Methane coupling in nanosecond pulsed plasmas: correlation between temperature and pressure and effects on product selectivity

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Supporting Information

1. Carbon and hydrogen balance

Table S1 Carbon and hydrogen balance

Pressure (bar)	Carbon recovery (%)	H Recovery (%)
1	90.5	97.1
2	81.0	98.1
3	77.7	94.4
4	74.7	95.4
5	77.2	90.7

Carbon and hydrogen recoveries (C_{out}/C_{in} and H_{out}/H_{in}) were calculated on the basis of the chromatographic data of C_2 species produced by the plasma reactor and methane/hydrogen fed into the plasma reactor using the equations below. Heavy species with minor selectivity, *i.e.*, C_3–C_6 were also formed but not quantified. At higher conversions (2 – 5 bar), carbon and hydrogen balance of ~ 75 – 80% and ~ 90 – 95%, respectively, were calculated. The majority of the missing carbon must be attributed to C_3 or longer hydrocarbons. Based upon the weight of all solid matter collected following the experiment and assuming that it consists of only carbon, about 5 – 10% of the missing carbon is related to the formation of carbon black and other solid carbonaceous products deposited on the reactor wall or collected by the filter.

$$C\ recovery = \frac{v_{out} \times \left([CH_4]_{out} + 2 \times ([C_2H_2] + [C_2H_4] + [C_2H_6])\right)}{v_{in} \times [CH_4]_{in}} \times 100\%$$

$$H\ recovery = \frac{v_{out} \times \left[4 \times ([CH_4]_{out} + [C_2H_4]) + 2 \times ([H_2] + [C_2H_2]) + 6 \times [C_2H_6]\right]}{4 \times v_{in} \times [CH_4]_{in} + 2 \times v_{in} \times [H_2]_{in}} \times 100\%$$

2. Power deposition characteristics

The current and voltage waveforms, power pulses and energy curves of the co-axial reactor operating at applied pressure in the 1 to 5 bar pressure range are presented in Figure S1.

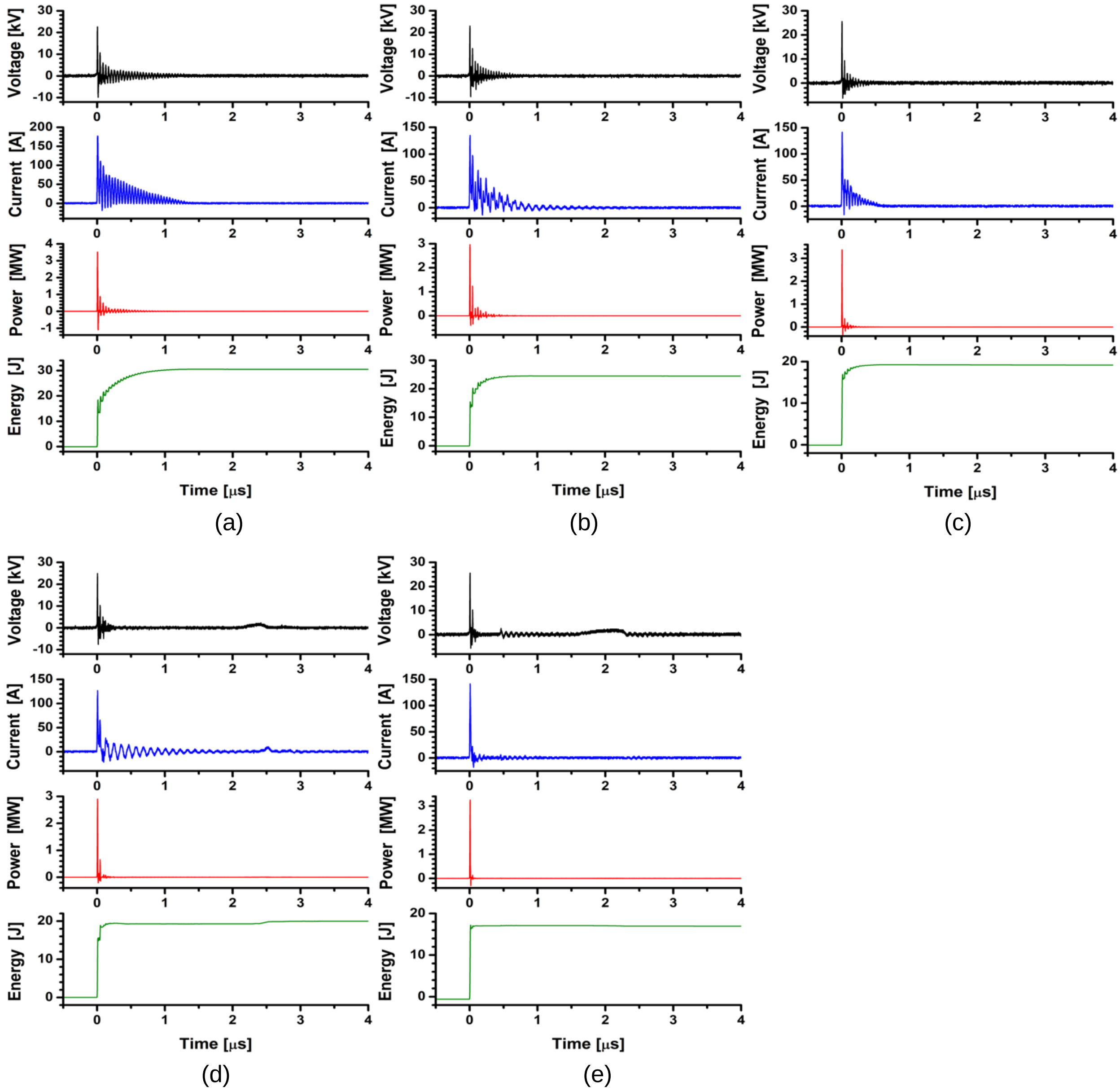

Figure S1 Experimental profiles of voltage (black), current (blue), peak of derived instantaneous power (red) and curve of delivered energy (green) at the applied pressures of (a) 1 bar, (b) 2 bar, (c) 3 bar, (d) 4 bar and (e) 5 bar. Pulses were generated by the nanosecond pulsed power supply NPG-18/100k, Megaimpulse Ltd. in the co-axial plasma reactor operating at 200 sccm (CH_4:H_2=1:1 molar basis), discharge gap 2.5 mm, pulse frequency 3 kHz (continuous mode).

3. Gas temperature calculations

The balance equation to solve the gas temperature in the system is as follows

$$N \frac{yk}{y-1}\frac{dT_{gas}}{dt} = Pe,el + \sum j \; R_j \, \Delta H_j - P_{ext}$$

where $N = \sum n_i$ is the total neutral species density, γ is the specific heat ratio of the total gas mixture, k is the Boltzmann constant (in J K^{-1}), Pe,el is the gas heating power density due to elastic electron-neutral collisions (in W m^{-3}), R_j is the rate of reaction j (in m^{-3} s^{-1}), ΔH_j is the heat released (or consumed when this value is negative) by reaction j (in Joules) and P_{ext} is the heat loss due to energy exchange with the surroundings (in W m^{-3}). The latter is expressed by the equation:

$$P_{ext} = \frac{8\lambda_{CH_4}}{R^2}\left(T_{gas} - T_{gas}, i\right) x_{CH_4} + \frac{8\lambda_{H_2}}{R^2}\left(T_{gas} - T_{gas}, i\right) x_{H_2}$$

With R being the radius of the plasma zone, T_{gas} the plasma gas temperature and T_{gas}, i the gas temperature at the edge of the plasma zone, which is assumed to be the average between room temperature and plasma temperature, according to Berthelot.[1] λ is the gas thermal conductivity of each gas (in W cm^{-1} K^{-1}) and x is the fraction of each gas (CH_4 and H_2). The thermal conductivity of CH_4 and H_2 taken respectively from Hepburn et al.[2] and Edlmann et al.[3] can be expressed as:

$$\lambda_{CH_4} = (1.49\ x\ 10^{-6}) * T_{gas} - 9.92\ x\ 10^{-5}$$

$$\lambda_{H_2} = (4.90\ x\ 10^{-6}) * T_{gas} + 3.85\ x\ 10^{-4}$$

It is important to note that the model developed in this study investigates the gas temperature in the plasma volume confined within the reactor volume. Thus, the gas temperatures calculated by the model may not reflect the gas temperature in the whole reactor body. Moreover, the model is concerned with a finite element volume and does not account for conductive or convective losses in the reactor.

4. Vibrational kinetics of H_2

Alongside ground state H_2, 14 vibrational levels of H_2 are included in the model with ascending energy from the ground state (0 eV) up to the dissociation limit (4.48 eV). The energy of each level is calculated using the anharmonic oscillator theory for a diatomic molecule, where the first two vibrational constants, ω_e = 4401.213 cm^{-1} $\omega_e x_e$ = 121.336 cm^{-1}, of the hydrogen molecule are used in this work[4]. The energy values are H_2 = 0.00 eV, H_2(v1) = 0.516 eV, H_2(v2) = 1.001 eV, H_2(v3) = 1.457 eV, H_2(v4) = 1.882 eV, H_2(v5) = 2.277 eV, H_2(v6) = 2.642 eV, H_2(v7) = 2.977 eV, H_2(v8) = 3.282 eV, H_2(v9) = 3.557 eV, H_2(v10) = 3.802 eV, H_2(v11) = 4.017 eV, H_2(v12) = 4.201 eV, H_2(v13) = 4.356 eV and H_2(v14) = 4.480 eV.

(a) VV-relaxation between H_2 molecules

The rate coefficient of H_2–H_2 relaxation processes of vibrationally excited states, i.e., $H_2(v+1) + H_2(w) \rightarrow H_2(v) + H_2(w+1)$, were scaled with the approach proposed by Matveyev and Silakov,[5] and Loureiro and Ferreira.[6] In this approach, the rate coefficient of the lowest levels $k_{1,0}^{0,1}$ (in cm^3 s^{-1}) is used to determine the rate coefficient of reactions involving higher levels $k_{v+1,v}^{w,w+1}$:

$$k_{v+1,v}^{w,w+1} = k_{1,0}^{0,1}\,(v+1)(w+1)\left[\frac{3}{2} - \frac{1}{2}\exp(-\delta\,(w-v)\right]\exp[\Delta_1(w-v) - \Delta_2(w-v)^2]\quad w > v$$

With $k_{1,0}^{0,1} = 4.23\,x\,10^{-15}\left(\frac{300}{T_{gas}}\right)^{\frac{1}{3}}$, $\delta = 0.21\sqrt{\left(\frac{T_{gas}}{300}\right)}$, $\Delta_1 = 0.236\left(\frac{Tgas}{300}\right)^{\frac{1}{4}}$ and $\Delta_2 = 0.0572\left(\frac{300}{T_{gas}}\right)^{\frac{1}{3}}$

Detailed balance is then applied to this equation to calculate reverse reaction rates.

