Supporting Information for:

Computational Investigation of the Mechanism of Addition of Singlet Carbenes to Bicyclobutanes

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Table S1. Enthalpies of transition structures and products in Scheme 5 at levels of theory including geometry optimization (ΔH(0 K), relative to reactants, kcal/mol).

Reaction of **1** and **2**	**Gas-Phase**				**PCM**	
	HF/ 6-31G*	**CBS-4**	**QCISD/ 6-31G***	**CCSD/ 6-31G***	**HF/ 6-31G***	**CBS-4**
TS **17** (A)	12.6	-1.0	2.1	2.1	11.1	-1.1
TS **18** (B)	12.1	0.3	3.3	3.2	10.9	0.1
TS **20** (C)	33.0	18.1	24.8	25.7	31.1	16.2
TS/Int **19**	4.1	-2.3	N/A	-0.3	-3.0	-6.6
product **3**	-94.8	-96.0	-96.6	-97.3	-94.5	-95.6
product **4**	-67.7	-78.9	-75.0	-75.8	-67.6	-78.6

Table S2. Free energies of transition structures and products in Scheme 5 at levels of theory including geometry optimization (ΔG(298 K), relative to reactants, kcal/mol).

Reaction of **1** and **2**	**Gas-Phase**				**PCM**	
	HF/ 6-31G*	**CBS-4**	**QCISD/ 6-31G***	**CCSD/ 6-31G***	**HF/ 6-31G***	**CBS-4**
TS **17** (A)	23.6	9.6	12.9	12.9	22.0	9.3
TS **18** (B)	23.0	10.7	14.0	13.9	21.6	10.4
TS **20** (C)	44.8	28.5	36.7	37.0	42.9	26.6
TS/Int **19**	15.7	9.0	N/A	11.0	8.7	4.6
product **3**	-84.5	-85.9	-86.6	-87.3	-84.2	-85.6
product **4**	-54.8	-66.1	-62.1	-63.0	-54.7	-65.8

Table S3. Enthalpies and free energies of transition structures and products in Scheme 5 from single-point calculations at the CCSD/6-31G* optimized geometries (relative to reactants, kcal/mol; CCSD/6-31G* unscaled thermodynamic corrections; gas-phase).

Reaction of **1** and **2**	**ΔH (0 K)**			**ΔH (298 K)**			**ΔG (298 K)**		
	CC1	**CC2**	**G3**	**CC1**	**CC2**	**G3**	**CC1**	**CC2**	**G3**
TS **17** (A)	-1.1	-3.0	-2.7	-1.5	-3.3	-3.1	9.7	7.9	8.4
TS **18** (B)	0.3	-1.7	-1.0	0.0	-2.0	-1.4	11.0	8.9	9.9
TS **20** (C)	21.5	18.2	15.3	20.9	17.7	14.3	32.8	29.5	27.1
TS/Int **19**	-2.4	-5.4	-5.7	-2.7	-5.7	-6.4	8.9	5.9	6.0
product **3**	-97.2	-96.5	-95.9	-97.3	-96.6	-96.0	-87.2	-86.5	-85.7
product **4**	-76.1	-76.8	-75.1	-77.4	-78.2	-76.5	-63.2	-63.9	-62.2

Notes:

CC1 = CCSD(T)/6-31G*//CCSD/6-31G*.

CC2 = CCSD(T)/6-311+G**//CCSD/6-31G*.

G3 = G3 composite calculation using CCSD/6-31G* optimized geometry.

Table S4. Comparison of QCISD/6-31G* and CCSD/6-31G*enthalpies computed using QCISD/6-31G*, CCSD/6-31G*, and HF/6-31G* geometries (ΔH(0 K), relative to reactants, kcal/mol; gas-phase).

Reaction of **1** and **2**	**QCISD/6-31G*//**		**CCSD/6-31G*//**	
	QCISD/6-31G*	**HF/6-31G***	**CCSD/6-31G***	**HF/6-31G***
TS **17** (A)	2.1	2.2	2.1	2.2
TS **18** (B)	3.3	3.5	3.2	3.5
TS **20** (C)	24.8	23.9	25.7	23.7
TS/Int **19**	N/A	0.8	-0.2	0.5
product **3**	-96.6	-95.9	-97.3	-96.5
product **4**	-75.0	-74.9	-75.8	-75.6

Table S5. Enthalpies and free energies of transition structures and products in Scheme 5 from single-point calculations at the HF/6-31G* optimized geometries (relative to reactants, kcal/mol; HF/6-31G* unscaled thermodynamic corrections; gas-phase).

Reaction of **1** and **2**	**ΔH (0 K)**		**ΔH (298 K)**		**ΔG (298 K)**	
	QCISD(T)	**CCSD(T)**	**QCISD(T)**	**CCSD(T)**	**QCISD(T)**	**CCSD(T)**
TS **17** (A)	-1.6	0.0	-2.0	-1.9	9.5	9.6
TS **18** (B)	0.4	-1.5	0.0	0.0	11.3	11.3
TS **20** (C)	20.8	0.4	19.9	19.8	32.7	32.6
TS/Int **19**	-1.1	-1.3	-1.8	-2.0	10.6	10.4
product **3**	-96.0	-96.3	-96.2	-96.5	-85.8	-86.1
product **4**	-75.7	-76.1	-77.1	-77.5	-62.8	-63.2

Note: Basis set is 6-31G* for all calculations.

Table S6. Calculated bond distances for the incipient C-C bond in transition structures in Scheme 6 (Å).

Reaction of **10** and **2**	**Gas-Phase**				**PCM**	
	HF/ 3-21G*	**HF/ 6-31G***	**QCISD/ 6-31G***	**CCSD/ 6-31G***	**HF/ 3-21G***	**HF/ 6-31G***
TS **21** (A)	2.25	2.05	2.18	2.18	2.30	2.12
TS **22** (B)	2.31	2.11	2.21	2.22	2.36	2.17
TS **23** (C)	2.15	2.06	2.08	2.08	2.20	2.09
TS **24** (D)	2.29	2.07	2.20	2.20	2.34	2.14
TS **25** (E)	2.25	2.03	2.15	2.15	2.30	2.09
TS **26** (F)	2.22	2.00	2.10	2.09	2.27	2.07
TS **27** (G)	2.29	2.09	2.14	2.14	2.34	2.15
Int. **16**	N/A	1.56	N/A	1.62	N/A	1.55

Table S7. Enthalpies of transition structures and products in Scheme 6 at levels of theory including geometry optimization (ΔH(0 K), relative to reactants, kcal/mol).

Reaction of **10** and **2**	**Gas-Phase**				**PCM**	
	HF/ 6-31G*	**CBS-4**	**QCISD/ 6-31G***	**CCSD/ 6-31G***	**HF/ 6-31G***	**CBS-4**
TS **21** (A)	13.8	-3.0	1.8	1.9	12.6	-3.1
TS **22** (B)	11.3	-3.2	0.7	1.1	10.7	-3.0
TS **23** (C)	31.7	11.6	18.8	18.8	30.9	11.1
TS **24** (D)	12.9	-3.1	1.4	1.5	12.0	-3.0
TS **25** (E)	19.7	-1.1	4.8	4.9	18.8	-0.9
TS **26** (F)	22.3	0.9	7.1	7.2	21.1	0.8
TS **27** (G)	17.1	-2.0	4.2	4.1	16.4	-1.8
Int. **16**	0.4	N/A	N/A	-5.6	-5.6	N/A
product **11**	-85.8	-93.1	-90.7	-91.2	-85.4	-92.7
product **12**	-93.0	-94.6	-94.2	-94.9	-92.6	-94.1
product **13**	-80.7	-89.4	-86.9	-87.5	-80.4	-89.0
product **14**	-96.1	-97.5	-97.1	-97.7	-95.7	-97.0
product **15**	-52.6	-69.6	-63.3	-64.1	-52.5	-69.4

Table S8. Free energies of transition structures and products in Scheme 6 at levels of theory including geometry optimization (ΔG(298 K), relative to reactants, kcal/mol).

Reaction of **10** and **2**	**Gas-Phase**				**PCM**	
	HF/ 6-31G*	**CBS-4**	**QCISD/ 6-31G***	**CCSD/ 6-31G***	**HF/ 6-31G***	**CBS-4**
TS **21** (A)	25.8	8.4	13.8	13.9	24.5	8.2
TS **22** (B)	23.1	8.0	12.4	12.8	22.3	8.1
TS **23** (C)	43.9	23.7	31.0	31.0	43.1	23.1
TS **24** (D)	24.6	8.0	13.1	13.2	23.6	8.1
TS **25** (E)	32.1	10.7	17.2	17.3	31.1	10.7
TS **26** (F)	34.6	12.6	19.5	19.5	33.3	12.5
TS **27** (G)	29.3	9.5	16.3	16.3	28.5	9.6
Int. **16**	12.1	N/A	N/A	6.0	6.1	N/A
product **11**	-74.3	-81.4	-79.1	-79.7	-73.9	-81.1
product **12**	-82.8	-84.6	-84.1	-84.7	-82.5	-84.2
product **13**	-68.6	-77.3	-74.9	-75.5	-68.4	-77.0
product **14**	-85.6	-87.1	-86.6	-87.3	-85.2	-86.6
product **15**	-39.5	-56.6	-50.2	-51.0	-39.5	-56.4

Note: For QCISD/6-31G* and CCSD/6-31G*, the zero-point energy and thermal corrections are derived from the corresponding HF/6-31G* optimizations and frequency calculations.

Table S9. Enthalpies and free energies of transition structures and products in Scheme 6 from single-point calculations at the CCSD/6-31G* optimized geometries (relative to reactants, kcal/mol; CCSD/6-31G* unscaled thermodynamic corrections; gas-phase).

Reaction of **10** and **2**	**ΔH (0 K)**			**ΔH (298 K)**			**ΔG (298 K)**		
	CC1	**CC2**	**G3**	**CC1**	**CC2**	**G3**	**CC1**	**CC2**	**G3**
TS **21** (A)	-1.8	-5.7	-4.7	-2.1	-6.0	-5.0	10.2	6.4	7.3
TS **22** (B)	-1.9	-5.8	-4.4	-2.1	-6.0	-4.6	9.8	5.9	7.3
TS **23** (C)	14.5	10.0	9.4	14.2	9.7	9.0	26.6	22.2	21.5
TS **24** (D)	-2.0	-5.9	-4.8	-2.3	-6.1	-5.0	9.7	5.8	6.9
TS **25** (E)	0.4	-4.5	-3.5	0.1	-4.9	-3.9	12.9	7.9	8.9
TS **26** (F)	2.4	-2.6	-1.9	2.0	-3.1	-2.4	14.8	9.7	10.4
TS **27** (G)	0.2	-5.0	-3.7	-0.2	-5.3	-4.1	12.4	7.2	8.5
Int. **16**	-8.1	-13.3	-12.9	-8.1	-13.3	-13.0	3.5	-1.6	-1.3
product **11**	-91.8	-94.7	-93.2	-92.1	-95.0	-93.5	-80.2	-83.2	-81.7
product **12**	-94.8	-94.9	-94.5	-94.6	-94.7	-94.3	-84.6	-84.7	-84.3
product **13**	-88.3	-90.9	-89.8	-88.6	-91.2	-90.1	-76.2	-78.8	-77.8
product **14**	-97.6	-97.6	-97.2	-97.5	-97.5	-97.1	-87.1	-87.1	-86.8
product **15**	-65.0	-68.5	-66.6	-66.0	-69.5	-67.6	-51.9	-55.4	-53.5

Notes:

CC1 = CCSD(T)/6-31G*//CCSD/6-31G*.

