313,0.5991526491
C,0,-1.0300382956,-3.476580369,1.3657251529
H,0,-2.0403089722,-1.8453041947,0.3892069252
C,0,0.201324565,-4.0298331195,1.751240018
H,0,2.3484540085,-3.7605839526,1.7511026897
H,0,-1.9574070569,-4.0125504161,1.5765199798
H,0,0.2363067222,-4.9960804691,2.2574404396

*Diphenyl 1st TS 2+2 (Similar to 10) BPW91/6-311+G***



key distances 1.903 3.200
E(RB-PW91) = -808.880726010

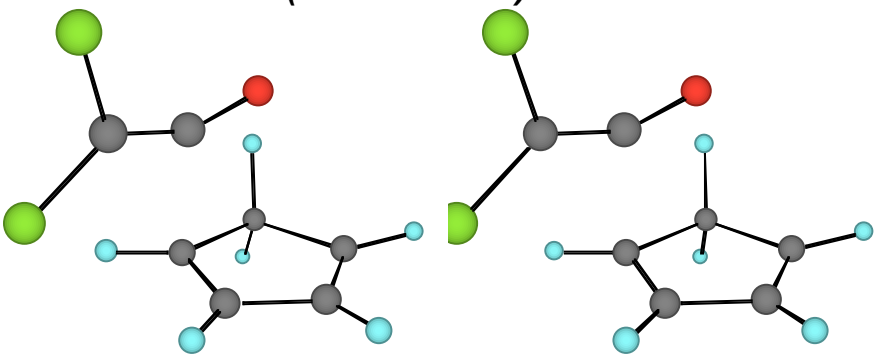
Zero-point correction=	0.281608 (Hartree/Particle)
Thermal correction to Energy=	0.298368
Thermal correction to Enthalpy=	0.299312
Thermal correction to Gibbs Free Energy=	0.236095
Sum of electronic and zero-point Energies=	-808.599118
Sum of electronic and thermal Energies=	-808.582358
Sum of electronic and thermal Enthalpies=	-808.581414
Sum of electronic and thermal Free Energies=	-808.644631

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	187.229	67.044	133.051

C,0,-0.0525624775,0.7680705395,-2.6472157296
C,0,1.347797851,0.8857924702,-2.4374450583
C,0,1.6299289321,2.0631365123,-1.675466468
C,0,0.4750648398,2.7900021043,-1.5335017529
C,0,-0.6400206043,2.1385427461,-2.2925952577
C,0,-0.9706438598,-0.3559454002,-1.4155850609
O,0,-2.009081545,-0.6716876262,-1.9567513756
C,0,-0.4172221121,-0.4555274932,-0.1304030617
H,0,-0.4046657369,0.2514799857,-3.5409615303
H,0,2.100256929,0.2042721724,-2.8248310521
H,0,2.606549345,2.3291092028,-1.275519147
H,0,0.3735389788,3.7278160223,-0.9885233263
H,0,-0.8219752786,2.7014540374,-3.2307228285
H,0,-1.6012411263,2.1186249328,-1.7616974488
C,0,1.020645737,-0.5809271341,0.1051366401
C,0,1.8286139503,-1.380239861,-0.7411933235
C,0,1.65999605,0.0542051153,1.2022684229
C,0,3.2038150947,-1.533595574,-0.5096804057
H,0,1.3537408732,-1.9364239555,-1.5510546362
C,0,3.0247936979,-0.0984311065,1.4302412048
H,0,1.0667680831,0.6866164347,1.86388984
C,0,3.8085191574,-0.8945147682,0.5739644821

```
H,0,3.7952229242,-2.170240167,-1.1707582296
H,0,3.4910233912,0.4111917065,2.2758719015
H,0,4.8764292884,-1.0171195557,0.7619819321
C,0,-1.3821467005,-0.4803791303,0.995607099
C,0,-1.0533298493,-1.1363577672,2.2085165288
C,0,-2.6680171405,0.1041746093,0.9076373511
C,0,-1.9555371782,-1.1879484753,3.2738080223
H,0,-0.0874014081,-1.6324534822,2.3030416994
C,0,-3.5676303756,0.0477374738,1.9737439744
H,0,-2.9702311219,0.6071482166,-0.0109146015
C,0,-3.2189521165,-0.59324926,3.1695587427
H,0,-1.6712987496,-1.7122926096,4.1885377481
H,0,-4.5498735034,0.512936175,1.8693101055
H,0,-3.9228679045,-0.6358917099,4.0019824777
```

*Dichloro 1st TS (similar to 18) BPW91/6-311+G***



key distances OC 3.012 CC 2.288 CC 3.176
E(RB-PW91) = -1265.97703588

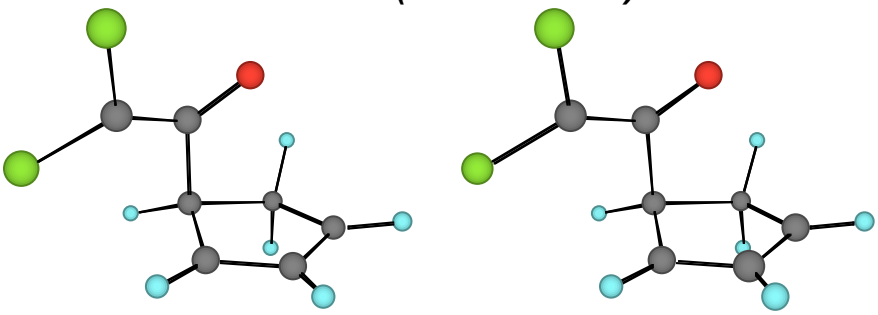
Zero-point correction=	0.106089 (Hartree/Particle)
Thermal correction to Energy=	0.116018
Thermal correction to Enthalpy=	0.116963
Thermal correction to Gibbs Free Energy=	0.069537
Sum of electronic and zero-point Energies=	-1265.870947
Sum of electronic and thermal Energies=	-1265.861017
Sum of electronic and thermal Enthalpies=	-1265.860073
Sum of electronic and thermal Free Energies=	-1265.907499

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	72.803	35.421	99.817

```
C,0,-1.391063558,0.7786003879,-0.6958893959
C,0,-1.5603028426,1.0159569298,0.65883681
C,0,-2.633738873,0.1856913239,1.1645106907
C,0,-3.1580114617,-0.5371892155,0.1346327008
C,0,-2.4717646734,-0.165683057,-1.1470719871
O,0,-0.4128926776,-1.7732112193,0.0516031689
C,0,0.1833411465,-0.7377149946,-0.0193805992
C,0,1.3554995114,-0.0690762486,0.020671701
Cl,0,1.6184468162,1.6485512567,-0.0809270261
Cl,0,2.8083268451,-1.0537737109,0.0883922829
H,0,-0.7723296459,1.362938162,-1.3716890013
H,0,-0.9780687041,1.7172253196,1.2533832053
H,0,-2.9345862143,0.1303631661,2.2088276123
```

```
H,0,-3.951314204,-1.2791011809,0.2047396934
H,0,-3.162803812,0.3601908098,-1.832758523
H,0,-2.096663736,-1.0406555564,-1.7000972245
```

*Dichloro Intermediate (similar to 19) BPW91/6-311+G***



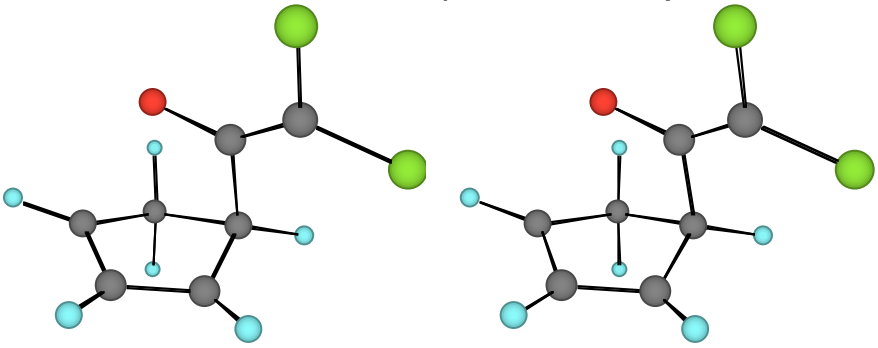
```
key distances OC 2.859 CC 2.762
E(RB-PW91) = -1265.98733358
```

Zero-point correction=	0.108038 (Hartree/Particle)
Thermal correction to Energy=	0.117569
Thermal correction to Enthalpy=	0.118513
Thermal correction to Gibbs Free Energy=	0.072104
Sum of electronic and zero-point Energies=	-1265.879295
Sum of electronic and thermal Energies=	-1265.869765
Sum of electronic and thermal Enthalpies=	-1265.868820
Sum of electronic and thermal Free Energies=	-1265.915229

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.776	35.129	97.676

```
C,0,-1.129222366,0.5729267354,-0.7883334313
C,0,-1.3689903997,0.9614031289,0.6185504076
C,0,-2.4073314985,0.1570522354,1.14367326
C,0,-2.9552638565,-0.5998039943,0.1293001139
C,0,-2.3921607888,-0.1938097162,-1.200420031
O,0,-0.3650932175,-1.7131618572,-0.3473190579
C,0,-0.0327927188,-0.5212290923,-0.3751650864
C,0,1.1817012106,0.0210730054,0.1308176392
Cl,0,1.7119886075,1.6533906322,-0.2274900375
Cl,0,2.4519877736,-1.0605536044,0.5965956016
H,0,-0.7414522161,1.3304771233,-1.474562161
H,0,-0.7945436248,1.7080931337,1.1603423359
H,0,-2.6880745528,0.1082888531,2.1941093981
H,0,-3.7305976237,-1.3548835875,0.2538824298
H,0,-3.0930721452,0.4910955895,-1.7133118949
H,0,-2.1947500712,-1.0416795415,-1.8672394663
```

