Supporting Information for:

A Computational Investigation of the Reactions of Methylene, Chlorocarbene, and Dichlorocarbene with Cyclopropane

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Table S1. Absolute Energies (hartrees), Zero-point Energies (kcal/mol), Heat Capacity Corrections (kcal/mol), and Entropies (cal/mol•K) at B3LYP/6-31G(d) Geometries[a]

	PG	B3LYP/a	ZPE	Cp(298K)	Entropy	MP2/b	QCI/b	MP2/c	[QCI/c]	G3B3 •H(298K)
1	D_{3h}	-117.89521	51.30	2.70	56.61	-117.45508	-117.50337	-117.60868	-117.65697	-117.76590
CH_2	C_{2v}	-39.12825	10.42	2.37	45.23	-38.97541	-39.00353	-39.02796	-39.05608	-39.10025
4	C_s	-498.76056	7.05	2.43	56.20	-498.03717	-498.07819	-498.16949	-498.21051	-498.59511
5	C_{2v}	-958.38306	2.49	2.75	63.49	-957.09314	-957.14612	-957.30408	-957.35706	
$H_2C{=}CH_2$	D_{2h}	-78.58746	32.15	2.50	52.32	-78.29106	-78.32788	-78.39325	-78.43007	-78.50526
10	C_s	-538.18539	26.89	2.81	63.00	-537.32321	-537.37128	-537.50445	-537.55252	-537.97088
11	C_{2v}	-997.77529	21.17	3.28	68.79	-996.34995	-996.40888	-996.61205	-996.67098	
CP1a	C_s	-157.03132	64.44	4.59	76.81	-156.43753	-156.51255	-156.64577	-156.72079	-156.86977
CP1b	C_s	-157.03183	64.65	4.51	76.10	-156.43688	-156.51164	-156.64543	-156.72019	-156.86886
TS1-2	C_1	-157.02772	63.79	4.17	74.50	-156.43179	-156.50711	-156.64196	-156.71728	-156.86778
TS1-3	C_s	-157.02982	65.61	3.78	69.96	-156.43404	-156.50519	-156.64563	-156.71678	-156.86508
2	C_s	-157.21202	69.07	3.50	67.55	-156.62545	-156.68990	-156.83075	-156.89520	-157.03951
3	D_{2d}	-157.21315	69.93	3.18	62.92	-156.62389	-156.68983	-156.82920	-156.89514	-157.03860
CP4	C_1	-616.65820	59.25	5.57	93.42	-615.49633	-615.58529	-615.78333	-615.87229	-616.36307
TS4-6	C_1	-616.65169	58.64	4.38	79.17	-615.48701	-615.57067	-615.77851	-615.86217	-616.35552
TS4-10	C_1	-616.64255	60.39	4.40	78.31	-615.47896	-615.56176	-615.77081	-615.85361	-616.34400
6	C_1	-616.80812	63.84	4.01	75.23	-615.65737	-615.73357	-615.94148	-616.01768	-616.50466
CP5	C_1	-1076.27914	54.08	6.33	110.61	-1074.55264	-1074.65381	-1074.91792	-1075.01403	
TS5-7	C_1	-1076.24902	52.91	5.03	85.93	-1074.52655	-1074.61951	-1074.89910	-1075.01909	
TS5-11	C_s	-1076.25249	54.43	5.16	86.03	-1074.52606	-1074.62082	-1074.89758	-1074.99206	
7	C_1	-1076.39644	57.96	4.60	81.51	-1074.68511	-1074.77236	-1075.04962	-1075.13687	
TS5-14(0.36)[b,c]	C_s	-1076.24104	53.51	4.90	84.00					
14(0.90)[b]	C_s	-1076.31623	54.67	5.45	88.02					
TS14-11(0.54)[b]	C_s	-1076.31212	54.06	5.24	86.91					
Cyclobutane	C_s	-1076.40522	58.15	4.41	79.31	-1074.69450	-1074.78256	-1075.05847	-1075.14653	

a) Basis set "a" is 6-31G(d), basis set "b" is 6-31+G(d), and basis set "c" is 6-311+G(3df,2p). The square brackets indicate the use of the additivity approximation (i.e. [QCI/c]=QCI/b+MP2/c-MP2/b).

b) The number in parentheses is the spin squared value of the singlet at the UB3LYP/6-31G(d) level.
c) The "SS" indicates that there are two imaginary frequencies.

TABLE S2. Cartesian Coordinates of the Species listed in Tables 1 and 2.

