

## Supporting Information: Afterglow quenching in plasma-based dry reforming of methane: a detailed analysis of the post-plasma chemistry via kinetic modelling.

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### S1 Model equations

The mass balance equation (Eq. 1 in the main paper) requires the rate ( $R_i$ ) for each reaction  $i$  (as given by Eq. S1), which is the product of the rate coefficient  $k_i$  and number densities of the reactants  $n_s$ . These rate coefficients are given by analytical equations, e.g., modified Arrhenius equations or fall-off functions. A complete list of all reactions in the kinetics scheme, with the corresponding rate coefficients or cross sections and references, is given in Table S3 at the end of the document.

$$R_i = k_i \prod_s n_s^{a_s^L} \quad (\text{Eq. S1})$$

The correction for the gas expansion is added to the mass balance equation of each species (see last term in Eq. 1 in the main paper) and consists of two terms, i.e., reactive expansion and thermal expansion. The former term accounts for the total number density increase or decrease caused by chemical reactions and the latter for changes due to temperature changes. This correction parameter is given in Eq. S2, in which  $n_s$  is the number density of the species  $s$  for which the mass balance is solved,  $n_j$  the number density of all species in the model  $j$ ,  $a_{j,i}^R$  and  $a_{j,i}^L$  the coefficients of  $j$  in reaction  $i$ ,  $R_i$  the rate of reaction  $i$ ,  $R_{\text{mix}}$  the rate of gas mixing (when applicable),  $\partial T/\partial t$  the temperature change with respect to time,  $k_B$  the Boltzmann constant,  $P_0$  the pressure (1 atm) and  $T$  the gas temperature.

$$R_{\text{expansion}} = -\frac{n_s}{\sum_j n_j} \left( \sum_j \sum_{i=1}^j [(a_{j,i}^R - a_{j,i}^L) \cdot R_i] + R_{\text{mix}} \right) - \frac{n_s}{\sum_j n_j} \frac{\partial T}{\partial t} \frac{P_0}{k_B T^2} \quad (\text{Eq. S2})$$

Furthermore, as explained in the main paper, the heat balance equation is solved in the post-plasma region (see Eq. 4 in the main paper). The isobaric heat capacity of the gas mixture  $C_{p,\text{mix}}$ , used in the self-consistent temperature calculation, is given in Eq. S3. This is calculated as the sum of the heat capacity  $C_{p,i}$  of the individual species  $i$  (obtained from McBride et al.[1] and Burcat et al.[2]) weighted to the number density  $n_i$  of the species  $i$  over the total number density  $n_{\text{tot}}$ .

$$C_{p,\text{mix}}(T) = \sum_i C_{p,i}(T) \frac{n_i}{n_{\text{tot}}} \quad (\text{Eq. S3})$$

The temperature-dependent reaction enthalpy  $\epsilon$  is calculated for reaction  $i$  using Eq. S4, in which  $a_{s,i}^R$  and  $a_{s,i}^L$  are the coefficients of species  $s$  in reaction  $i$  at the right and left side of the reaction, respectively, and  $\Delta H_s^f$  the temperature-dependent enthalpy of formation of species  $s$  (obtained from McBride et al.[1] and Burcat et al.[2]).

$$\epsilon_i(T) = \sum_s [a_s^R - a_s^L] H_s^f(T) \quad (\text{Eq. S4})$$

To calculate the thermal loss, a thermal conductivity is required and this is calculated as the mixture-averaged conductivity using the Mason Saxena equation (Eq. S5),[3] in which  $i$  and  $k$  are the species in the model,  $\lambda_i$  is their temperature-dependent thermal conductivity (obtained from the polynomials provided by McBride et al.[4]),  $x_i$  and  $x_k$  are their molar fractions and  $G_{ik}$  is a factor calculated using Eq. S6.

$$\lambda_{\text{mix}}(T) = \sum_i \lambda_i(T) \left[ 1 + \sum_k G_{ik} \frac{x_k}{x_i} \right]^{-1} \quad (\text{Eq. S5})$$

The factor  $G_{ik}$  for species  $i$  respective to species  $k$  is given in Eq. S6, in which  $M$  is the molar mass and  $\mu$  the viscosity (obtained from the polynomials provided by McBride et al.[4]).

$$G_{ik} = \frac{1.065}{2\sqrt{2}} \left( 1 + \frac{M_i}{M_k} \right)^{-\frac{1}{2}} \left[ 1 + \left( \frac{\mu_i M_k}{\mu_k M_i} \right)^{\frac{1}{2}} \left( \frac{M_i}{M_k} \right)^{\frac{1}{4}} \right] \quad (\text{Eq. S6})$$

## S2 Chemistry

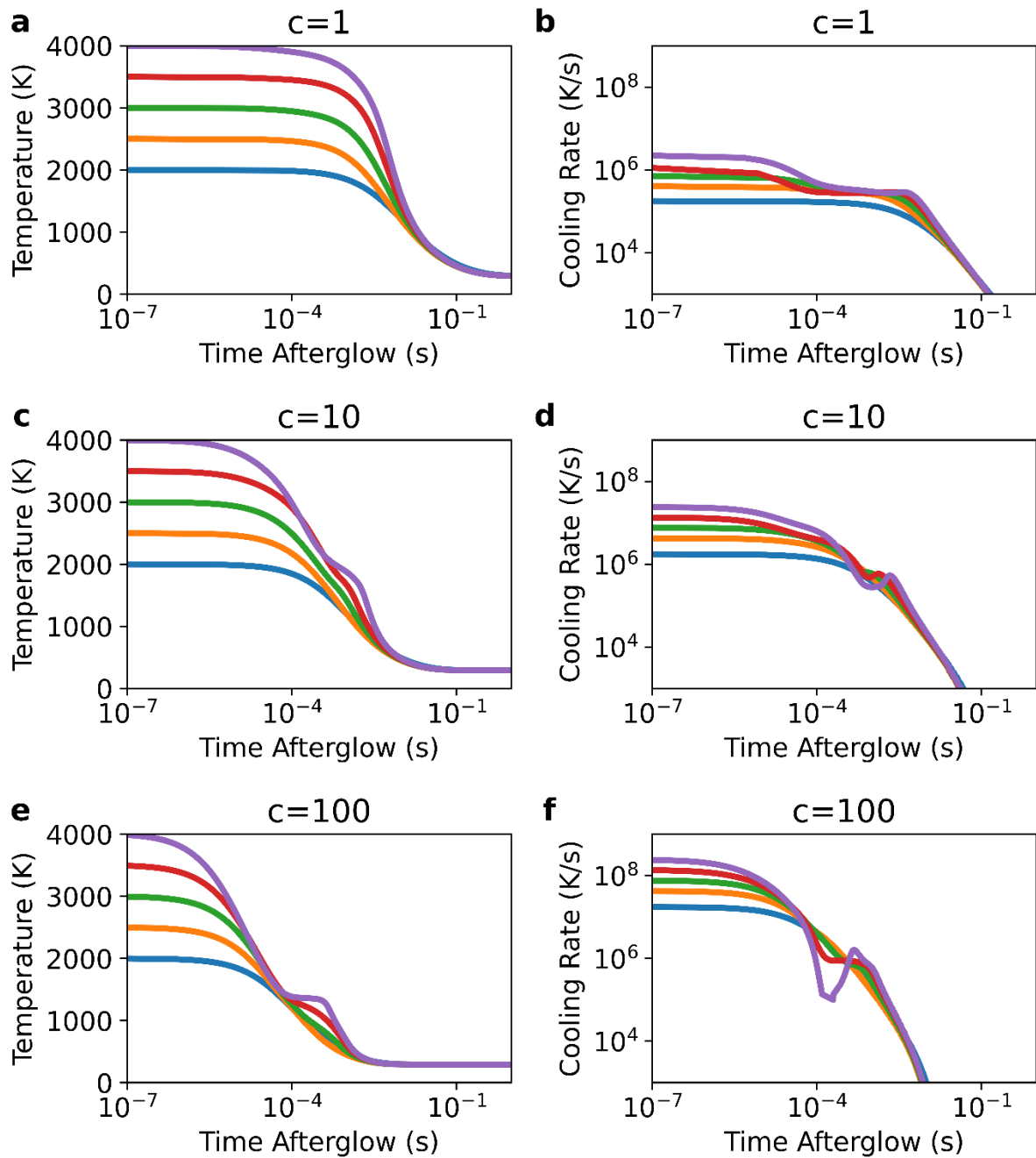
In this work we use a subset of the reaction scheme used in our previous work,[5] more specifically we only use the thermal reactions (i.e., electrons and ions and their respective reactions are not included), as we demonstrated before that the thermal chemistry is dominant at the conditions under study here. Most rate coefficients are obtained directly from literature sources, with some exceptions. Indeed, for reverse reactions between neutral species for which no reliable source could be found in literature, detailed balancing is used to obtain the rate coefficients. The equilibrium constant  $K_{eq}$  is calculated using Eq. S7, with  $p$  the reference pressure (1 bar),  $\Delta v$  the change in number of species in the reaction and  $\Delta G_r$  the Gibbs free energy of the reaction, calculated using thermodynamic data from McBride et al. [1] and Burcat et al.[2].