*Dichloro 2nd TS 4+2 side (similar to 20) BPW91/6-311+G***



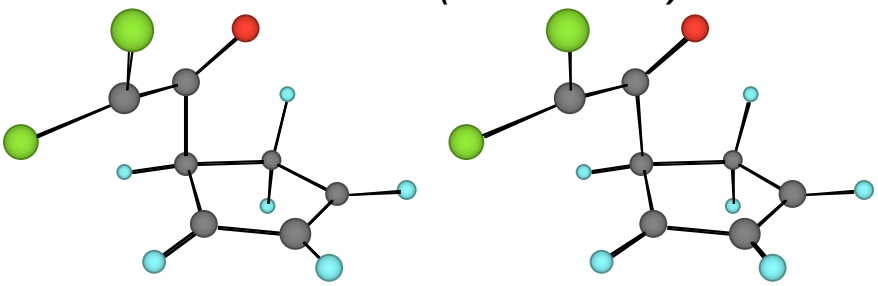
key distances OC 2.237 CC 3.013
E(RB-PW91) = -1265.98525915

Zero-point correction=	0.108517 (Hartree/Particle)
Thermal correction to Energy=	0.117098
Thermal correction to Enthalpy=	0.118042
Thermal correction to Gibbs Free Energy=	0.073903
Sum of electronic and zero-point Energies=	-1265.876743
Sum of electronic and thermal Energies=	-1265.868161
Sum of electronic and thermal Enthalpies=	-1265.867217
Sum of electronic and thermal Free Energies=	-1265.911356

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.480	32.637	92.899

C,0,2.3663661481,0.1410107553,-1.1151882835
C,0,1.1385731132,0.8627707159,-0.5357547185
C,0,1.4749026108,1.0161981718,0.9063102419
C,0,2.3781189274,0.0168905463,1.2530950155
C,0,2.7055643993,-0.6959202119,0.0845262216
C,0,0.114014409,-0.3384936714,-0.319540881
C,0,-1.1996389855,-0.0446925892,0.0116624057
O,0,0.6559095031,-1.4874634257,-0.3339962746
Cl,0,-2.3598028865,-1.3155926192,0.2332707617
Cl,0,-1.8815008259,1.56096175,-0.1471195891
H,0,0.7304643343,1.7256704094,-1.0664802703
H,0,0.9578492881,1.691714643,1.5849966627
H,0,2.6553081551,-0.2688212438,2.265535945
H,0,3.3067355188,-1.6028196277,0.0488462849
H,0,3.170428539,0.871766625,-1.3125167861
H,0,2.1666975176,-0.4356609243,-2.0236415833

*Dichloro 2nd TS 2+2 side (similar to 21) BPW91/6-311+G***



key distances CC 2.459 OC 2.998

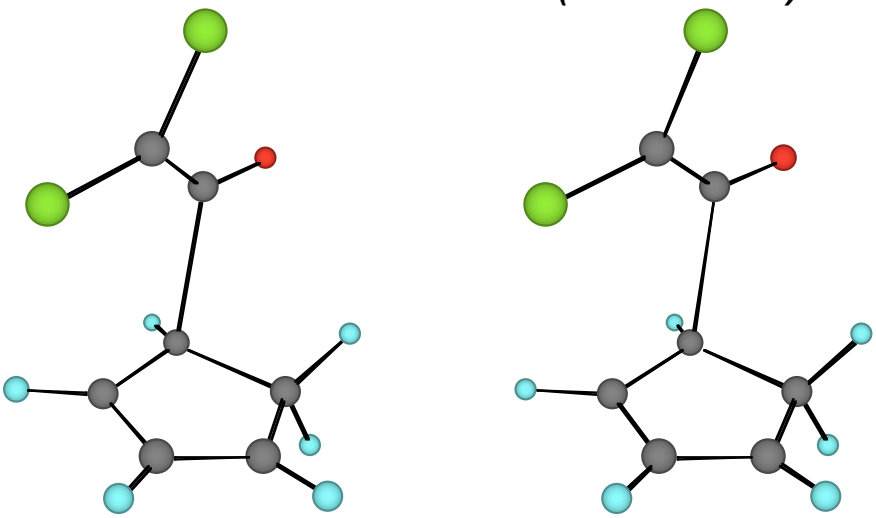
E(RB-PW91) = -1265.98670643

Zero-point correction=	0.108075 (Hartree/Particle)
Thermal correction to Energy=	0.116703
Thermal correction to Enthalpy=	0.117648
Thermal correction to Gibbs Free Energy=	0.073793
Sum of electronic and zero-point Energies=	-1265.878631
Sum of electronic and thermal Energies=	-1265.870003
Sum of electronic and thermal Enthalpies=	-1265.869059
Sum of electronic and thermal Free Energies=	-1265.912913

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	73.233	33.046	92.300

C,0,-1.1398244731,0.5775894634,-0.8574292182
C,0,-1.1824912507,0.8758601033,0.6085387825
C,0,-2.1805149269,0.0465071975,1.2001186954
C,0,-2.8822959225,-0.6072523655,0.2202067904
C,0,-2.4607135944,-0.1504320927,-1.1503423254
O,0,-0.2544850567,-1.710056597,-0.7120285962
C,0,-0.0187665,-0.5078131051,-0.6187669534
C,0,1.0870020242,0.0567027531,0.1323634172
Cl,0,1.7302367416,1.6489828968,-0.2590981908
Cl,0,2.2557571969,-1.0205037085,0.8284673824
H,0,-0.8487612799,1.3859968793,-1.5336475714
H,0,-0.6462860099,1.680638962,1.1026478983
H,0,-2.3379420149,-0.061360822,2.2718409134
H,0,-3.6771311887,-1.3322195416,0.3938147121
H,0,-3.2045845808,0.5542948496,-1.5636494004
H,0,-2.3456835656,-0.9780154754,-1.8621891696

*Dichloro Alternative TS for 2+2 (similar to 10) BPW91/6-311+G***



key distances 2.017 3.090
E(RB-PW91) = -1265.96141832

Zero-point correction=	0.105929 (Hartree/Particle)
Thermal correction to Energy=	0.115878
Thermal correction to Enthalpy=	0.116822
Thermal correction to Gibbs Free Energy=	0.068544

```
 Sum of electronic and zero-point Energies=          -1265.855489
 Sum of electronic and thermal Energies=             -1265.845540
 Sum of electronic and thermal Enthalpies=           -1265.844596
 Sum of electronic and thermal Free Energies=        -1265.892874

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   72.714             35.104            101.610

 C,0,-0.3945199446,-0.5171171527,-1.6823048935
 C,0,-1.3668987606,0.4868870905,-1.5481779692
 C,0,-2.5452727194,-0.0391187669,-0.9169846672
 C,0,-2.3926020414,-1.3900582395,-0.7584137983
 C,0,-1.0770945213,-1.8300421897,-1.316430045
 C,0,1.0768133121,-0.4544895986,-0.3039224861
 O,0,1.8161299768,-1.3681810531,-0.596079593
 C,0,0.9255432265,0.4873150001,0.6707900775
 Cl,0,-0.1192476417,1.8732846207,0.6821606079
 Cl,0,1.8423127091,0.2361418331,2.145915634
 H,0,0.3442984174,-0.4608483993,-2.4816676086
 H,0,-1.2604384028,1.508936483,-1.905010906
 H,0,-3.4101840605,0.550319148,-0.618665392
 H,0,-3.1110392612,-2.0647141397,-0.2944458847
 H,0,-1.2387082286,-2.4288480411,-2.2343117226
 H,0,-0.5008857337,-2.4799031988,-0.6418951637
```

*Cyclopentadiene (1) HF/6-311+G***

```
E(RHF) = -192.839556311

 Zero-point correction=                           0.098543 (Hartree/Particle)
 Thermal correction to Energy=                    0.102457
 Thermal correction to Enthalpy=                  0.103401
 Thermal correction to Gibbs Free Energy=         0.072051
 Sum of electronic and zero-point Energies=          -192.741013
 Sum of electronic and thermal Energies=             -192.737100
 Sum of electronic and thermal Enthalpies=           -192.736156
 Sum of electronic and thermal Free Energies=        -192.767505

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                   64.292             14.109             65.981

 C,0,0.2858698357,-0.151975256,-1.1725584918
 C,0,-0.6434958307,0.8571214422,-0.5526808638
 C,0,-0.6758702636,0.6829550327,0.7650064507
 C,0,0.2144421895,-0.4377537552,1.1273197707
 C,0,0.7725626407,-0.9256288256,0.0236165616
 H,0,-1.186014248,1.594971161,-1.1131861487
 H,0,-1.251133159,1.2558411533,1.4683941979
 H,0,0.3737796639,-0.7896161812,2.1296594416
 H,0,1.4658167572,-1.7435516728,-0.0339615718
 H,0,1.10542121,0.3261307533,-1.7073648473
 H,0,-0.2289216541,-0.7920870431,-1.8877616361
```

*Diphenylketene (2) HF/6-311+G***

```
E(RHF) = -610.959930871
```

```
Zero-point correction=                           0.208244 (Hartree/Particle)
Thermal correction to Energy=                    0.219457
Thermal correction to Enthalpy=                  0.220401
Thermal correction to Gibbs Free Energy=         0.168472
Sum of electronic and zero-point Energies=           -610.751687
Sum of electronic and thermal Energies=              -610.740474
Sum of electronic and thermal Enthalpies=            -610.739530
Sum of electronic and thermal Free Energies=         -610.791459

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  137.711             42.874           109.294

C,0,2.0220822209,0.7816761522,0.0404057867
O,0,3.082848274,1.1917313225,0.0615969048
C,0,0.7987759372,0.3087841323,0.015965795
C,0,0.1257826125,0.0180870532,1.3168331878
C,0,-1.2031707552,0.3893047081,1.5104622009
C,0,0.800844548,-0.6093331108,2.358028048
C,0,-1.8342552166,0.1416259262,2.7155196393
H,0,-1.7404664772,0.874028339,0.7157254354
C,0,0.171787864,-0.8409649815,3.5718183258
H,0,1.8190201989,-0.9284704395,2.2200139005
C,0,-1.1481570355,-0.4701105495,3.7544803458
H,0,-2.8607378094,0.4346266511,2.8471146902
H,0,0.7125824483,-1.3235786076,4.3663233887
H,0,-1.6397117828,-0.657795331,4.6921393009
C,0,0.1509361021,0.0888852012,-1.3113006553
C,0,-0.575209606,-1.0768846383,-1.5460484376
C,0,0.2642662877,1.0211838937,-2.3366896539
C,0,-1.1664679698,-1.3017265156,-2.7755333014
H,0,-0.6740824306,-1.8076180242,-0.7640614629
C,0,-0.314399137,0.7859492166,-3.5746182772
H,0,0.7976086412,1.9401733964,-2.1676275778
C,0,-1.0345101561,-0.3736401342,-3.7980974605
H,0,-1.7237484026,-2.2070493651,-2.9388188022
H,0,-0.21152668,1.5174713305,-4.356222747
H,0,-1.4915580751,-0.5526566515,-4.754714624
```

