Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supporting Information for: "The $C(^3P) + CH_2(^3B_1)$ Reaction: Accurate electronic structure calculations and Kinetics for Astrochemical Modeling"

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Ab initio calculations data

HEAT345-Q geometries

Here, optimized geometries obtained at the UHF-CCSD(T)/cc-pVQZ level used in the HEAT345-Q scheme.

Table S1: Atomic coordinates of $CH_2(^3B_1)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
H	0.000000	0.000000	1.074362
H	0.776290	0.000000	-0.742716

Table S2: Atomic coordinates of $C_2H(^2\Sigma^+)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.205320
H	0.000000	0.000000	-1.061871

Table S3: Atomic coordinates of $CCH_2(^1A_1)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.298686
H	0.937375	0.000000	1.841536
H	-0.937375	0.000000	1.841536

Table S4: Atomic coordinates of TS1 (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.253140
H	0.000000	0.000000	-1.069405
H	-1.110454	0.215254	0.860121

Table S5: Atomic coordinates of HCCH($^1\Sigma_g^+$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.204100
H	0.000000	0.000000	-1.061263
H	0.000000	0.000000	2.265363

Table S6: Atomic coordinates of CCH_2($^3B_2$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.315199
H	0.931062	0.000000	1.873723
H	-0.931062	0.000000	1.873723

Table S7: Atomic coordinates of t-HCCH(^3B_u) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.376682
H	0.000000	0.933370	-0.562554
H	0.000000	-0.933370	1.939236

Table S8: Atomic coordinates of c-HCCH($^3B_2$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.332207
H	0.000000	0.856863	-0.668782
H	0.000000	0.856863	2.000989

HEAT345-Q Anharmonicity Constants.

$$X_{\mathrm{CH_2}(^3\mathrm{B_1})} = \begin{bmatrix} -39.7953 & & \\ -5.2416 & -28.2642 & \\ -3.1239 & -110.3652 & -456.0258 \end{bmatrix}$$

$$X_{\mathrm{CCH}(^2\Sigma^+)} = \begin{bmatrix} 21.041 & & \\ -79.357 & -8.962 & \\ -0.216 & -9.464 & -52.816 \end{bmatrix}$$

$$X_{\mathrm{CCH_2}(^1\mathrm{A_1})} = \begin{bmatrix} -18.251 & & & & & \\ -11.734 & 3.041 & & & & \\ -10.885 & -17.850 & -4.702 & & & \\ 14.323 & -3.563 & -7.292 & -6.894 & & \\ -9.239 & -10.421 & -16.296 & -11.244 & -27.143 & \\ -21.485 & -15.554 & -23.692 & 0.194 & -136.234 & -32.142 \end{bmatrix}$$

$$X_{TS1} = \begin{bmatrix} -169.418 & & & & & \\ -1.450 & 2.265 & & & & \\ -16.513 & 32.110 & -0.418 & & & \\ -3.573 & -6.772 & -3.989 & -8.978 & & \\ -60.796 & -0.280 & 0.348 & -5.221 & -25.986 & \\ 2.670 & -10.705 & -17.235 & -11.950 & -1.713 & -54.784 \end{bmatrix}$$

$$X_{\mathrm{HCCH}(^1\Sigma_g^+)} = \begin{bmatrix} 21.936 & & & & & & \\ 33.119 & 21.936 & & & & & \\ 1.093 & -3.575 & -5.836 & & & & \\ -3.576 & 1.092 & -2.048 & -5.836 & & & \\ -12.802 & -12.802 & -0.678 & -0.678 & -6.356 & & \\ -2.473 & -2.473 & -8.787 & -8.787 & -4.228 & -25.674 & \\ -10.815 & -10.815 & -10.889 & -10.889 & -10.233 & -101.314 & -24.721 \end{bmatrix}$$

$$X_{\mathrm{CCH_2}(^3\mathrm{B_2})} = \begin{bmatrix} -1.189 & & & & & \\ -8.871 & -4.842 & & & & \\ -10.292 & -5.201 & -8.449 & & & \\ 5.121 & -1.880 & -12.128 & 22.024 & & \\ -9.901 & -13.970 & -7.504 & -92.427 & -30.443 & \\ -7.971 & -21.757 & 6.104 & -4.791 & -136.307 & -39.507 \end{bmatrix}$$