$$K_{eq} = \left(\frac{p}{RT}\right)^{\Delta v} e^{\left(\frac{-\Delta G_r}{RT}\right)} \quad (\text{Eq. S7})$$

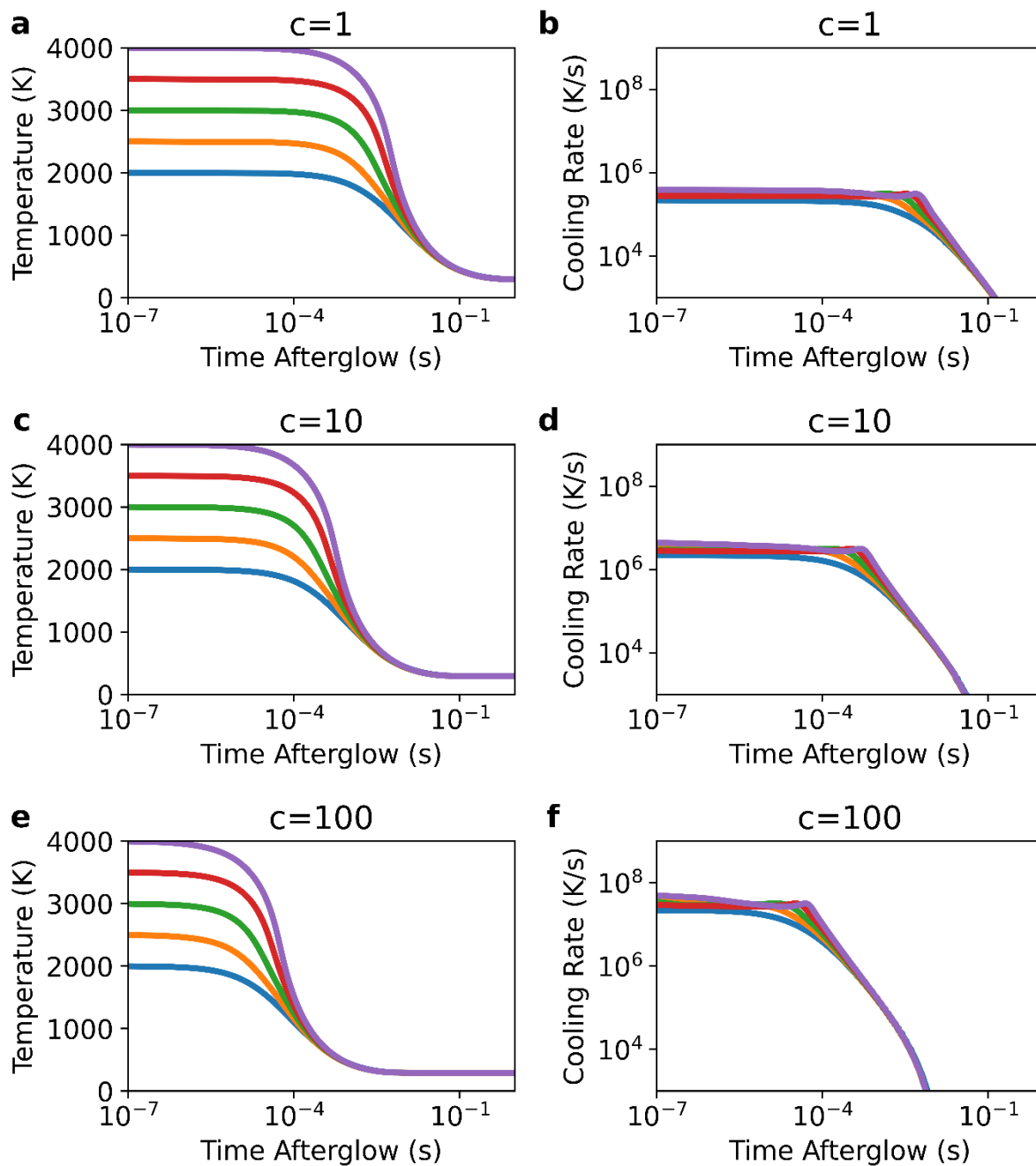
For the full list of the included reactions with the corresponding rate coefficients and respective references, see Table S3, at the end of this document.