*Diphenyl 4+2 product (3) HF/6-311+G***

```
E(RHF) = -803.799060173

Zero-point correction=                           0.314684 (Hartree/Particle)
Thermal correction to Energy=                    0.328867
Thermal correction to Enthalpy=                  0.329811
Thermal correction to Gibbs Free Energy=         0.271329
Sum of electronic and zero-point Energies=           -803.484376
Sum of electronic and thermal Energies=              -803.470194
Sum of electronic and thermal Enthalpies=            -803.469249
Sum of electronic and thermal Free Energies=         -803.527731

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                  206.367             57.079           123.084

C,0,2.2478631905,1.013494325,0.2786413031
```

```
C,0,2.9903767166,1.0102820964,-1.0584898236
C,0,3.6664763132,-0.1233235677,-1.1327182394
C,0,3.351356224,-0.8765062685,0.1509340301
C,0,3.2798184215,0.2693926951,1.1580548059
O,0,1.9644384275,-1.2599847519,0.0793157148
C,0,1.2327132438,-0.1163294733,0.1432198174
C,0,-0.092660557,-0.0783755283,0.0828314927
H,0,1.8584890293,1.9569987736,0.6169982636
H,0,2.8824745623,1.76561677,-1.814034469
H,0,4.2362490031,-0.503597287,-1.9590462187
H,0,3.9299156201,-1.7546514171,0.3835993014
H,0,4.208749261,0.8098665315,1.2731922208
H,0,2.8912179112,-0.0429407218,2.1210708516
C,0,-0.8068491031,1.2351140154,0.2164434926
C,0,-0.8388176781,1.9272779385,1.4212099682
C,0,-1.483846516,1.7770884176,-0.873520632
C,0,-1.5085233815,3.1376515804,1.5322958142
H,0,-0.3408585251,1.5134646504,2.2805095662
C,0,-2.1526818342,2.9838427495,-0.7668938679
H,0,-1.4839183979,1.2472183723,-1.809588378
C,0,-2.1660109966,3.6709535848,0.4379605872
H,0,-1.5199327822,3.6566282947,2.4746375775
H,0,-2.6636907045,3.3880438142,-1.622911818
H,0,-2.6874616106,4.6078498318,0.5217959157
C,0,-0.9353731,-1.2982570249,-0.1164879839
C,0,-2.1363083262,-1.4365096866,0.5763764283
C,0,-0.5719707997,-2.3088967269,-1.004309999
C,0,-2.9378922077,-2.552447999,0.4039074226
H,0,-2.4495483378,-0.6657215052,1.2566756187
C,0,-1.3765041859,-3.4213866147,-1.1827592469
H,0,0.3440696231,-2.2253851447,-1.5557957213
C,0,-2.561736293,-3.5517709365,-0.4775221324
H,0,-3.8568041372,-2.6373875239,0.9568809537
H,0,-1.0760852068,-4.1865696833,-1.8769497098
H,0,-3.1849475113,-4.4173171999,-0.6165990955
```

*Diphenyl 2+2 product (4) HF/6-311+G***

```
E(RHF) = -803.818294978

 Zero-point correction=                           0.313448 (Hartree/Particle)
 Thermal correction to Energy=                    0.328137
 Thermal correction to Enthalpy=                  0.329082
 Thermal correction to Gibbs Free Energy=         0.269679
 Sum of electronic and zero-point Energies=           -803.504847
 Sum of electronic and thermal Energies=              -803.490158
 Sum of electronic and thermal Enthalpies=            -803.489213
 Sum of electronic and thermal Free Energies=         -803.548616

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                 205.909             58.335            125.024

 C,0,-2.1841909085,-1.2798698941,-0.3335199099
 C,0,-1.5400917331,-0.0293074235,-0.9924954791
 C,0,-2.5095972684,1.060440364,-0.5997673468
 C,0,-3.6023659286,0.5900238262,-0.0257141982
 C,0,-3.6080408177,-0.9159265933,0.1064934748
```

```
C,0,-1.1119006332,-1.1735360579,0.7401872397
O,0,-1.0132391847,-1.6383285275,1.8182380716
C,0,-0.260605883,-0.1797305168,-0.0818406364
H,0,-2.1001377137,-2.2075229225,-0.8863953938
H,0,-1.3664724791,-0.0548078013,-2.0582511454
H,0,-2.3195874054,2.1015521721,-0.7857131546
H,0,-4.4214881593,1.200583807,0.3116983438
H,0,-4.3596072433,-1.3652129728,-0.5377873246
H,0,-3.8136119493,-1.2472742211,1.1197624409
C,0,0.2647019087,1.0769341027,0.6036351893
C,0,0.7204407501,2.1363267505,-0.1784087595
C,0,0.3137000197,1.2043048051,1.9836006115
C,0,1.202909332,3.2932199436,0.4018799639
H,0,0.7024305658,2.0565597872,-1.2512218847
C,0,0.803648465,2.3662143876,2.5679624844
H,0,-0.0241250223,0.4024083486,2.6106395055
C,0,1.2471243442,3.4131900007,1.7840513758
H,0,1.5478460148,4.0992697076,-0.2214315007
H,0,0.8339920593,2.4449472763,3.6403268335
H,0,1.6248894164,4.3116262844,2.2386103067
C,0,0.8922522198,-0.9496869786,-0.7474177569
C,0,1.1880716192,-0.8314041163,-2.099183165
C,0,1.7113672856,-1.7574416944,0.037967974
C,0,2.2684456909,-1.5024159131,-2.6534983889
H,0,0.5896957324,-0.2100480103,-2.7383312111
C,0,2.7865749939,-2.4302620816,-0.5140832001
H,0,1.5076915883,-1.8609601138,1.0878316745
C,0,3.070499692,-2.3063783287,-1.8649053741
H,0,2.4782882872,-1.3929363773,-3.7027926881
H,0,3.4023855373,-3.0506632847,0.112442841
H,0,3.9060653573,-2.8290609523,-2.2949568075
```

*Dichloroketene (5) HF/6-311+G***

```
E(RHF) = -1069.58479345

 Zero-point correction=                           0.017068 (Hartree/Particle)
 Thermal correction to Energy=                    0.021888
 Thermal correction to Enthalpy=                  0.022832
 Thermal correction to Gibbs Free Energy=        -0.012459
 Sum of electronic and zero-point Energies=          -1069.567725
 Sum of electronic and thermal Energies=             -1069.562906
 Sum of electronic and thermal Enthalpies=           -1069.561961
 Sum of electronic and thermal Free Energies=        -1069.597253

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  13.735             14.658            74.277

 C,0,1.2152325414,-0.5287817795,-0.2374108151
 C,0,0.0366698691,-0.0159503091,-0.0071324837
 O,0,2.2376222745,-0.9736572323,-0.4371741422
 Cl,0,-1.2915596821,-1.0379244897,0.3968772748
 Cl,0,-0.2032869448,1.6883745129,-0.1048388672
```

*Dichloro 2+2 product (7) HF/6-311+G***

```
E(RHF) = -1262.47759460
```

```
Zero-point correction=                           0.122026 (Hartree/Particle)
Thermal correction to Energy=                    0.130229
Thermal correction to Enthalpy=                  0.131173
Thermal correction to Gibbs Free Energy=         0.087786
Sum of electronic and zero-point Energies=          -1262.355568
Sum of electronic and thermal Energies=             -1262.347366
Sum of electronic and thermal Enthalpies=           -1262.346422
Sum of electronic and thermal Free Energies=        -1262.389808

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   81.720             30.085             91.315

C,0,-0.6480257891,-0.9142669357,-1.126912891
C,0,-0.4053817558,0.6105027378,-0.9023052846
C,0,-1.7444458264,1.0744206779,-0.3865850432
C,0,-2.6696986078,0.1358364012,-0.4661154504
C,0,-2.1596833365,-1.1670232273,-1.0355592805
C,0,0.1364711057,-1.170941621,0.1592498569
O,0,0.2423946506,-2.0662753696,0.9013176061
C,0,0.6600382514,0.2812018203,0.1796426453
Cl,0,2.3080575704,0.3105707201,-0.5081887246
Cl,0,0.6219388391,1.1379240553,1.7179330309
H,0,-0.1625131901,-1.3554677472,-1.987308172
H,0,-0.0225014552,1.206935434,-1.7179858757
H,0,-1.9037193785,2.0699110198,-0.0165002903
H,0,-3.6949301118,0.269843493,-0.1699805368
H,0,-2.593261222,-1.3661893441,-2.0114965715
H,0,-2.3878150569,-2.0176202006,-0.4014099228
```

*Dichloro 4+2 product (8) HF/6-311+G***

```
E(RHF) = -1262.44626284

Zero-point correction=                           0.123541 (Hartree/Particle)
Thermal correction to Energy=                    0.131202
Thermal correction to Enthalpy=                  0.132146
Thermal correction to Gibbs Free Energy=         0.089739
Sum of electronic and zero-point Energies=          -1262.322722
Sum of electronic and thermal Energies=             -1262.315061
Sum of electronic and thermal Enthalpies=           -1262.314117
Sum of electronic and thermal Free Energies=        -1262.356524

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   82.331             28.847             89.253

C,0,1.3396466755,0.6142484404,0.4978993226
C,0,2.0666936909,0.8466822729,-0.82691361
C,0,2.432191888,-0.3370271971,-1.2880949569
C,0,1.933864689,-1.3533288141,-0.273538837
C,0,2.1412478635,-0.5958594172,1.0361282009
O,0,0.4878285688,-1.3509759783,-0.3551837814
C,0,0.0868400215,-0.1484268819,0.0951052049
C,0,-1.1765016583,0.2186274909,0.144009375
Cl,0,-1.6635833524,1.7748323609,0.7360252501
Cl,0,-2.4657911622,-0.8068199674,-0.3732156024
```

```
H,0,1.1841960935,1.4653143604,1.1373922326
H,0,2.1583376974,1.8012221573,-1.3092576505
H,0,2.8913307746,-0.5683122492,-2.2298521853
H,0,2.266916476,-2.3729826407,-0.361404694
H,0,3.1739548267,-0.3561922658,1.2448973347
H,0,1.6781033086,-1.086947588,1.8843630063
```