$$X_{t-\mathrm{HCCH}(^3\mathrm{B}_u)} = \begin{bmatrix} -1.351 & & & & & \\ -8.226 & -6.961 & & & & \\ -5.748 & -0.326 & -9.977 & & & \\ 37.411 & 19.815 & 126.532 & -234.932 & & \\ -28.580 & -5.272 & -1.548 & -25.449 & -33.265 & \\ -17.634 & 24.123 & 221.026 & -115.025 & -268.695 & -58.422 \end{bmatrix}$$

$$X_{c-\mathrm{HCCH}(^3\mathrm{B_2})} = \begin{bmatrix} 0.704 & & & & & \\ -3.822 & 1.058 & & & & \\ 55.313 & -12.054 & -49.457 & & & \\ -5.172 & -5.299 & -94.966 & -8.829 & & \\ 16.066 & -1.657 & -12.724 & -1.777 & -35.299 & \\ -10.490 & -5.162 & -3.597 & 1.426 & -135.998 & -32.457 \end{bmatrix}$$

Table S9: Energies and ZPEs for each stationary point at the UHF-CCSD(T)/cc-pVQZ geometry.

Specie	Energy (a.u.)	Harmonic Zero-Point Energy (a.u.)	Anharmonic Zero-Point Energy
H (^{2}S) (HF)	-0.49982118		
C (^{3}P)	-37.78323705		
$CH_2(^3B_1)$	-39.11559874	0.01743851	0.01647815
$CCH(^2\Sigma^+)$	-76.544169496	0.0136686	0.0135181
$CCH_2(^1A_1)$	-77.194543182	0.0234193	0.0229984
TS1	-77.19067946	0.0.0229758	0.0204061
$HCCH(^1\Sigma_g^+)$	-77.267446702863	0.02652865	0.02634941
$CCH_2(^3B_2)$	-77.0634532	0.0270814	0.0266415
t-$HCCH(^3B_u)$	-77.099586889	0.0261557	0.0256925
c-$HCCH(^3B_2)$	-77.1233397764	0.0243955	0.0239843

Table S10: Harmonic vibrational frequencies for each stationary point at the UHF-CCSD(T)/cc-pVQZ geometry.

Molecule	Frequencies (cm^{-1})						
$CH_2(^3B_1)$	1087.35	3171.74	3395.52				
$CCH(^2\Sigma^+)$	447.48	2077.48	3474.04				
$CCH_2(^1A_1)$	333.62	735.98	1219.96	1658.37	3123.56	3212.71	
TS1	942.24i	565.44	890.91	1796.86	2540.06	3345.14	
$HCCH(^1\Sigma_g^+)$	597.08	597.08	756.50	756.50	2012.56	3415.84	3509.15
$CCH_2(^3B_2)$	994.83	1406.28	1588.92	1647.28	3084.28	3165.99	
t-$HCCH(^3B_u)$	837.21	1120.69	1413.79	1850.36	3117.86	3133.12	
c-$HCCH(^3B_2)$	764.93	845.40	1216.93	1602.88	3125.99	3148.51	

MRCI+Q/aug-cc-pVTZ optimized geometries, energies and harmonic frequencies

Here, geometries optimized with the MRCI+Q/aug-cc-pVTZ method are reported, along with their calculated energies and harmonic frequencies that were used in densities and sum of states calculations.

Table S11: Atomic coordinates of $CH_2(^3B_1)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0000000000	0.0000000000	-0.2837740226
H	0.0000000000	0.9916627249	0.1418870113
H	0.0000000000	-0.9916627249	0.1418870113

Table S12: Atomic coordinates of $C_2H(^2\Sigma^+)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0000000000	-0.5291024261	-1.0337467960
C	0.0000000000	0.0271233603	0.0405799149
H	0.0000000000	0.5019790657	0.9931668812

Table S13: Atomic coordinates of $CCH_2(^1A_1)$ (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0528702279	0.0138161084	0.0056111322
C	-1.2101728375	-0.2879404540	-0.1470512794
H	0.7911380633	-0.3656448828	-0.6936119753
H	0.3661645463	0.6397692284	0.8350521225

Table S14: Atomic coordinates of TS1 (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0000214779	0.2686749504	-0.2586224550
C	-0.0000894072	0.2972354976	1.0026127999
H	0.0001167425	0.2666905058	-1.3280728653
H	-0.0000478132	-0.8326009537	0.5840825204

Table S15: Atomic coordinates of HCCH($^1\Sigma_g^+$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0000000000	0.0000000000	0.6053765462
C	0.0000000000	0.0000000000	-0.6053765462
H	0.0000000000	0.0000000000	1.6690698966
H	0.0000000000	0.0000000000	-1.6690698966