## S3 Additional results

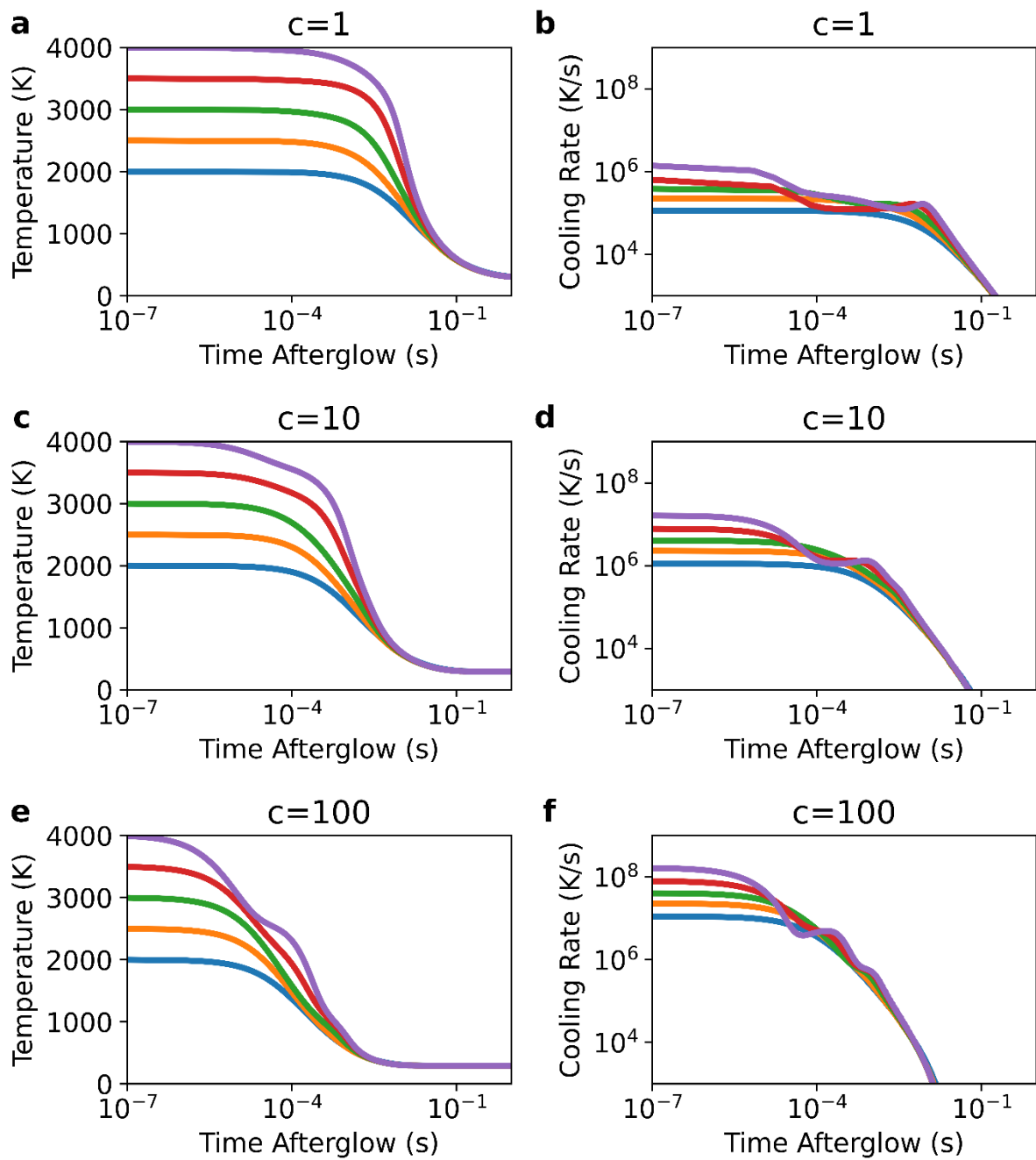
### S3.1 Post-plasma conductive cooling



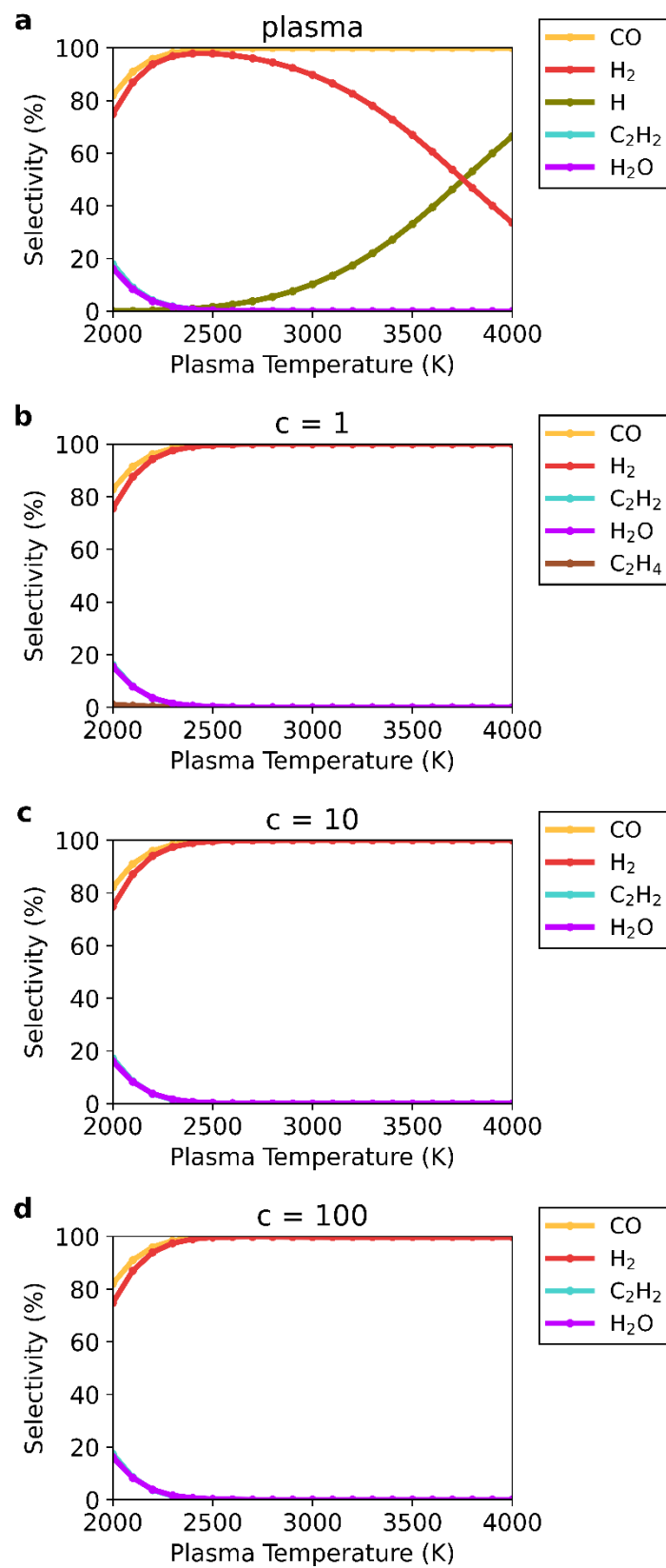
**Figure S1.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 50/50  $\text{CO}_2/\text{CH}_4$  gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for quenching with c-factors of 1 (a, b), 10 (c, d) and 100 (e, f).