CC2 = CCSD(T)/6-311+G**//CCSD/6-31G*.

G3 = G3 composite calculation using CCSD/6-31G* optimized geometry.

Table S10. Enthalpies and free energies of transition structures and products in Scheme 6 from single-point calculations at the HF/6-31G* optimized geometries (relative to reactants, kcal/mol; HF/6-31G* unscaled thermodynamic corrections; gas-phase).

Reaction of **10** and **2**	**ΔH (0 K)**		**ΔH (298 K)**		**ΔG (298 K)**	
	QCISD(T)	**CCSD(T)**	**QCISD(T)**	**CCSD(T)**	**QCISD(T)**	**CCSD(T)**
TS **21** (A)	-2.5	-2.5	-2.8	-2.8	9.5	9.6
TS **22** (B)	-2.7	-2.7	-2.9	-2.9	9.1	9.1
TS **23** (C)	15.2	15.2	14.9	14.9	27.3	27.4
TS **24** (D)	-3.0	-2.9	-3.2	-3.1	8.7	8.8
TS **25** (E)	-0.1	0.0	-0.5	-0.4	12.3	12.4
TS **26** (F)	2.3	2.5	1.9	2.0	14.7	14.8
TS **27** (G)	0.2	0.2	-0.2	-0.1	12.4	12.4
Int. **16**	-7.2	-7.3	-7.2	-7.3	4.5	4.4
product **11**	-91.0	-91.3	-91.3	-91.6	-79.5	-79.8
product **12**	-94.1	-94.4	-94.0	-94.3	-84.0	-84.3
product **13**	-87.6	-87.9	-87.9	-88.2	-75.6	-75.8
product **14**	-97.0	-97.3	-96.9	-97.2	-86.6	-86.9
product **15**	-65.1	-65.4	-66.1	-66.4	-52.0	-52.3

Note: Basis set is 6-31G* for all calculations.

Table S11. Calculated energies in Hartrees (page 1).

Species	**HF/6-31G***			
	Energy	**ZPE**	**H (298 K)**	**G (298 K)**
BCB:				
1 (BCB)	-154.87177	0.09311	0.09757	0.06845
2 (CCl_2)	-956.71226	0.00457	0.00884	-0.02107
1 + **2** (reactants)	-1111.58403	0.09769	0.10641	0.04738
TS **17** (A)	-1111.56591	0.09960	0.10763	0.06692
TS **18** (B)	-1111.56642	0.09936	0.10748	0.06647
TS **20** (C)	-1111.53215	0.09837	0.10560	0.06694
TS/Int **19**	-1111.58085	0.10099	0.10862	0.06927
product **3**	-1111.74046	0.10311	0.11162	0.06912
product **4**	-1111.70091	0.10669	0.11321	0.07693
TM122BCB:	-271.98147	0.18295	0.19144	0.15206
10 (TM122BCB)	-956.71226	0.00457	0.00884	-0.02107
2 (CCl_2)	-1228.69373	0.18753	0.20028	0.13099
10 + **2** (reactants)	-1228.67327	0.18907	0.20135	0.15170
TS **21** (A)	-1228.67685	0.18873	0.20115	0.15093
TS **22** (B)	-1228.64352	0.18791	0.20018	0.15078
TS **23** (C)	-1228.67456	0.18898	0.20134	0.15108
TS **24** (D)	-1228.66412	0.18933	0.20148	0.15256
TS **25** (E)	-1228.66039	0.18975	0.20174	0.15285
TS **26** (F)	-1228.66821	0.18930	0.20152	0.15218
TS **27** (G)	-1228.69599	0.19049	0.20317	0.15250
Int. **16**	-1228.83625	0.19334	0.20562	0.15516
product **11**	-1228.84751	0.19317	0.20617	0.15280
product **12**	-1228.82811	0.19334	0.20559	0.15598
product **13**	-1228.85255	0.19322	0.20614	0.15332
product **14**	-1228.78576	0.19570	0.20678	0.16000
product **15**	-271.98147	0.18295	0.19144	0.15206

Note: Enthalpies and free energies (H and G) are thermodynamic *corrections*, to be added to the electronic energies.

Table S11, continued. Calculated energies in Hartrees (page 2).

Species	**CCSD/6-31G***			
	Energy	**ZPE**	**H (298 K)**	**G (298 K)**
BCB:				
1 (BCB)	-155.42461	0.08815	0.09277	0.06341
2 (CCl_2)	-957.12111	0.00432	0.00863	-0.02138
1 + **2** (reactants)	-1112.54572	0.09247	0.10140	0.04203
TS **17** (A)	-1112.54393	0.09409	0.10246	0.06087
TS **18** (B)	-1112.54191	0.09382	0.10229	0.06038
TS **20** (C)	-1112.50641	0.09412	0.10219	0.06165
TS/Int **19**	-1112.54923	0.09558	0.10399	0.06309
product **3**	-1112.70532	0.09706	0.10589	0.06258
product **4**	-1112.67487	0.10075	0.10753	0.07084
TM122BCB:				
10 (TM122BCB)	-272.96695	0.17387	0.18267	0.14275
2 (CCl_2)	-957.12111	0.00432	0.00863	-0.02138
10 + **2** (reactants)	-1230.08806	0.17818	0.19130	0.12137
TS **21** (A)	-1230.08661			
TS **22** (B)	-1230.08755			
TS **23** (C)	-1230.05845			
TS **24** (D)	-1230.08714			
TS **25** (E)	-1230.08201			
TS **26** (F)	-1230.07876			
TS **27** (G)	-1230.08323			
Int. **16**	-1230.10000			
product **11**	-1230.23928			
product **12**	-1230.24488			
product **13**	-1230.23328			
product **14**	-1230.24943			
product **15**	-1230.19831			

Note: Enthalpies and free energies (H and G) are thermodynamic *corrections*, to be added to the electronic energies.

Table S11, continued. Calculated energies in Hartrees (page 3).

Species	**CCSD(T)/6-31G***	**CCSD(T)/6-311+G****	**CCSD/6-31G***	**CCSD(T)/6-31G***
	//CCSD/6-31G*	**//CCSD/6-31G***	**//HF/6-31G***	**//HF/6-31G*)**
	Energy	**Energy**	**Energy**	**Energy**
BCB:				
1 (BCB)	-155.44467	-155.55134	-155.42352	-155.44309
2 (CCl_2)	-957.13669	-957.22605	-957.12087	-957.13623
1 + **2** (reactants)	-1112.58136	-1112.77739	-1112.54438	-1112.57932
TS **17** (A)	-1112.58480	-1112.78371	-1112.54276	-1112.58363
TS **18** (B)	-1112.58223	-1112.78152	-1112.54055	-1112.58039
TS **20** (C)	-1112.54879	-1112.75003	-1112.50731	-1112.54693
TS/Int **19**	-1112.58830	-1112.78910	-1112.54689	-1112.58465
product **3**	-1112.74083	-1112.93579	-1112.70351	-1112.73824
product **4**	-1112.71092	-1112.90808	-1112.67393	-1112.70956
TM122BCB:				
10 (TM122BCB)	-273.00193	-273.20283	-272.96531	-272.99965
2 (CCl_2)	-957.13669	-957.22605	-957.12087	-957.13623
10 + **2** (reactants)	-1230.13862	-1230.42888	-1230.08618	-1230.13588
TS **21** (A)	-1230.14306	-1230.43944	-1230.08493	-1230.14133
TS **22** (B)	-1230.14290	-1230.43935	-1230.08606	-1230.14133
TS **23** (C)	-1230.11597	-1230.41331	-1230.05612	-1230.11204
TS **24** (D)	-1230.14331	-1230.43968	-1230.08571	-1230.14191
TS **25** (E)	-1230.13972	-1230.43789	-1230.08006	-1230.13765
TS **26** (F)	-1230.13695	-1230.43521	-1230.07657	-1230.13419
TS **27** (G)	-1230.14012	-1230.43856	-1230.08109	-1230.13730
Int. **16**	-1230.15447	-1230.45298	-1230.09716	-1230.15040
product **11**	-1230.29067	-1230.58557	-1230.23673	-1230.28715
product **12**	-1230.29529	-1230.58571	-1230.24257	-1230.29203
product **13**	-1230.28508	-1230.57949	-1230.23086	-1230.28173
product **14**	-1230.29982	-1230.59005	-1230.24719	-1230.29666
product **15**	-1230.25031	-1230.54619	-1230.19681	-1230.24826

Table S11, continued. Calculated energies in Hartrees (page 4).

Species	**QCISD/6-31G***			
	Energy	**ZPE**	**H (298 K)**	**G (298 K)**
BCB:				
1 (BCB)	-155.42550	0.08805	0.09267	0.06330
2 (CCl_2)	-957.12325	0.00426	0.00858	-0.02146
1 + **2** (reactants)	-1112.54875	0.09230	0.10125	0.04185
TS **17** (A)	-1112.54697	0.09390	0.10230	0.06063
TS **18** (B)	-1112.54481	0.09363	0.10213	0.06014
TS **20** (C)	-1112.50956	0.09259	0.10016	0.06112
TS/Int **19**				
product **3**	-1112.70735	0.09693	0.10576	0.06246
product **4**	-1112.67656	0.10061	0.10740	0.07069
TM122BCB:				
10 (TM122BCB)	-272.96859	0.17367	0.18248	0.14255
2 (CCl_2)	-957.12325	0.00426	0.00858	-0.02146
10 + **2** (reactants)	-1230.09183	0.17793	0.19106	0.12110
TS **21** (A)	-1230.09049			
TS **22** (B)	-1230.09197			
TS **23** (C)	-1230.06225			
TS **24** (D)	-1230.09101			
TS **25** (E)	-1230.08593			
TS **26** (F)	-1230.08267			
TS **27** (G)	-1230.08699			
Int. **16**				
product **11**	-1230.24211			
product **12**	-1230.24765			
product **13**	-1230.23616			
product **14**	-1230.25222			
product **15**	-1230.20087			

Note: Enthalpies and free energies (H and G) are thermodynamic *corrections*, to be added to the electronic energies.

Table S11, continued. Calculated energies in Hartrees (page 5).