(b) VT-relaxation of H_2 molecules

For VT relaxation processes, i.e, $H_2(v) + M \rightarrow H_2(v \pm 1) + M$, we also employed the approach proposed by Matveyev and Silakov, [5] in which the rate coefficient of $k_{v,v-1}$ levels (upon VT relaxation from higher levels) can be determined using the rate coefficient of the $k_{1,0}$ process, or the $H_2(v1) + M \rightarrow H_2 + M$ reaction.

$$k_{v,v-1} = k_{1,0}\, v \exp\left[0.97\left(\frac{300}{T_{gas}}\right)^{\frac{1}{3}}(v-1)\right]$$

The rate expression of $k_{1,0}$ is taken from Capitelli et al.[7]

$$k_{1,0} = 7.47\,x10^{-12}\,T_{gas}^{0.50}\exp\left(-93.87\,T_{gas}^{-\frac{1}{3}}\right)\left[1-\exp\left(-\frac{E_{1,0}}{T_{gas}}\right)\right]^{-1}$$

With $E_{1,0} = 5983\,K$. The reverse processes are included using detailed balance.

The H_2 VT reactions in which H atoms are collision partners, $H_2(v) + H \rightarrow H_2(v \pm 1) + H$, are divided into two distinct processes, one of non-reactive character (i) and another of reactive character (ii), depending on the occurrence (ii) or not (i) of atomic exchange between the H_2 and H species. These reactions were described by Gorse et al.[8] for $w < v < 10$ and the proposed rate coefficient is:

$$k = A_{nr}\exp\left(-\frac{E_{a,nr}}{T_{gas}}\right) + A_r\exp\left(-\frac{E_{a,r}}{T_{gas}}\right)$$

Where the pre-exponential factors A_{nr} and A_r (in $cm^3\,s^{-1}$) and activation energies $E_{a,nr}$ and $E_{a,r}$ (in K) are given in Gorse et al. for the relaxation reactions from all levels $v < 10$ to all levels $w \leq v-1$.

5. Vibrational kinetics of CH_4

The lowest energy level of the four degenerate vibrational modes of CH_4 are considered in the model: the $v1$ singly degenerate symmetric stretch mode (at 0.362 eV), the $v2$ doubly degenerate scissoring bend mode (at 0.190 eV), the $v3$ triply degenerate asymmetric stretch mode (at 0.374 eV) and the $v4$ triply degenerate umbrella bend mode (at 0.162 eV).[9] The relaxation processes between these modes were studied by Menard-Bourcin et al.[10] who determined the reaction rates at gas temperature of 193 and 296 K. Based on earlier works of Capitelli et al.,[7] Wang and Springer[11] and Richards and Sigafoos,[12] it is possible to express the rate constants of these relaxation processes at any given gas temperatures T_1 and T_2 (in Kelvin, $T_1 > T_2$) as follows

$$\frac{k_{T_2}}{k_{T_1}} = exp\left(-\ \alpha T_2^{-\left(\frac{1}{3}\right)} +\ \alpha T_1^{-\left(\frac{1}{3}\right)}\right)$$

Where k_{T_1} and k_{T_2} are the rate coefficients (in cm^3 s^{-1}) at gas temperatures T_1 and T_2 and α is a constant derived from the rates calculated by Menard-Bourcin et al. at 193 and 296 K. The reverse reactions are also included in the model and their rate coefficients were defined by the detailed balance approach suggested by Menard-Bourcin et al.[10]

6. Full chemistry of CH_4 and H_2

The chemical reactions included in the model are divided in different types and are listed in the tables below.

Table S2 Electron impact reactions with neutral species and corresponding rate coefficients. The rate coefficients are evaluated using cross section data $f(\sigma)$, or an analytical expression with T_{gas} and T_e in Kelvin. The rate coefficients for two-body and three-body reactions are given in cm^3 s^{-1} or cm^6 s^{-1}, respectively. References are shown in the last column.

$e^- + CH_4 \rightarrow e^- + CH_4$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH_4(v1-v4) \leftrightarrow e^- + CH_4(v1-v4)$	f(σ)	[13]
$e^- + CH_3 \rightarrow e^- + CH_3$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH_2 \rightarrow e^- + CH_2$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH \rightarrow e^- + CH$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C \rightarrow e^- + C$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_s \rightarrow e^- + C_s$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H_6 \rightarrow e^- + C_2H_6$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H_5 \rightarrow e^- + C_2H_5$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H_4 \rightarrow e^- + C_2H_4$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H_3 \rightarrow e^- + C_2H_3$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H_2 \rightarrow e^- + C_2H_2$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2H \rightarrow e^- + C_2H$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_3H_8 \rightarrow e^- + C_3H_8$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_3H_7 \rightarrow e^- + C_3H_7$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_3H_6 \rightarrow e^- + C_3H_6$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_3H_5 \rightarrow e^- + C_3H_5$	f(σ)	IST Lisbon database – Lxcat net

$e^- + H \rightarrow e^- + H$	f(σ)	IST Lisbon database – Lxcat net
$e^- + H_2 \rightarrow e^- + H_2$	f(σ)	IST Lisbon database – Lxcat net
$e^- + H_2(v1 - 14) \leftrightarrow e^- + H_2(v1 - 14)$	f(σ)	[14]
$e^- + H_2^* \rightarrow e^- + H_2^*$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH_4(v) \leftrightarrow e^- + CH_4(w)$	f(σ)	[13]
$e^- + CH_4 \rightarrow CH_2^- + H_2$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH \rightarrow CH^-$	f(σ)	Itikawa database – Lxcat net
$e^- + H_2 \rightarrow e^- + H_2(v1 - 14)$	f(σ)	[14]
$e^- + H_2(v) \leftrightarrow e^- + H_2(w)$	f(σ)	[14]
$e^- + H_2 \rightarrow e^- + H_2^*$	f(σ)	IST Lisbon database – Lxcat net
$e^- + CH_4 \rightarrow e^- + e^- + CH_4^+$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + e^- + CH_3^+ + H$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + e^- + CH_2^+ + H_2$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + CH_3 + H$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + CH_2 + H_2$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + CH_2 + H + H$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + CH + H_2 + H$	f(σ)	[15]
$e^- + CH_4 \rightarrow e^- + C + H_2 + H_2$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + e^- + CH_3^+$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + e^- + CH_2^+ + H$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + e^- + CH^+ + H_2$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + CH_2 + H$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + CH + H_2$	f(σ)	[15]
$e^- + CH_3 \rightarrow e^- + C + H_2 + H$	f(σ)	[15]
$e^- + CH_2 \rightarrow e^- + e^- + CH_2^+$	f(σ)	[15]
$e^- + CH_2 \rightarrow e^- + CH + H$	f(σ)	[15]
$e^- + CH_2 \rightarrow e^- + C + H_2$	f(σ)	[15]
$e^- + CH_2 \rightarrow e^- + C + H + H$	f(σ)	[15]
$e^- + CH \rightarrow e^- + e^- + CH^+$	f(σ)	[15]
$e^- + CH \rightarrow e^- + C + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + e^- + C_2H_6^+$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + e^- + C_2H_5^+$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + e^- + C_2H_4^+$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + e^- + C_2H_3^+$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + e^- + C_2H_2^+$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + e^- + C_2H_5^+ + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + e^- + C_2H_4^+ + H_2$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow 2\,e^- + C_2H_3^+ + H_2 + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + e^- + C_2H_2^+ + 2\,H_2$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + e^- + CH_3^+ + CH_3$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + e^- + C_2H_4^+ + H$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + e^- + C_2H_3^+ + H_2$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow 2\,e^- + C_2H_2^+ + H_2 + H$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + e^- + C_2H_3^+ + H$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + e^- + C_2H_2^+ + H_2$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + e^- + C_2H_2^+ + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + C_2H_5 + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + C_2H_4 + H_2$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + C_2H_3 + H_2 + H$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + C_2H_2 + 2\,H_2$	f(σ)	[15]

$e^- + C_2H_6 \rightarrow e^- + CH_4 + CH_2$	f(σ)	[15]
$e^- + C_2H_6 \rightarrow e^- + CH_3 + CH_3$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + C_2H_4 + H$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + C_2H_3 + H_2$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + C_2H_3 + 2\,H$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + C_2H_2 + H_2 + H$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + C_2H + 2\,H_2$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + CH_4 + CH$	f(σ)	[15]
$e^- + C_2H_5 \rightarrow e^- + CH_3 + CH_2$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + C_2H_3 + H$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + C_2H_2 + H_2$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + C_2H_2 + 2\,H$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + C_2H + H_2 + H$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + CH_3 + CH$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + CH_2 + CH_2$	f(σ)	[15]
$e^- + C_2H_4 \rightarrow e^- + C + CH_4$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + C_2H + H + H$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + C_2 + H_2 + H$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + CH_2 + CH$	f(σ)	[15]
$e^- + C_2H_3 \rightarrow e^- + C + CH_3$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + C_2H + H$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + C_2 + H_2$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + C_2 + 2\,H$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + CH + CH$	f(σ)	[15]
$e^- + C_2H_2 \rightarrow e^- + C + CH_2$	f(σ)	[15]
$e^- + C_2H \rightarrow e^- + C_2 + H$	f(σ)	[15]
$e^- + C_2H \rightarrow e^- + C + CH$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + e^- + C_2H_5^+ + CH_3$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + e^- + C_2H_4^+ + CH_4$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + e^- + C_2H_5^+ + CH_2$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + e^- + C_2H_4^+ + CH_3$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + e^- + C_2H_3^+ + CH_4$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + e^- + CH_3^+ + C_2H_4$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + e^- + C_2H_5^+ + CH$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + e^- + C_2H_4^+ + CH_2$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + e^- + C_2H_3^+ + CH_3$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + e^- + C_2H_2^+ + CH_4$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + e^- + CH_3^+ + C_2H_3$	f(σ)	[15]
$e^- + C_3H_5 \rightarrow e^- + e^- + C_2H_3^+ + CH_2$	f(σ)	[15]
$e^- + C_3H_5 \rightarrow e^- + e^- + C_2H_2^+ + CH_3$	f(σ)	[15]
$e^- + C_3H_5 \rightarrow e^- + e^- + CH_3^+ + C_2H_2$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + C_3H_7 + H$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + C_3H_6 + H_2$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + C_2H_4 + CH_4$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + C_2H_6 + CH_2$	f(σ)	[15]
$e^- + C_3H_8 \rightarrow e^- + C_2H_5 + CH_3$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + C_3H_6 + H$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + C_2H_4 + CH_3$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + C_2H_3 + CH_4$	f(σ)	[15]
$e^- + C_3H_7 \rightarrow e^- + C_3H_5 + H_2$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + C_2H_2 + CH_4$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + C_3H_5 + H$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + C_2H_3 + CH_3$	f(σ)	[15]
$e^- + C_3H_6 \rightarrow e^- + C_2H_4 + CH_2$	f(σ)	[15]