1
H -0.00000 0.91096 1.46342
C -0.00000 0.00000 0.87102
H 1.26736 0.91096 -0.73171
C -0.75433 0.00000 -0.43551
H -0.00000 -0.91096 1.46342
C 0.75433 0.00000 -0.43551
H -1.26736 0.91096 -0.73171
H -1.26736 -0.91096 -0.73171
H 1.26736 -0.91096 -0.73171

CH_2
H 0.00000 0.85898 0.53771
C 0.00000 0.00000 -0.17924
H 0.00000 -0.85898 0.53771

4
Cl 0.11176 0.00000 0.50297
C -0.41108 0.00000 -1.14412
H 0.56659 0.00000 -1.68585

5
Cl 0.00000 1.42954 -0.15209
C 0.00000 0.00000 0.86186
Cl 0.00000 -1.42954 -0.15209

10
H 1.56860 0.00000 0.66499
C 0.48695 0.00000 0.59094
C -0.33239 0.00000 1.63522
Cl -0.06864 0.00000 -1.07005
H 0.08321 0.00000 2.63863
H -1.41226 0.00000 1.53023

11
Cl 1.46691 0.00000 0.52002
C 0.00000 0.00000 -0.42459
C 0.00000 0.00000 -1.75372
Cl -1.46691 0.00000 0.52002
H 0.93298 0.00000 -2.30532
H -0.93298 0.00000 -2.30532

CP1a

H 1.02535 0.13449 1.27711
C 0.07894 0.30252 0.77304
C -0.08504 1.58102 0.00000
C 0.07894 0.30252 -0.77304
H -0.78885 -0.09603 1.28556
H 0.74758 2.27943 0.00000
H -1.06529 2.04865 0.00000
C -0.25198 -2.17081 0.00000
H -0.78885 -0.09603 -1.28556
H 0.45981 -2.24824 -0.85688
H 0.45981 -2.24824 0.85688
H 1.02535 0.13449 -1.27711

CP1b
H 0.96706 0.28960 1.26032
C 0.59235 -0.39497 0.50704
C -0.64219 -1.17540 0.81699
C -0.74998 -0.04949 -0.19522
H 1.36532 -0.87641 -0.08238
H -1.11331 -1.02090 1.78346
H -0.71098 -2.19112 0.43824
C 0.65343 1.65078 -1.21231
H -0.89256 -0.33044 -1.23108
H 1.04441 2.10250 -0.26956
H 1.51631 1.00779 -1.50720
H -1.29795 0.83350 0.10923

TS1-2
C 2.289497 0.176327 -0.153321
H 2.577998 -0.422404 0.745644
H 2.435940 -0.591471 -0.958766
C -0.088518 -0.369686 0.422506
C -0.828581 0.865157 0.000257
C -1.432547 -0.482870 -0.278987
H -1.263281 1.475998 0.786321
H -0.413063 1.430017 -0.827288
H -0.014295 -0.617234 1.475854
H 0.756256 -0.749284 -0.179030
H -2.276597 -0.817685 0.318601
H -1.442059 -0.841505 -1.304065

TS1-3
C 0.28576 -1.82308 0.00000
C -0.86302 0.23340 0.00000
C -0.04136 1.45463 0.00000
C 0.76499 0.12204 0.00000

H -0.38763 -1.95670 -0.87070
H -0.38763 -1.95670 0.87070
H 1.32661 -0.01035 0.91458
H 1.32661 -0.01035 -0.91458
H 0.00685 2.03782 0.91497
H 0.00685 2.03782 -0.91497
H -1.38492 -0.03175 -0.91025
H -1.38492 -0.03175 0.91025

2
H 0.73946 0.94514 -1.38305
C 0.80105 0.88193 -0.29902
C -0.48074 1.01844 0.49053
C 0.19381 -0.32685 0.37118
H 1.71112 1.30675 0.11639
H -1.40433 1.17346 -0.06252
H -0.44634 1.53653 1.44534
C -0.43290 -1.42959 -0.45570
H 0.70823 -0.67430 1.26641
H 0.32134 -2.14567 -0.80549
H -0.93494 -1.01915 -1.34042
H -1.18185 -1.98639 0.12140

3
H 0.00000 1.96538 0.52566
C 0.00000 1.08432 -0.12452
C -1.08432 0.00000 0.12452
C 1.08432 0.00000 0.12452
C 0.00000 -1.08432 -0.12452
H 0.00000 -1.96538 0.52566
H 0.00000 -1.42315 -1.16646
H 0.00000 1.42315 -1.16646
H 1.96538 0.00000 -0.52566
H 1.42315 0.00000 1.16646
H -1.96538 0.00000 -0.52566
H -1.42315 0.00000 1.16646

CP4
H -0.22722 -0.35027 1.48102
C -0.38748 -1.22453 0.85724
C -1.59543 -2.08155 1.14213
C -1.57305 -1.21723 -0.09078
H 0.52546 -1.71703 0.53342
H -2.24628 -1.78866 1.96112
H -1.49903 -3.15631 1.01331
C -0.03461 1.48807 -0.58643

H -1.46058 -1.70652 -1.05481
Cl 1.69986 1.54914 -0.60194
H -0.24374 0.92756 -1.52680
H -2.20286 -0.33266 -0.10729

TS4-6
C 0.17454 1.16634 0.51998
H 0.94611 0.71159 1.15760
Cl 1.04505 1.68554 -0.94418
C -0.38468 -0.95894 0.00207
C -0.40590 -1.89792 1.15968
C -1.64496 -1.72472 0.31040
H 0.17135 -2.81573 1.08238
H -0.43398 -1.47328 2.16141
H 0.19884 -1.13692 -0.89381
H -0.66654 0.24679 0.22757
H -1.93351 -2.50830 -0.38587
H -2.48215 -1.18680 0.74896