Species	**QCISD/6-31G***	**QCISD(T)/6-31G***	**CBS-4M**		
	//HF/6-31G*	**//HF/6-31G***			
	Energy	**Energy**	**ΔH (0 K)**	**ΔH (298 K)**	**ΔG (298 K)**
BCB:					
1 (BCB)	-155.42434	-155.44340	-155.66981	-155.66517	-155.69456
2 (CCl_2)	-957.12287	-957.13719	-957.42164	-957.41721	-957.44742
1 + **2** (reactants)	-1112.54721	-1112.58059	-1113.09146	-1113.08238	-1113.14198
TS **17** (A)	-1112.54565	-1112.58500	-1113.09303	-1113.08421	-1113.12669
TS **18** (B)	-1112.54329	-1112.58167	-1113.09101	-1113.08213	-1113.12487
TS **20** (C)	-1112.50988	-1112.54811	-1113.06267	-1113.05405	-1113.09654
TS/Int **19**	-1112.54925	-1112.58567	-1113.09508	-1113.08668	-1113.12759
product **3**	-1112.70544	-1112.73903	-1113.24445	-1113.23556	-1113.27885
product **4**	-1112.67557	-1112.71029	-1113.21718	-1113.21013	-1113.24728
TM122BCB:					
10 (TM122BCB)	-272.96687	-273.00027	-273.40000	-273.39093	-273.43138
2 (CCl_2)	-957.12287	-957.13719	-957.42164	-957.41721	-957.44742
10 + **2** (reactants)	-1230.08974	-1230.13745	-1230.82164	-1230.80814	-1230.87880
TS **21** (A)	-1230.08868	-1230.14306	-1230.82647	-1230.81302	-1230.86534
TS **22** (B)	-1230.08965	-1230.14297	-1230.82673	-1230.81323	-1230.86599
TS **23** (C)	-1230.05972	-1230.11366	-1230.80310	-1230.79001	-1230.84100
TS **24** (D)	-1230.08942	-1230.14362	-1230.82658	-1230.81309	-1230.86598
TS **25** (E)	-1230.08386	-1230.13941	-1230.82337	-1230.80998	-1230.86180
TS **26** (F)	-1230.08036	-1230.13594	-1230.82025	-1230.80703	-1230.85872
TS **27** (G)	-1230.08466	-1230.13893	-1230.82484	-1230.81146	-1230.86368
Int. **16**	-1230.10085	-1230.15183			
product **11**	-1230.23944	-1230.28828	-1230.97001	-1230.95703	-1231.00854
product **12**	-1230.24521	-1230.29312	-1230.97234	-1230.95865	-1231.01363
product **13**	-1230.23362	-1230.28287	-1230.96405	-1230.95110	-1231.00201
product **14**	-1230.24986	-1230.29775	-1230.97700	-1230.96344	-1231.01759
product **15**	-1230.19930	-1230.24934	-1230.93259	-1230.92065	-1230.96893

Table S11, continued. Calculated energies in Hartrees (page 6).

Species	**HF/6-31G* PCM(solvent=cyclohexane)**			
	Energy	**ZPE**	**H (298 K)**	**G (298 K)**
BCB:				
1 (BCB)	-154.87274	0.09289	0.09735	0.06823
2 (CCl_2)	-956.71369	0.00454	0.00881	-0.02110
1 + **2** (reactants)	-1111.58642	0.09743	0.10616	0.04713
TS **17** (A)	-1111.57043	0.09918	0.10731	0.06623
TS **18** (B)	-1111.57059	0.09890	0.10714	0.06575
TS **20** (C)	-1111.53755	0.09818	0.10542	0.06670
TS/Int **19**	-1111.59450	0.10079	0.10845	0.06903
product **3**	-1111.74239	0.10288	0.11140	0.06884
product **4**	-1111.70316	0.10643	0.11298	0.07667
TM122BCB:				
10 (TM122BCB)	-271.98204	0.18277	0.19126	0.15188
2 (CCl_2)	-956.71369	0.00454	0.00881	-0.02110
10 + **2** (reactants)	-1228.69573	0.18731	0.20008	0.13078
TS **21** (A)	-1228.67709	0.18875	0.20111	0.15117
TS **22** (B)	-1228.67981	0.18840	0.20090	0.15039
TS **23** (C)	-1228.64681	0.18771	0.20000	0.15054
TS **24** (D)	-1228.67800	0.18866	0.20108	0.15059
TS **25** (E)	-1228.66742	0.18901	0.20125	0.15201
TS **26** (F)	-1228.66429	0.18944	0.20150	0.15238
TS **27** (G)	-1228.67120	0.18898	0.20127	0.15168
Int. **16**	-1228.70764	0.19031	0.20299	0.15237
product **11**	-1228.83770	0.19315	0.20544	0.15495
product **12**	-1228.84891	0.19298	0.20599	0.15255
product **13**	-1228.82967	0.19315	0.20542	0.15576
product **14**	-1228.85395	0.19305	0.20597	0.15319
product **15**	-1228.78763	0.19548	0.20657	0.15977

Note: Enthalpies and free energies (H and G) are thermodynamic *corrections*, to be added to the electronic energies.

Table S11, continued. Calculated energies in Hartrees (page 7).

Species	**CBS-4M PCM(solvent=cyclohexane)**		
	ΔH (0 K)	**ΔH (298 K)**	**ΔG (298 K)**
BCB:			
1 (BCB)	-155.67119	-155.66654	-155.69594
2 (CCl_2)	-957.42269	-957.41825	-957.44846
1 + **2** (reactants)	-1113.09388	-1113.08479	-1113.14440
TS **17** (A)	-1113.09571	-1113.08682	-1113.12958
TS **18** (B)	-1113.09366	-1113.08471	-1113.12777
TS **20** (C)	-1113.06804	-1113.05940	-1113.10202
TS/Int **19**	-1113.10441	-1113.09595	-1113.13700
product **3**	-1113.24627	-1113.23736	-1113.28073
product **4**	-1113.21918	-1113.21211	-1113.24929
TM122BCB:			
10 (TM122BCB)	-273.40092	-273.39184	-273.43230
2 (CCl_2)	-957.42269	-957.41825	-957.44846
10 + **2** (reactants)	-1230.82361	-1230.81009	-1230.88076
TS **21** (A)	-1230.82857	-1230.81507	-1230.86763
TS **22** (B)	-1230.82836	-1230.81480	-1230.86782
TS **23** (C)	-1230.80588	-1230.79275	-1230.84387
TS **24** (D)	-1230.82832	-1230.81477	-1230.86792
TS **25** (E)	-1230.82504	-1230.81157	-1230.86369
TS **26** (F)	-1230.82231	-1230.80903	-1230.86086
TS **27** (G)	-1230.82652	-1230.81309	-1230.86544
Int. **16**			
product **11**	-1230.97136	-1230.95837	-1231.00995
product **12**	-1230.97358	-1230.95988	-1231.01491
product **13**	-1230.96544	-1230.95247	-1231.00343
product **14**	-1230.97823	-1230.96465	-1231.01881
product **15**	-1230.93421	-1230.92225	-1230.97056

Table S12. Calculation of G3-CCSD energies (Hartrees) (page 1).

Species	**HF/6-31G(d) ZPE**	**MP2/ 6-31G(d)**	**MP2/ 6-31+G(d)**	**MP2/ 6-31G(2df,p)**	**MP2/ G3Large**
BCB:					
1 (BCB)	0.09311	-155.38989	-155.39857	-155.52318	-155.75087
2 (CCl_2)	0.00457	-957.08623	-957.09428	-957.21444	-957.96303
1 + **2** (reactants)	0.09769	-1112.47611	-1112.49284	-1112.73762	-1113.71389
TS **17** (A)	0.10669	-1112.61923	-1112.63227	-1112.88296	-1113.85541
TS **18** (B)	0.09960	-1112.48582	-1112.50365	-1112.75029	-1113.72623
TS **20** (C)	0.09936	-1112.48366	-1112.50212	-1112.74811	-1113.72385
TS/Int **19**	0.09837	-1112.44968	-1112.46695	-1112.72018	-1113.69705
product **3**	0.10099	-1112.49092	-1112.51063	-1112.75676	-1113.73371
product **4**	0.10311	-1112.63930	-1112.65578	-1112.89654	-1113.87644
TM122BCB:					
10 (TM122BCB)	0.18295	-272.90102	-272.91411	-273.14707	-273.54612
2 (CCl_2)	0.00457	-957.08623	-957.09428	-957.21444	-957.96303
10 + **2** (reactants)	0.18753	-1229.98725	-1230.00838	-1230.36151	-1231.50914
TS **21** (A)	0.18907	-1229.99863	-1230.02319	-1230.37650	-1231.52502
TS **22** (B)	0.18873	-1229.99808	-1230.02291	-1230.37569	-1231.52381
TS **23** (C)	0.18791	-1229.97242	-1229.99624	-1230.35406	-1231.50289
TS **24** (D)	0.18898	-1229.99900	-1230.02339	-1230.37653	-1231.52506
TS **25** (E)	0.18933	-1229.99618	-1230.02192	-1230.37491	-1231.52420
TS **26** (F)	0.18975	-1229.99419	-1230.01942	-1230.37364	-1231.52282
TS **27** (G)	0.18930	-1229.99695	-1230.02280	-1230.37631	-1231.52506
Int. **16**	0.19049	-1230.01062	-1230.03691	-1230.39007	-1231.53980
product **11**	0.19334	-1230.14438	-1230.16875	-1230.51691	-1231.66928
product **12**	0.19317	-1230.14823	-1230.16918	-1230.51861	-1231.67025
product **13**	0.19334	-1230.13885	-1230.16258	-1230.51163	-1231.66401
product **14**	0.19322	-1230.15304	-1230.17410	-1230.52319	-1231.67491
product **15**	0.19570	-1230.11255	-1230.13276	-1230.49056	-1231.63636

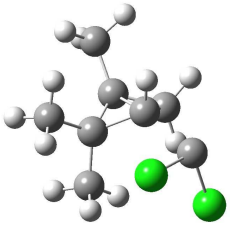
Table S12, continued. Calculation of G3-CCSD energies (Hartrees) (page 2).