$e^- + C_3H_5 \rightarrow e^- + C_2H_2 + CH_3$	f(σ)	15
$e^- + C_3H_5 \rightarrow e^- + C_2H + CH_4$	f(σ)	15
$e^- + H_2 \rightarrow e^- + H + H$	f(σ)	16
$e^- + H_2(v1 - 14) \rightarrow e^- + H + H$	f(σ)	16
$e^- + H_2^* \rightarrow e^- + H + H$	f(σ)	16
$e^- + H_2 \rightarrow e^- + e^- + H_2^+$	f(σ)	16
$e^- + H_2(v1 - 14) \rightarrow e^- + e^- + H_2^+$	f(σ)	16
$e^- + H_2^* \rightarrow e^- + e^- + H_2^+$	f(σ)	16
$e^- + H^+ \rightarrow H$	See reference	17
$e^- + H_3^+ \rightarrow H_2 + H$	f(σ)	18,19
$e^- + H_3^+ \rightarrow e^- + H_2 + H^+$	f(σ)	18,19
$e^- + H_3^+ \rightarrow H + H + H$	f(σ)	18,19
$e^- + H_2^+ \rightarrow e^- + H + H^+$	f(σ)	17
$e^- + H_3^+ \rightarrow e^- + H + H + H^+$	f(σ)	18,19
$e^- + H \rightarrow e^- + e^- + H^+$	f(σ)	IST Lisbon database – Lxcat net
$e^- + H^- \rightarrow e^- + e^- + H$	f(σ)	Itikawa database – Lxcat net
$e^- + CH_4 \rightarrow CH_3 + H^-$	f(σ)	Itikawa database – Lxcat net
$e^- + CH_4 \rightarrow CH_2^- + H_2$	f(σ)	IST Lisbon database – Lxcat net
$e^- + H_2 \rightarrow H + H^-$	f(σ)	Itikawa database – Lxcat net
$e^- + H_2(v1 - 14) \rightarrow H + H^-$	f(σ)	IST Lisbon database – Lxcat net
$e^- + H_2^* \rightarrow H + H^-$	f(σ)	Itikawa database – Lxcat net
$e^- + CH_4 \rightarrow CH_2^- + H_2$	f(σ)	Itikawa database – Lxcat net
$e^- + H_2^+ \rightarrow H + H$	See reference	17
$e^- + C \rightarrow e^- + e^- + C^+$	f(σ)	IST Lisbon database – Lxcat net
$e^- + C_2 \rightarrow e^- + e^- + C_2^+$	f(σ)	15
$e^- + C_2 \rightarrow e^- + C + C$	f(σ)	15
$e^- + C_2^+ \rightarrow e^- + C^+ + C$	f(σ)	15
$e^- + C_2^+ \rightarrow C + C$	f(σ)	15
$e^- + C_3 \rightarrow e^- + C_2 + C$	f(σ)	15
$e^- + C_3 \rightarrow e^- + C + C + C$	f(σ)	15
$e^- + CH_5^+ \rightarrow CH_3 + H + H$	$2.57 \times 10^{-7}\ T_e^{-0.30}$	15,20
$e^- + CH_5^+ \rightarrow CH_2 + H_2 + H$	$6.61 \times 10^{-8}\ T_e^{-0.30}$	15,20
$e^- + CH_4^+ \rightarrow CH_3 + H$	$3.50 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + CH_4^+ \rightarrow CH_2 + H + H$	$3.50 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + CH_4^+ \rightarrow CH + H_2 + H$	$1.41 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + CH_3^+ \rightarrow CH_2 + H$	$3.50 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + CH_3^+ \rightarrow CH + H_2$	$7.88 \times 10^{-8}\ T_e^{-0.50}$	15,20
$e^- + CH_3^+ \rightarrow CH + H + H$	$9.00 \times 10^{-8}\ T_e^{-0.50}$	15,20
$e^- + CH_3^+ \rightarrow C + H_2 + H$	$1.69 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + CH_2^+ \rightarrow CH + H$	$6.25 \times 10^{-8}\ T_e^{-0.50}$	15,20
$e^- + CH_2^+ \rightarrow C + H_2$	$5.78 \times 10^{-9}\ T_e^{-0.50}$	15,20
$e^- + CH_2^+ \rightarrow C + H + H$	$1.59 \times 10^{-9}\ T_e^{-0.50}$	15,20
$e^- + CH^+ \rightarrow C + H$	$2.53 \times 10^{-7}\ T_e^{-0.50}$	15,20
$e^- + C_2H_6^+ \rightarrow C_2H_5 + H$	$2.19 \times 10^{-8}\ T_e^{-0.71}$	21
$e^- + C_2H_6^+ \rightarrow C_2H_4 + H + H$	$3.36 \times 10^{-8}\ T_e^{-0.71}$	21
$e^- + C_2H_5^+ \rightarrow C_2H_4 + H$	$7.70 \times 10^{-9}\ T_e^{-0.71}$	21
$e^- + C_2H_5^+ \rightarrow C_2H_3 + H + H$	$1.92 \times 10^{-8}\ T_e^{-0.71}$	21
$e^- + C_2H_5^+ \rightarrow C_2H_2 + H_2 + H$	$1.60 \times 10^{-8}\ T_e^{-0.71}$	21

$e^- + C_2H_5^+ \rightarrow C_2H_2 + H + H + H$	$8.98 \times 10^{-9}\ T_e^{-0.71}$	21
$e^- + C_2H_5^+ \rightarrow CH_3 + CH_2$	$9.62 \times 10^{-9}\ T_e^{-0.71}$	21
$e^- + C_2H_4^+ \rightarrow C_2H_3 + H$	$6.16 \times 10^{-8}\ T_e^{-0.76}$	21
$e^- + C_2H_4^+ \rightarrow C_2H_2 + H_2$	$3.36 \times 10^{-8}\ T_e^{-0.76}$	21
$e^- + C_2H_4^+ \rightarrow C_2H_2 + H + H$	$3.70 \times 10^{-7}\ T_e^{-0.71}$	21
$e^- + C_2H_4^+ \rightarrow C_2H + H_2 + H$	$5.60 \times 10^{-8}\ T_e^{-0.76}$	21
$e^- + C_2H_4^+ \rightarrow CH_3 + CH$	$1.12 \times 10^{-8}\ T_e^{-0.76}$	21
$e^- + C_2H_4^+ \rightarrow CH_2 + CH_2$	$2.24 \times 10^{-8}\ T_e^{-0.76}$	21
$e^- + C_2H_3^+ \rightarrow C_2H_2 + H$	$1.45 \times 10^{-7}\ T_e^{-0.84}$	21
$e^- + C_2H_3^+ \rightarrow C_2H + H + H$	$2.95 \times 10^{-7}\ T_e^{-0.84}$	21
$e^- + C_2H_3^+ \rightarrow C_2 + H + H_2$	$2.87 \times 10^{-8}\ T_e^{-1.38}$	21
$e^- + C_2H_3^+ \rightarrow C_2H + H_2$	$3.00 \times 10^{-8}\ T_e^{-0.84}$	21
$e^- + C_2H_3^+ \rightarrow CH_2 + CH$	$1.50 \times 10^{-8}\ T_e^{-0.84}$	21
$e^- + C_2H_2^+ \rightarrow C_2H + H$	$9.00 \times 10^{-8}\ T_e^{-0.50}$	21
$e^- + C_2H_2^+ \rightarrow CH + CH$	$9.00 \times 10^{-8}\ T_e^{-0.50}$	21
$e^- + C_2H_2^+ \rightarrow C_2 + H + H$	$9.00 \times 10^{-8}\ T_e^{-0.50}$	21
$e^- + C_2H^+ \rightarrow C_2 + H$	$1.16 \times 10^{-7}\ T_e^{-0.76}$	21
$e^- + C_2H^+ \rightarrow CH + C$	$1.53 \times 10^{-7}\ T_e^{-0.76}$	21

Table S3 Neutral-neutral pressure-dependent recombination reactions with low pressure (k_0) and high pressure ($k\infty$) limit rate coefficients. T_{gas} is given in units of Kelvin. The respective rate coefficients (in $cm^3\ s^{-1}$) k_0 and $k\infty$ of each reaction are also given alongside the falloff curve expression (F_C) which incorporates the Troe parameters. k_0, $k\infty$ and F_C were used to calculate the rate coefficients of pressure dependent reactions (see details in [22]). References are shown in the last column.

$CH_3 + H \rightarrow CH_4$	$k_0 = 1.0 \times 10^{-26} * \exp\left(-\frac{T_{gas}}{21220}\right)^2$ $k\infty = (3.34 \times 10^{-10}) * \left(\frac{T_{gas}}{298.15}\right)^{-0.186} * \exp\left(-\frac{T_{gas}}{25200}\right)$ $F_C = (0.710) * \exp\left(-\frac{T_{gas}}{3079}\right) + 0.290 * \exp\left(-\frac{T_{gas}}{54}\right)$	23
$CH_3 + CH_3 \rightarrow C_2H_6$	$k_0 = (3.50 \times 10^{-7}) * (T_{gas})^{-7.0} * \exp\left(-\frac{1390}{T_{gas}}\right)$ $k\infty = (6.00 \times 10^{-11})$ $F_C = 0.381 * \exp\left(-\frac{T_{gas}}{73}\right) + 0.619 * \exp\left(-\frac{T_{gas}}{1180}\right)$	24
$CH_3 + C_2H_5 \rightarrow C_3H_8$	$k_0 = (7.50 \times 10^{-17}) * (T_{gas})^{-3.0} * \exp\left(-\frac{300}{T_{gas}}\right)$ $k\infty = 6.64 \times 10^{-11}$ $F_C = (1 - 0.153) * \exp\left(-\frac{T_{gas}}{291}\right) + 0.153 * \exp\left(-\frac{T_{gas}}{2742}\right) + \exp\left(-\frac{7748}{T_{gas}}\right)$	22
$CH_2 + H \rightarrow CH_3$	$k_0 = (9.00 \times 10^{-32}) * \exp\left(-\frac{550}{T_{gas}}\right)$ $k\infty = (8.55 \times 10^{-12}) * (T_{gas})^{0.15}$ $F_C = (1 - 0.562) * \exp\left(-\frac{T_{gas}}{91}\right) + 0.562 * \exp\left(-\frac{T_{gas}}{5836}\right) + \exp\left(-\frac{8552}{T_{gas}}\right)$	24
$CH + H_2 \rightarrow CH_3$	$k = (4.70 \times 10^{-26}) * T_{gas}^{-1.60}$	24