*Diphenyl 1st TS (Similar to 9, but later) HF/6-311+G***

```
E(RHF) = -803.738877702

 Zero-point correction=                           0.310028 (Hartree/Particle)
 Thermal correction to Energy=                    0.324652
 Thermal correction to Enthalpy=                  0.325596
 Thermal correction to Gibbs Free Energy=         0.266438
 Sum of electronic and zero-point Energies=           -803.428849
 Sum of electronic and thermal Energies=              -803.414226
 Sum of electronic and thermal Enthalpies=            -803.413282
 Sum of electronic and thermal Free Energies=         -803.472439

                     E (Thermal)             CV                S
                      KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  203.722             58.444            124.508

 C,0,2.3437997607,-0.4356498686,0.247754922
 C,0,2.5647364365,-0.3884048078,-1.1723574654
 C,0,3.076402257,-1.6037475018,-1.6297914567
 C,0,3.3147754307,-2.3860836412,-0.5351736224
 C,0,3.2114864682,-1.5961244389,0.7215861422
 O,0,0.8270123086,-2.3037506624,0.1511038165
 C,0,0.7931988063,-1.0797432795,0.1657740312
 C,0,-0.2283907707,-0.1719844965,0.1023279518
 H,0,2.3731099606,0.4911012103,0.7892555874
 H,0,2.2815541488,0.4404325332,-1.7917960004
 H,0,3.1545194098,-1.9058752058,-2.6547793283
 H,0,3.6012475272,-3.4211183202,-0.5683931803
 H,0,4.2043277886,-1.2274249068,0.9796281079
 H,0,2.8112338256,-2.1563642631,1.5504703179
 C,0,-1.6501271853,-0.6036551944,0.1559825217
 C,0,-2.0356603082,-1.9529302619,0.1918912951
 C,0,-2.6786814667,0.3476216686,0.1624276551
 C,0,-3.3704587341,-2.3145593515,0.2219928477
 H,0,-1.2846953366,-2.7138092287,0.1980847075
 C,0,-4.0126011153,-0.0223978481,0.1936832688
 H,0,-2.443503835,1.3938383542,0.1406071779
 C,0,-4.3727566414,-1.3575994481,0.2227092478
 H,0,-3.6266164468,-3.3597668454,0.2480803194
 H,0,-4.7700147023,0.7423307935,0.1961890866
 H,0,-5.4085013032,-1.6466579072,0.2481729837
 C,0,0.0366416787,1.3072516896,0.1118174608
 C,0,0.0706320196,2.0421284466,-1.0698481699
 C,0,0.2042031401,1.9996708778,1.3098167224
 C,0,0.2960491348,3.4111639801,-1.0620337299
 H,0,-0.0998765898,1.5361868896,-2.0044174365
 C,0,0.4345390065,3.365859036,1.3251428412
 H,0,0.1488039952,1.4576110735,2.237683231
 C,0,0.4856152342,4.0776423345,0.1366936854
 H,0,0.3163814077,3.954852032,-1.9904019586
```

```
H,0,0.5655491071,3.8749883065,2.263930932
H,0,0.6599636645,5.1389334142,0.1464780277
```

*Diphenyl 2nd TS Claisen Rearrangement (Similar to 11) HF/6-311+G***

E(RHF) = -803.738361541

Zero-point correction=	0.310544 (Hartree/Particle)
Thermal correction to Energy=	0.324861
Thermal correction to Enthalpy=	0.325806
Thermal correction to Gibbs Free Energy=	0.268111
Sum of electronic and zero-point Energies=	-803.427818
Sum of electronic and thermal Energies=	-803.413500
Sum of electronic and thermal Enthalpies=	-803.412556
Sum of electronic and thermal Free Energies=	-803.470251

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	203.854	58.052	121.429

```
C,0,2.2199504816,0.883207841,-2.902155815
C,0,1.4074227196,1.1385624978,-1.637231838
C,0,2.3268183562,0.842245765,-0.5493917109
C,0,3.4118906181,0.0777858889,-1.0317553246
C,0,3.3202630976,0.0161162463,-2.3807698469
C,0,0.5505252415,-0.198142944,-1.322372096
C,0,-0.1711690071,-0.181734613,-0.1331122201
O,0,0.7756324863,-1.1243031737,-2.088704076
H,0,0.8516239283,2.0552306641,-1.5783508895
H,0,2.1925624012,1.1624284931,0.4628012277
H,0,4.1409701963,-0.414968791,-0.4200025636
H,0,3.9755526713,-0.5531957082,-3.0147216108
H,0,2.6464748998,1.8144622986,-3.2731531549
H,0,1.6571605961,0.4110063615,-3.6923476896
C,0,-0.4813337385,1.0953143908,0.5914918913
C,0,-1.2464966726,2.0986327781,0.0032605404
C,0,-0.0672956108,1.28678281,1.9102770816
C,0,-1.5559689293,3.2644978784,0.6889736079
H,0,-1.6157492427,1.9587559517,-0.997539303
C,0,-0.3767222781,2.4457767768,2.6005141843
H,0,0.4947854652,0.5105182797,2.4000903187
C,0,-1.1193571822,3.4451751281,1.9895252012
H,0,-2.1490764452,4.0229005626,0.2087273455
H,0,-0.0419122629,2.5672428051,3.6157396991
H,0,-1.3620229113,4.3459085282,2.524621123
C,0,-0.9038541656,-1.3930677384,0.3236076849
C,0,-2.037422328,-1.284077635,1.1346573426
C,0,-0.4732365722,-2.6860165202,-0.0069544369
C,0,-2.7077132415,-2.4047538877,1.597859466
H,0,-2.4098472253,-0.3155746832,1.4083485143
C,0,-1.1384411646,-3.8009939972,0.4655277297
H,0,0.3749378363,-2.8079638243,-0.6476538945
C,0,-2.2613388153,-3.6716914022,1.2699902814
H,0,-3.5806381532,-2.2809866612,2.2147274066
H,0,-0.7799144415,-4.7795920182,0.1974592704
H,0,-2.7790920557,-4.5434624509,1.6292364706
```

*Dichloro 1st TS (similar to 18) HF/6-311+G***

E(RHF) = -1262.38593504

Zero-point correction=	0.117638 (Hartree/Particle)
Thermal correction to Energy=	0.126432
Thermal correction to Enthalpy=	0.127376
Thermal correction to Gibbs Free Energy=	0.082593
Sum of electronic and zero-point Energies=	-1262.268297
Sum of electronic and thermal Energies=	-1262.259503
Sum of electronic and thermal Enthalpies=	-1262.258559
Sum of electronic and thermal Free Energies=	-1262.303342

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	79.337	31.494	94.254

C,0,-1.2202442283,0.643043371,-0.6810215723
C,0,-1.4753711712,0.9644395057,0.6508572349
C,0,-2.5485894192,0.1701080036,1.158022534
C,0,-3.040409301,-0.563587509,0.1427828615
C,0,-2.3806294371,-0.207667486,-1.1492041174
O,0,-0.4136818431,-1.6958770169,-0.0613966629
C,0,0.0607336475,-0.6100035443,-0.1366439246
C,0,1.2647218406,-0.0302752202,0.0220198631
Cl,0,1.6349539561,1.6574715801,-0.1397781344
Cl,0,2.6471009555,-1.0564413337,0.2357832171
H,0,-0.7145583361,1.3184575872,-1.3422718664
H,0,-0.9123588542,1.6770070264,1.2225256254
H,0,-2.8503687878,0.1288004082,2.1854026151
H,0,-3.8120809206,-1.3057403194,0.228812844
H,0,-3.0553443746,0.4077363988,-1.7440387606
H,0,-2.102039068,-1.0731018798,-1.7322208367

*Dichloro intermediate (similar to 19) HF/6-311+G***

E(RHF) = -1262.38848133

Zero-point correction=	0.119049 (Hartree/Particle)
Thermal correction to Energy=	0.128015
Thermal correction to Enthalpy=	0.128959
Thermal correction to Gibbs Free Energy=	0.083452
Sum of electronic and zero-point Energies=	-1262.269432
Sum of electronic and thermal Energies=	-1262.260466
Sum of electronic and thermal Enthalpies=	-1262.259522
Sum of electronic and thermal Free Energies=	-1262.305029

	E (Thermal) KCal/Mol	CV Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	80.331	32.081	95.777

C,0,-1.1188868549,0.5768919837,-0.7351968356
C,0,-1.411986466,0.9667678307,0.6321533623
C,0,-2.4530123887,0.1859789076,1.1498792289
C,0,-2.9421002438,-0.5808732211,0.1366539336
C,0,-2.3557714885,-0.1957898655,-1.1781195106
O,0,-0.4171056454,-1.6770654905,-0.2567330117
C,0,-0.0099869981,-0.5299708357,-0.3087749867

```
C,0,1.1990989641,-0.014659211,0.0634685957
Cl,0,1.6778393985,1.645700764,-0.1802904692
Cl,0,2.5047028432,-1.0745178495,0.46120544
H,0,-0.7256612084,1.331590862,-1.3933405509
H,0,-0.8499013595,1.6992430901,1.1784630271
H,0,-2.747673575,0.1440961519,2.1789734038
H,0,-3.6894145915,-1.3447867447,0.251986326
H,0,-3.0511453668,0.4701225436,-1.6880663075
H,0,-2.1467039877,-1.0439250572,-1.8100890331
```