Table S16: Atomic coordinates of CCH_2($^3B_2$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0506892534	0.0122753437	0.0060181871
C	-1.2315466956	-0.2927203041	-0.1498495364
H	0.8021661904	-0.3607118861	-0.6897211202
H	0.3786912519	0.6411568465	0.8335524695

Table S17: Atomic coordinates of TS2 (Ångstroms)

Atomic Symbol	X	Y	Z
C	-0.2673645055	0.0250353874	-0.4285579025
C	-0.2111641620	0.1224401987	0.9875121761
H	0.2897684550	0.8007203223	-1.0234647628
H	0.1887602125	-0.9481959084	0.4645104892

Table S18: Atomic coordinates of t-HCCH(^3B_u) (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0600968054	-0.2957491529	0.6038059072
C	-0.0601050874	0.2957479551	-0.6038162040
H	-0.5148891726	-1.0714254317	1.0924712600
H	0.5148974546	1.0714266295	-1.0924609633

Table S19: Atomic coordinates of TS3 (Ångstroms)

Atomic Symbol	X	Y	Z
C	-0.0038236143	0.0024950144	0.0000000000
C	0.0005816790	1.3505675321	0.0000000000
H	-0.0919159619	2.4129184836	0.0000000000
H	0.8477808972	-0.6800500301	0.0000000000

Table S20: Atomic coordinates of c-HCCH($^3B_2$) (Ångstroms)

Atomic Symbol	X	Y	Z
C	-0.6709881987	-0.0292811630	0.4268303757
C	0.6709862661	-0.0292817818	0.4268333796
H	-1.3477486437	0.0292820681	-0.4268348923
H	1.3477505763	0.0292808767	-0.4268288629

Table S21: Atomic coordinates of TS4 (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0000000000	-0.5913346761	-0.2362202257
C	0.0000000000	0.6485154618	0.0309675676
H	0.0000000000	-1.7289326267	1.3132258807
H	0.0000000000	1.4509339849	0.7572478843

Table S22: Atomic coordinates of TS5 (Ångstroms)

Atomic Symbol	X	Y	Z
C	0.0001663913	-0.3127702407	0.1588252057
C	-0.0013470404	-0.1311826822	1.3875889492
H	-0.0005865040	1.3397598321	-0.7980292229
H	0.0017671532	-0.8958069093	-0.7483849320

Table S23: Energies and harmonic ZPEs for each stationary point at the MRCI+Q/aug-cc-pVTZ geometry.

Specie	Energy (a.u.)	Zero-Point Energy (a.u.)
H (^{2}S) (HF)	-0.49982118	
C (^{3}P)	-37.78323705	
$CH_2(^3B_1)$	-39.08069407	0.01727122
$CCH(^2\Sigma^+)$	-76.47368447	0.01343692
$CCH_2(^1A_1)$	-77.12247159	0.02359761
TS1	-77.11670749	0.02085331
$HCCH(^1\Sigma_g^+)$	-77.19237403	0.02635084
$CCH_2(^3B_2)$	-77.04961694	0.02483038
TS2	-76.9696288	0.01807277
t-$HCCH(^3B_u)$	-77.04162265	0.02391306
TS3	-77.03216087	0.02101876
c-$HCCH(^3B_2)$	-77.05293554	0.02367285
TS4	-76.97153172	0.01518912
TS5	-76.97192532	0.01572555

Table S24: Harmonic vibrational frequencies for each stationary point at the MRCI+Q/aug-cc-pVTZ geometry.

Molecule	Frequencies (cm^{-1})						
$CH_2(^3B_1)$	1093.36	3131.67	3356.16				
$CCH(^2\Sigma^+)$	405.94	2043.50	3448.69				
$CCH_2(^1A_1)$	357.62	742.87	1226.75	1656.42	3142.41	3232.08	
TS1	936.48i	560.86	896.53	1790.20	2531.52	3374.43	
$HCCH(^1\Sigma_g^+)$	591.90	591.90	748.18	748.18	1990.88	3395.13	3500.49
$CCH_2(^3B_2)$	772.31	1005.03	1406.71	1537.80	3049.69	3127.73	
TS2	1400.22i	811.35	974.81	1236.66	2197.13	2713.07	
t-$HCCH(^3B_u)$	743.60	816.05	1042.57	1503.55	3188.88	3201.88	
TS3	910.94i	285.96	974.96	1508.33	3053.76	3403.17	
c-$HCCH(^3B_2)$	754.34	804.67	1092.53	1563.40	3072.05	3104.18	
TS4	1153.64i	489.78	546.73	732.95	1634.09	3251.94	
TS5	1043.07i	493.27	519.13	802.28	1800.01	3288.03	