	$k\infty = (8.50 \times 10^{-11}) * (T_{gas})^{0.15}$ $F_C = (1 - 0.578) + \left(0.25 * \exp\left(-\frac{T_{gas}}{300}\right)\right)$	
$H + C_2H_4 \rightarrow C_2H_5$	$k_0 = (1.30 \times 10^{-29}) * \exp\left(-\frac{380}{T_{gas}}\right)$ $k\infty = (6.60 \times 10^{-15}) * (T_{gas})^{1.28} * \exp\left(-\frac{650}{T_{gas}}\right)$ $F_C = (0.240) * \exp\left(-\frac{T_{gas}}{40}\right) + 0.760 * \exp\left(-\frac{T_{gas}}{1025}\right)$	22
$C_2H_4 \rightarrow C_2H_2 + H_2$	$k_0 = (1.70 \times 10^{-6}) * T_{gas} * \exp\left(-\frac{39390}{T_{gas}}\right)$ $k\infty = (8.00 \times 10^{12}) * (T_{gas})^{0.44} * \exp\left(-\frac{88770}{T_{gas}}\right)$ $F_C = (1 - 0.735) * \exp\left(-\frac{T_{gas}}{180}\right) + 0.735 * \exp\left(-\frac{T_{gas}}{1035}\right) + \exp\left(-\frac{5417}{T_{gas}}\right)$	22
$H + C_2H_5 \rightarrow C_2H_6$	$k_0 = (4.00 \times 10^{-19}) * (T_{gas})^{-3.00} * \exp\left(-\frac{600}{T_{gas}}\right)$ $k\infty = (2.00 \times 10^{-10})$ $F_C = (1 - 0.842) * \exp\left(-\frac{T_{gas}}{125}\right) + 0.842 * \exp\left(-\frac{T_{gas}}{2219}\right) + \exp\left(-\frac{6682}{T_{gas}}\right)$	22
$H + C_2H_3 \rightarrow C_2H_4$	$k_0 = 1.75 \times 10^{-27} * (T_{gas})^{-0.347}$ $k\infty = 7.05 \times 10^{-11} * (T_{gas})^{0.180}$ $F_C = 0.0506 * (T_{gas})^{0.40}$	22
$H + C_2H_2 \rightarrow C_2H_3$	$k_0 = (1.60 \times 10^{-20}) * (T_{gas})^{-3.47} * \exp\left(-\frac{475}{T_{gas}}\right)$ $k\infty = (9.20 \times 10^{-16}) * (T_{gas})^{1.64} * \exp\left(-\frac{1055}{T_{gas}}\right)$ $F_C = 7.94 \times 10^{-4} * (T_{gas})^{0.78}$	22
$H + C_3H_7 \rightarrow C_3H_8$	$k_0 = (4.00 \times 10^{-19}) * (T_{gas})^{-3.00} * \exp\left(-\frac{600}{T_{gas}}\right)$ $K\infty = (2.49 \times 10^{-10})$ $F_C = (1 - 0.315) * \exp\left(-\frac{T_{gas}}{369}\right) + 0.315 * \exp\left(-\frac{T_{gas}}{3285}\right) + \exp\left(-\frac{6667}{T_{gas}}\right)$	22
$H + C_2H \rightarrow C_2H_2$	$k_0 = (1.26 \times 10^{-18}) * (T_{gas})^{-3.10} * \exp\left(-\frac{721}{T_{gas}}\right)$ $k\infty = (3.00 \times 10^{-10})$ $F_C = (1 - 0.646) * \exp\left(-\frac{T_{gas}}{132}\right) + 0.65 * \exp\left(-\frac{T_{gas}}{1315}\right) + \exp\left(-\frac{5566}{T_{gas}}\right)$	22
$C_2H_6 \rightarrow CH_3 + CH_3$	$k_0 = (2.60 \times 10^{25}) * (T_{gas})^{-8.37} * \exp\left(-\frac{47290}{T_{gas}}\right)$ $k\infty = (4.50 \times 10^{21}) * (T_{gas})^{-1.37} * \exp\left(-\frac{45900}{T_{gas}}\right)$	22

	$F_C = (0.38) * \exp\left(-\frac{T_{gas}}{73}\right) + 0.62 * \exp\left(-\frac{T_{gas}}{1180}\right)$	
$CH_4 \rightarrow H + CH_3$	$k_0 = (1.40 \times 10^{-6}) * \exp\left(-\frac{45700}{T_{gas}}\right)$ $k\infty = (2.40 \times 10^{16}) * \exp\left(-\frac{52800}{T_{gas}}\right)$ $F_C = (0.31) * \exp\left(-\frac{T_{gas}}{91}\right) + 0.69 * \exp\left(-\frac{T_{gas}}{2207}\right)$	23
$C_2H_3 \rightarrow C_2H_2 + H$	$k = (4.30 \times 10^{3}) * (T_{gas})^{-3.40} * \exp\left(-\frac{18020}{T_{gas}}\right)$ $k\infty = (3.90 \times 10^{8}) * (T_{gas})^{1.62} * \exp\left(-\frac{18650}{T_{gas}}\right)$ $F_C = (7.37 \times 10^{-4}) * (T_{gas})^{0.80}$	22
$C_2H_5 \rightarrow C_2H_4 + H$	$K_0 = (1.70 \times 10^{-6}) * \exp\left(-\frac{16800}{T_{gas}}\right)$ $K\infty = (8.20 \times 10^{13}) * \exp\left(-\frac{20070}{T_{gas}}\right)$ $F_C = (0.25) * \exp\left(-\frac{T_{gas}}{97}\right) + 0.75 * \exp\left(-\frac{T_{gas}}{1379}\right)$	22
$C_3H_7 \rightarrow C_3H_6 + H$	$k_0 = (3.56 \times 10^{-7}) * \exp\left(-\frac{14200}{T_{gas}}\right)$ $k\infty = (8.76 \times 10^{7}) * (T_{gas})^{1.76} * \exp\left(-\frac{17870}{T_{gas}}\right)$ $F_C = 0.35 \times 10^{0}$	22
$C_3H_8 \rightarrow CH_3 + C_2H_5$	$k_0 = (1.30 \times 10^{-5}) * \exp\left(-\frac{32700}{T_{gas}}\right)$ $k\infty = (4.00 \times 10^{23}) * (T_{gas})^{-1.87} * \exp\left(-\frac{45394}{T_{gas}}\right)$ $F_C = (0.24) * \exp\left(-\frac{T_{gas}}{1946}\right) + 0.76 * \exp\left(-\frac{T_{gas}}{38}\right)$	22
$H + H \rightarrow H_2$	$k_0 = (2.70 \times 10^{-31}) * (T_{gas})^{-0.60}$ $k\infty = (1.00 \times 10^{-11})$ $F_C = (0.0506) * (T_{gas})^{0.40}$	25
$CH_3 + C_2H_3 \rightarrow C_3H_6$	$k = (5.00 \times 10^{-27})$ $k\infty = (1.10 \times 10^{-10})$ $F_C = (0.0506) * (T_{gas})^{0.40}$	26
$CH_2 + C_2H_4 \rightarrow C_3H_6$	$k_0 = (1.5 \times 10^{-18}) * (T_{gas})^{-3} * \exp\left(-\frac{300}{T_{gas}}\right)$ $k\infty = (9.17 \times 10^{-12}) * \left(\frac{T_{gas}}{298.15}\right)^{0.00730} * \exp\left(-\frac{4410}{RT_{gas}}\right)$ $F_C = (0.0506) * (T_{gas})^{0.40}$	22

$H + C_3H_6 \rightarrow C_3H_7$	$k_0 = (1.30 \times 10^{-28}) * \exp\left(-\frac{380}{T_{gas}}\right)$ $k\infty = (9.47 \times 10^{-15}) * (T_{gas})^{1.16} * \exp\left(-\frac{440}{T_{gas}}\right)$ $F_C = (0.0506) * (T_{gas})^{0.40}$	27
$C + H_2 \rightarrow CH_2$	$k_0 = (7.00 \times 10^{-32})$ $k\infty = (2.06 \times 10^{-11}) * \exp\left(-\frac{57}{T_{gas}}\right)$ $F_C = (0.0506) * (T_{gas})^{0.40}$	28
$H + C_3H_5 \rightarrow C_3H_6$	$k_0 = (1.50 \times 10^{-29})$ $k\infty = (2.4 \times 10^{-10})$ $F_C = (0.0506) * (T_{gas})^{0.40}$	27

Table S4 Neutral-neutral molecular recombination reactions and respective rate coefficients (in $cm^3\ s^{-1}$ or $cm^6\ s^{-1}$). T_{gas} is given in Kelvin and R is the gas constant 8.314 J mol^{-1} K^{-1}. References are shown in the last column.

$CH_4 + CH_3 \rightarrow H + C_2H_6$	$4.95 \times 10^{-13}\left(\frac{T_{gas}}{298.15}\right)\exp\left(-\frac{188000}{RT_{gas}}\right)$	29
$CH_4 + CH_3 \rightarrow H_2 + C_2H_5$	$1.66 \times 10^{-11}\exp\left(\frac{-96450}{RT_{gas}}\right)$	29
$CH_4 + CH_2 \rightarrow CH_3 + CH_3$	$7.14 \times 10^{-12}\exp\left(-\frac{41990}{RT_{gas}}\right)$	30
$CH_4 + CH \rightarrow C_2H_4 + H$	$3.96 \times 10^{-8}\left(\frac{T_{gas}}{298.15}\right)^{-1.04}\exp\left(-\frac{36.1}{T_{gas}}\right)$	31
$CH_4 + C \rightarrow CH + CH_3$	$8.30 \times 10^{-11}\,exp\left(-\frac{24.015}{1.987 \times T_{gas}}\right)$	32
$CH_4 + C \rightarrow C_2H_4$	5.00×10^{-15}	32
$CH_4 + C_2H_5 \rightarrow C_2H_6 + CH_3$	$2.51 \times 10^{-15}\left(\frac{T_{gas}}{298.15}\right)^{2.84}\exp\left(-\frac{52550}{RT_{gas}}\right)$	33
$CH_4 + C_2H_3 \rightarrow C_2H_4 + CH_3$	$2.13 \times 10^{-14}\left(\frac{T_{gas}}{298.15}\right)^{4.02}\exp\left(-\frac{22860}{RT_{gas}}\right)$	33
$CH_4 + C_2H \rightarrow C_2H_2 + CH_3$	$3.01 \times 10^{-12}\exp\left(-\frac{2080}{RT_{gas}}\right)$	33
$CH_4 + C_3H_7 \rightarrow C_3H_8 + CH_3$	$3.54 \times 10^{-16}\left(\frac{T_{gas}}{298.15}\right)^{4.02}\exp\left(-\frac{45480}{RT_{gas}}\right)$	33
$CH_4 + C_3H_5 \rightarrow C_3H_6 + CH_3$	$1.71 \times 10^{-14}\left(\frac{T_{gas}}{298.15}\right)^{3.40}\exp\left(-\frac{97280}{RT_{gas}}\right)$	34
$CH_4 + H \rightarrow CH_3 + H_2$	$2.94 \times 10^{-10}\exp\left(-\frac{57650}{RT_{gas}}\right)$	35
$CH_3 + CH_3 \rightarrow C_2H_5 + H$	$1.46 \times 10^{-11}\left(\frac{T_{gas}}{298.15}\right)^{0.10}\exp\left(-\frac{44400}{RT_{gas}}\right)$	36
$CH_3 + CH_3 \rightarrow CH_2 + CH_4$	$1.16 \times 10^{-13}\left(\frac{T_{gas}}{298.15}\right)^{1.34}\exp\left(-\frac{67910}{RT_{gas}}\right)$	37