Species	**MP4SDTQ/ 6-31G(d)**	**MP4SDTQ/ 6-31+G(d)**	**MP4SDTQ/ 6-31G(2df,p)**	**QCISD(T)/ 6-31G***
BCB:				
1 (BCB)	-155.44396	-155.45292	-155.58446	-155.44501
2 (CCl_2)	-957.13588	-957.14443	-957.28110	-957.13772
1 + **2** (reactants)	-1112.57984	-1112.59736	-1112.86556	-1112.58273
TS **17** (A)	-1112.71251	-1112.72674	-1113.00045	-1112.71166
TS **18** (B)	-1112.58654	-1112.60545	-1112.87477	-1112.58624
TS **20** (C)	-1112.58382	-1112.60336	-1112.87205	-1112.58358
TS/Int **19**	-1112.54974	-1112.56799	-1112.84348	-1112.55020
product **3**	-1112.58870	-1112.60966	-1112.87853	-1112.58949
product **4**	-1112.73979	-1112.75681	-1113.02086	-1112.74166
TM122BCB:				
10 (TM122BCB)	-273.00114	-273.01535	-273.26097	-273.00258
2 (CCl_2)	-957.13588	-957.14443	-957.28110	-957.13772
10 + **2** (reactants)	-1230.13702	-1230.15978	-1230.54208	-1230.14030
TS **21** (A)	-1230.14549	-1230.17206	-1230.55366	-1230.14486
TS **22** (B)	-1230.14496	-1230.17182	-1230.55291	-1230.14464
TS **23** (C)	-1230.11870	-1230.14446	-1230.53030	-1230.11770
TS **24** (D)	-1230.14582	-1230.17225	-1230.55372	-1230.14509
TS **25** (E)	-1230.14263	-1230.17038	-1230.55156	-1230.14155
TS **26** (F)	-1230.14016	-1230.16741	-1230.54985	-1230.13877
TS **27** (G)	-1230.14286	-1230.17076	-1230.55235	-1230.14184
Int. **16**	-1230.15531	-1230.18375	-1230.56526	-1230.15604
product **11**	-1230.29003	-1230.31585	-1230.69272	-1230.29184
product **12**	-1230.29430	-1230.31664	-1230.69501	-1230.29643
product **13**	-1230.28460	-1230.30976	-1230.68748	-1230.28625
product **14**	-1230.29894	-1230.32144	-1230.69942	-1230.30095
product **15**	-1230.25243	-1230.27474	-1230.66112	-1230.25142

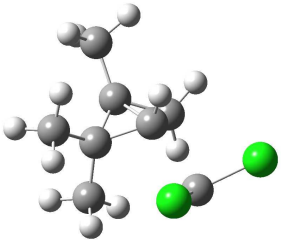
Table S12, continued. Calculation of G3-CCSD energies (Hartrees) (page 3).

Species	valence lone pairs	higher-level correction	G3 (0 K)	E(rel) (kcal/mol)
BCB:				
1 (BCB)	11	-0.07025	-155.80058	
2 (CCl_2)	9	-0.05747	-958.08543	
1 + **2** (reactants)	20	-0.12772	-1113.88601	0.0
TS **17** (A)	20	-0.12772	-1114.00571	-75.1
TS **18** (B)	20	-0.12772	-1113.89027	-2.7
TS **20** (C)	20	-0.12772	-1113.88762	-1.0
TS/Int **19**	20	-0.12772	-1113.86167	15.3
product **3**	20	-0.12772	-1113.89508	-5.7
product **4**	20	-0.12772	-1114.03882	-95.9
TM122BCB:				
10 (TM122BCB)	20	-0.12772	-273.62694	
2 (CCl_2)	9	-0.05747	-958.08543	
10 + **2** (reactants)	29	-0.18519	-1231.71237	0.0
TS **21** (A)	29	-0.18519	-1231.71992	-4.7
TS **22** (B)	29	-0.18519	-1231.71942	-4.4
TS **23** (C)	29	-0.18519	-1231.69747	9.4
TS **24** (D)	29	-0.18519	-1231.72001	-4.8
TS **25** (E)	29	-0.18519	-1231.71793	-3.5
TS **26** (F)	29	-0.18519	-1231.71543	-1.9
TS **27** (G)	29	-0.18519	-1231.71831	-3.7
Int. **16**	29	-0.18519	-1231.73298	-12.9
product **11**	29	-0.18519	-1231.86090	-93.2
product **12**	29	-0.18519	-1231.86289	-94.5
product **13**	29	-0.18519	-1231.85551	-89.8
product **14**	29	-0.18519	-1231.86726	-97.2
product **15**	29	-0.18519	-1231.81849	-66.6

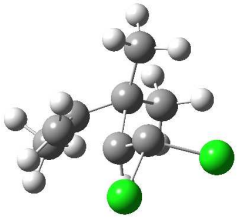
TS A (**21**):



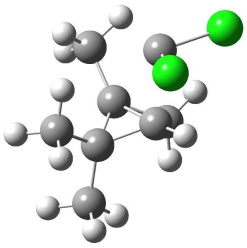
TS B (**22**):



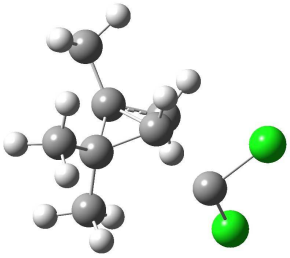
Int. (**16**):



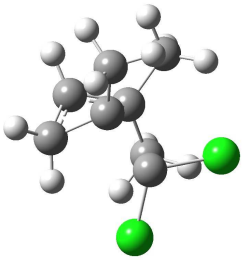
TS C (**23**):



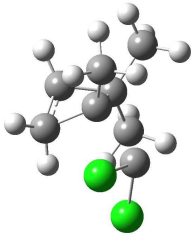
TS D (**24**):



TS E (**25**):



TS F (**26**):



TS G (**27**):

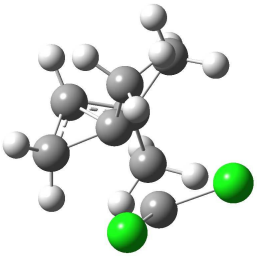


Figure S1. HF/6-31G* optimized structures of the transition structures and intermediate in Scheme 6.

Structure **1**
Bicyclobutane C2V HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.733478	.000000	-.323725
2	6	0	-.733478	.000000	-.323725
3	6	0	.000000	1.126267	.315114
4	6	0	.000000	-1.126267	.315114
5	1	0	1.436390	.000000	-1.130508
6	1	0	-1.436390	.000000	-1.130508
7	1	0	.000000	2.067914	-.210601
8	1	0	.000000	1.225588	1.392774
9	1	0	.000000	-2.067914	-.210601
10	1	0	.000000	-1.225588	1.392774

NImag = 0
E(HF/6-31G*) = -154.87177
ZPE(HF/6-31G*) = 0.09311

Structure **2**
Dichlorocarbene singlet C2V HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.000000	.000000	.831178
2	17	0	.000000	1.404467	-.146679
3	17	0	.000000	-1.404467	-.146679

NImag = 0
E(HF/6-31G*) = -956.71226094
ZPE(HF/6-31G*) = 0.00457

Structure **3**
1,1-Dichloropenta-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.408491	-.415161	.646029
2	6	0	-2.826705	.059447	.072138
3	1	0	-3.736559	.552082	.375533
4	6	0	-2.868950	-.798679	-.927510
5	6	0	-1.605773	.465175	.865770
6	1	0	-.519096	-1.449112	.920818
7	1	0	-1.996040	-1.314645	-1.286186
8	1	0	-3.792697	-1.011452	-1.434792
9	1	0	-1.369390	1.500786	.652813
10	1	0	-1.857074	.424475	1.924123
11	6	0	.762833	-.061473	.165025
12	17	0	1.171852	1.539117	-.350590
13	17	0	2.060700	-1.197823	-.007117

NImag = 0
E(HF/6-31G*) = -1111.74046
ZPE(HF/6-31G*) = 0.10311

Structure **4**
2,2-Dichlorobicyclo[1.1.1]pentane C2V HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.000000	.000000	.163312
2	6	0	.000000	1.057046	-1.680173
3	6	0	.000000	-1.057046	-1.680173
4	6	0	.944013	.000000	-1.050216
5	6	0	-.944013	.000000	-1.050216
6	17	0	.000000	1.430800	1.231446
7	17	0	.000000	-1.430800	1.231446
8	1	0	.000000	2.053074	-1.269270
9	1	0	.000000	1.082687	-2.761456
10	1	0	.000000	-2.053074	-1.269270
11	1	0	.000000	-1.082687	-2.761456
12	1	0	2.022668	.000000	-1.011464
13	1	0	-2.022668	.000000	-1.011464

NImag = 0
E(HF/6-31G*) = -1111.70091
ZPE(HF/6-31G*) = 0.10669

Structure **17**

TS A for dichlorocarbene addition to bicyclobutane C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.064873	-0.494602	-0.456337
2	6	0	2.515942	-0.369320	0.245243
3	1	0	3.254407	-1.102392	-0.011719
4	6	0	1.361196	-0.658777	1.055222
5	6	0	2.054191	0.655565	-0.670880
6	1	0	1.047107	-1.339323	-1.114287
7	1	0	0.914504	0.125729	1.647218
8	1	0	1.282122	-1.641103	1.486314
9	1	0	1.706735	1.596960	-0.275522
10	1	0	2.547122	0.730577	-1.624463
11	6	0	-0.847411	0.149438	-0.797805
12	17	0	-1.025835	1.545844	0.287918
13	17	0	-1.776797	-1.196684	-0.073812

NImag = 1
E(HF/6-31G*) = -1111.56591
ZPE(HF/6-31G*) = 0.09960

Structure **18**

TS B for dichlorocarbene addition to bicyclobutane Cs HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.544824	1.018700	0.000000
2	6	0	0.392388	2.612112	0.000000
3	1	0	1.285432	3.204984	0.000000
4	6	0	-0.066868	1.853231	1.139956
5	6	0	-0.066868	1.853231	-1.139956
6	1	0	1.571059	0.708070	0.000000
7	1	0	-1.120405	1.656228	1.261893
8	1	0	0.485231	1.946376	2.058485
9	1	0	-1.120405	1.656228	-1.261893
10	1	0	0.485231	1.946376	-2.058485
11	6	0	-0.688918	-0.645106	0.000000
12	17	0	-0.066868	-1.507978	1.432084
13	17	0	-0.066868	-1.507978	-1.432084

NImag = 1
E(HF/6-31G*) = -1111.56642
ZPE(HF/6-31G*) = 0.09936

Structure **19**
TS connecting to TS B for dichlorocarbene addition to bicyclobutane Cs HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.467672	.749477	.000000
2	6	0	.330025	2.445583	.000000
3	1	0	1.280386	2.950022	.000000
4	6	0	-.065427	1.762223	1.173235
5	6	0	-.065427	1.762223	-1.173235
6	1	0	1.522131	.529095	.000000
7	1	0	-1.089660	1.480979	1.328933
8	1	0	.531820	1.902746	2.054532
9	1	0	-1.089660	1.480979	-1.328933
10	1	0	.531820	1.902746	-2.054532
11	6	0	-.577228	-.422556	.000000
12	17	0	-.065427	-1.412596	1.472066
13	17	0	-.065427	-1.412596	-1.472066

NImag = 1
E(HF/6-31G*) = -1111.58085
ZPE(HF/6-31G*) = 0.10099

Structure **20**
TS C for dichlorocarbene addition to bicyclobutane Cs HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.504827	1.025883	0.000000
2	6	0	0.812677	1.874460	0.000000
3	6	0	-0.106596	2.005094	1.120000
4	6	0	-0.106596	2.005094	-1.120000
5	1	0	-1.385222	0.424448	0.000000
6	1	0	1.789215	1.440386	0.000000
7	1	0	0.184362	1.582068	2.065438
8	1	0	-0.703998	2.903158	1.183941
9	1	0	0.184362	1.582068	-2.065438
10	1	0	-0.703998	2.903158	-1.183941
11	6	0	0.615267	-0.641205	0.000000
12	17	0	-0.106596	-1.425037	-1.454928
13	17	0	-0.106596	-1.425037	1.454928