Varshni fit parameters for loose transition states

Table S25: Varshni fit parameters for loose transition states

Transition State	D (cm^{-1})	r_e (Ångstroms)	β (Ångstroms^{-2})
$C + CH_2 \rightleftharpoons CCH_2(^1A_1)$	57622	1.300	0.445
$H + C_2H \rightleftharpoons CCH_2(^1A_1)$	35658	1.119	0.570
$H + C_2H \rightleftharpoons HCCH(^1\Sigma_g^+)$	48287	1.078	0.437
$C + CH_2 \rightleftharpoons CCH_2(^3B_2)$	41806	1.358	0.425

Kinetic data in the collisionless case

Code availability

The code written and used to compute collisionless rate constants is available on Github (https://github.com/EldwinLorin/collisionless).

Singlet case

Kinetic calculations results are reported here for the collisionless scheme.

Table S26: Temperature-dependent rate constants and product formation percentages for the $C + CH_2 \longrightarrow H + C_2H$ reaction occurring on the singlet spin surface including J values from 1 to 80. Rate constants are in cm^3s^{-1}.

T (K)	$k_{bi}(T)$	$k_{prod}(T)$	$k_{prod}^{CCH_2}(T)$	$k_{prod}^{HCCH}(T)$	$k_{back}(T)$	Prod. formation (%)
10	6.310E-12	6.310E-12	2.418E-12	3.892E-12	1.136E-17	99.99982
20	2.282E-11	2.282E-11	8.738E-12	1.408E-11	5.477E-17	99.99976
30	3.293E-11	3.293E-11	1.261E-11	2.032E-11	1.087E-16	99.99967
40	3.877E-11	3.877E-11	1.484E-11	2.393E-11	1.628E-16	99.99958
50	4.261E-11	4.261E-11	1.631E-11	2.630E-11	2.216E-16	99.99949
60	4.546E-11	4.546E-11	1.740E-11	2.806E-11	2.819E-16	99.99938
70	4.776E-11	4.776E-11	1.828E-11	2.948E-11	3.486E-16	99.99927
80	4.972E-11	4.972E-11	1.904E-11	3.068E-11	4.176E-16	99.99916
90	5.145E-11	5.145E-11	1.970E-11	3.175E-11	4.939E-16	99.99905
100	5.300E-11	5.300E-11	2.029E-11	3.271E-11	5.724E-16	99.99893
110	5.465E-11	5.465E-11	2.093E-11	3.372E-11	6.503E-16	99.99880
120	5.600E-11	5.600E-11	2.145E-11	3.455E-11	7.392E-16	99.99868
130	5.728E-11	5.728E-11	2.194E-11	3.534E-11	8.248E-16	99.99856
140	5.850E-11	5.850E-11	2.241E-11	3.609E-11	9.126E-16	99.99843
150	5.966E-11	5.966E-11	2.286E-11	3.680E-11	1.008E-15	99.99831
160	6.078E-11	6.078E-11	2.329E-11	3.749E-11	1.106E-15	99.99818
170	6.186E-11	6.186E-11	2.371E-11	3.815E-11	1.206E-15	99.99805
180	6.289E-11	6.289E-11	2.410E-11	3.879E-11	1.314E-15	99.99791
190	6.389E-11	6.389E-11	2.449E-11	3.940E-11	1.418E-15	99.99778
200	6.486E-11	6.486E-11	2.487E-11	3.999E-11	1.531E-15	99.99764
210	6.579E-11	6.579E-11	2.523E-11	4.056E-11	1.645E-15	99.99750
220	6.669E-11	6.669E-11	2.558E-11	4.111E-11	1.767E-15	99.99735
230	6.756E-11	6.756E-11	2.591E-11	4.165E-11	1.892E-15	99.99721
240	6.841E-11	6.841E-11	2.624E-11	4.216E-11	2.018E-15	99.99705
250	6.922E-11	6.922E-11	2.656E-11	4.266E-11	2.146E-15	99.99690
260	7.001E-11	7.001E-11	2.687E-11	4.314E-11	2.282E-15	99.99674
270	7.078E-11	7.078E-11	2.717E-11	4.361E-11	2.428E-15	99.99657
273	7.101E-11	7.101E-11	2.726E-11	4.375E-11	2.471E-15	99.99652
280	7.151E-11	7.151E-11	2.745E-11	4.406E-11	2.574E-15	99.99640
290	7.223E-11	7.223E-11	2.773E-11	4.450E-11	2.723E-15	99.99623
300	7.292E-11	7.292E-11	2.800E-11	4.492E-11	2.880E-15	99.99605

pTS results at various pressures are shown in Fig S1.