*Dichloro 2nd TS 4+2 side (similar to 20) HF/6-311+G***

```
E(RHF) = -1262.38833767

 Zero-point correction=                           0.119125 (Hartree/Particle)
 Thermal correction to Energy=                    0.127250
 Thermal correction to Enthalpy=                  0.128195
 Thermal correction to Gibbs Free Energy=         0.084806
 Sum of electronic and zero-point Energies=          -1262.269213
 Sum of electronic and thermal Energies=             -1262.261087
 Sum of electronic and thermal Enthalpies=           -1262.260143
 Sum of electronic and thermal Free Energies=        -1262.303532

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
 Total                  79.851             29.940             91.320

 C,0,2.3649386128,0.0806382791,-1.0963048042
 C,0,1.1304240588,0.7657106463,-0.5166172827
 C,0,1.4471991309,0.9095226382,0.8974596847
 C,0,2.4403867058,0.013511027,1.2625788247
 C,0,2.8660846367,-0.6166308228,0.1178715488
 C,0,0.0510825423,-0.4318544736,-0.3339374647
 C,0,-1.2129468565,-0.048098744,-0.0320510671
 O,0,0.5405082105,-1.5548118444,-0.4049177412
 Cl,0,-2.4794964191,-1.2167088092,0.102314631
 Cl,0,-1.75602251,1.6097583567,0.0071474722
 H,0,0.7358435011,1.6271671005,-1.0252395583
 H,0,0.8943787038,1.5399235053,1.5684256778
 H,0,2.7260123919,-0.2349839478,2.2646414065
 H,0,3.5316953539,-1.4596498001,0.0920789537
 H,0,3.0997935825,0.8285577864,-1.3922125132
 H,0,2.1690195935,-0.5811534991,-1.923204428
```

*Dichloro 2nd TS 2+2 side (similar to 21) HF/6-311+G***

```
E(RHF) = -1262.38830671

 Zero-point correction=                           0.119156 (Hartree/Particle)
 Thermal correction to Energy=                    0.127162
 Thermal correction to Enthalpy=                  0.128106
 Thermal correction to Gibbs Free Energy=         0.085316
 Sum of electronic and zero-point Energies=          -1262.269151
 Sum of electronic and thermal Energies=             -1262.261145
 Sum of electronic and thermal Enthalpies=           -1262.260200
 Sum of electronic and thermal Free Energies=        -1262.302991

                    E (Thermal)             CV                S
```

	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	79.795	29.921	90.060

```
C,0,-1.1380077056,0.5681330364,-0.7530072254
C,0,-1.2859193538,0.8897092418,0.6667988213
C,0,-2.30164757,0.0923454898,1.235112502
C,0,-2.9212486667,-0.5809542417,0.2372382979
C,0,-2.4258474582,-0.1667784986,-1.1106188497
O,0,-0.3489993486,-1.6884315213,-0.4997273826
C,0,-0.0162263564,-0.5237873552,-0.4510143001
C,0,1.146238375,0.0127641434,0.0802352853
Cl,0,1.6489092016,1.6640317877,-0.1904966004
Cl,0,2.444791557,-1.0426637692,0.5114438999
H,0,-0.8114801585,1.3585410748,-1.4067451001
H,0,-0.706557088,1.6244381535,1.1876254335
H,0,-2.5043681865,0.006515776,2.2836467505
H,0,-3.7029213927,-1.3047223481,0.3811886547
H,0,-3.1444056318,0.5166539769,-1.5599388712
H,0,-2.2752332359,-1.0058216726,-1.7725290866
```

*Dichloro Alternative TS for 2+2 (similar to 10) HF/6-311+G***

E(RHF) = -1262.36481937

Zero-point correction=	0.116821 (Hartree/Particle)
Thermal correction to Energy=	0.125933
Thermal correction to Enthalpy=	0.126877
Thermal correction to Gibbs Free Energy=	0.080630
Sum of electronic and zero-point Energies=	-1262.247999
Sum of electronic and thermal Energies=	-1262.238886
Sum of electronic and thermal Enthalpies=	-1262.237942
Sum of electronic and thermal Free Energies=	-1262.284189

	E (Thermal)	CV	S
	KCal/Mol	Cal/Mol-Kelvin	Cal/Mol-Kelvin
Total	79.024	31.865	97.335

```
C,0,-0.3981850567,-0.5500081603,-1.5463275133
C,0,-1.3828712813,0.4374893514,-1.4461277785
C,0,-2.6099173396,-0.090465513,-0.9366750363
C,0,-2.475052276,-1.4254865237,-0.8504044741
C,0,-1.1267926341,-1.8704585507,-1.310822754
C,0,0.9562122776,-0.5208931241,-0.2351820141
O,0,1.6378239868,-1.459033611,-0.4644381881
C,0,0.913927708,0.4742774055,0.6692806606
Cl,0,-0.208035515,1.7871798329,0.8056770301
Cl,0,2.157942764,0.4786112743,1.8869433594
H,0,0.306786186,-0.4630915282,-2.3555747702
H,0,-1.2498720362,1.4568441589,-1.7516205867
H,0,-3.4722842069,0.4907420479,-0.6776580604
H,0,-3.2286777772,-2.1010413713,-0.4877397645
H,0,-1.2267749043,-2.4227168331,-2.2444930341
H,0,-0.6441207771,-2.5336457198,-0.604401443
```

*TS for Claisen Rearrangment of allyl vinyl ether, mPW1K/6-31+G***

Key distances: OC 1.825, CC 2.184

E(RmPW+HF-PW91) = -270.389380845

```
Zero-point correction=                           0.120500 (Hartree/Particle)
Thermal correction to Energy=                    0.126232
Thermal correction to Enthalpy=                  0.127177
Thermal correction to Gibbs Free Energy=         0.091690
Sum of electronic and zero-point Energies=           -270.268881
Sum of electronic and thermal Energies=              -270.263149
Sum of electronic and thermal Enthalpies=            -270.262204
Sum of electronic and thermal Free Energies=         -270.297691

                    E (Thermal)             CV                S
                     KCal/Mol        Cal/Mol-Kelvin    Cal/Mol-Kelvin
Total                   79.212             21.610             74.688

O,0,-0.4774594235,-1.3392553893,-0.2378251765
C,0,-1.2592878654,-0.461813222,0.26394953
C,0,-1.4046418704,0.7910674689,-0.2853067918
C,0,0.6073832701,1.3947358465,0.3122547977
C,0,1.3455826717,0.4078040883,-0.3055530973
C,0,1.2453553554,-0.8999866429,0.1743490414
H,0,-1.1828373484,0.9440173297,-1.3290637997
H,0,-2.0813874064,1.496383404,0.1775627533
H,0,0.5648279225,2.3919128808,-0.1027295502
H,0,0.4132441124,1.3402381199,1.3732262562
H,0,1.6578484472,0.5539569802,-1.3301358862
H,0,1.7328175019,-1.702989759,-0.3556132129
H,0,1.1525690902,-1.0638749375,1.2381523782
H,0,-1.6437562989,-0.6364461363,1.2730415931
```

Programs for Trajectories Calculations

The programs below are either Unix shell scripts or awk programs. Gaussian98 or Gaussian03 were used to calculate the forces at each point in trajectories.

An older version of the program used for dynamics was initially described in Supporting Information for a previous publication (3). The latest version of this program may be obtained for free by emailing D. Singleton: singleton@mail.chem.tamu.edu