NImag = 2 (-720.1 and -19.3 cm^{-1})
E(HF/6-31G*) = -1111.53215
ZPE(HF/6-31G*) = 0.09837

Structure **10**

1,2,2-Trimethylbicyclobutane C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.257490	-.540880	1.053450
2	6	0	.777038	-.016402	-.219485
3	6	0	-.697553	.030005	.053224
4	6	0	1.056911	-1.428905	.168178
5	6	0	1.758092	1.058016	-.585321
6	6	0	-1.704953	-.826630	-.702413
7	6	0	-1.274140	1.394039	.405685
8	1	0	.443979	-.240489	2.065818
9	1	0	2.069809	-1.623085	.488531
10	1	0	.610499	-2.268992	-.341291
11	1	0	2.709513	.894178	-.087422
12	1	0	1.944527	1.066321	-1.655400
13	1	0	1.399357	2.042450	-.306298
14	1	0	-1.313062	-1.796029	-.978547
15	1	0	-2.592565	-.988488	-.096527
16	1	0	-2.014787	-.324598	-1.615395
17	1	0	-.592484	1.980463	1.011704
18	1	0	-1.504331	1.963997	-.490230
19	1	0	-2.197769	1.278813	.965144

NImag = 0

E(HF/6-31G*) = -271.98147

ZPE(HF/6-31G*) = 0.18295

Structure **11**

1,1-Dichloro-3,3,4-trimethylpenta-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.328272	.114592	-.036080
2	6	0	-.296520	.927701	.039487
3	6	0	1.176050	.681496	-.302260
4	6	0	1.762747	-.511417	.469247
5	6	0	2.495589	-1.448069	-.106999
6	6	0	1.305433	.539871	-1.830688
7	6	0	1.952111	1.953633	.110164
8	6	0	1.518981	-.554177	1.962782
9	17	0	-2.929236	.654207	.370988
10	17	0	-1.272293	-1.542167	-.520040
11	1	0	-.539070	1.925841	.358984
12	1	0	2.927358	-2.244209	.473315
13	1	0	2.692909	-1.478631	-1.161063
14	1	0	.827836	-.358904	-2.197284
15	1	0	.840731	1.390600	-2.317257
16	1	0	2.348134	.521199	-2.127381
17	1	0	3.009092	1.827522	-.093404
18	1	0	1.598460	2.812117	-.453001
19	1	0	1.835848	2.181015	1.163388
20	1	0	.462069	-.643159	2.189334
21	1	0	2.026927	-1.401697	2.405681
22	1	0	1.878988	.341844	2.458652

NImag = 0

E(HF/6-31G*) = -1228.83625

ZPE(HF/6-31G*) = 0.19334

Structure **12**
1,1-Dichloro-4,5-dimethylhexa-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.827597	-.230872	.060434
2	6	0	.569469	-.551153	.271614
3	6	0	-.494624	.284608	.937590
4	6	0	-1.688862	.514227	.017323
5	6	0	-2.791873	-.228277	.053566
6	6	0	-4.008621	.011043	-.814844
7	6	0	-2.990315	-1.419619	.967758
8	6	0	-1.459827	1.675755	-.926634
9	17	0	2.929080	-1.315998	-.725395
10	17	0	2.552520	1.272020	.524574
11	1	0	.262237	-1.522151	-.074566
12	1	0	-.789641	-.210814	1.853654
13	1	0	-.085264	1.243353	1.228406
14	1	0	-3.998891	.958175	-1.332446
15	1	0	-4.111002	-.778524	-1.556245
16	1	0	-4.906804	-.016497	-.203155
17	1	0	-3.740561	-1.200241	1.724290
18	1	0	-3.364001	-2.263998	.394145
19	1	0	-2.093333	-1.746146	1.473532
20	1	0	-.467211	1.609117	-1.362566
21	1	0	-2.166210	1.719849	-1.741863
22	1	0	-1.504180	2.621234	-.390069

NImag = 0
E(HF/6-31G*) = -1228.84751
ZPE(HF/6-31G*) = 0.19317

Structure **13**

1,1-Dichloro-2,3,3-trimethylpenta-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.140955	-0.116388	-0.013152
2	6	0	0.179454	0.795886	-0.043098
3	6	0	-1.331697	0.454001	0.094675
4	6	0	-1.740577	-0.664823	-0.854948
5	6	0	-2.598529	-1.635951	-0.618137
6	6	0	0.535237	2.265439	-0.142038
7	6	0	-1.628973	0.141478	1.572914
8	6	0	-2.215874	1.657149	-0.318933
9	17	0	2.840147	0.252969	-0.154819
10	17	0	0.915768	-1.822131	0.198894
11	1	0	-1.319340	-0.581385	-1.844478
12	1	0	-2.864790	-2.333271	-1.392186
13	1	0	-3.057739	-1.793712	0.340877
14	1	0	1.597836	2.434603	-0.160366
15	1	0	0.110404	2.706773	-1.035698
16	1	0	0.129973	2.801651	0.709430
17	1	0	-2.693851	0.011334	1.730641
18	1	0	-1.122704	-0.754357	1.906008
19	1	0	-1.306280	0.966590	2.199825
20	1	0	-2.059204	1.940171	-1.354140
21	1	0	-3.254158	1.367955	-0.215494
22	1	0	-2.050677	2.528657	0.302611

NImag = 0

E(HF/6-31G*) = -1228.82811

ZPE(HF/6-31G*) = 0.19334

Structure **14**

1,1-Dichloro-2,5-dimethylhexa-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.685913	-.022679	-.068911
2	6	0	.545662	.573580	-.366686
3	6	0	-.628820	-.169103	-.984044
4	6	0	-1.639035	-.567666	.067290
5	6	0	-2.906466	-.197107	.180914
6	6	0	-3.762185	-.726495	1.307872
7	6	0	-3.637406	.740978	-.749295
8	6	0	.291656	2.038902	-.114822
9	17	0	3.054490	.783626	.634420
10	17	0	1.993237	-1.713051	-.331975
11	1	0	-1.247581	-1.249992	.804844
12	1	0	-1.070852	.476253	-1.732341
13	1	0	-.285596	-1.055697	-1.500018
14	1	0	-3.209261	-1.396297	1.955089
15	1	0	-4.149259	.088869	1.914512
16	1	0	-4.622400	-1.265461	.917828
17	1	0	-4.482627	.232334	-1.206386
18	1	0	-4.041738	1.582967	-.192834
19	1	0	-3.019160	1.134508	-1.543742
20	1	0	1.044941	2.504523	.500747
21	1	0	.248086	2.569331	-1.062507
22	1	0	-.671822	2.156418	.369322

NImag = 0

E(HF/6-31G*) = -1228.85255

ZPE(HF/6-31G*) = 0.19322

Structure **15**

2,2-Dichloro-1,4,4-trimethyl[1.1.1]bicyclopentane C1 HF/6-31G* freq

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.414617	-.644903	.610897
2	6	0	-.714762	.054791	-.191007
3	6	0	.336571	-.317448	-1.255643
4	6	0	1.466822	.146300	-.267762
5	6	0	.385738	-1.693089	-.541332
6	6	0	.433511	-.888194	2.094840
7	6	0	1.745162	1.653463	-.026423
8	6	0	2.865466	-.483630	-.431180
9	17	0	-1.173273	1.749237	.133294
10	17	0	-2.308585	-.788309	-.277820
11	1	0	.252816	-.119917	-2.314763
12	1	0	1.267877	-2.285742	-.683996
13	1	0	-.480826	-2.323884	-.616264
14	1	0	-.432127	-1.466211	2.400358
15	1	0	1.325537	-1.438233	2.377073
16	1	0	.425292	.049359	2.641079
17	1	0	1.288041	2.286329	-.773300
18	1	0	1.404623	1.990223	.943049
19	1	0	2.811764	1.836663	-.066828
20	1	0	2.907322	-1.547677	-.595526
21	1	0	3.370752	-.008128	-1.266161
22	1	0	3.451761	-.272313	.457880

NImag = 0

E(HF/6-31G*) = -1228.78576

ZPE(HF/6-31G*) = 0.19570

Structure **16**
Intermediate along pathway B for dichlorocarbene addition to
1,2,2-tri methylbicyclobutane C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.111437	-.358529	-.218185
2	6	0	-1.759924	-.823305	.157648
3	6	0	-2.687576	-1.362453	-.888079
4	6	0	-1.352468	.564823	.278026
5	6	0	-.690391	-1.626275	.633853
6	6	0	-1.141927	1.172790	1.662472
7	6	0	-1.915123	1.578764	-.704284
8	1	0	-.075142	-.505962	-1.287769
9	1	0	-2.219482	-2.145284	-1.471599
10	1	0	-3.513820	-1.812622	-.341819
11	1	0	-3.088803	-.604926	-1.541668
12	1	0	-.277596	-1.486586	1.614427
13	1	0	-.599075	-2.621573	.239395
14	1	0	-.817158	.459854	2.402327
15	1	0	-.399770	1.954697	1.611314
16	1	0	-2.087699	1.602938	1.980478
17	1	0	-1.894324	1.228102	-1.727837
18	1	0	-2.935929	1.842315	-.444493
19	1	0	-1.311933	2.475216	-.657997
20	6	0	1.217556	.052621	.489316
21	17	0	2.384058	-1.289822	-.033543
22	17	0	1.725852	1.550011	-.486419

NImag = 0
E(HF/6-31G*) = -1228.69599
ZPE(HF/6-31G*) = 0.19049

Structure **21**
TS A for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-4,5-dimethylhexa-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.504484	-.263621	-.662262
2	6	0	-1.966532	-.615430	-.030061
3	6	0	-3.255954	-.476110	-.787359
4	6	0	-1.163694	.451544	.562569
5	6	0	-1.008235	-1.668634	-.302226
6	6	0	-.511474	.257474	1.926401
7	6	0	-1.610790	1.890418	.359135
8	1	0	-.675101	.133570	-1.643868
9	1	0	-3.211208	-.991835	-1.740483
10	1	0	-4.048601	-.936978	-.203621
11	1	0	-3.532766	.554337	-.960012
12	1	0	-.446960	-2.136961	.488293
13	1	0	-1.250005	-2.340503	-1.108661
14	1	0	-.241221	-.767766	2.129297
15	1	0	.380121	.864298	2.013037
16	1	0	-1.214037	.575015	2.691460
17	1	0	-1.937657	2.084635	-.654525
18	1	0	-2.421524	2.139711	1.036955
19	1	0	-.783405	2.556286	.569812
20	6	0	1.530964	-.294609	-.934963
21	17	0	2.184154	-1.263682	.406640
22	17	0	1.952526	1.415446	-.606939