$CH_3 + CH_3 \rightarrow C_2H_4 + H_2$	$1.66 \times 10^{-8} \exp\left(-\frac{138000}{RT_{gas}}\right)$	38
$CH_3 + CH_2 \rightarrow C_2H_4 + H$	5.01×10^{-11}	39
$CH_3 + C_2H_6 \rightarrow C_2H_5 + CH_4$	$1.74 \times 10^{-16} \left(\frac{T_{gas}}{298}\right)^{6.00} \exp\left(-\frac{25280}{RT_{gas}}\right)$	33
$CH_3 + C_2H_5 \rightarrow C_2H_4 + CH_4$	$1.88 \times 10^{-12} \left(\frac{T_{gas}}{298.0}\right)^{-0.5}$	33
$CH_3 + C_2H_5 \rightarrow C_2H_6 + CH_2$	$3.0 \times 10^{-44} (T_{gas})^{9.0956}$	33
$CH_3 + C_2H_4 \rightarrow C_2H_3 + CH_4$	$6.91 \times 10^{-12} \exp\left(-\frac{46560}{RT_{gas}}\right)$	33
$CH_3 + C_2H_4 \rightarrow C_3H_7$	$3.50 \times 10^{-13} \exp\left(-\frac{3700}{T_{gas}}\right)$	22
$CH_3 + C_2H_3 \rightarrow C_2H_2 + CH_4$	$1.5 \times 10^{-11} \exp\left(\frac{3200}{RT_{gas}}\right)$	26
$CH_3 + C_2H_3 \rightarrow C_3H_5 + H$	$2.59 \times 10^{-9} \left(\frac{T_{gas}}{298.0}\right)^{-1.25} \exp\left(-\frac{32100}{RT_{gas}}\right)$	26
$CH_3 + C_2H_2 \rightarrow CH_4 + C_2H$	$3.01 \times 10^{-13} \exp\left(-\frac{72340}{RT_{gas}}\right)$	33
$CH_3 + C_2H_2 \rightarrow C_3H_5$	$1.00 \times 10^{-12} \exp\left(-\frac{3900}{T_{gas}}\right)$	22
$CH_3 + C_3H_8 \rightarrow C_3H_7 + CH_4$	$1.50 \times 10^{-24} (T_{gas})^{3.65} \exp\left(-\frac{7154}{1.987 \times T_{gas}}\right)$	33
$CH_3 + C_3H_7 \rightarrow C_3H_6 + CH_4$	$3.07 \times 10^{-12} \left(\frac{T_{gas}}{298}\right)^{-0.32}$	33
$CH_3 + C_3H_7 \rightarrow C_2H_5 + C_2H_5$	$\left(\frac{1.93 \times 10^{13}}{6.0223 \times 10^{23}}\right) (T_{gas})^{-0.32}$	33
$CH_3 + C_3H_6 \rightarrow C_3H_5 + CH_4$	$1.68 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.50} \exp\left(-\frac{23780}{RT_{gas}}\right)$	37
$CH_3 + H_2 \rightarrow CH_4 + H$	$2.52 \times 10^{-14} \left(\frac{T_{gas}}{298}\right)^{3.12} \exp\left(\frac{36420}{RT_{gas}}\right)$	35
$CH_3 + H \rightarrow CH_2 + H_2$	$1.00 \times 10^{-10} \exp\left(-\frac{63190}{RT_{gas}}\right)$	35
$CH_3 \rightarrow H_2 + CH$	$8.30 \times 10^{-9} \exp\left(-\frac{356000}{RT_{gas}}\right)$	22
$CH_3 \rightarrow CH_2 + H$	$1.69 \times 10^{-8} \exp\left(-\frac{379000}{RT_{gas}}\right)$	22
$CH_2 + CH_2 \rightarrow C_2H_2 + H + H$	$3.32 \times 10^{-10} \exp\left(-\frac{45980}{RT_{gas}}\right)$	30
$CH_2 + CH_2 \rightarrow C_2H_2 + H_2$	$2.62 \times 10^{-9} \exp\left(-\frac{49970}{RT_{gas}}\right)$	30
$CH_2 + CH_3 \rightarrow C_2H_5$	$7.00 \times 10^{-23} (T_{gas})^{3.6337}$	30
$CH_2 + C_2H_6 \rightarrow C_2H_5 + CH_3$	$9.0 \times 10^{-33} (T_{gas})^{6.4162}$	30
$CH_2 + C_2H_6 \rightarrow C_3H_8$	4.80×10^{-12}	30
$CH_2 + C_2H_5 \rightarrow C_2H_4 + CH_3$	8.01×10^{-11}	30
$CH_2 + C_2H_3 \rightarrow C_2H_2 + CH_3$	8.01×10^{-11}	30

$CH_2 + C_2H_4 \rightarrow C_3H_5 + H$	$4.25 \times 10^{-12} \exp\left(-\frac{2658}{T_{gas}}\right)$	30
$CH_2 + C_2H \rightarrow C_2H_2 + CH$	3.01×10^{-11}	30
$CH_2 + C_3H_8 \rightarrow C_3H_7 + CH_3$	$1.61 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.65} \exp\left(-\frac{29930}{RT_{gas}}\right)$	30
$CH_2 + C_3H_7 \rightarrow C_2H_4 + C_2H_5$	3.01×10^{-11}	30
$CH_2 + C_3H_7 \rightarrow C_3H_6 + CH_3$	3.01×10^{-11}	30
$CH_2 + C_3H_6 \rightarrow C_3H_5 + CH_3$	$1.20 \times 10^{-12} \exp\left(-\frac{25940}{RT_{gas}}\right)$	30
$CH_2 + H_2 \rightarrow CH_3 + H$	$3.59 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{2.30} \exp\left(-\frac{30760}{RT_{gas}}\right)$	30
$CH_2 + H \rightarrow CH + H_2$	$1.00 \times 10^{-11} \exp\left(\frac{7480}{RT_{gas}}\right)$	37
$CH_2 \rightarrow C + H_2$	$5.00 \times 10^{-10} \exp\left(-\frac{32600}{T_{gas}}\right)$	30
$CH_2 \rightarrow CH + H$	$1.56 \times 10^{-8} \exp\left(-\frac{44880}{T_{gas}}\right)$	30
$CH + H_2 \rightarrow CH_2 + H$	$1.48 \times 10^{-11} \left(\frac{T_{gas}}{298.0}\right)^{1.79} \exp\left(-\frac{6980}{RT_{gas}}\right)$	40
$CH + H \rightarrow C + H_2$	$6.50 \times 10^{-10} (T_{gas})^{0.01} \exp\left(-\frac{22330}{RT_{gas}}\right)$	38
$CH + CH_3 \rightarrow C_2H_3 + H$	$\left(\frac{3.0 \times 10^{13}}{6.0223 \times 10^{23}}\right)$	40
$CH + CH_2 \rightarrow C_2H_2 + H$	$\left(\frac{4.0 \times 10^{13}}{6.0223 \times 10^{23}}\right)$	40
$CH + CH \rightarrow C_2H_2$	1.99×10^{-10}	40
$CH + C_2H_2 \rightarrow C_2H + CH_2$	$3.80 \times 10^{-8} (T_{gas})^{-0.859} \exp\left(-\frac{33.5}{T_{gas}}\right)$	31
$CH + C_2H_3 \rightarrow CH_2 + C_2H_2$	8.3×10^{-11}	31
$CH + C_2H_4 \rightarrow C_3H_5$	$2.84 \times 10^{-10} \left(\frac{T_{gas}}{298.15}\right)^{-0.310}$	31
$CH + C_2H_4 \rightarrow C_2H_2 + CH_3$	$0.50 \times 1.59 \times 10^{-9} (T_{gas})^{-0.546} \exp\left(-\frac{29.6}{T_{gas}}\right)$	31
$CH + C_2H_4 \rightarrow CH_4 + C_2H$	$0.50 \times 1.59 \times 10^{-9} (T_{gas})^{-0.546} \exp\left(-\frac{29.6}{T_{gas}}\right)$	31
$CH + C_2H_5 \rightarrow C_3H_5 + H$	$3.80 \times 10^{-8} (T_{gas})^{-0.859} \exp\left(-\frac{33.5}{T_{gas}}\right)$	31
$CH + C_2H_6 \rightarrow C_2H_4 + CH_3$	$3.80 \times 10^{-8} (T_{gas})^{-0.859} \exp\left(-\frac{53.2}{T_{gas}}\right)$	41
$CH + C_2H_6 \rightarrow C_3H_6 + H$	$6.17 \times 10^{-11} (T_{gas})^{-0.52} \exp\left(-\frac{29.2}{T_{gas}}\right)$	41
$CH + C_2H_6 \rightarrow C_3H_7$	1.60×10^{-10}	41
$CH \rightarrow C + H$	$3.16 \times 10^{-10} \exp\left(-\frac{280000}{RT_{gas}}\right)$	40
$C_2H_6 + C_2H_3 \rightarrow C_2H_5 + C_2H_4$	$1.46 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{3.30} \exp\left(-\frac{43900}{RT_{gas}}\right)$	42