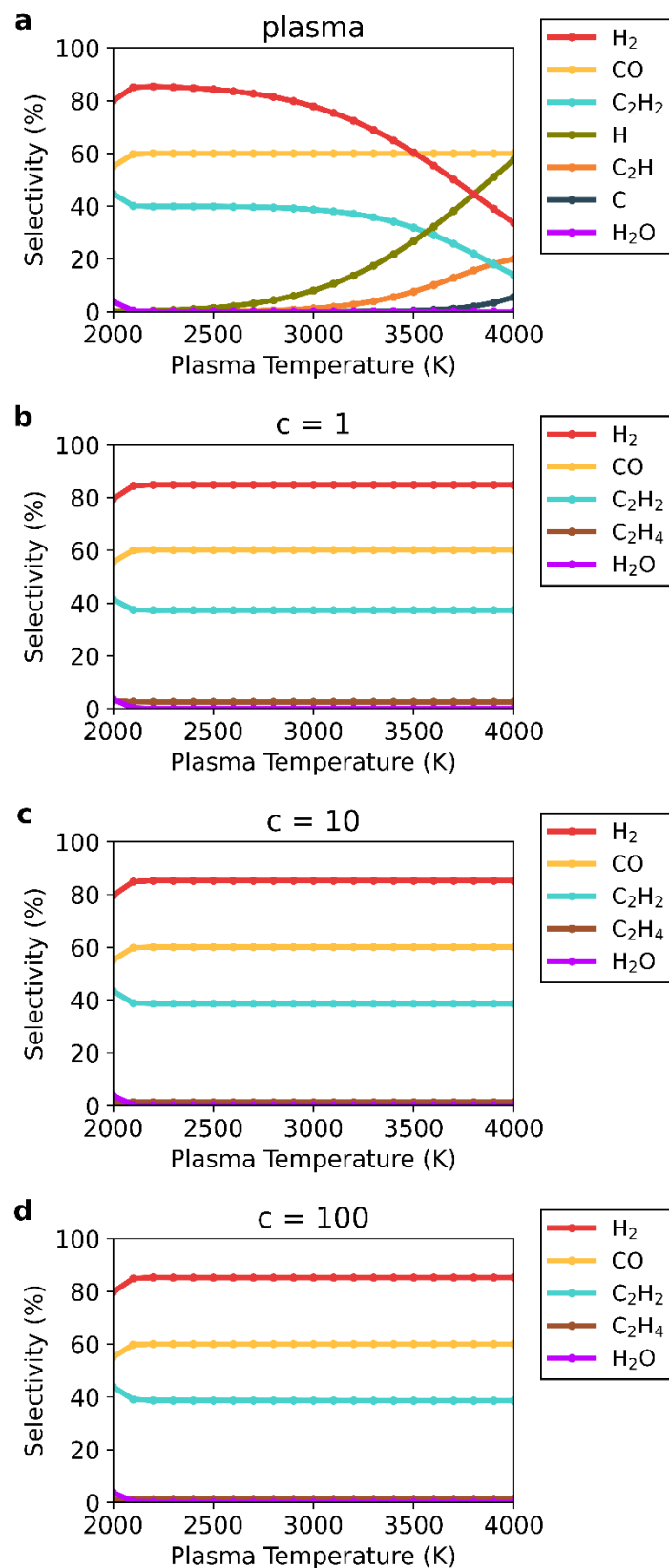
**Figure S2.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 30/70  $\text{CO}_2/\text{CH}_4$  gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for quenching with c-factors of 1 (a, b), 10 (c, d) and 100 (e, f).



**Figure S3.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 70/30  $\text{CO}_2/\text{CH}_4$  gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for quenching with  $c$ -factors of 1 (a, b), 10 (c, d) and 100 (e, f).

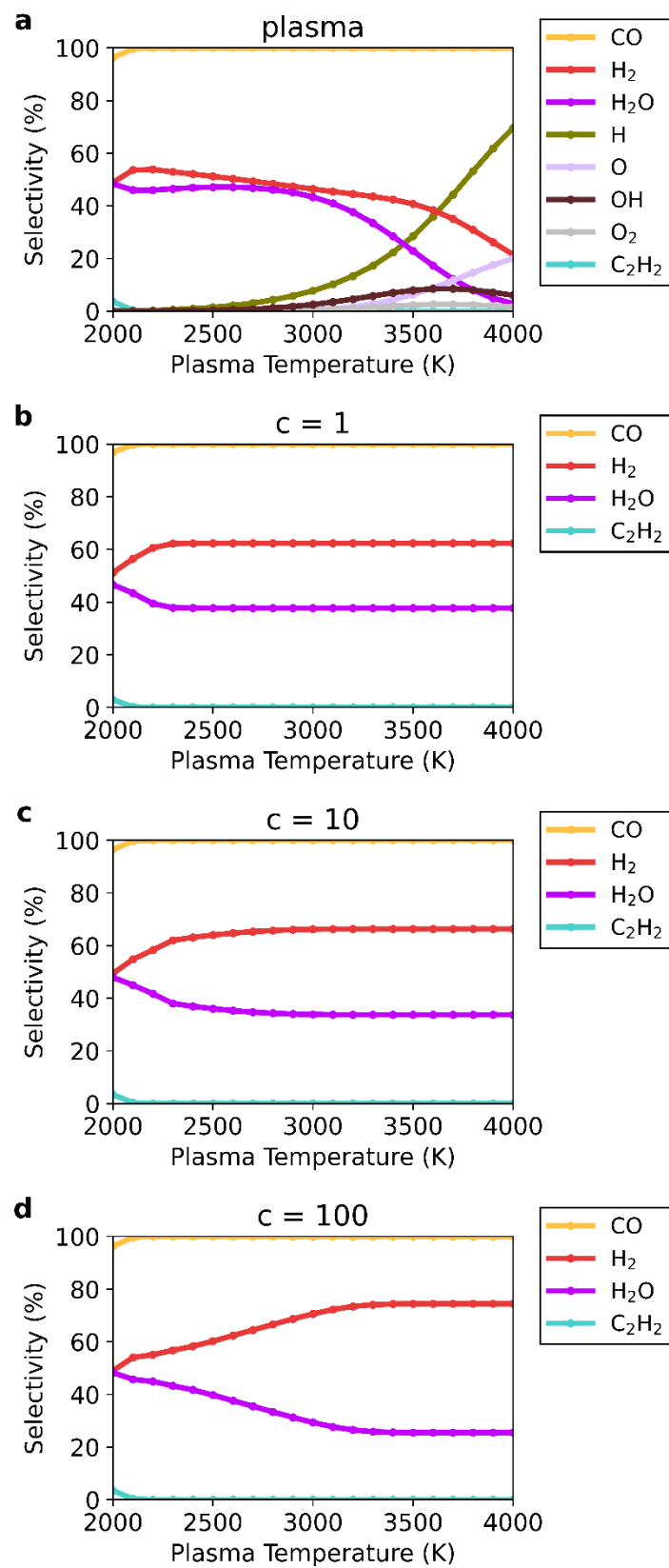


**Figure S4.** Selectivity of the main species (above 1%), as a function of the plasma temperature for the 50/50 CO<sub>2</sub>/CH<sub>4</sub> ratio, at the end of the plasma (a), and at the end of the afterglow (b, c, d), for c-factors of 1 (b), 10 (c) and 100 (d). The H<sub>2</sub> and CO selectivity curves and the H<sub>2</sub>O and C<sub>2</sub>H<sub>2</sub> selectivity curves overlap.