TS4-10
C -0.80834 0.50515 -0.94462
C -0.61885 0.52311 0.95766
C 0.46239 0.52410 2.30459
C 0.95119 0.59098 0.95322
H 1.41949 -0.28188 0.50693
H 1.34651 1.53719 0.59421
H -1.14149 -0.41453 1.08661
H -1.19974 1.42650 1.08790
H 0.43673 -0.42136 2.83292
H 0.38234 1.42272 2.90571
Cl -0.06556 -1.02257 -1.61135
H -0.04763 1.25502 -1.24653

6
H 1.21847 1.77072 -1.55131
C 1.31546 1.70623 -0.47017
C 0.06011 1.79464 0.35976
C 0.77056 0.47271 0.22298
H 2.23230 2.14104 -0.08227
H -0.88735 1.91390 -0.15988
H 0.10619 2.30002 1.32000
C 0.18185 -0.61939 -0.61865
H 1.32037 0.12179 1.09339
H 0.93087 -1.35132 -0.92829
H -0.31680 -0.22181 -1.50567
Cl -1.09247 -1.57644 0.28532

CP5
Cl 0.35350 1.55847 1.43625
C -0.62331 1.31586 0.00046
C -1.03530 -1.99571 -0.01511
C 0.45777 -2.23005 -0.00023
C -0.48922 -3.40296 -0.01255
H -0.59073 -3.98949 0.89653
H -0.57185 -3.98553 -0.92608
Cl 0.36877 1.56740 -1.42327
H 1.02010 -2.01652 -0.90547
H 1.00135 -2.02045 0.91729
H -1.48923 -1.62336 -0.92896
H -1.50801 -1.62730 0.89077

TS5-7
C 0.12194 0.59161 -0.87913
C 0.36322 0.55162 1.37476
C 1.58628 0.02578 2.05555
C 0.32323 -0.80848 1.95466
H -0.29612 -0.95965 2.83621
H 0.35443 -1.66412 1.27957
H -0.24530 1.37233 1.74393
H 0.70413 0.98116 0.06659
H 1.87900 0.47086 3.00443
H 2.42417 -0.28633 1.43439
Cl -1.60093 0.95815 -0.90550
Cl 0.47220 -1.08035 -1.29451

TS5-11
C -0.69672 0.71342 -0.33898
Cl -0.88508 0.86499 1.46761
C 1.19845 0.49215 -0.68966
C 1.55977 -0.76145 0.14024
C 2.78725 -0.36117 -0.48930
H 1.44564 -0.59944 1.21050
H 1.05754 -1.65774 -0.21914
H 1.45607 1.47327 -0.31261
H 1.06326 0.40214 -1.75959
H 3.50105 0.26828 0.02935
H 3.10653 -0.80751 -1.42393
Cl -1.51037 -0.84009 -0.83576

7
H 1.36229 1.85935 -1.08348
C 1.49724 1.74592 -0.01263

C 0.27087 1.84890 0.85948
C 0.93001 0.51215 0.65151
H 2.44459 2.11912 0.36604
H -0.67994 2.02365 0.36557
H 0.36020 2.30204 1.84222
C 0.29703 -0.61272 -0.12480
H 1.49573 0.11716 1.49308
H 1.03765 -1.32071 -0.49281
Cl -0.61468 -0.06630 -1.58829
Cl -0.79658 -1.58465 0.95700

TS5-14
C -1.78622 -2.59708 0.00000
C -2.05612 -1.15813 0.00000
C -0.55800 -1.16337 0.00000
H -0.03491 -1.40543 0.91735
H -0.03491 -1.40543 -0.91735
H -2.48988 -0.73057 0.90409
H -2.48988 -0.73057 -0.90409
H -1.74356 -3.15719 0.92705
H -1.74356 -3.15719 -0.92705
C 0.00000 0.77919 0.00000
Cl 1.02761 1.04184 -1.46236
Cl 1.02761 1.04184 1.46236

14
C -0.40897 0.64956 0.00000
Cl -1.27570 0.29372 1.47205
Cl -1.27570 0.29372 -1.47205
C 1.06400 0.47701 0.00000
C 1.53196 -1.05209 0.00000
C 2.99953 -1.18173 0.00000
H 1.08872 -1.51872 0.88678
H 1.08872 -1.51872 -0.88678
H 1.47605 0.96747 0.88708
H 1.47605 0.96747 -0.88708
H 3.56261 -1.12020 0.92695
H 3.56261 -1.12020 -0.92695

TS14-11
C 0.37813 0.65518 0.00000
Cl -0.32645 1.27384 1.47019
Cl -0.32645 1.27384 -1.47019
C 0.98257 -0.63262 0.00000
C -0.28732 -1.94724 0.00000
C 0.32161 -3.22302 0.00000

H -0.83850 -1.68621 0.90498
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