1. Program progdynstarterHP

```
#!/bin/tcsh
# This is the master control program for dynamics, in the form of a Unix
Shell Script.
#
# Necessary input files:
# freqinHP          - This is the standard output from a Gaussian 98 or 03
frequency calculation using freq=hpmodes.
# progdyn.conf — This is a file giving a variety of configuration options,
called on by many of the subprograms.
#
# Optional input:
# isomernumber     - A number in file isomernumber provides a start for
numbering runs.
# detour — A signal file that, by existing, signals the program to do a side
calculations
```

```
# nogo – A signal file that, by existing, signals the program to stop between
points
#
# Programs called:
#  proggenHP     - An awk program that starts a trajectory, giving each mode
its zero point energy plus random additional excitations depending on the
temperature.
#  prog1stpoint – Awk program that creates the first Gaussian input file for
each run
#  prog2ndpoint – Awk program that creates the second Gaussian input file for
each run
#  progdynb – Creates subsequent Gaussian input files until run is completed,
used the awk
# proganal – A program to analyze the latest point and see if a run is done.
# randgen – A program that generates random numbers between 0 and 1.  These
are generated all at once and stored in a file for use by proggenHP.
#
# Output files
# isomernumber – A running tab of the run number
# geoRecord – A record of all the starting positions and velocities.
# geoPlusVel – Created by proggen, this gives starting position and
velocities for current run.
# g03.com – Created by prog1stpoint, prog2ndpoint, and progdynb, this is the
latest input
#       file for Gaussian03 for current run and latest point.
# olddynrun and olderdynrun – files containing the last two outputs from
Gaussian, for creation
# of the next point
# dyn  - A record of all of the Gaussian outputs.
# dynfollowfile – A short record of the runs and their results.
# skipstart - A signal file that, by existing, tells progdynstarter that we
are in the middle of a run.
# A number of files starting with 'temp' are created then later erased.


#!/bin/bash
#progdynstarterHP, made to use high=precision modes from Gaussian freq output
#updated to create a random number file temp811 that is used by proggenHP
#version September 16, 2005, made for Cosmos

#                                        OUTLINE
# A. initilize to perform Gaussian jobs and know where we are
#    start loop
# B. if no file named "skipstart" then generate a new isomer.  Get rid of
skipstart to start new isomer.
#
#  AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
origdir=`pwd`
export g03root=/usr/local/g03/c02.scsl
source $g03root/g03/bsd/g03.profile

rm -f nogo    # assume that if someone is starting a job, they want it to go.
rm -f diagnostics # contains extra info from start of progFS

while (true)
do
#  BBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBBB
if (test -f skipstart) then
```

```
  echo "skipping start and continuing from previous runs"
else
# change from older versions - freqin and most other files are in origdir.
Advantage is compartmentalization.
# Also allows separate configurations for separate runs, so we can move to
using config files.
# Disadvantage is multiple copies of files.
   cd $origdir
   echo 3 > runpointnumber
   randgen > temp811
# lets keep the next 8 lines as the only difference between progdynstarter
and progdynstarterHP
    awk '/        1         2         3         4/,/Harmonic frequencies/
{print}' freqinHP > temp401
    awk '/Frequencies --/ {print $3;print $4;print $5;print $6;print $7}'
temp401 > tempfreqs
    awk '/Reduced masses/ {print $4;print $5;print $6;print $7;print $8}'
temp401 > tempredmass
    awk '/Force constants/ {print $4;print $5;print $6;print $7;print $8}'
temp401 > tempfrc
    awk '/0/ && ((length($1) < 2) && ($1 < 4)) {print}' temp401 > tempmodes
    awk '/has atomic number/ {print}' freqinHP > tempmasses
    awk '/Standard orientation:/,/tional const/ {if ($3==0) print}' freqinHP
> tempstangeos
    awk -f proggenHP freqinHP > geoPlusVel
   if (test -f isomernumber) then
      cp isomernumber temp533
      awk 'BEGIN {getline;i=$1+1;print i}' temp533 > isomernumber
      rm temp533
   else
      echo 1 > isomernumber
   fi
   rm g03.com
   awk -f prog1stpoint geoPlusVel > g03.com
# TO DO - put error checking in prog1stpoint, prog2ndpoint, and progdynb  so
no g03.com unless things are ok
   if (test -s g03.com) then
      rm tempfreqs tempredmass tempfrc tempmodes tempstangeos tempmasses
temp401 temp811
      cat isomernumber >> geoRecord
      cat geoPlusVel >> geoRecord
      cat g03.com
      rm -f goingwell
      cd $TMPDIR
      $g03root/g03/g03 < $origdir/g03.com > $origdir/g03.log
      cd $origdir
      grep 'Normal termination' g03.log > goingwell
      if (test -s goingwell) then
         cat g03.log >> dyn
         cp g03.log olderdynrun
      else
         break
      fi
   else
      break
   fi
   rm g03.com
   awk -f prog2ndpoint g03.log > g03.com
```

```
   if (test -s g03.com) then
      rm -f goingwell
      cd $TMPDIR
      $g03root/g03/g03 < $origdir/g03.com > $origdir/g03.log
      cd $origdir
      grep 'Normal termination' g03.log > goingwell
      if (test -s goingwell) then
         cp g03.log olddynrun
         cat g03.log >> dyn
# old program progdyn replaced here with commands from progdyn
         awk '/Input orientation/,/Distance matrix/ {print}' olddynrun >
temp101
         awk '/   0   / {print}' temp101 > old
         awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun >
temp102
         awk '/   0   / {print}' temp102 > older
         awk -f progdynb olddynrun > g03.com
         rm -f temp101 temp102 old older tempchk
      else
         break
      fi
   else
      break
   fi
# we've just completed a start, so lets skipstart until instructed otherwise
   echo "skipping start" > skipstart
fi

while (true)
do
#increment runpointnumber
   if (test -f runpointnumber) then
      cp runpointnumber temp533
      awk 'BEGIN {getline;i=$1+1;print i}' temp533 > runpointnumber
      rm temp533
   else
      echo 4 > runpointnumber
   fi
# this loop always starts with a g03.com in place - because of the loss of
former program progdyn, I
# may have to worry about how each it is to restart from a bad run
   rm -f goingwell
   cd $TMPDIR
   $g03root/g03/g03 < $origdir/g03.com > $origdir/g03.log
   cd $origdir
   grep 'Normal termination' g03.log > goingwell
   if (test -s goingwell) then
      cp olddynrun olderdynrun
      cp g03.log olddynrun
# old program progdyn replaced here too
      awk '/Input orientation/,/Distance matrix/ {print}' olddynrun > temp101
      awk '/   0   / {print}' temp101 > old
      awk '/Input orientation/,/Distance matrix/ {print}' olderdynrun >
temp102
      awk '/   0   / {print}' temp102 > older
      awk -f progdynb olddynrun > g03.com
      rm -f temp101 temp102 old older tempchk
#     cat g03.log >> dyn
```

```
   else
      break
   fi

# here is a cool link that lets you interupt the dynamics with a short job,
then
# it automatically goes back to the dynamics  just make the file 'detour' and
it
# will delete detour, run run.com, then go back to dynamics
   if (test  -f detour) then
      rm detour
      date >> docslog
      cat run.com >> docslog
      cp run.log temp.log
      cd $TMPDIR
      $g03root/g03/g03 < $origdir/run.com > $origdir/run.log
      cd $origdir
   fi

#stop it all nicely by creating a nogo file
   if (test  -f nogo) then
      break
   fi

#figure out if this isomer is done
   awk -f proganal g03.log >> dynfollowfile
   rm -f tempdone
   awk -f proganal g03.log > temp281
   awk '/XXXX/ {print}' temp281 > tempdone
   rm temp281
   if (test  -s tempdone) then
      rm -f skipstart
      rm -f olddynrun
      rm -f olderdynrun
      rm -f geoPlusVel
      break
   fi
done

# We've got to break a second time to get out of this loop
# if we really want to quit.  Otherwise, it will start over
# at the top
if (test  -f nogo) then
   break
fi
if (test  -s goingwell) then
   echo "probably starting a new point"
else
   break
fi
done
exit 0
```

2. Program proggenHP

```
BEGIN {
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.
   i=1;j=1;k=1
# Danger — initialDis seems really attractive but it can go wrong for low-
energy rotational
#modes, whose excitation has the effect of stretching the bonds.  Check for
reasonable starting
#structures
#
#
# version Sept 16, 2005 - incorportates searchdir but not yet rotation
# now reads random numbers from temp811, starting at a random place
# The input files are generated before this and are tempfreqs, tempredmass,
# tempfrc, tempmodes, and tempstangeos.
# It will count the number of atoms.

# Gets from progdyn.conf
# timestep, scaling, temp, and initialdis.
# default values
initialDis=0
timeStep=1E-15
scaling=1.0
temp=298.15

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
   getline < "progdyn.conf"
   if ($1=="method") method=$2
   if ($1=="charge") charge=$2
   if ($1=="multiplicity") multiplicity=$2
   if ($1=="memory") memory=$2
   if ($1=="processors") processors=$2
   if ($1=="checkpoint") checkpoint=$2
   if ($1=="diagnostics") diag=$2
   if ($1=="initialdis") initialDis=$2
   if ($1=="timestep") timeStep=$2
   if ($1=="scaling") scaling=$2
   if ($1=="temperature") temp=$2
   if ($1=="searchdir") searchdir=$2
   if ($1=="title") {
      title1=$2
      title2=$3
      title3=$4
      title4=$5
      }
   blankLineTester=length($0)
   }

if (diag==1) print "***************** starting proggen ****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print
"processors,checkpoint,title,initialdis,timestep,scaling,temperature" >>
"diagnostics"
```

```
if (diag==1) print
processors,checkpoint,title1,title2,title3,title4,initialDis,timeStep,scaling
,temp >> "diagnostics"

i=1;j=1;k=1
c=29980000000
h=6.626075E-34
avNum=6.02E23
numAtoms=0

# put geometries into array, also figure out number of atoms
# note that this picks out the last geometry in a file, assuming
# that if there is an optimization followed by a freq, nothing else follows
# kludgy - repeats last line twice - must be a better way
do {
   getline < "tempstangeos"
   if (oldline==$0) $0=""
   oldline=$0
   atom = $1
   if (atom>numAtoms) numAtoms=atom
   atNum[atom]=$2
   geoArr[atom,1]=$4
   geoArr[atom,2]=$5
   geoArr[atom,3]=$6
   velArr[atom,1]=0
   velArr[atom,2]=0
   velArr[atom,3]=0
   }
while (length($0) > 0)

#output the number of atoms - this will help in reading the file later
print numAtoms

# put in atomic symbols and atomic weights - this will have to be edited for
isotopic labeling
for (i=1;i<=numAtoms;i++) {
   getline < "tempmasses"
   atWeight[i]=$9
   if (atNum[i]==6) atSym[i]="C"
   if (atNum[i]==1) atSym[i]="H"
   if (atNum[i]==8) atSym[i]="O"
   if (atNum[i]==7) atSym[i]="N"
   if (atNum[i]==5) atSym[i]="B"
   if (atNum[i]==9) atSym[i]="F"

#   print atNum[i],atSym[i],atWeight[i],geoArr[i,1],geoArr[i,2],geoArr[i,3]
   }

# read in frequencies, scale them, read in Reduced masses, read in force
#constants, replace negative frequencies by 10
numFreq=3*numAtoms-6
for (i=1;i<=numFreq;i++) {
   getline < "tempfreqs"
   freq[i]=$0*scaling
   if (freq[i]<0) freq[i]=10
   }
for (i=1;i<=numFreq;i++) {
   getline < "tempredmass"
```

```
   redMass[i]=$0
   }
for (i=1;i<=numFreq;i++) {
   getline < "tempfrc"
   frc[i]=$0
#   print freq[i],redMass[i],frc[i]
   }

# read in the modes
#the next 10 lines are commented for low precision modes, uncommented for
high precision modes
for (i=1;i<=numFreq;i+=5) {
   for (j=1;j<=(3*numAtoms);j++) {
      getline < "tempmodes"
      mode[i,$2,$1]=$4
      mode[i+1,$2,$1]=$5
      mode[i+2,$2,$1]=$6
      mode[i+3,$2,$1]=$7
      mode[i+4,$2,$1]=$8
      }
   }
#the next 14 lines are uncommented for low precision modes, commented for
high precision modes
#for (i=1;i<=numFreq;i+=3) {
#  for (j=1;j<=numAtoms;j++) {
#     getline < "tempmodes"
#     mode[i,j,1]=$3
#     mode[i,j,2]=$4
#     mode[i,j,3]=$5
#     mode[i+1,j,1]=$6
#     mode[i+1,j,2]=$7
#     mode[i+1,j,3]=$8
#     mode[i+2,j,1]=$9
#     mode[i+2,j,2]=$10
#     mode[i+2,j,3]=$11
#     }
#  }
for (i=1;i<=numFreq;i++) {
#  print mode[i,1,1],mode[i,1,2],mode[i,1,3]
   }

#convert freqs to units used in spreedsheat, pick a random number,
#and decide vibrational quantum state and energy
srand()
# want to read from temp811, starting at a random place
tester=rand()*1000
for (i=1;i<=tester;i++) {
   getline < "temp811"
   }
for (i=1;i<=numFreq;i++) {
   getline < "temp811"
   randArr[i]=$1
   getline < "temp811"
   randArrB[i]=$1
   getline < "temp811"
   randArrC[i]=$1
}
for (i=1;i<=numFreq;i++) {
```

```
   zpeJ[i]=0.5*h*c*freq[i]
   zpeK[i]=zpeJ[i]*avNum*0.239/1000
#program so that if the temp is too low, it just acts like 0 K
   if (temp<10) {
      vibN[i]=0
      }
   if (temp>=10) {
      zpeRat[i]=exp((-2*zpeK[i])/(0.001987*temp))
      Q[i]=1/(1-zpeRat[i])
      newRand=randArr[i]
#     print newRand
      vibN[i]=0
      tester=1/Q[i]
      for (j=1;j<=(50*zpeRat[i]+2);j++) {
         if (newRand>tester) vibN[i]++
         tester=tester+((zpeRat[i]^j)/Q[i])
         }
      }
   }

# figure out mode energies and maximum classical shift and then
# actual shift
for (i=1;i<=numFreq;i++) {
   modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i]+1)
# no 1/2 hv for imaginary frequencies
# treating modes with frequencies <15 as translations, ignoring their zero
point energies
   if (freq[i]<15) modeEn[i]=(zpeJ[i]*1E18)*(2*vibN[i])
   maxShift[i]=(2*modeEn[i]/frc[i])^0.5
   if (initialDis==1) shift[i]=maxShift[i]*(2*(randArrC[i]-0.5))
   if (initialDis==0) shift[i]=0
# no displacements along imaginary frequencies and very low ones - it is
better to treat these
# as translations - employing a shift can give you initial weird geometries
   if (freq[i]<15) shift[i]=0
   }
for (i=1;i<=numFreq;i++) {
#   print
zpeJ[i],zpeK[i],zpeRat[i],Q[i],vibN[i],modeEn[i],maxShift[i],shift[i]
   }

# multiply each of the modes by its shift and add them up
for (i=1;i<=numFreq;i++) {
   for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
         shiftMode[i,j,k]=mode[i,j,k]*shift[i]
         geoArr[j,k]=geoArr[j,k]+shiftMode[i,j,k]
         }
      }
   }

#output the new geometry.
for (j=1;j<=numAtoms;j++) {
   print atSym[j],geoArr[j,1],geoArr[j,2],geoArr[j,3],atWeight[j]
   }

#now start toward velocities
for (i=1;i<=numFreq;i++) {
```

```
   kinEn[i]=100000*(modeEn[i]-0.5*frc[i]*shift[i]^2)
   vel[i]=(2*kinEn[i]/(redMass[i]/avNum))^0.5
#it is tricky here to set the velocities for modes along reaction coordinate
#I think I would like to have them all going the same direction, but setting
#the right direction is difficult.  I guess the thing to do is pick one
direction
#and go with it, and if there is a problem the program will have to be
changed here.
#use searchdir in progdyn.conf to change directions
   if (freq[i]>15) {
      if (randArrB[i]<0.5) vel[i]=-vel[i]
      }
   if (freq[i]<15) {
      if (searchdir=="negative") vel[i]=-vel[i]
      }
#   print vel[i]
   }

# multiply each of the modes by its velocity and add them up
for (i=1;i<=numFreq;i++) {
   for (j=1;j<=numAtoms;j++) {
      for (k=1;k<=3;k++) {
         velMode[i,j,k]=mode[i,j,k]*vel[i]*timeStep
         velArr[j,k]=velArr[j,k]+velMode[i,j,k]
         }
      }
   }

#output the velocities.  The markers let a later program grab these
velocities.
for (j=1;j<=numAtoms;j++) {
   print velArr[j,1],velArr[j,2],velArr[j,3]
   }

#anything else I add to the file is not going to be read but will be useful
#for error checking
for (i=1;i<=numFreq;i++) {
   print randArr[i],vibN[i],vel[i]
   }
print "temp ",temp
print "initialDis",initialDis
print "timeStep",timeStep

}
```