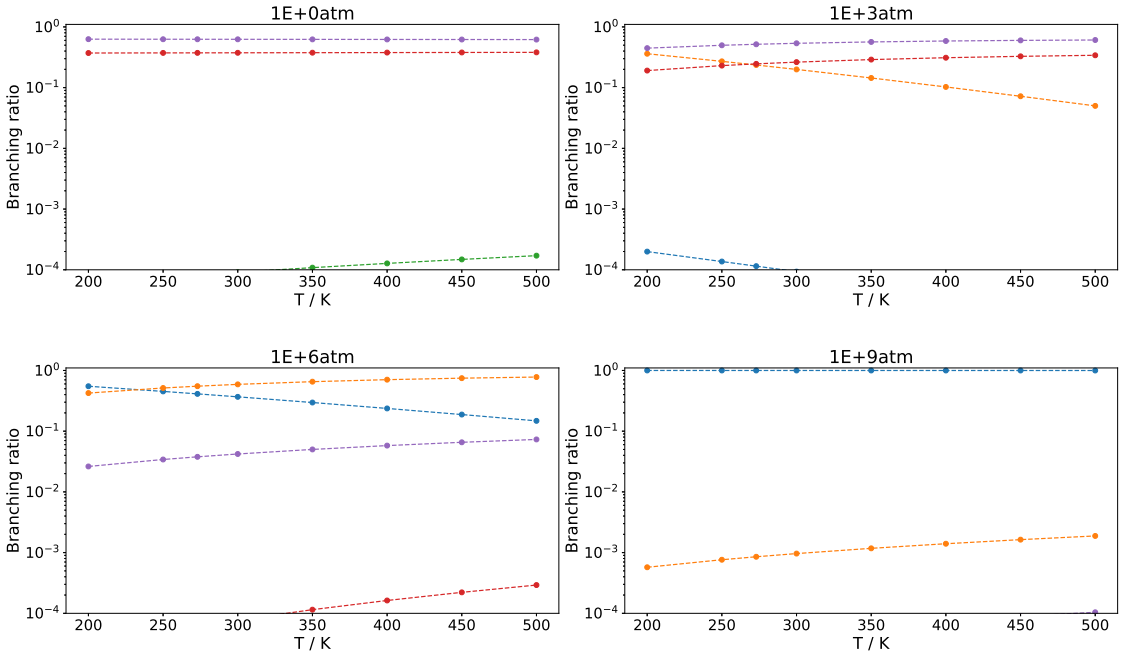

Figure S1: Branching ratios for individual channels as a function of temperature at various pressures, on the singlet surface. Blue: CCH_2 formation, Orange: HCCH formation, Purple: $H + C_2H$ formation from CCH_2 dissociation, Red: $H + C_2H$ formation directly from HCCH dissociation, Green: Backdissociation. A curve not being visible means that the branching ratio is lower than 10^{-4}.

Triplet case

Table S27: Temperature-dependent rate constants and product formation percentages for the $C + CH_2 \longrightarrow H + C_2H$ reaction occurring on the triplet spin surface including J values from 1 to 80. Rate constants are in cm^3s^{-1}.