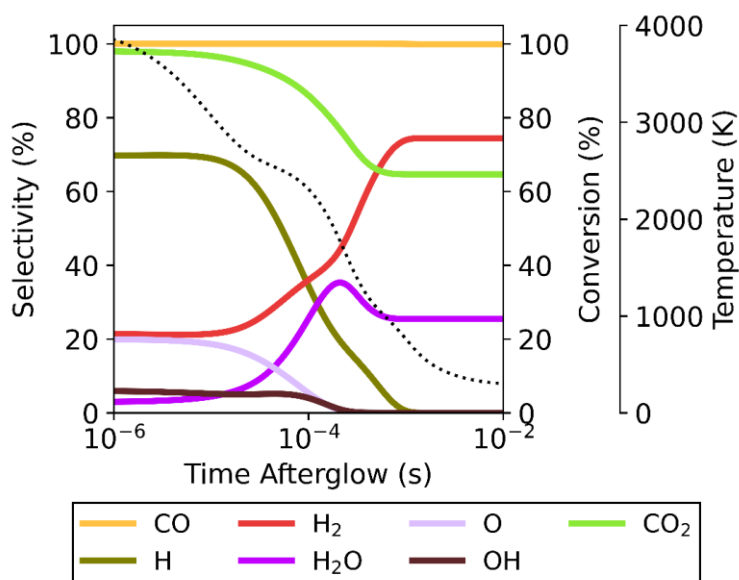


**Figure S5.** Selectivity of the main species (above 1%), as a function of the plasma temperature for the 30/70 CO<sub>2</sub>/CH<sub>4</sub> ratio, at the end of the plasma (a), and at the end of the afterglow (b, c, d), for c-factors of 1 (b), 10 (c) and 100 (d). The H<sub>2</sub>O and C<sub>2</sub>H<sub>4</sub> selectivity curves overlap.

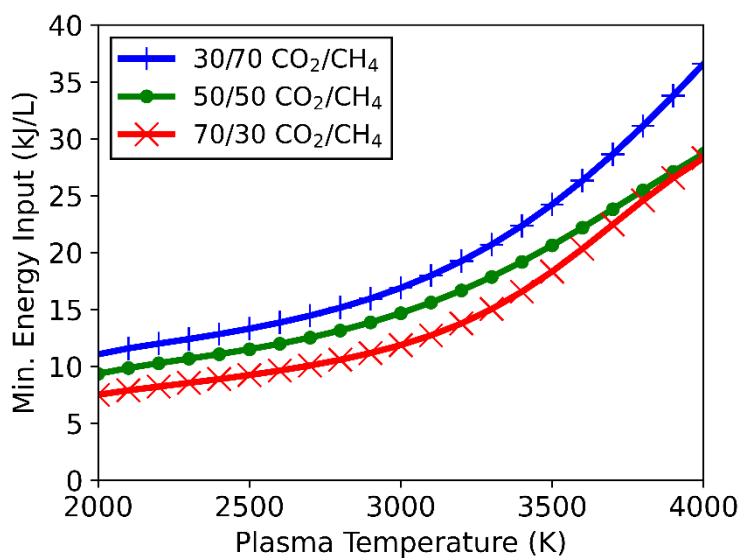




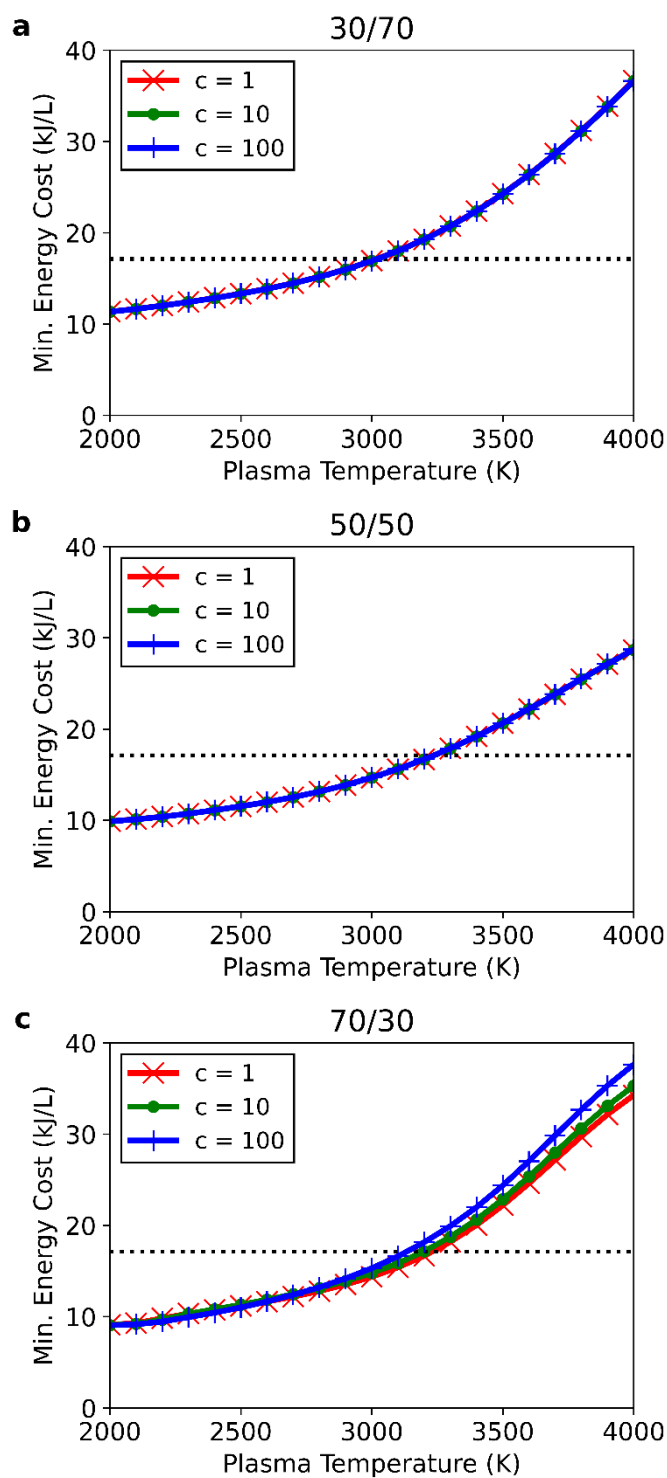
**Figure S6.** Selectivity of the main species (above 1%), as a function of the plasma temperature for the 70/30 CO<sub>2</sub>/CH<sub>4</sub> ratio, at the end of the plasma (a), and at the end of the afterglow (b, c, d), for c-factors of 1 (b), 10 (c) and 100 (d).