NImag = 1
E(HF/6-31G*) = -1228.67327
ZPE(HF/6-31G*) = 0.18907

Structure **22**
TS B for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane
C1 HF/6-31G* freq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.386069	-.430803	-.249068
2	6	0	-1.906570	-.756406	.121967
3	6	0	-2.936084	-1.268832	-.845266
4	6	0	-1.406088	.613446	.267478
5	6	0	-.837436	-1.578302	.657424
6	6	0	-1.164528	1.215013	1.646312
7	6	0	-1.881478	1.660307	-.727054
8	1	0	-.199146	-.565202	-1.297386
9	1	0	-2.590038	-2.166026	-1.347022
10	1	0	-3.835493	-1.528556	-.293263
11	1	0	-3.209575	-.536408	-1.592022
12	1	0	-.494012	-1.483144	1.673634
13	1	0	-.768205	-2.580886	.270484
14	1	0	-.823170	.492787	2.371774
15	1	0	-.423158	2.001519	1.589956
16	1	0	-2.094494	1.647208	2.005496
17	1	0	-1.928727	1.280576	-1.740031
18	1	0	-2.864068	2.032387	-.453283
19	1	0	-1.195364	2.498551	-.722521
20	6	0	1.506779	.054185	.549562
21	17	0	2.447389	-1.336204	-.048746
22	17	0	1.934629	1.445353	-.480310

NImag = 1
E(HF/6-31G*) = -1228.67685
ZPE(HF/6-31G*) = 0.18873

Structure **23**
TS D for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-3,4,4-trimethylpenta-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.394543	-.476361	.048187
2	6	0	1.827415	-.363998	-.710903
3	6	0	2.875588	-1.439495	-.702420
4	6	0	1.488307	.566805	.371862
5	6	0	.603066	-.462615	-1.476209
6	6	0	1.179206	2.028765	.073382
7	6	0	2.185323	.412255	1.713359
8	1	0	.381659	-1.401870	.588661
9	1	0	2.470198	-2.388456	-1.036084
10	1	0	3.663351	-1.158123	-1.396508
11	1	0	3.328994	-1.575100	.269506
12	1	0	.162938	.395601	-1.956457
13	1	0	.448691	-1.380176	-2.019059
14	1	0	.754490	2.184294	-.906986
15	1	0	.486098	2.420626	.806785
16	1	0	2.100850	2.600515	.132092
17	1	0	2.312969	-.623857	2.000567
18	1	0	3.160163	.889900	1.703176
19	1	0	1.585627	.892204	2.477990
20	6	0	-1.467060	.162629	.694122
21	17	0	-2.078845	1.189161	-.622938
22	17	0	-2.354941	-1.390542	.579881

NImag = 1
E(HF/6-31G*) = -1228.67456
ZPE(HF/6-31G*) = 0.18898

Structure **24**
TS C for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 2,2-dichloro-1,4,4-trimethyl[1.1.1]bicyclobutane C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.405067	-.122006	-.747374
2	6	0	1.219393	-.947648	.343460
3	6	0	.880884	-1.438348	1.708778
4	6	0	1.722300	.366198	-.114866
5	6	0	.885699	-1.566727	-.935792
6	6	0	2.967416	.473269	-.996462
7	6	0	1.656224	1.526559	.869150
8	1	0	-.199203	.401829	-1.454673
9	1	0	.720225	-.633764	2.407991
10	1	0	.007803	-2.075176	1.693362
11	1	0	1.733361	-2.030293	2.038034
12	1	0	1.652990	-1.735702	-1.672558
13	1	0	.133534	-2.336935	-.917902
14	1	0	3.076811	-.331273	-1.708835
15	1	0	2.931282	1.404210	-1.552124
16	1	0	3.859201	.493153	-.376664
17	1	0	2.534841	1.523334	1.508071
18	1	0	1.646059	2.467319	.329951
19	1	0	.774454	1.492201	1.490562
20	6	0	-1.222450	.115572	.488072
21	17	0	-1.803339	1.740311	-.055853
22	17	0	-2.311870	-1.097965	-.266206

NImag = 1
E(HF/6-31G*) = -1228.64352
ZPE(HF/6-31G*) = 0.18791

Structure **25**
TS E for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,5-dimethylhexa-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.988393	-1.062683	-.067647
2	6	0	-.690380	-.396190	.667292
3	6	0	-1.031927	.175538	2.040366
4	6	0	-1.406617	.104804	-.681764
5	6	0	-.896253	-1.898304	.373352
6	6	0	-.644245	-.022307	-1.992359
7	6	0	-2.194847	1.399511	-.595978
8	1	0	-2.906602	-1.009052	.483079
9	1	0	-2.065185	.026985	2.338902
10	1	0	-.389942	-.290624	2.774859
11	1	0	-.825175	1.238023	2.065600
12	1	0	-.203136	-2.318797	-.334450
13	1	0	-1.091455	-2.538939	1.217161
14	1	0	-.115885	-.958184	-2.085858
15	1	0	-1.365909	.034564	-2.801973
16	1	0	.065283	.783341	-2.115614
17	1	0	-2.804611	1.452863	.297410
18	1	0	-1.517847	2.245483	-.596792
19	1	0	-2.847023	1.493353	-1.458033
20	6	0	1.298284	-.023585	.788979
21	17	0	2.150416	-1.065918	-.373164
22	17	0	1.460981	1.664759	.198003

NImag = 1
E(HF/6-31G*) = -1228.66412
ZPE(HF/6-31G*) = 0.18933

Structure **26**
TS F for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,3,3-trimethylpenta-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.689562	-.483174	1.227602
2	6	0	.497909	-.623156	.108981
3	6	0	.451317	-2.039602	-.462567
4	6	0	1.796642	.246550	-.034000
5	6	0	.337423	-.356885	1.663458
6	6	0	1.695954	1.766632	-.040529
7	6	0	2.846492	-.225138	-1.030736
8	1	0	2.250543	-1.377844	1.417268
9	1	0	1.420527	-2.518557	-.511112
10	1	0	-.194897	-2.665581	.138192
11	1	0	.041102	-2.008618	-1.463890
12	1	0	-.099435	.605660	1.867714
13	1	0	-.066231	-1.156465	2.259564
14	1	0	1.065846	2.158827	.740770
15	1	0	2.693503	2.169392	.105174
16	1	0	1.319837	2.123010	-.990683
17	1	0	3.081354	-1.276733	-.941256
18	1	0	2.499773	-.040832	-2.041786
19	1	0	3.765784	.332027	-.888555
20	6	0	-1.128159	.135747	-.773371
21	17	0	-1.507073	1.729378	-.066601
22	17	0	-2.428253	-.957033	-.147776

NImag = 1
E(HF/6-31G*) = -1228.66039
ZPE(HF/6-31G*) = 0.18975

Structure **27**
TS G for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,5-dimethylhexa-1,4-diene C1 HF/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.854352	-1.308625	-.114616
2	6	0	-.471132	-.629981	.330301
3	6	0	-.167005	-.734625	1.817211
4	6	0	-1.740944	.125119	-.267263
5	6	0	-.611518	-1.884914	-.562152
6	6	0	-1.625093	.759189	-1.645076
7	6	0	-2.550219	.982660	.690003
8	1	0	-2.435428	-1.753614	.670180
9	1	0	-.553253	-1.652826	2.251702
10	1	0	.901161	-.720411	1.990803
11	1	0	-.590703	.098619	2.362367
12	1	0	-.260518	-1.746155	-1.570001
13	1	0	-.330999	-2.827594	-.124020
14	1	0	-1.053066	.166444	-2.339783
15	1	0	-2.629836	.883556	-2.039626
16	1	0	-1.161846	1.734872	-1.581279
17	1	0	-2.765763	.475923	1.622572
18	1	0	-2.014531	1.898340	.914231
19	1	0	-3.494300	1.254837	.230378
20	6	0	1.101267	.286675	-.697597
21	17	0	2.457454	-.793652	-.262065
22	17	0	1.301549	1.771006	.280160

NImag = 1
E(HF/6-31G*) = -1228.66821
ZPE(HF/6-31G*) = 0.18930

Structure **1**
Bicyclobutane C2V CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.746439	.000000	-.317310
2	6	0	-.746439	.000000	-.317310
3	6	0	.000000	1.134608	.313412
4	6	0	.000000	-1.134608	.313412
5	1	0	1.430689	.000000	-1.155598
6	1	0	-1.430689	.000000	-1.155598
7	1	0	.000000	2.083905	-.223865
8	1	0	.000000	1.240987	1.402853
9	1	0	.000000	-2.083905	-.223865
10	1	0	.000000	-1.240987	1.402853

NImag = 0
E(CCSD/6-31G*) = -155.4246145
ZPE(CCSD/6-31G*) = 0.088153

Structure **2**
Dichlorocarbene singlet C2V CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.000000	.000000	.844652
2	17	0	.000000	1.413593	-.149056
3	17	0	.000000	-1.413593	-.149056

NImag = 0
E(CCSD/6-31G*) = -957.1211059
ZPE(CCSD/6-31G*) = 0.004318

Structure **3**

1,1-Dichloropenta-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.410657	-.445373	.690956
2	6	0	-2.807035	.033859	.058857
3	1	0	-3.747536	.513582	.335839
4	6	0	-2.784486	-.807997	-.980715
5	6	0	-1.617815	.420509	.911503
6	1	0	-.497398	-1.493888	.972954
7	1	0	-1.873239	-1.304072	-1.308162
8	1	0	-3.686348	-1.024329	-1.548501
9	1	0	-1.371197	1.475563	.738898
10	1	0	-1.904817	.345645	1.971954
11	6	0	.759390	-.058747	.176069
12	17	0	1.107147	1.557451	-.351856
13	17	0	2.083686	-1.167216	-.018909

NImag = 0

E(CCSD/6-31G*) = -1112.7053206

ZPE(CCSD/6-31G*) = 0.097060

Structure **4**

2,2-Dichlorobicyclo[1.1.1]pentane C2V CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.000000	.000000	.169550
2	6	0	.000000	1.062555	-1.680899
3	6	0	.000000	-1.062555	-1.680899
4	6	0	.949959	.000000	-1.049316
5	6	0	-.949959	.000000	-1.049316
6	17	0	.000000	1.438545	1.230619
7	17	0	.000000	-1.438545	1.230619
8	1	0	.000000	2.068926	-1.260557
9	1	0	.000000	1.087110	-2.775135
10	1	0	.000000	-2.068926	-1.260557
11	1	0	.000000	-1.087110	-2.775135
12	1	0	2.042162	.000000	-1.012195
13	1	0	-2.042162	.000000	-1.012195

NImag = 0

E(CCSD/6-31G*) = -1112.6748704

ZPE(CCSD/6-31G*) = 0.100752

Structure **17**
TS A for dichlorocarbene addition to bicyclobutane C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.147760	-.477578	-.496816
2	6	0	2.570250	-.375987	.266459
3	1	0	3.350561	-1.078689	-.004141
4	6	0	1.345070	-.731262	.993208
5	6	0	2.080735	.710983	-.603047
6	1	0	1.122334	-1.273537	-1.230695
7	1	0	.880803	.021039	1.639966
8	1	0	1.245815	-1.752227	1.359775
9	1	0	1.709973	1.625646	-.131916
10	1	0	2.596005	.877596	-1.548475
11	6	0	-.902594	.160151	-.803765
12	17	0	-1.047068	1.542100	.295359
13	17	0	-1.797215	-1.197257	-.073050