$C_2H_6 + C_2H \rightarrow C_2H_2 + C_2H_5$	$3.50 \times 10^{-11} \exp\left(\frac{20}{RT_{gas}}\right)$	22
$C_2H_6 + C_3H_7 \rightarrow C_3H_8 + C_2H_5$	$1.19 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.82} \exp\left(-\frac{37830}{RT_{gas}}\right)$	43
$C_2H_6 + C_3H_5 \rightarrow C_3H_6 + C_2H_5$	$5.71 \times 10^{-14} \left(\frac{T_{gas}}{298}\right)^{3.30} \exp\left(-\frac{83060}{RT_{gas}}\right)$	34
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	$1.23 \times 10^{-11} \left(\frac{T_{gas}}{298}\right)^{1.50} \exp\left(-\frac{31010}{RT_{gas}}\right)$	37
$H + C_2H_6 \rightarrow CH_4 + CH_3$	$8.97 \times 10^{-20} \exp\left(-\frac{48640}{RT_{gas}}\right)$	38
$C_2H_6 \rightarrow C_2H_5 + H$	$8.11 \times 10^{17} \left(\frac{T_{gas}}{298}\right)^{-1.23} \exp\left(-\frac{427000}{RT_{gas}}\right)$	44
$C_2H_6 \rightarrow C_2H_4 + H_2$	$1.32 \times 10^{15} \exp\left(-\frac{306000}{RT_{gas}}\right)$	44
$C_2H_5 + C_2H_3 \rightarrow C_2H_6 + C_2H_2$	2.40×10^{-11}	45
$C_2H_5 + C_2H_3 \rightarrow C_2H_4 + C_2H_4$	9.60×10^{-11}	45
$C_2H_5 + C_2H_5 \rightarrow C_2H_6 + C_2H_4$	2.41×10^{-12}	22
$C_2H_5 + C_2H_4 \rightarrow C_2H_6 + C_2H_3$	$5.83 \times 10^{-14} \left(\frac{T_{gas}}{298}\right)^{3.13} \exp\left(-\frac{75330}{RT_{gas}}\right)$	22
$C_2H_5 + C_2H_2 \rightarrow C_2H_6 + C_2H$	$4.50 \times 10^{-13} \exp\left(-\frac{98110}{RT_{gas}}\right)$	42
$C_2H_5 + C_2H \rightarrow C_2H_4 + C_2H_2$	3.01×10^{-12}	42
$C_2H_5 + C_3H_8 \rightarrow C_2H_6 + C_3H_7$	$1.61 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.65} \exp\left(-\frac{38250}{RT_{gas}}\right)$	43
$C_2H_5 + C_3H_7 \rightarrow C_3H_8 + C_2H_4$	1.91×10^{-12}	43
$C_2H_5 + C_3H_7 \rightarrow C_3H_6 + C_2H_6$	2.41×10^{-12}	43
$C_2H_5 + C_3H_6 \rightarrow C_3H_5 + C_2H_6$	$1.69 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.50} \exp\left(-\frac{27770}{RT_{gas}}\right)$	46
$C_2H_5 + C_3H_5 \rightarrow C_3H_6 + C_2H_4$	$4.30 \times 10^{-12} \exp\left(\frac{550}{RT_{gas}}\right)$	34
$C_2H_5 + H_2 \rightarrow C_2H_6 + H$	$5.10 \times 10^{-24} \left(\frac{T_{gas}}{298}\right)^{3.60} \exp\left(-\frac{35340}{RT_{gas}}\right)$	22
$H + C_2H_5 \rightarrow CH_3 + CH_3$	$1.79 \times 10^{-10} \exp\left(-\frac{3640}{RT_{gas}}\right)$	22
$H + C_2H_5 \rightarrow C_2H_4 + H_2$	3.32×10^{-12}	42
$C_2H_5 \rightarrow CH_2 + CH_3$	$1.0 \times 10^{-118} (T_{gas})^{37.47}$	44
$C_2H_4 + C_2H \rightarrow C_2H_2 + C_2H_3$	1.40×10^{-10}	42
$C_2H_4 + C_2H_2 \rightarrow C_2H_3 + C_2H_3$	$4.0 \times 10^{-11} \exp\left(-\frac{286000}{RT_{gas}}\right)$	42
$C_2H_4 + C_3H_6 \rightarrow C_3H_5 + C_2H_5$	$9.6 \times 10^{-11} \exp\left(-\frac{216000}{RT_{gas}}\right)$	46
$C_2H_4 + C_3H_6 \rightarrow C_2H_3 + C_3H_7$	$1.0 \times 10^{-10} \exp\left(-\frac{316000}{RT_{gas}}\right)$	46
$C_2H_4 + C_2H_4 \rightarrow C_2H_5 + C_2H_3$	$8.0 \times 10^{-10} \exp\left(-\frac{299000}{RT_{gas}}\right)$	42

$C_2H_4 + H \rightarrow C_2H_3 + H_2$	$8.41 \times 10^{-17} \left(T_{gas}\right)^{1.93} \exp\left(-\frac{6518}{T_{gas}}\right)$	37
$C_2H_4 + H_2 \rightarrow C_2H_5 + H$	$1.69 \times 10^{-11} \exp\left(-\frac{285000}{RT_{gas}}\right)$	42
$C_2H_4 + H_2 \rightarrow C_2H_6$	$4.75 \times 10^{-16} \exp\left(-\frac{180000}{RT_{gas}}\right)$	42
$C_2H_4 + C \rightarrow C_2H_2 + CH_2$	1.24×10^{-11}	47
$C_2H_4 \rightarrow C_2H_3 + H$	$2.00 \times 10^{16} \exp\left(-\frac{461000}{RT_{gas}}\right)$	44
$C_2H_3 + C_2H_3 \rightarrow C_2H_4 + C_2H_2$	3.50×10^{-11}	42
$C_2H_3 + C_2H \rightarrow C_2H_2 + C_2H_2$	3.15×10^{-11}	42
$C_2H_3 + C_3H_8 \rightarrow C_2H_4 + C_3H_7$	$1.46 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{3.30} \exp\left(-\frac{43900}{RT_{gas}}\right)$	43
$C_2H_3 + C_3H_7 \rightarrow C_3H_8 + C_2H_2$	2.01×10^{-12}	43
$C_2H_3 + C_3H_7 \rightarrow C_3H_6 + C_2H_4$	2.01×10^{-12}	43
$C_2H_3 + C_3H_6 \rightarrow C_3H_5 + C_2H_4$	$1.68 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.50} \exp\left(-\frac{19620}{RT_{gas}}\right)$	46
$C_2H_3 + C_3H_5 \rightarrow C_3H_6 + C_2H_2$	8.00×10^{-12}	34
$C_2H_3 + H_2 \rightarrow C_2H_4 + H$	$1.61 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{2.63} \exp\left(-\frac{35750}{RT_{gas}}\right)$	48
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	$1.50 \times 10^{-12} \left(T_{gas}\right)^{0.50}$	22
$C_2H_2 + C_3H_7 \rightarrow C_3H_5 + C_2H_4$	$1.20 \times 10^{-12} \exp\left(-\frac{37700}{RT_{gas}}\right)$	43
$C_2H_2 + C_3H_6 \rightarrow C_2H_3 + C_3H_5$	$6.71 \times 10^{-11} \exp\left(-\frac{196000}{RT_{gas}}\right)$	46
$C_2H_2 + C_2H_2 \rightarrow C_2H + C_2H_3$	$1.6 \times 10^{-11} \exp\left(-\frac{353000}{RT_{gas}}\right)$	42
$C_2H_2 + H_2 \rightarrow C_2H_4$	$5.0 \times 10^{-13} \exp\left(-\frac{163000}{RT_{gas}}\right)$	42
$C_2H_2 + H_2 \rightarrow C_2H_3 + H$	$1.33 \times 10^{-12} \exp\left(-\frac{236000}{RT_{gas}}\right)$	42
$C_2H_2 + H \rightarrow C_2H + H_2$	$2.77 \times 10^{-10} \left(\frac{T_{gas}}{298.0}\right)^{1.32} \exp\left(-\frac{128000}{RT_{gas}}\right)$	38
$C_2H_2 \rightarrow C_2H + H$	$2.63 \times 10^{15} \exp\left(-\frac{519000}{RT_{gas}}\right)$	44
$C_2H + C_3H_8 \rightarrow C_2H_2 + C_3H_7$	1.79×10^{-11}	43
$C_2H + C_3H_7 \rightarrow C_3H_6 + C_2H_2$	2.01×10^{-11}	43
$C_2H + C_3H_6 \rightarrow C_3H_5 + C_2H_2$	1.79×10^{-11}	46
$C_2H + C_2H \rightarrow C_2H_2 + C_2$	3.01×10^{-12}	42
$C_2H + H_2 \rightarrow C_2H_2 + H$	$1.59 \times 10^{-11} \left(\frac{T_{gas}}{298}\right)^{0.90} \exp\left(-\frac{8310}{RT_{gas}}\right)$	42
$H + C_2H \rightarrow H_2 + C_2$	$5.99 \times 10^{-11} \exp\left(-\frac{118000}{RT_{gas}}\right)$	37
$C_3H_8 + C_3H_5 \rightarrow C_3H_6 + C_3H_7$	$5.71 \times 10^{-14} \left(\frac{T_{gas}}{298}\right)^{3.30} \exp\left(-\frac{83060}{RT_{gas}}\right)$	34

$C_3H_8 + H \rightarrow C_3H_7 + H_2$	$4.23 \times 10^{-12} \left(\frac{T_{gas}}{298}\right)^{2.54} \exp\left(-\frac{28270}{RT_{gas}}\right)$	38
$C_3H_8 \rightarrow C_3H_7 + H$	$1.58 \times 10^{16} \exp\left(-\frac{408000}{RT_{gas}}\right)$	44
$C_3H_7 + C_3H_7 \rightarrow C_3H_6 + C_3H_8$	2.81×10^{-12}	27
$C_3H_7 + C_3H_6 \rightarrow C_3H_5 + C_3H_8$	$1.69 \times 10^{-15} \left(\frac{T_{gas}}{298}\right)^{3.50} \exp\left(-\frac{27770}{RT_{gas}}\right)$	27
$C_3H_7 + C_3H_5 \rightarrow C_3H_6 + C_3H_6$	$2.41 \times 10^{-12} \exp\left(\frac{550}{RT_{gas}}\right)$	27
$C_3H_7 + H_2 \rightarrow C_3H_8 + H$	$3.19 \times 10^{-14} \left(\frac{T_{gas}}{298}\right)^{2.84} \exp\left(-\frac{38250}{RT_{gas}}\right)$	27
$C_3H_7 + H \rightarrow C_3H_6 + H_2$	3.01×10^{-12}	27
$C_3H_7 + H \rightarrow CH_3 + C_2H_5$	$6.74 \times 10^{-18} (T_{gas})^{2.19} \exp\left(-\frac{890}{1.987\, T_{gas}}\right)$	27
$C_3H_7 \rightarrow C_2H_4 + CH_3$	$1.31 \times 10^{13} \left(\frac{T_{gas}}{298}\right)^{0.87} \exp\left(-\frac{127000}{RT_{gas}}\right)$	27
$C_3H_6 + C_3H_6 \rightarrow C_3H_7 + C_3H_5$	$4.2 \times 10^{-10} \exp\left(-\frac{231000}{RT_{gas}}\right)$	37
$C_3H_6 + H \rightarrow C_3H_5 + H_2$	$4.40 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{2.50} \exp\left(-\frac{10390}{RT_{gas}}\right)$	38
$C_3H_6 + H \rightarrow C_2H_4 + CH_3$	$7.51 \times 10^{-11} \exp\left(-\frac{17300}{RT_{gas}}\right)$	38
$C_3H_6 \rightarrow C_3H_5 + H$	$2.50 \times 10^{15} \exp\left(\frac{-410000}{RT_{gas}}\right)$	37
$C_3H_6 \rightarrow CH_3 + C_2H_3$	$1.18 \times 10^{18} \left(\frac{T_{gas}}{298}\right)^{-1.20} \exp\left(-\frac{409000}{RT_{gas}}\right)$	37
$C_3H_6 \rightarrow CH_4 + C_2H_2$	$3.50 \times 10^{12} \exp\left(\frac{-293000}{RT_{gas}}\right)$	44
$C_3H_6 \rightarrow CH_2 + C_2H_4$	$5.03 \times 10^{15} \exp\left(\frac{-808000}{RT_{gas}}\right)$	44
$C_3H_5 + H_2 \rightarrow C_3H_6 + H$	$1.39 \times 10^{-13} \left(\frac{T_{gas}}{298}\right)^{2.38} \exp\left(-\frac{79490}{RT_{gas}}\right)$	34
$C_3H_5 + H \rightarrow C_2H_3 + CH_3$	4.00×10^{-12}	34
$C_3H_5 \rightarrow C_2H_2 + CH_3$	$1.26 \times 10^{13} \exp\left(-\frac{140000}{RT_{gas}}\right)$	44
$C + C \rightarrow C_2$	2.20×10^{-12}	49
$C_2 \rightarrow C + C_s$	$1.5 \times 10^{16} \exp\left(-\frac{594630}{RT_{gas}}\right)$	50
$C_3 \rightarrow C_2 + C_s$	$3.48 \times 10^{11} (T_{gas})^{1.1256} \exp\left(-\frac{131430}{RT_{gas}}\right)$	50
$C_2 + C_2 \rightarrow C + C_3$	5.31×10^{-10}	50
$C + H_2 \rightarrow CH + H$	$6.64 \times 10^{-10} \exp\left(-\frac{97280}{RT_{gas}}\right)$	32
$C + CH_2 \rightarrow CH + CH$	$2.69 \times 10^{-12} \exp\left(-\frac{196000}{RT_{gas}}\right)$	51