**Figure S7.** Time-evolution of the selectivity of the main species in the afterglow, starting from a plasma temperature of 4000 K for the 70/30 CO<sub>2</sub>/CH<sub>4</sub> ratio and c-factor = 100. The evolution of the CO<sub>2</sub> conversion (lime green curve) and the gas temperature (dotted line) are also plotted, and shown on the right axis.

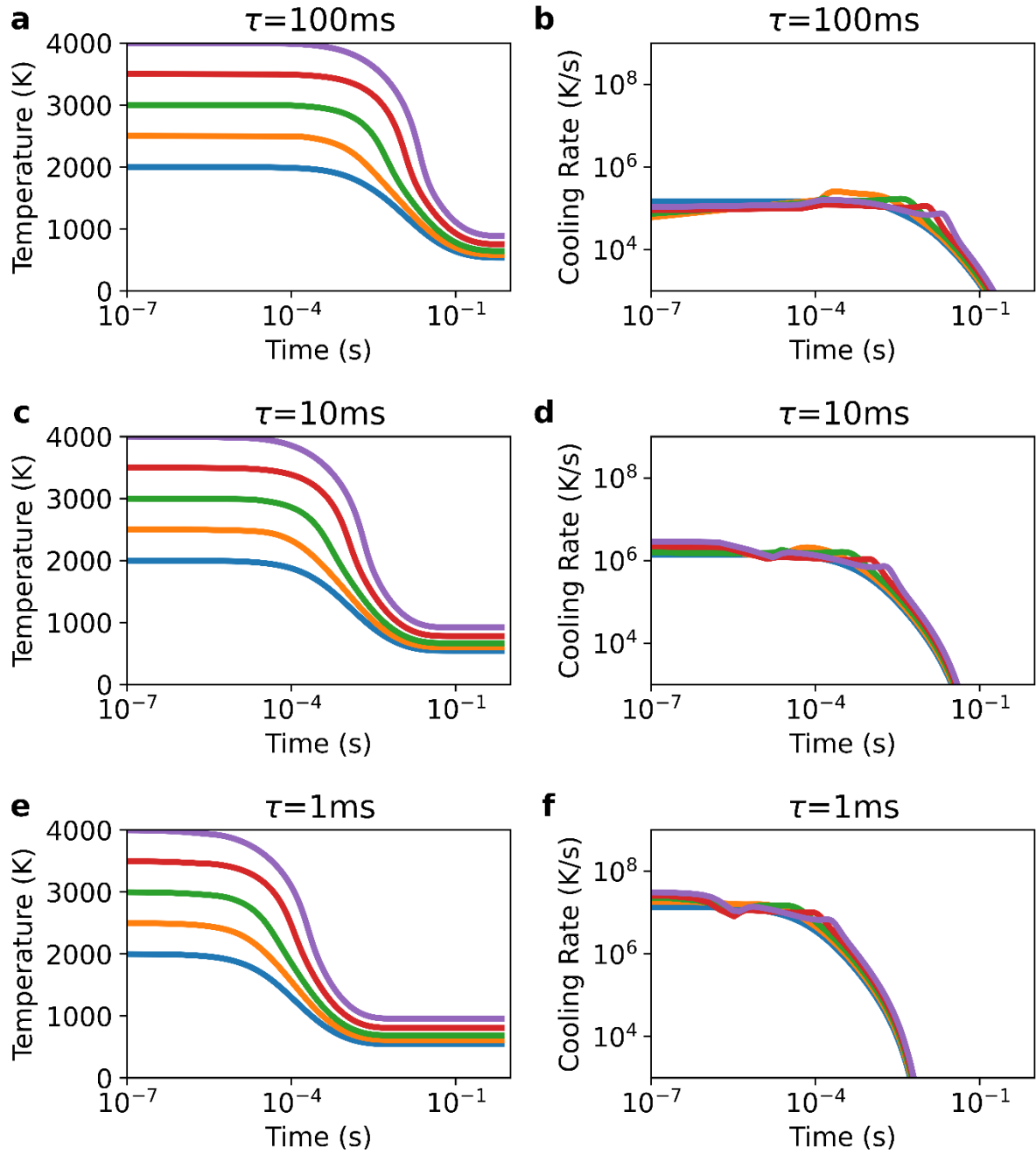


**Figure S8.** Minimum energy input required to achieve the final species distribution at the end of the plasma as a function of plasma temperature for the three different CO<sub>2</sub>/CH<sub>4</sub> ratios (70/30, 50/50, 30/70).