NImag = 1
E(CCSD/6-31G*) = -1112.5439302
ZPE(CCSD/6-31G*) = 0.094091

Structure **18**
TS B for dichlorocarbene addition to bicyclobutane Cs CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.541759	1.057797	.000000
2	6	0	.404983	2.663077	.000000
3	1	0	1.309800	3.261915	.000000
4	6	0	-.066866	1.866045	1.139466
5	6	0	-.066866	1.866045	-1.139466
6	1	0	1.570045	.711908	.000000
7	1	0	-1.139945	1.692072	1.256752
8	1	0	.484444	1.939156	2.075970
9	1	0	-1.139945	1.692072	-1.256752
10	1	0	.484444	1.939156	-2.075970
11	6	0	-.695575	-.672280	.000000
12	17	0	-.066866	-1.527070	1.435921
13	17	0	-.066866	-1.527070	-1.435921

NImag = 1
E(CCSD/6-31G*) = -1112.5419092
ZPE(CCSD/6-31G*) = 0.093822

Structure **19**
TS connecting to TS B for dichlorocarbene addition to bicyclobutane CS CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	.458390	.777360	.000000
2	6	0	.357680	2.473295	.000000
3	1	0	1.314818	2.994972	.000000
4	6	0	-.060965	1.749886	1.165505
5	6	0	-.060965	1.749886	-1.165505
6	1	0	1.518311	.518812	.000000
7	1	0	-1.111169	1.487816	1.299343
8	1	0	.525476	1.862241	2.073867
9	1	0	-1.111169	1.487816	-1.299343
10	1	0	.525476	1.862241	-2.073867
11	6	0	-.625629	-.447214	.000000
12	17	0	-.060965	-1.412740	1.473033
13	17	0	-.060965	-1.412740	-1.473033

NImag = 0
E(CCSD/6-31G*) = -1112.5492253
ZPE(CCSD/6-31G*) = 0.095578

Structure **20**
TS C for dichlorocarbene addition to bicyclobutane Cs CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-.805401	1.157586	.000000
2	6	0	.818742	1.364158	.000000
3	6	0	-.090770	1.855590	1.108245
4	6	0	-.090770	1.855590	-1.108245
5	1	0	-1.565668	.384751	.000000
6	1	0	1.898338	1.278708	.000000
7	1	0	-.028721	1.356011	2.074318
8	1	0	-.235173	2.939456	1.178186
9	1	0	-.028721	1.356011	-2.074318
10	1	0	-.235173	2.939456	-1.178186
11	6	0	.715085	-.618572	.000000
12	17	0	-.090770	-1.292368	-1.458491
13	17	0	-.090770	-1.292368	1.458491

NImag = 1
E(CCSD/6-31G*) = -1112.5064132
ZPE(CCSD/6-31G*) = 0.094120

Structure **10**

1,2,2-Trimethylbicyclobutane C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.253575	-0.549754	1.059472
2	6	0	0.775791	-0.018832	-0.238147
3	6	0	-0.703272	0.031396	0.052693
4	6	0	1.064600	-1.434574	0.164272
5	6	0	1.754339	1.064608	-0.580986
6	6	0	-1.710436	-0.829634	-0.696260
7	6	0	-1.269630	1.399450	0.404259
8	1	0	0.463835	-0.220566	2.071677
9	1	0	2.091936	-1.623002	0.484763
10	1	0	0.615823	-2.288931	-0.347230
11	1	0	2.707300	0.902230	-0.059679
12	1	0	1.962512	1.081710	-1.659059
13	1	0	1.375056	2.053679	-0.298143
14	1	0	-1.308958	-1.813047	-0.958241
15	1	0	-2.609254	-0.983491	-0.083719
16	1	0	-2.016426	-0.331851	-1.626669
17	1	0	-0.570095	1.983600	1.013681
18	1	0	-1.499713	1.974824	-0.502494
19	1	0	-2.201819	1.288884	0.973297

NImag = 0

E(CCSD/6-31G*) = -272.9669505

ZPE(CCSD/6-31G*) = 0.173865

Structure **11**
1,1-Dichloro-3,3,4-trimethylpenta-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.323729	0.123273	-0.044106
2	6	0	-0.289700	0.961774	0.072211
3	6	0	1.177179	0.708456	-0.263590
4	6	0	1.726017	-0.526021	0.463022
5	6	0	2.522288	-1.423909	-0.134702
6	6	0	1.316897	0.622078	-1.794541
7	6	0	1.976690	1.941040	0.214582
8	6	0	1.386104	-0.663818	1.931138
9	17	0	-2.944085	0.625383	0.348753
10	17	0	-1.209237	-1.523311	-0.566572
11	1	0	-0.545402	1.966513	0.409480
12	1	0	2.937574	-2.259678	0.425708
13	1	0	2.782431	-1.382447	-1.187987
14	1	0	0.819078	-0.267064	-2.193694
15	1	0	0.863330	1.508253	-2.254954
16	1	0	2.373076	0.595640	-2.087721
17	1	0	3.041746	1.800764	-0.002868
18	1	0	1.632021	2.844254	-0.305976
19	1	0	1.864355	2.107951	1.291920
20	1	0	0.315573	-0.854442	2.072798
21	1	0	1.940912	-1.496842	2.376145
22	1	0	1.631310	0.244635	2.495980

E(CCSD/6-31G*) = -1230.2392758

Structure **12**
1,1-Dichloro-4,5-dimethylhexa-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.812397	-0.246088	0.076652
2	6	0	0.554948	-0.606136	0.349013
3	6	0	-0.501303	0.236972	1.014251
4	6	0	-1.652649	0.516329	0.056250
5	6	0	-2.778705	-0.224981	0.026991
6	6	0	-3.955142	0.063556	-0.880405
7	6	0	-3.011726	-1.443991	0.894537
8	6	0	-1.374317	1.695728	-0.850768
9	17	0	2.920948	-1.320074	-0.723614
10	17	0	2.494194	1.300177	0.477637
11	1	0	0.255275	-1.605623	0.035148
12	1	0	-0.846869	-0.272698	1.920765
13	1	0	-0.068755	1.189926	1.340580
14	1	0	-3.916913	1.051766	-1.343946
15	1	0	-4.026616	-0.688986	-1.679144
16	1	0	-4.889135	0.004122	-0.304543
17	1	0	-3.778384	-1.240938	1.656353
18	1	0	-3.391309	-2.269706	0.276665
19	1	0	-2.113764	-1.802702	1.403967
20	1	0	-0.339414	1.645692	-1.214406
21	1	0	-2.027730	1.734710	-1.725410
22	1	0	-1.474817	2.644355	-0.303535

E(CCSD/6-31G*) = -1230.2448823

Structure **13**
1,1-Dichloro-2,3,3-trimethylpenta-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.145752	-0.126167	-0.016336
2	6	0	0.180225	0.810299	-0.050031
3	6	0	-1.321587	0.466800	0.086508
4	6	0	-1.717251	-0.673595	-0.841788
5	6	0	-2.621105	-1.625846	-0.587865
6	6	0	0.547097	2.276251	-0.127572
7	6	0	-1.618351	0.172022	1.567892
8	6	0	-2.205342	1.658785	-0.353101
9	17	0	2.851396	0.231345	-0.151583
10	17	0	0.881102	-1.829780	0.194416
11	1	0	-1.263933	-0.628656	-1.834872
12	1	0	-2.889987	-2.356220	-1.347839
13	1	0	-3.109895	-1.735466	0.377436
14	1	0	1.625217	2.429970	-0.160298
15	1	0	0.108600	2.745410	-1.015199
16	1	0	0.158123	2.806823	0.751086
17	1	0	-2.694497	0.037299	1.730125
18	1	0	-1.098515	-0.729099	1.907227
19	1	0	-1.291696	1.016411	2.188087
20	1	0	-2.040936	1.920488	-1.405483
21	1	0	-3.254836	1.364261	-0.244528
22	1	0	-2.036748	2.550880	0.259857

E(CCSD/6-31G*) = -1230.2332809

Structure **14**
1,1-Dichloro-2,5-dimethylhexa-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.680803	-0.016353	-0.069035
2	6	0	0.518507	0.561036	-0.403798
3	6	0	-0.619558	-0.223098	-1.031874
4	6	0	-1.617768	-0.639250	0.023120
5	6	0	-2.881747	-0.211085	0.184150
6	6	0	-3.733009	-0.744626	1.312651
7	6	0	-3.584324	0.793601	-0.697703
8	6	0	0.220529	2.017761	-0.157444
9	17	0	3.012414	0.833124	0.662803
10	17	0	2.018878	-1.707089	-0.315553
11	1	0	-1.229339	-1.370178	0.736276
12	1	0	-1.085950	0.408645	-1.796940
13	1	0	-0.236549	-1.111487	-1.545506
14	1	0	-3.184902	-1.469154	1.924852
15	1	0	-4.072241	0.071961	1.965682
16	1	0	-4.634831	-1.236487	0.921411
17	1	0	-4.473108	0.339356	-1.157685
18	1	0	-3.937402	1.643934	-0.097482
19	1	0	-2.952742	1.186024	-1.499191
20	1	0	0.961658	2.502707	0.480389
21	1	0	0.177412	2.558355	-1.113070
22	1	0	-0.764581	2.105804	0.317611

E(CCSD/6-31G*) = -1230.2494262

Structure **15**
2,2-Dichloro-1,4,4-trimethyl[1.1.1]bicyclopentane C1 CCSD/6-31G* freq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.410793	-0.642142	0.615710
2	6	0	-0.718556	0.057111	-0.195488
3	6	0	0.335405	-0.329578	-1.264878
4	6	0	1.469711	0.141553	-0.272918
5	6	0	0.379207	-1.705365	-0.532480
6	6	0	0.430215	-0.865496	2.100855
7	6	0	1.742370	1.649726	-0.042558
8	6	0	2.865201	-0.496703	-0.419427
9	17	0	-1.159884	1.758369	0.127568
10	17	0	-2.313165	-0.789733	-0.272356
11	1	0	0.254424	-0.140159	-2.339675
12	1	0	1.271277	-2.308439	-0.670837
13	1	0	-0.502414	-2.338982	-0.602100
14	1	0	-0.448745	-1.441536	2.415422
15	1	0	1.330590	-1.419579	2.394104
16	1	0	0.423498	0.092695	2.635850
17	1	0	1.256687	2.284110	-0.787165
18	1	0	1.416533	1.985960	0.946173
19	1	0	2.818979	1.841708	-0.109000
20	1	0	2.901794	-1.575745	-0.570353
21	1	0	3.383238	-0.028739	-1.266339
22	1	0	3.449898	-0.272739	0.482411