3. Program prog1stpoint

```
BEGIN {
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not
yet methodfile or rotation
# this program creates the first input file for g03
# the title should be changed as appropriate
# the isomer number comes from a file isomernumber

# read progdyn.conf for configuration info
```

```
blankLineTester=10
while (blankLineTester>1) {
   getline < "progdyn.conf"
   if ($1=="method") method=$2
   if ($1=="method2") meth2=$2
   if ($1=="charge") charge=$2
   if ($1=="multiplicity") multiplicity=$2
   if ($1=="memory") memory=$2
   if ($1=="processors") processors=$2
   if ($1=="checkpoint") checkpoint=$2
   if ($1=="diagnostics") diag=$2
   if ($1=="method3") meth3=$2
   if ($1=="method4") meth4=$2
   if ($1=="method5") meth5=$2
   if ($1=="method6") meth6=$2
   if ($1=="title") {
      title1=$2
      title2=$3
      title3=$4
      title4=$5
      }
   blankLineTester=length($0)
   }

if (diag==1) print "***************** starting prog1stpoint
*****************" >> "diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >>
"diagnostics"

getline < "isomernumber"
isomernum = $1
print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint 1"
print "runisomer ", isomernum
print ""
print charge,multiplicity
}

(/C / || /H / || /O / || /N / || /B / || /F /) {
   printf("%s %.7f %.7f %.7f",$1,$2,$3,$4)
   print ""
   }

END {
print ""
```

```
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
print ""
}
```

4. Program prog2ndpoint

```
BEGIN {
# version Sept 9, 2005 - incorportates meth3, meth4, meth5, meth6, but not
yet methodfile or rotation
# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
   getline < "progdyn.conf"
   if ($1=="method") method=$2
   if ($1=="method2") meth2=$2
   if ($1=="charge") charge=$2
   if ($1=="multiplicity") multiplicity=$2
   if ($1=="memory") memory=$2
   if ($1=="processors") processors=$2
   if ($1=="checkpoint") checkpoint=$2
   if ($1=="diagnostics") diag=$2
   if ($1=="method3") meth3=$2
   if ($1=="method4") meth4=$2
   if ($1=="method5") meth5=$2
   if ($1=="method6") meth6=$2
   if ($1=="title") {
      title1=$2
      title2=$3
      title3=$4
      title4=$5
      }
   blankLineTester=length($0)
   }

if (diag==1) print "***************** starting prog2ndpoint
*****************" >> "diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >>
"diagnostics"

# TO DO : move timestep to progdyn.conf
i=1;j=1;k=1
timestep=1E-15
avNum=6.02E23

#get the isomer number from file
getline < "isomernumber"
isomernum = $1

print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "#p " method " force scf=(tight,nosym) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
```

```
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check,
sometimes faster, sometimes not
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
print ""
# make the title four words exactly, leaving out spaces if necessary
print title1,title2,title3,title4
print "runpoint 2"
print "runisomer ", isomernum
print ""
print charge,multiplicity

# ok, now we have to figure the second point.  this should be
# x(t) = x + v*t + 1/2*F*t^2/m
# so we need to set up arrays for position, velocity, and force
getline < "geoPlusVel"
numAtoms=$1
# first the geometry
for (i=1;i<=numAtoms;i++) {
   getline < "geoPlusVel"
   weight[i]=$5
   atSym[i]=$1
   for (j=1;j<=3;j++) {
      arr[i,j]=$(1+j)
      }
   }
#now we go ahead and add the velocities
for (i=1;i<=numAtoms;i++) {
   getline < "geoPlusVel"
   for (j=1;j<=3;j++) {
      arr[i,j]=$j+arr[i,j]
      }
#   print arr[i,1],arr[i,2],arr[i,3]
   }
# first end the BEGIN
}
# now we go ahead and translate the forces and add them
(/          6    / || /          1    / || /          8    / || /          9
/) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
   forceArr[i,j]=$(2+j)
   }
#   print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]
}

END {
# turn the forces into motion
for (i=1;i<=numAtoms;i++) {
   for (j=1;j<=3;j++) {

forceArr[i,j]=0.5*1E10*forceArr[i,j]*627.509*(4184/(0.5292*avNum))*1E10*(time
step^2)/(weight[i]/(avNum*1000))
      arr[i,j]=arr[i,j]+forceArr[i,j]
      }
#   print forceArr[i,1],forceArr[i,2],forceArr[i,3]
   printf("%s %.7f %.7f %.7f",atSym[i],arr[i,1],arr[i,2],arr[i,3])
```

```
   print ""
   }
print ""
if (length(meth5)>2) print meth5
if (length(meth6)>2) print meth6
print ""
}
```