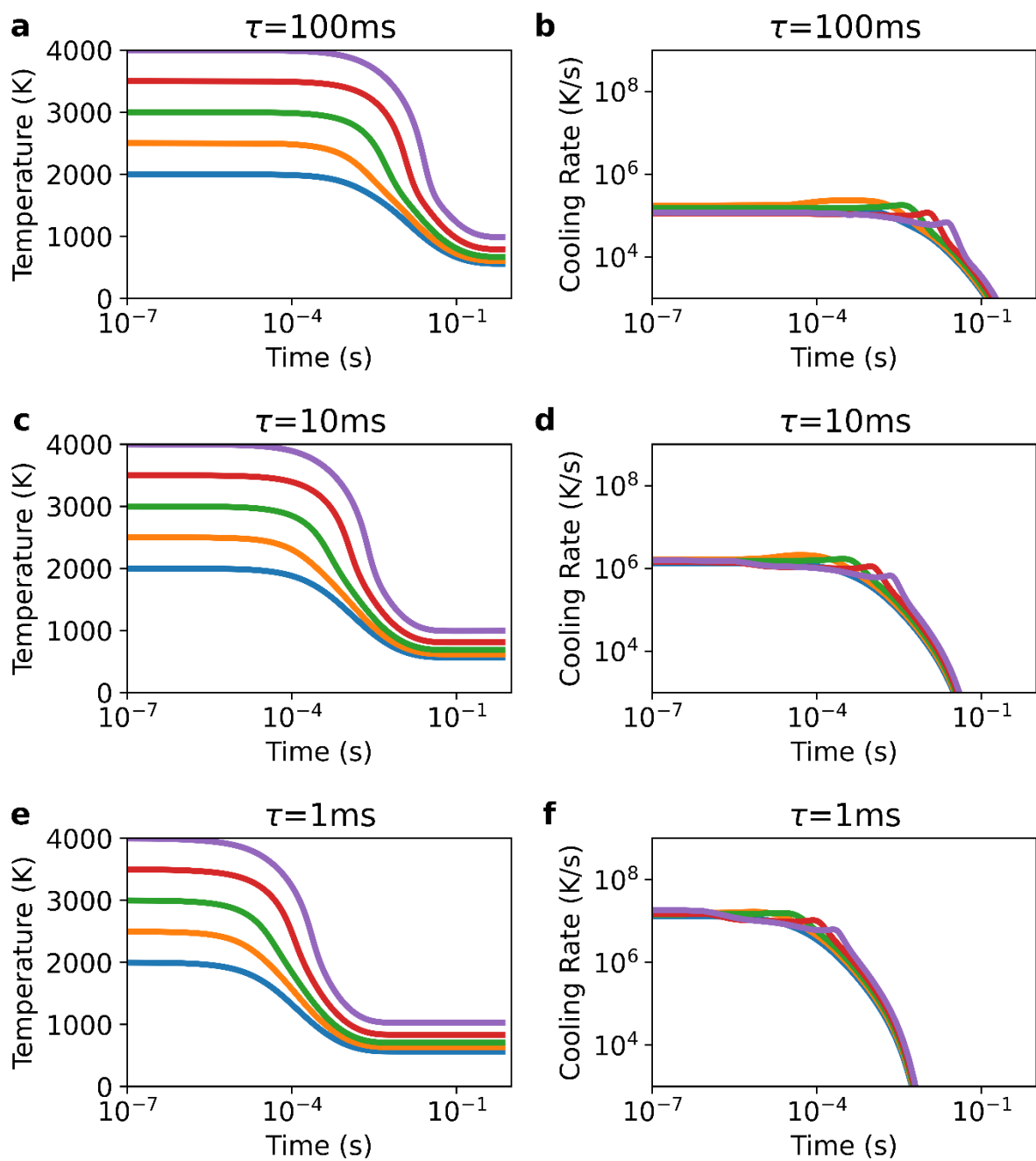


**Figure S9.** Minimum energy cost of conversion for c-factors of 1, 10 and 100 as a function of plasma temperature for CO<sub>2</sub>/CH<sub>4</sub> ratios of 30/70 (a), 50/50 (b) and 70/30 (c). The horizontal dotted black line indicates the target energy cost value of 17.1 kJ/L (4.27 eV/molecule) proposed by Snoeckx and Bogaerts for plasma-based DRM to be competitive with existing technologies.[6]