E(CCSD/6-31G*) = -1230.1983122

Structure **16**
Intermediate along pathway B for dichlorocarbene addition to
1,2,2-tri methylbicyclobutane C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.135054	-0.397261	-0.199927
2	6	0	-1.775189	-0.816288	0.158689
3	6	0	-2.712686	-1.336006	-0.889793
4	6	0	-1.343092	0.568993	0.291656
5	6	0	-0.684738	-1.634306	0.630510
6	6	0	-1.101236	1.165314	1.672894
7	6	0	-1.861813	1.593007	-0.699452
8	1	0	-0.074759	-0.532740	-1.283903
9	1	0	-2.217216	-2.051508	-1.556221
10	1	0	-3.503840	-1.881022	-0.355075
11	1	0	-3.178270	-0.543763	-1.478441
12	1	0	-0.279276	-1.517052	1.635194
13	1	0	-0.598282	-2.638242	0.219736
14	1	0	-0.790832	0.428975	2.414880
15	1	0	-0.323540	1.930141	1.615402
16	1	0	-2.041729	1.629525	1.998786
17	1	0	-1.869983	1.213108	-1.726061
18	1	0	-2.875274	1.917601	-0.430817
19	1	0	-1.200409	2.464456	-0.675035
20	6	0	1.236811	0.056698	0.521335
21	17	0	2.380332	-1.288948	-0.050303
22	17	0	1.691161	1.546572	-0.496398

E(CCSD/6-31G*) = -1230.1000013

Structure **21**
TS A for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-4,5-dimethylhexa-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.587645	-0.296627	-0.681307
2	6	0	-2.019343	-0.599227	0.014021
3	6	0	-3.343720	-0.477994	-0.682689
4	6	0	-1.145827	0.488290	0.520315
5	6	0	-1.045024	-1.675286	-0.249721
6	6	0	-0.461983	0.340392	1.874059
7	6	0	-1.564345	1.924075	0.250839
8	1	0	-0.723848	0.065360	-1.694906
9	1	0	-3.334961	-1.002931	-1.647021
10	1	0	-4.125341	-0.939196	-0.063324
11	1	0	-3.628809	0.564689	-0.853783
12	1	0	-0.472339	-2.131064	0.561127
13	1	0	-1.312573	-2.386406	-1.032924
14	1	0	-0.188431	-0.693108	2.100588
15	1	0	0.445386	0.951967	1.918454
16	1	0	-1.150757	0.688376	2.654805
17	1	0	-1.959564	2.055114	-0.762275
18	1	0	-2.328119	2.248369	0.969260
19	1	0	-0.694591	2.581866	0.359425
20	6	0	1.579815	-0.293729	-0.944589
21	17	0	2.184586	-1.309881	0.375633
22	17	0	1.992025	1.400328	-0.558868

E(CCSD/6-31G*) = -1230.0869951

Structure **22**
TS B for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane
C1 CCSD/6-31G* freq

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.452669	-0.464120	-0.256501
2	6	0	-1.974834	-0.730084	0.121749
3	6	0	-3.048216	-1.195827	-0.819529
4	6	0	-1.389037	0.628779	0.266343
5	6	0	-0.898633	-1.589023	0.654023
6	6	0	-1.119811	1.217053	1.644419
7	6	0	-1.810057	1.690278	-0.736238
8	1	0	-0.222564	-0.594106	-1.310108
9	1	0	-2.732643	-2.095924	-1.362998
10	1	0	-3.951243	-1.453131	-0.249087
11	1	0	-3.323244	-0.425944	-1.547301
12	1	0	-0.562105	-1.517052	1.689883
13	1	0	-0.857067	-2.603839	0.255498
14	1	0	-0.794414	0.465752	2.367497
15	1	0	-0.338482	1.982603	1.582779
16	1	0	-2.039277	1.686761	2.018672
17	1	0	-1.903805	1.286459	-1.750357
18	1	0	-2.769483	2.139787	-0.449613
19	1	0	-1.056636	2.486267	-0.760247
20	6	0	1.552443	0.024167	0.551974
21	17	0	2.469681	-1.363361	-0.074118
22	17	0	1.965370	1.431304	-0.457768

E(CCSD/6-31G*) = -1230.0875521

Structure **23**
TS D for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-3,4,4-trimethylpenta-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.462335	-0.501737	0.049332
2	6	0	1.877994	-0.355330	-0.711584
3	6	0	2.963079	-1.392638	-0.727989
4	6	0	1.496152	0.566348	0.394120
5	6	0	0.615047	-0.465429	-1.461124
6	6	0	1.157070	2.022120	0.104110
7	6	0	2.189797	0.405679	1.736059
8	1	0	0.402850	-1.430172	0.607387
9	1	0	2.571259	-2.372144	-1.031685
10	1	0	3.733353	-1.104488	-1.456650
11	1	0	3.451112	-1.496295	0.246219
12	1	0	0.166550	0.399803	-1.956419
13	1	0	0.460777	-1.396328	-2.009580
14	1	0	0.714146	2.165682	-0.884480
15	1	0	0.449660	2.397610	0.852249
16	1	0	2.074676	2.622675	0.156874
17	1	0	2.350911	-0.646341	1.995537
18	1	0	3.159317	0.919937	1.742536
19	1	0	1.563222	0.851490	2.517911
20	6	0	-1.530220	0.169842	0.688919
21	17	0	-2.097319	1.174021	-0.656686
22	17	0	-2.401819	-1.386053	0.585454

E(CCSD/6-31G*) = -1230.0876055

Structure **24**
TS C for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 2,2-dichloro-1,4,4-trimethyl[1.1.1]bicyclobutane C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.452290	-0.090388	-0.761259
2	6	0	1.262933	-0.963787	0.314020
3	6	0	0.880551	-1.446368	1.667570
4	6	0	1.743994	0.391547	-0.097319
5	6	0	0.914119	-1.521082	-1.011949
6	6	0	3.001343	0.544454	-0.949971
7	6	0	1.627129	1.499881	0.939331
8	1	0	-0.232687	0.468491	-1.386455
9	1	0	-0.038023	-0.924881	1.985274
10	1	0	0.698348	-2.525345	1.658615
11	1	0	1.679857	-1.216510	2.381851
12	1	0	1.696452	-1.684201	-1.755878
13	1	0	0.137774	-2.287389	-1.028222
14	1	0	3.115780	-0.238364	-1.704518
15	1	0	2.974920	1.511958	-1.466928
16	1	0	3.891018	0.529918	-0.306374
17	1	0	2.507380	1.493362	1.596161
18	1	0	1.587454	2.477578	0.443781
19	1	0	0.726660	1.390402	1.548574
20	6	0	-1.212418	0.137122	0.456957
21	17	0	-1.903366	1.725778	-0.089696
22	17	0	-2.259256	-1.155384	-0.222667

E(CCSD/6-31G*) = -1230.0584515

Structure **25**
TS E for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,5-dimethylhexa-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.081881	-1.030849	-0.135815
2	6	0	-0.787190	-0.417771	0.646131
3	6	0	-1.078185	0.142130	2.029276
4	6	0	-1.392288	0.154444	-0.674590
5	6	0	-0.976364	-1.890953	0.315085
6	6	0	-0.617834	0.023608	-1.979098
7	6	0	-2.112781	1.486407	-0.563013
8	1	0	-3.028728	-0.968853	0.392750
9	1	0	-0.851697	1.213573	2.057272
10	1	0	-2.118347	0.001355	2.350496
11	1	0	-0.415199	-0.345020	2.750057
12	1	0	-0.283716	-2.318942	-0.412769
13	1	0	-1.182804	-2.559314	1.152561
14	1	0	-0.118214	-0.942771	-2.078127
15	1	0	-1.328189	0.123538	-2.809772
16	1	0	0.135011	0.811796	-2.074673
17	1	0	-2.747484	1.536444	0.328430
18	1	0	-1.382197	2.303023	-0.514204
19	1	0	-2.743486	1.648040	-1.445739
20	6	0	1.328227	-0.044190	0.797286
21	17	0	2.150150	-1.109268	-0.353396
22	17	0	1.518958	1.636337	0.217640

E(CCSD/6-31G*) = -1230.0821597

Structure **26**
TS F for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,3,3-trimethylpenta-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.760000	-0.458293	1.251567
2	6	0	0.559663	-0.628073	0.133413
3	6	0	0.488369	-2.033943	-0.446873
4	6	0	1.811286	0.260673	-0.046429
5	6	0	0.358394	-0.346625	1.640627
6	6	0	1.671069	1.777248	-0.053530
7	6	0	2.846282	-0.195529	-1.064553
8	1	0	2.346180	-1.351072	1.453921
9	1	0	1.466104	-2.520782	-0.513398
10	1	0	-0.161372	-2.663956	0.168629
11	1	0	0.056534	-1.991759	-1.452739
12	1	0	-0.076074	0.630289	1.867846
13	1	0	-0.058709	-1.154344	2.242656
14	1	0	1.025117	2.151322	0.742016
15	1	0	2.667345	2.216158	0.085518
16	1	0	1.268848	2.122776	-1.012141
17	1	0	3.100545	-1.255202	-0.969493
18	1	0	2.471024	-0.020802	-2.080718
19	1	0	3.768595	0.384483	-0.941536
20	6	0	-1.169904	0.136384	-0.767708
21	17	0	-1.555530	1.717225	-0.052246
22	17	0	-2.434182	-0.988882	-0.151851

E(CCSD/6-31G*) = -1230.0787645

Structure **27**
TS G for dichlorocarbene addition to 1,2,2-trimethylbicyclobutane yielding 1,1-dichloro-2,5-dimethylhexa-1,4-diene C1 CCSD/6-31G*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.915807	-1.310496	-0.102071
2	6	0	-0.512275	-0.645491	0.329260
3	6	0	-0.171028	-0.728453	1.804586
4	6	0	-1.729900	0.139868	-0.262744
5	6	0	-0.647337	-1.892771	-0.547271
6	6	0	-1.607084	0.746666	-1.652058
7	6	0	-2.496485	1.039164	0.691094
8	1	0	-2.513893	-1.741550	0.697212
9	1	0	-0.624227	0.095428	2.364364
10	1	0	-0.513165	-1.674460	2.245201
11	1	0	0.912592	-0.669825	1.954751
12	1	0	-0.309141	-1.772403	-1.577430
13	1	0	-0.357738	-2.842893	-0.097081
14	1	0	-1.045419	0.115818	-2.342537
15	1	0	-2.619026	0.896488	-2.051257
16	1	0	-1.104664	1.718311	-1.602404
17	1	0	-2.731668	0.539077	1.636830
18	1	0	-1.910186	1.940494	0.909495
19	1	0	-3.439579	1.353842	0.228392
20	6	0	1.119246	0.278134	-0.710435
21	17	0	1.303419	1.767162	0.269509
22	17	0	2.462472	-0.809401	-0.249962

E(CCSD/6-31G*) = -1230.0832341