5. Program progdynb

```
BEGIN { #this is the main routine for generating new .com files by the Verlet
algorithym
# version Sept 11, 2005 - incorportates meth3, meth4, meth5, meth6, but not
yet methodfile or rotation

# read progdyn.conf for configuration info
blankLineTester=10
while (blankLineTester>1) {
   getline < "progdyn.conf"
   if ($1=="method") method=$2
   if ($1=="method2") meth2=$2
   if ($1=="charge") charge=$2
   if ($1=="multiplicity") multiplicity=$2
   if ($1=="memory") memory=$2
   if ($1=="processors") processors=$2
   if ($1=="checkpoint") checkpoint=$2
   if ($1=="diagnostics") diag=$2
   if ($1=="method3") meth3=$2
   if ($1=="method4") meth4=$2
   if ($1=="method5") meth5=$2
   if ($1=="method6") meth6=$2
   if ($1=="title") {
      title1=$2
      title2=$3
      title3=$4
      title4=$5
      }
   blankLineTester=length($0)
   }

if (diag==1) print "***************** starting progdynb *****************" >>
"diagnostics"
if (diag==1) print "method,charge,multiplicity,memory" >> "diagnostics"
if (diag==1) print method,charge,multiplicity,memory >> "diagnostics"
if (diag==1) print "processors,checkpoint,title" >> "diagnostics"
if (diag==1) print processors,checkpoint,title1,title2,title3,title4 >>
"diagnostics"

OFS="     ";i=1;j=1;k=1
# TO DO - move timestep to progdyn.conf
timestep=1E-15
avNum=6.02E23

# get number of atoms and weights from geoPlusVel
getline < "geoPlusVel"
numAtoms=$1
```

```
for (i=1;i<=numAtoms;i++) {
   getline < "geoPlusVel"
   weight[i]=$5
   atSym[i]=$1
   }

for (at=1;at<=numAtoms;at++) {
   getline < "old"
   oldarr[at,1]=$4
   oldarr[at,2]=$5
   oldarr[at,3]=$6
   }

for (at=1;at<=numAtoms;at++) {
   getline < "older"
   olderarr[at,1]=$4
   olderarr[at,2]=$5
   olderarr[at,3]=$6
   }
}

#must adjust next line for weird atoms
(/          6    / || /          1    / || /          8    / || /          7
/ || /          9    /) && length($3) > 9 {
i=$1
for (j=1;j<=3;j++) {
   forceArr[i,j]=$(2+j)
   }
#  print i,weight[i],forceArr[i,1],forceArr[i,2],forceArr[i,3]
}

END {
for (i=1;i<=numAtoms;i++) {
   for (j=1;j<=3;j++) {

forceArr[i,j]=1E10*forceArr[i,j]*627.509*(4184/(0.5292*avNum))*1E10*(timestep
^2)/(weight[i]/(avNum*1000))
      arr[i,j]=arr[i,j]+forceArr[i,j]
      }
   }
getline < "isomernumber"
isomernum = $1
getline < "runpointnumber"
runpointnum = $1
print "%nproc=" processors
print "%mem=" memory
print "%chk=" checkpoint
print "# " method " force scf=(maxcycle=200) "
#print "IOp(3/76=0572004280)" #for mPW1K in g03
if (meth2=="unrestricted") print "guess=mix" #for unrestricted calculations
if (meth2=="read") print "guess=tcheck" #for reading orbitals from check,
sometimes faster, sometimes not
print "pop=none "
if (length(meth3)>2) print meth3
if (length(meth4)>2) print meth4
#print "pop=none IOP(2/9=10,6/12=2)" #old IOPs for g98
print ""
print  title1,title2,title3,title4
```

```
print "runpoint ",runpointnum
print "runisomer ",isomernum
print ""
print charge,multiplicity
for (i=1;i<=numAtoms;i++) {
   for (j=1;j<=3;j++) {
      newarr[i,j]=2*oldarr[i,j]-olderarr[i,j]+forceArr[i,j]
      }
   printf("%s %.7f %.7f %.7f",atSym[i],newarr[i,1],newarr[i,2],newarr[i,3])
   print ""
   }
   print ""
   if (length(meth5)>2) print meth5
   if (length(meth6)>2) print meth6
   print ""
}
```

6. Program randgen

```
# c program
# this can be replaced by a more reliable random number
# generator when available on a system
#include <stdio.h>
#include <stdlib.h>

int a,b,c;
double d;

int product(int x, int y);

int main(void)
{
   int count=1;
   srand48(time (0));
   while (count<=10000)
   {
      d = drand48();
      printf ("%.20f\n", d);
      count++;
   }
   return 0;
}
```

7. Program proganal

```
# pronounced pro-ganal
# this program requires serious rewriting for new molecules
# or for reordered atoms
#  sept 9, 2005
/ diphenylketene BBdis/ {
   printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
   runpoint=$8
   }
```

```
/    1  C    0.000000/,/     6  O    0.000000/ {
   if (($1==6) && ($2=="O") && ($3>.5)) {
      C4O6=$6
      }
   }
/    1  C    0.000000/,/     6  O    0.000000/ {
   if (($1==7) && ($2=="C") && ($3>.5)) {
      C1C7=$3
      }
   }
/    1  C    0.000000/,/     6  O    0.000000/ {
   if (($1==8) && ($2=="C") && ($3>.5)) {
      C2C8=$4
      }
   }
END {
      printf("%s %.3f  %s %.3f %s %.3f ","4+2 ",C4O6,"  SM ",C1C7," 2+2
",C2C8)
      if (runpoint>500) {
         print "   Too many points.  XXXX"
         }
      if ((C1C7<1.7) && (C2C8<1.7)) {
         print "   XXXX Formed 2+2 Product Look at this file XXXX"
         }
      if ((C1C7<1.7) && (C4O6<1.7)) {
         print "   Formed 4+2 Product XXXX"
         }
      if (C1C7>2.4)  {
         print "    Returned to SM XXXX"
         }
     print " "
   }
```

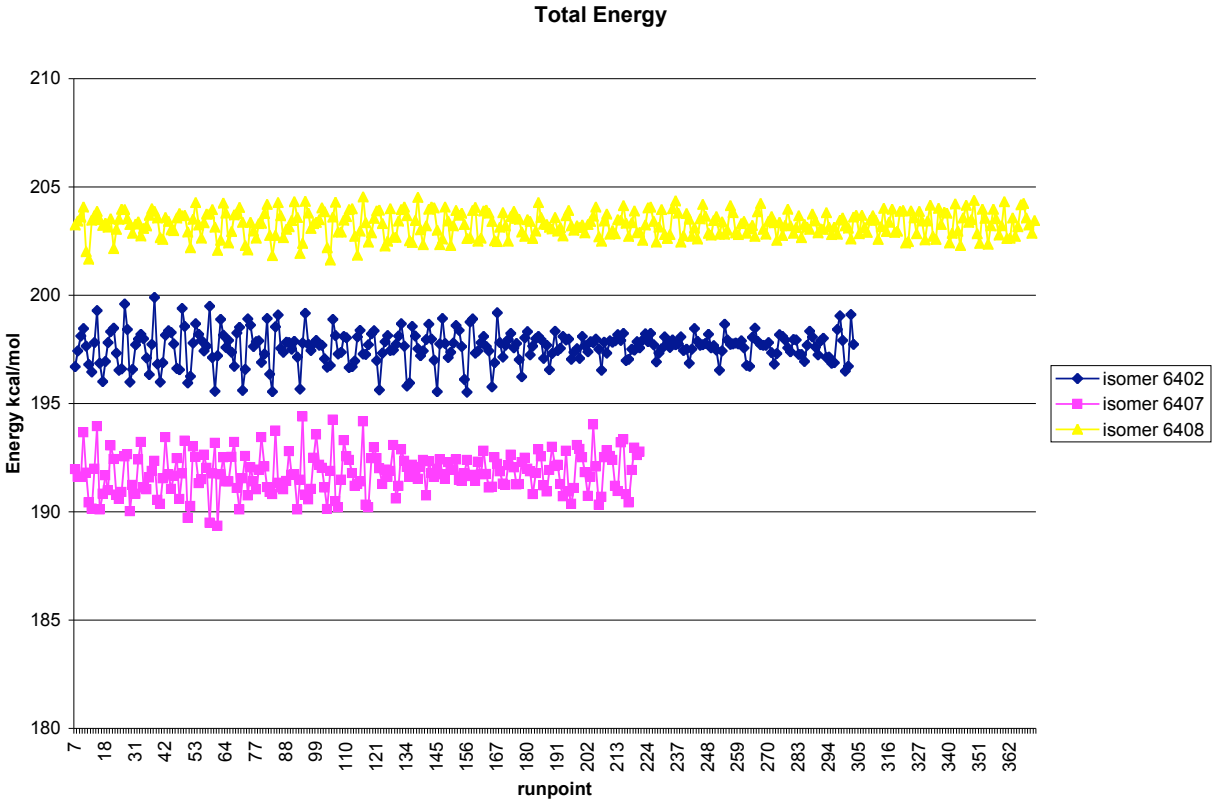
8. progdyn.conf

```
conf file for dynamics.  This is read by awk programs prog1stpoint,
prog2ndpoint, and progdynb.
The programs won't read anything past the first blank line,
and this file must end with a blank line.  You can add to these comments but
don't use keywords as the first word on a line.  Don't delete lines - the
program
has no built in default values if they aren't here.
values here are read repeatedly and can be changed in the middle of runs
```

```
method B3LYP/6-31G*
method2 restricted #The options here are restricted, unrestricted, and read.
#If the method is U..., put unrestricted here and the .com files will have in
them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which
sometimes makes things faster, sometimes not.
charge 0
multiplicity 1
memory 80000000
checkpoint g98.chk #uses one checkpoint file repeatedly
processors 2
diagnostics 1 # 1 prints out extra stuff to a file "diagnostics"
title diphenylketene BB 273.15 dis # the title must be exactly four words
initialdis 0
timestep 1E-15
scaling 1.0
temperature 0
#add extra lines to .com files to implement things like the iop for mPW1k
#Leave the second word blank if you are not going to use them. otherwise any
word you put in will end up in the com file
#only a single term with no spaces can be added, one per method line
method3
method4
#method5 and method6 are placed at the end of the file instead of in the
keyword section
method5
method6
#searchdir says what direction to follow the mode associated with the
imaginary frequency.
#put as values the words "negative" or "positive"
searchdir negative
#to be implemented:
#for more complicated ends of .com files, it will have to learn to use a file
methodfile
rotation 0 #use 1 to turn on rotational modes
#since displacements run into a problem with easy rotation modes such as a
methyl group,
#it would be easy to turn off displacements for particular modes.  Sometimes
this would be
#the right thing to do but it would be awkward to explain it in a paper.
numberlimitedmodes 0
limitedmodes 3 5

#updated Sept 9, 2005 and believed to incorporate everything as of that date
```

Energy Conservation in Trajectories

The graph below illustrates the conservation of energy in the trajectories employing the Verlet algorithm, but giving the total of potential energy plus kinetic energy for three long trajectories at varying energies. Overall, the energy doesn't change significantly across a run, which is the key observation. There is some apparent oscillation, which is due to a problem in calculating the kinetic energy at each point – velocities are calculated assuming a linear path of atoms from point to point, while the Verlet algorithm propagating the trajectories makes no such assumption and the trajectories taken are actually curved.



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