$C + CH_2 \rightarrow H + C_2H$	8.30×10^{-11}	52
$C + CH_3 \rightarrow H + C_2H_2$	8.30×10^{-11}	52
$C_2 + H_2 \rightarrow C_2H_2$	$1.77 \times 10^{-10} \exp\left(-\frac{1470}{T_{gas}}\right)$	38
$C_2 + H_2 \rightarrow C_2H + H$	$1.10 \times 10^{-10} \exp\left(-\frac{33260}{RT_{gas}}\right)$	38
$C_2 + CH_4 \rightarrow C_2H + CH_3$	$5.05 \times 10^{-11} \exp\left(-\frac{297}{T_{gas}}\right)$	38
$H_2 + M \rightarrow H + H + M$	$3.64 \times 10^{-8} \left(\frac{T_{gas}}{298.15}\right)^{-1.00} \exp\left(-\frac{431000}{RT_{gas}}\right)$	25
$H + H \rightarrow e^- + H + H^+$	See reference	53

Table S5 Negative and positive ion-ion and ion-neutral molecular recombination reactions and respective rate coefficients (in cm^3 s^{-1} or cm^6 s^{-1}). T_{gas} is given in Kelvin. References are shown in the last column.

$CH_5^+ + CH_2 \rightarrow CH_3^+ + CH_4$	0.960×10^{-9}	54
$CH_5^+ + CH \rightarrow CH_2^+ + CH_4$	0.690×10^{-9}	54
$CH_5^+ + C \rightarrow CH^+ + CH_4$	0.120×10^{-8}	54
$CH_5^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2 + CH_4$	0.225×10^{-9}	54
$CH_5^+ + C_2H_4 \rightarrow C_2H_5^+ + CH_4$	0.150×10^{-8}	54
$CH_5^+ + C_2H_2 \rightarrow C_2H_3^+ + CH_4$	0.160×10^{-8}	54
$CH_5^+ + C_2H \rightarrow C_2H_2^+ + CH_4$	0.900×10^{-9}	54
$CH_5^+ + C_2 \rightarrow C_2H^+ + CH_4$	0.950×10^{-9}	54
$CH_5^+ + H \rightarrow CH_4^+ + H_2$	0.150×10^{-9}	55
$CH_4^+ + CH_4 \rightarrow CH_5^+ + CH_3$	0.15×10^{-8}	56
$CH_4^+ + C_2H_6 \rightarrow C_2H_4^+ + CH_4 + H_2$	0.19×10^{-8}	56
$CH_4^+ + C_2H_4 \rightarrow C_2H_5^+ + CH_3$	1.38×10^{-9}	56
$CH_4^+ + C_2H_4 \rightarrow C_2H_4^+ + CH_4$	0.42×10^{-9}	56
$CH_4^+ + C_2H_2 \rightarrow C_2H_3^+ + CH_3$	6.27×10^{-10}	56
$CH_4^+ + C_2H_2 \rightarrow C_2H_2^+ + CH_4$	0.55×10^{-9}	56
$CH_4^+ + H_2 \rightarrow CH_5^+ + H$	$4.89 \times 10^{-11} \left(\frac{300}{T_{gas}}\right)^{0.14} \exp\left(-\frac{36.10}{T_{gas}}\right)$	57
$CH_4^+ + H \rightarrow CH_3^+ + H_2$	0.10×10^{-10}	55
$CH_3^+ + CH_4 \rightarrow CH_4^+ + CH_3$	0.136×10^{-9}	56
$CH_3^+ + CH_4 \rightarrow C_2H_5^+ + H_2$	0.120×10^{-8}	56
$CH_3^+ + CH_2 \rightarrow C_2H_3^+ + H_2$	0.990×10^{-9}	56
$CH_3^+ + CH \rightarrow C_2H_2^+ + H_2$	0.710×10^{-9}	56
$CH_3^+ + C \rightarrow C_2H^+ + H_2$	1.200×10^{-9}	56
$CH_3^+ + C_2H_6 \rightarrow C_2H_5^+ + CH_4$	1.48×10^{-9}	56
$CH_3^+ + C_2H_4 \rightarrow C_2H_3^+ + CH_4$	0.35×10^{-9}	56
$CH_3^+ + C_2H_3 \rightarrow C_2H_3^+ + CH_3$	0.300×10^{-9}	56

$CH_3^+ + H_2 \rightarrow CH_4^+ + H$	1.58×10^{-9}	57
$CH_2^+ + CH_4 \rightarrow CH_3^+ + CH_3$	0.138×10^{-9}	54
$CH_2^+ + CH_4 \rightarrow C_2H_5^+ + H$	0.360×10^{-9}	54
$CH_2^+ + CH_4 \rightarrow C_2H_4^+ + H_2$	0.84×10^{-9}	54
$CH_2^+ + CH_4 \rightarrow C_2H_3^+ + H_2 + H$	0.231×10^{-9}	54
$CH_2^+ + CH_4 \rightarrow C_2H_2^+ + 2\,H_2$	0.397×10^{-9}	54
$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	0.16×10^{-8}	57
$CH_2^+ + C \rightarrow C_2H^+ + H$	0.12×10^{-8}	54
$CH^+ + CH_2 \rightarrow C_2H^+ + H_2$	0.10×10^{-8}	54
$CH^+ + CH \rightarrow C_2^+ + H_2$	0.740×10^{-9}	54
$CH^+ + C \rightarrow C_2^+ + H$	1.2×10^{-9}	54
$CH^+ + H \rightarrow C^+ + H_2$	7.50×10^{-10}	55
$CH^+ + CH_4 \rightarrow C_2H_4^+ + H$	0.65×10^{-10}	54
$CH^+ + CH_4 \rightarrow C_2H_3^+ + H_2$	0.109×10^{-8}	54
$CH^+ + CH_4 \rightarrow C_2H_2^+ + H_2 + H$	0.143×10^{-9}	54
$CH^+ + H_2 \rightarrow CH_2^+ + H$	1.58×10^{-9}	57
$C_2H_6^+ + C_2H_4 \rightarrow C_2H_4^+ + C_2H_6$	1.15×10^{-9}	56
$C_2H_6^+ + C_2H_2 \rightarrow C_2H_5^+ + C_2H_3$	2.47×10^{-10}	56
$C_2H_6^+ + H \rightarrow C_2H_5^+ + H_2$	1.00×10^{-10}	58
$C_2H_5^+ + H \rightarrow C_2H_4^+ + H_2$	1.00×10^{-10}	55
$C_2H_4^+ + C_2H_3 \rightarrow C_2H_5^+ + C_2H_2$	5.00×10^{-10}	56
$C_2H_4^+ + C_2H_3 \rightarrow C_2H_3^+ + C_2H_4$	5.00×10^{-10}	56
$C_2H_4^+ + H \rightarrow C_2H_3^+ + H_2$	3.00×10^{-10}	55
$C_2H_3^+ + C_2H_6 \rightarrow C_2H_5^+ + C_2H_4$	2.91×10^{-10}	56
$C_2H_3^+ + C_2H_4 \rightarrow C_2H_5^+ + C_2H_2$	8.90×10^{-10}	56
$C_2H_3^+ + C_2H_3 \rightarrow C_2H_5^+ + C_2H$	5.00×10^{-10}	59
$C_2H_3^+ + C_2H \rightarrow C_2H_2^+ + C_2H_2$	3.30×10^{-10}	59
$C_2H_3^+ + H \rightarrow C_2H_2^+ + H_2$	6.80×10^{-11}	55
$C_2H_2^+ + CH_4 \rightarrow C_2H_3^+ + CH_3$	4.10×10^{-9}	56
$C_2H_2^+ + C_2H_6 \rightarrow C_2H_5^+ + C_2H_3$	1.31×10^{-10}	56
$C_2H_2^+ + C_2H_6 \rightarrow C_2H_4^+ + C_2H_4$	2.48×10^{-10}	56
$C_2H_2^+ + C_2H_4 \rightarrow C_2H_4^+ + C_2H_2$	4.14×10^{-10}	56
$C_2H_2^+ + C_2H_3 \rightarrow C_2H_3^+ + C_2H_2$	3.30×10^{-10}	56
$C_2H_2^+ + H_2 \rightarrow C_2H_3^+ + H$	1.00×10^{-11}	57
$C_2H^+ + CH_2 \rightarrow CH_3^+ + C_2$	4.40×10^{-10}	59
$C_2H^+ + CH \rightarrow CH_2^+ + C_2$	3.20×10^{-10}	59
$C_2H^+ + CH_4 \rightarrow C_2H_2^+ + CH_3$	3.74×10^{-10}	59
$C_2H^+ + H_2 \rightarrow C_2H_2^+ + H$	1.10×10^{-9}	57
$H_3^+ + CH_4 \rightarrow CH_5^+ + H_2$	2.40×10^{-9}	60