T (K)	$k_{bi}(T)$	$k_{prod}(T)$	$k_{prod}^{CCH_2}(T)$	$k_{prod}^{c-HCCH}(T)$	$k_{back}(T)$	Prod. formation (%)
10	1.282E-11	1.282E-11	1.640E-12	1.118E-11	2.051E-17	99.99985
20	4.603E-11	4.603E-11	5.830E-12	4.020E-11	9.666E-17	99.99979
30	6.663E-11	6.663E-11	8.370E-12	5.826E-11	1.866E-16	99.99973
40	7.851E-11	7.851E-11	9.790E-12	6.872E-11	2.748E-16	99.99965
50	8.630E-11	8.630E-11	1.070E-11	7.562E-11	3.797E-16	99.99956
60	9.207E-11	9.207E-11	1.130E-11	8.075E-11	4.788E-16	99.99947
70	9.672E-11	9.672E-11	1.180E-11	8.490E-11	5.997E-16	99.99938
80	1.007E-10	1.007E-10	1.220E-11	8.846E-11	7.150E-16	99.99928
90	1.042E-10	1.042E-10	1.260E-11	9.160E-11	8.440E-16	99.99919
100	1.073E-10	1.073E-10	1.290E-11	9.439E-11	9.764E-16	99.99908
110	1.107E-10	1.107E-10	1.330E-11	9.744E-11	1.129E-15	99.99898
120	1.135E-10	1.135E-10	1.350E-11	9.996E-11	1.283E-15	99.99887
130	1.161E-10	1.161E-10	1.380E-11	1.023E-10	1.440E-15	99.99876
140	1.186E-10	1.186E-10	1.400E-11	1.046E-10	1.601E-15	99.99865
150	1.209E-10	1.209E-10	1.430E-11	1.066E-10	1.777E-15	99.99852
160	1.232E-10	1.232E-10	1.450E-11	1.087E-10	1.959E-15	99.99841
170	1.254E-10	1.254E-10	1.470E-11	1.107E-10	2.157E-15	99.99829
180	1.275E-10	1.275E-10	1.490E-11	1.126E-10	2.346E-15	99.99816
190	1.295E-10	1.295E-10	1.510E-11	1.144E-10	2.551E-15	99.99802
200	1.314E-10	1.314E-10	1.530E-11	1.161E-10	2.773E-15	99.99789
210	1.333E-10	1.333E-10	1.550E-11	1.178E-10	2.999E-15	99.99775
220	1.351E-10	1.351E-10	1.560E-11	1.195E-10	3.229E-15	99.99761
230	1.369E-10	1.369E-10	1.580E-11	1.211E-10	3.477E-15	99.99746
240	1.385E-10	1.385E-10	1.600E-11	1.225E-10	3.726E-15	99.99731
250	1.402E-10	1.402E-10	1.610E-11	1.241E-10	3.996E-15	99.99715
260	1.417E-10	1.417E-10	1.630E-11	1.254E-10	4.265E-15	99.99699
270	1.432E-10	1.432E-10	1.640E-11	1.268E-10	4.554E-15	99.99682
280	1.437E-10	1.437E-10	1.640E-11	1.273E-10	4.814E-15	99.99665
290	1.447E-10	1.447E-10	1.650E-11	1.282E-10	5.108E-15	99.99647
300	1.461E-10	1.461E-10	1.660E-11	1.294E-10	5.435E-15	99.99629

Overall results

Table S28: Temperature-dependent total rate constants and product formation percentages for the $C + CH_2 \longrightarrow H + C_2H$ reaction including both the singlet and triplet surfaces. Rate constants are in cm^3s^{-1}.

T (K)	$k_{bi}(T)$	$k_{prod}(T)$	Prod. formation (%)
10	1.913E-11	1.913E-11	99.99984
20	6.885E-11	6.885E-11	99.99978
30	9.956E-11	9.956E-11	99.99971
40	1.173E-10	1.173E-10	99.99963
50	1.289E-10	1.289E-10	99.99954
60	1.375E-10	1.375E-10	99.99944
70	1.445E-10	1.445E-10	99.99934
80	1.504E-10	1.504E-10	99.99924
90	1.557E-10	1.557E-10	99.99914
100	1.603E-10	1.603E-10	99.99903
110	1.654E-10	1.654E-10	99.99892
120	1.695E-10	1.695E-10	99.99881
130	1.734E-10	1.734E-10	99.99869
140	1.771E-10	1.771E-10	99.99858
150	1.806E-10	1.806E-10	99.99845
160	1.840E-10	1.840E-10	99.99833
170	1.873E-10	1.873E-10	99.99821
180	1.914E-10	1.914E-10	99.99803
190	1.944E-10	1.944E-10	99.99789
200	1.972E-10	1.972E-10	99.99776
210	2.000E-10	2.000E-10	99.99762
220	2.027E-10	2.027E-10	99.99748
230	2.053E-10	2.053E-10	99.99732
240	2.077E-10	2.077E-10	99.99717
250	2.102E-10	2.102E-10	99.99701
260	2.125E-10	2.125E-10	99.99685
270	2.142E-10	2.142E-10	99.99672
280	2.152E-10	2.152E-10	99.99657
290	2.169E-10	2.169E-10	99.99639
300	2.190E-10	2.190E-10	99.99621