$H_3^+ + CH_3 \rightarrow CH_4^+ + H_2$	2.10×10^{-9}	61
$H_3^+ + CH_2 \rightarrow CH_3^+ + H_2$	1.70×10^{-9}	60
$H_3^+ + CH \rightarrow CH_2^+ + H_2$	1.20×10^{-9}	60
$H_3^+ + C \rightarrow CH^+ + H_2$	2.00×10^{-9}	60
$H_3^+ + C_2H \rightarrow C_2H_2^+ + H_2$	1.70×10^{-9}	61
$H_3^+ + C_2 \rightarrow C_2H^+ + H_2$	1.80×10^{-9}	60
$H_3^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2 + H_2$	2.40×10^{-9}	60
$H_3^+ + C_2H_5 \rightarrow C_2H_6^+ + H_2$	1.40×10^{-9}	61
$H_3^+ + C_2H_4 \rightarrow C_2H_5^+ + H_2$	1.15×10^{-9}	60
$H_3^+ + C_2H_4 \rightarrow C_2H_3^+ + H_2 + H_2$	1.15×10^{-9}	60
$H_3^+ + C_2H_3 \rightarrow C_2H_4^+ + H_2$	2.00×10^{-9}	61
$H_3^+ + C_2H_2 \rightarrow C_2H_3^+ + H_2$	3.50×10^{-9}	60
$H_3^+ + C_3H_6 \rightarrow C_2H_3^+ + CH_4 + H_2$	9.00×10^{-10}	61
$H_2^+ + CH_4 \rightarrow CH_5^+ + H$	1.14×10^{-10}	60
$H_2^+ + CH_4 \rightarrow CH_4^+ + H_2$	1.40×10^{-9}	60
$H_2^+ + CH_4 \rightarrow CH_3^+ + H_2 + H$	2.30×10^{-9}	60
$H_2^+ + CH_2 \rightarrow CH_3^+ + H$	1.00×10^{-9}	60
$H_2^+ + CH_2 \rightarrow CH_2^+ + H_2$	1.00×10^{-9}	60
$H_2^+ + CH \rightarrow CH_2^+ + H$	7.10×10^{-10}	60
$H_2^+ + CH \rightarrow CH^+ + H_2$	7.10×10^{-10}	60
$H_2^+ + C \rightarrow CH^+ + H$	2.40×10^{-9}	60
$H_2^+ + C_2H \rightarrow C_2H_2^+ + H$	1.00×10^{-9}	60
$H_2^+ + C_2H \rightarrow C_2H^+ + H_2$	1.00×10^{-9}	60
$H_2^+ + C_2 \rightarrow C_2H^+ + H$	1.10×10^{-9}	60
$H_2^+ + C_2 \rightarrow C_2^+ + H_2$	1.10×10^{-9}	60
$H_2^+ + C_2H_6 \rightarrow C_2H_6^+ + H_2$	2.94×10^{-9}	60
$H_2^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2 + H$	1.37×10^{-9}	60
$H_2^+ + C_2H_6 \rightarrow C_2H_4^+ + H_2 + H_2$	2.35×10^{-9}	60
$H_2^+ + C_2H_6 \rightarrow C_2H_3^+ + 2\,H_2 + H$	6.86×10^{-9}	60
$H_2^+ + C_2H_6 \rightarrow C_2H_2^+ + 3\,H_2$	1.96×10^{-9}	60
$H_2^+ + C_2H_4 \rightarrow C_2H_4^+ + H_2$	2.21×10^{-9}	60
$H_2^+ + C_2H_4 \rightarrow C_2H_3^+ + H_2 + H$	1.81×10^{-9}	60
$H_2^+ + C_2H_4 \rightarrow C_2H_2^+ + H_2 + H_2$	8.82×10^{-10}	60
$H_2^+ + C_2H_2 \rightarrow C_2H_3^+ + H$	4.80×10^{-10}	60
$H_2^+ + C_2H_2 \rightarrow C_2H_2^+ + H_2$	4.82×10^{-9}	60
$H^+ + CH_4 \rightarrow CH_4^+ + H$	1.50×10^{-9}	62
$H^+ + CH_4 \rightarrow CH_3^+ + H_2$	2.30×10^{-9}	62
$H^+ + CH_3 \rightarrow CH_3^+ + H$	3.40×10^{-9}	60
$H^+ + CH_2 \rightarrow CH_2^+ + H$	1.40×10^{-9}	60

$H^+ + CH_2 \rightarrow CH^+ + H_2$	1.40×10^{-9}	60
$H^+ + CH \rightarrow CH^+ + H$	1.90×10^{-9}	60
$H^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2$	1.30×10^{-9}	62
$H^+ + C_2H_6 \rightarrow C_2H_4^+ + H_2 + H$	1.40×10^{-9}	62
$H^+ + C_2H_6 \rightarrow C_2H_3^+ + H_2 + H_2$	2.80×10^{-9}	62
$H^+ + C_2H_5 \rightarrow C_2H_4^+ + H_2$	1.65×10^{-9}	60
$H^+ + C_2H_5 \rightarrow C_2H_3^+ + H_2 + H$	3.06×10^{-9}	60
$H^+ + C_2H_4 \rightarrow C_2H_4^+ + H$	1.00×10^{-9}	62
$H^+ + C_2H_4 \rightarrow C_2H_3^+ + H_2$	3.00×10^{-9}	62
$H^+ + C_2H_4 \rightarrow C_2H_2^+ + H_2 + H$	1.00×10^{-9}	62
$H^+ + C_2H_3 \rightarrow C_2H_3^+ + H$	2.00×10^{-9}	59
$H^+ + C_2H_3 \rightarrow C_2H_2^+ + H_2$	2.00×10^{-9}	59
$H^+ + C_2H_2 \rightarrow C_2H_2^+ + H$	5.40×10^{-10}	62
$H^+ + C_2H \rightarrow C_2H^+ + H$	1.50×10^{-9}	60
$H^+ + C_2H \rightarrow C_2^+ + H_2$	1.50×10^{-9}	60
$H^+ + C_2 \rightarrow C_2^+ + H$	3.10×10^{-9}	60
$C^+ + H^- \rightarrow C + H$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	63
$C^+ + CH_4 \rightarrow C_2H_3^+ + H$	1.43×10^{-9}	64
$C^+ + CH_4 \rightarrow C_2H_2^+ + H_2$	3.30×10^{-10}	64
$C^+ + CH_3 \rightarrow C_2H_2^+ + H$	1.30×10^{-9}	64
$C^+ + CH_3 \rightarrow C_2H^+ + H_2$	1.00×10^{-9}	64
$C^+ + CH_2 \rightarrow CH_2^+ + C$	5.20×10^{-10}	64
$C^+ + CH_2 \rightarrow C_2H^+ + H$	5.20×10^{-10}	64
$C^+ + CH \rightarrow CH^+ + C$	3.80×10^{-10}	64
$C^+ + CH \rightarrow C_2^+ + H$	3.80×10^{-10}	64
$C^+ + C_2H_6 \rightarrow C_2H_5^+ + CH$	2.31×10^{-10}	64
$C^+ + C_2H_6 \rightarrow C_2H_4^+ + CH_2$	1.16×10^{-10}	64
$C^+ + C_2H_6 \rightarrow C_2H_3^+ + CH_3$	4.95×10^{-10}	64
$C^+ + C_2H_6 \rightarrow C_2H_2^+ + CH_4$	8.25×10^{-11}	64
$C^+ + C_2H_5 \rightarrow C_2H_5^+ + C$	5.00×10^{-10}	64
$C^+ + C_2H_4 \rightarrow C_2H_4^+ + C$	1.70×10^{-11}	64
$C^+ + C_2H_4 \rightarrow C_2H_3^+ + CH$	8.50×10^{-11}	64
$C^+ + C_3H_6 \rightarrow C_2H_2^+ + C_2H_4$	6.00×10^{-10}	64
$C^+ + C_3H_6 \rightarrow C_2H_3^+ + C_2H_3$	6.00×10^{-10}	64
$C_2^+ + C \rightarrow C_2 + C^+$	1.10×10^{-10}	60
$C_2^+ + CH_4 \rightarrow C_2H_2^+ + CH_2$	1.82×10^{-10}	65
$C_2^+ + CH_4 \rightarrow C_2H^+ + CH_3$	2.38×10^{-10}	65
$C_2^+ + H_2 \rightarrow C_2H^+ + H$	1.40×10^{-9}	57
$C_2^+ + CH_2 \rightarrow CH_2^+ + C_2$	4.50×10^{-10}	65

$C_2^+ + CH \rightarrow CH^+ + C_2$	3.20×10^{-10}	65
$H^+ + 2\,H_2 \rightarrow H_2 + H_3^+$	$3.10 \times 10^{-29} \left(\frac{300}{T_{gas}}\right)^{0.5}$	17
$H^+ + H + M \rightarrow H_2^+ + M$	1.00×10^{-34}	17
$H_2^+ + H_2 \rightarrow H_2 + H^+ + H$	$1.00 \times 10^{-8} \exp\left(-\frac{84100.0}{T_{gas}}\right)$	57
$H_2^+ + H_2 \rightarrow H + H_3^+$	2.11×10^{-9}	57
$H_2^+ + H \rightarrow H_3^+$	2.10×10^{-9}	66
$H_2^+ + H \rightarrow H_2 + H^+$	6.39×10^{-10}	66
$H^- + M \rightarrow H + e^- + M$	$2.70 \times 10^{-10} \left(\frac{T_{gas}}{300}\right)^{-0.50} \exp\left(-\frac{5590.0}{T_{gas}}\right)$	63
$H^- + H_2^+ \rightarrow H + H + H$	$2.0 \times 10^{-7} \left(\frac{300}{T_{gas}}\right)^{0.50}$	67
$H^- + H_3^+ \rightarrow H_2 + H + H$	$2.0 \times 10^{-7} \left(\frac{300}{T_{gas}}\right)^{0.50}$	67
$H^- + H_3^+ \rightarrow H_2 + H_2$	$2.0 \times 10^{-7} \left(\frac{300}{T_{gas}}\right)^{0.50}$	67
$H^+ + H^- \rightarrow H + H$	$2.00 \times 10^{-7} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	67
$H_2^+ + H^- \rightarrow H_2 + H$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	68
$H + H^- \rightarrow e^- + H_2$	$\frac{1.43 \times 10^{15} \left(\frac{T_{gas}}{300}\right)^{-0.146} \exp\left(-\frac{815}{T_{gas}}\right)}{(6.022 \times 10^{23})}$	69
$H^- + CH_3 \rightarrow CH_4 + e^-$	1.00×10^{-9}	60
$H^- + CH_2 \rightarrow CH_3 + e^-$	1.00×10^{-9}	60
$H^- + CH \rightarrow CH_2 + e^-$	1.00×10^{-10}	60
$H^- + C \rightarrow CH + e^-$	1.00×10^{-9}	60
$H^- + C_2H \rightarrow C_2H_2 + e^-$	1.00×10^{-9}	60
$H^- + C_2 \rightarrow C_2H + e^-$	1.00×10^{-9}	60
$H^- + CH_4^+ \rightarrow H + CH_4$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	67
$H^- + CH_3^+ \rightarrow H + CH_3$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	67
$H^- + C_2H_2^+ \rightarrow H + C_2H_2$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$H^- + C_2H_3^+ \rightarrow H + C_2H_3$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$H^- + C_2H^+ \rightarrow H + C_2H$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70

$H^- + C_2H_4^+ \rightarrow H + C_2H_4$	$6.23 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$H^- + C_2H_5^+ \rightarrow H + C_2H_5$	$5.16 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$H^- + C_2H_6^+ \rightarrow H + C_2H_6$	$6.04 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH_2^- + M \rightarrow CH_2 + e^- + M$	$2.70 \times 10^{-10} \left(\frac{T_{gas}}{300}\right)^{-0.50} \exp\left(-\frac{5590.0}{T_{gas}}\right)$	71
$CH_2 + H^- \rightarrow CH^- + H_2$	$8.87 \times 10^{-11} \left(\frac{T_{gas}}{300}\right)^{2.65} \exp\left(-\frac{416.51}{T_{gas}}\right)$	72
$CH^- + C \rightarrow C_2H + e^-$	1.00×10^{-9}	65
$CH^- + H \rightarrow CH_2 + e^-$	1.00×10^{-10}	65
$CH^- + H^+ \rightarrow CH + H$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH^- + H_3^+ \rightarrow CH + H_2 + H$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH^- + C^+ \rightarrow C + CH$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH^- + CH_3^+ \rightarrow CH + CH_3$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH^- + C_2H_2^+ \rightarrow CH + C_2H_2$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70
$CH^- + C_2H_3^+ \rightarrow CH + C_2H_3$	$7.51 \times 10^{-8} \left(\frac{T_{gas}}{300}\right)^{-0.50}$	70

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