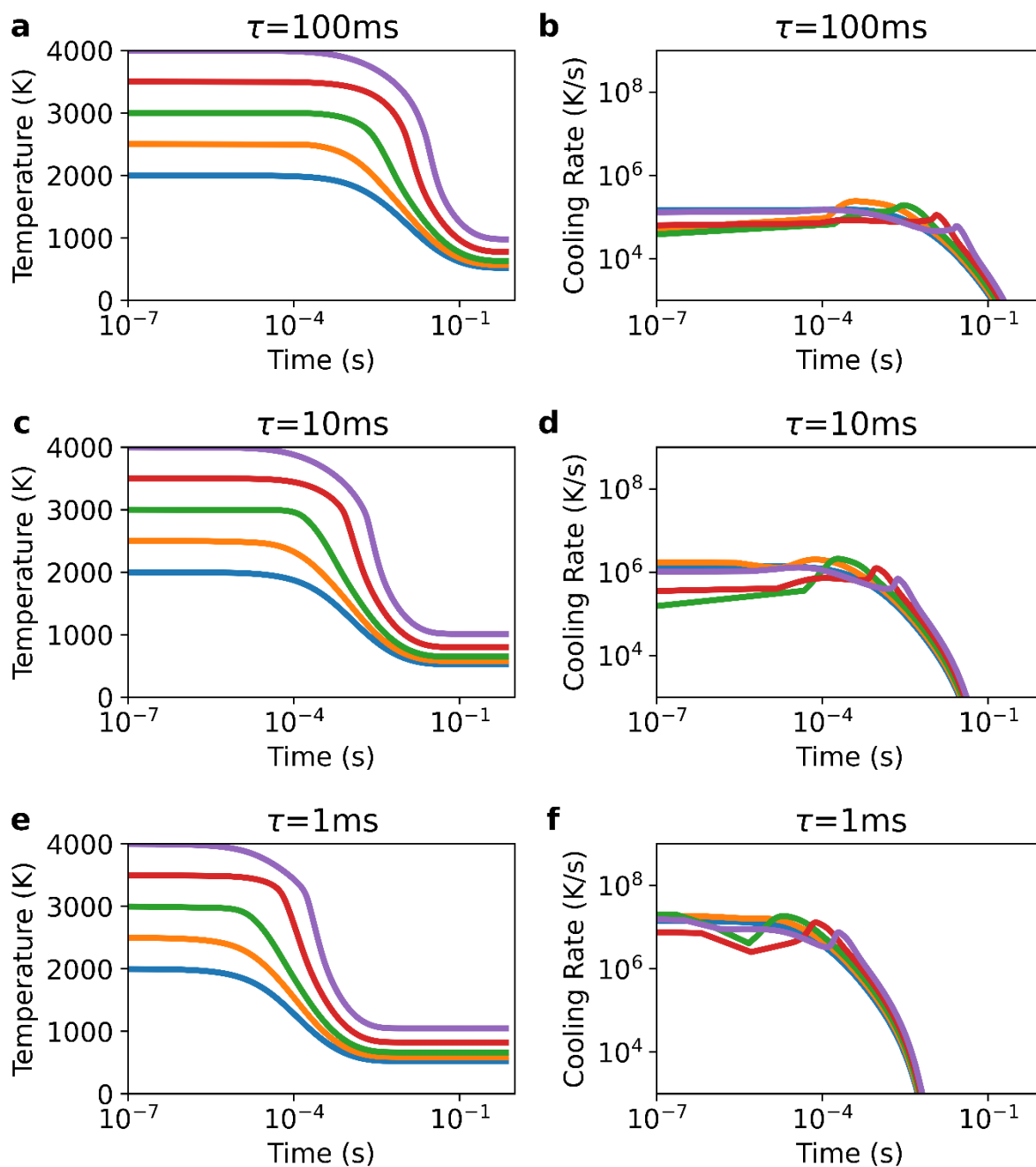
### S3.2 Post-plasma mixing



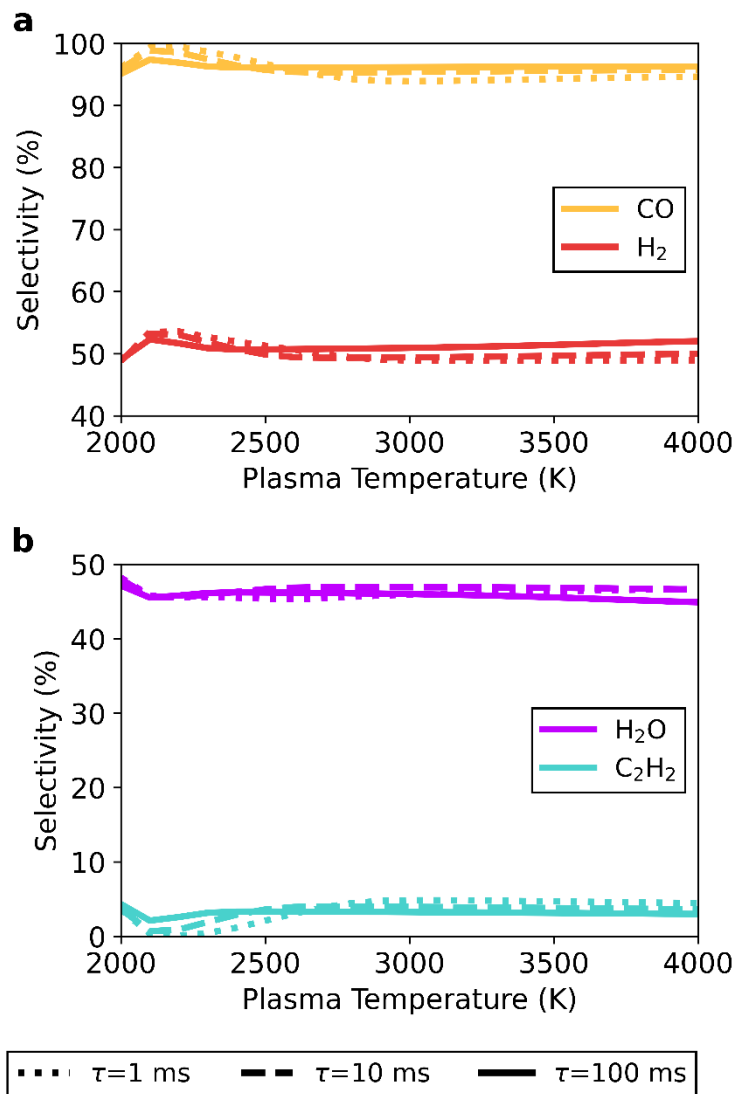
**Figure S10.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 50/50 CO<sub>2</sub>/CH<sub>4</sub> gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for characteristic mixing times of  $\tau_{\text{mix}} = 100$  ms (a, b), 10 ms (c, d) and 1 ms (e, f).



**Figure S11.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 30/70  $\text{CO}_2/\text{CH}_4$  gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for characteristic mixing times of  $\tau_{\text{mix}} = 100$  ms (a, b), 10 ms (c, d) and 1 ms (e, f).



**Figure S12.** Gas temperature profiles (left panels a, c, e) and cooling rates (right panels b, d, f) as a function of time in the afterglow for the 70/30  $\text{CO}_2/\text{CH}_4$  gas mixture, starting from plasma temperatures of 2000, 2500, 3000, 3500 and 4000 K, for characteristic mixing times of  $\tau_{\text{mix}} = 100$  ms (a, b), 10 ms (c, d) and 1 ms (e, f).



**Figure S13.** Selectivity at the end of the afterglow towards the main product species (H<sub>2</sub> and CO in panel a, and C<sub>2</sub>H<sub>2</sub> and H<sub>2</sub>O in panel b) as a function of the plasma temperature, at the 70/30 CO<sub>2</sub>/CH<sub>4</sub> ratio and  $\tau_{\text{mix}} = 1$  (dotted line), 10 (dashed line) and 100 (solid line) ms.

Table S1. CO<sub>2</sub> conversion obtained at the end of the plasma (Plasma), end of the afterglow (Afterglow) and relative additional conversion, calculated using equation 12 (Additional (Relative)) for plasma temperatures between 2000 and 4000 K and three different CO<sub>2</sub>/CH<sub>4</sub> ratios (70/30, 50/50, 30/70) at  $\tau_{\text{mix}} = 10$  ms.

| T <sub>plasma</sub> | CO <sub>2</sub> conversion (%) |           |                          |        |           |                          |        |           |                          |
|---------------------|--------------------------------|-----------|--------------------------|--------|-----------|--------------------------|--------|-----------|--------------------------|
|                     | 70/30                          |           |                          | 50/50  |           |                          | 30/70  |           |                          |
|                     | Plasma                         | Afterglow | Additional (Relative, %) | Plasma | Afterglow | Additional (Relative, %) | Plasma | Afterglow | Additional (Relative, %) |
| 2000                | 77                             | 7.7       | -0.65                    | 93     | 9.3       | -0.32                    | 98     | 9.8       | -0.070                   |
| 2100                | 81                             | 8.1       | -0.30                    | 97     | 9.7       | 0.59                     | 100    | 10        | 1.2                      |
| 2200                | 82                             | 8.3       | 0.70                     | 99     | 10        | 2.4                      | 100    | 10        | 3.4                      |
| 2300                | 83                             | 8.5       | 2.6                      | 99     | 10        | 5.0                      | 100    | 11        | 6.5                      |
| 2400                | 83                             | 8.8       | 5.0                      | 100    | 11        | 8.5                      | 100    | 11        | 10                       |
| 2500                | 84                             | 9.1       | 8.3                      | 100    | 11        | 12                       | 100    | 11        | 14                       |
| 2600                | 84                             | 9.5       | 12                       | 100    | 12        | 17                       | 100    | 12        | 19                       |
| 2700                | 84                             | 9.9       | 17                       | 100    | 12        | 22                       | 100    | 12        | 24                       |
| 2800                | 85                             | 10        | 23                       | 100    | 13        | 28                       | 100    | 13        | 31                       |
| 2900                | 85                             | 11        | 29                       | 100    | 14        | 35                       | 100    | 14        | 38                       |
| 3000                | 86                             | 12        | 37                       | 100    | 14        | 44                       | 100    | 15        | 47                       |
| 3100                | 87                             | 13        | 46                       | 100    | 15        | 53                       | 100    | 16        | 56                       |
| 3200                | 88                             | 14        | 57                       | 100    | 16        | 64                       | 100    | 17        | 68                       |
| 3300                | 89                             | 15        | 69                       | 100    | 18        | 77                       | 100    | 18        | 81                       |
| 3400                | 90                             | 17        | 84                       | 100    | 19        | 90                       | 100    | 20        | 96                       |
| 3500                | 92                             | 19        | 101                      | 100    | 21        | 105                      | 100    | 21        | 114                      |
| 3600                | 93                             | 21        | 121                      | 100    | 22        | 122                      | 100    | 23        | 133                      |
| 3700                | 95                             | 23        | 141                      | 100    | 24        | 139                      | 100    | 25        | 155                      |
| 3800                | 96                             | 25        | 161                      | 100    | 26        | 156                      | 100    | 28        | 178                      |
| 3900                | 97                             | 27        | 180                      | 100    | 27        | 174                      | 100    | 30        | 204                      |
| 4000                | 98                             | 29        | 197                      | 100    | 29        | 190                      | 100    | 33        | 230                      |



Table S2. CH<sub>4</sub> conversion obtained at the end of the plasma (Plasma), end of the afterglow (Afterglow) and relative additional conversion, calculated using equation 12 (Additional (Relative)) for plasma temperatures between 2000 and 4000 K and three different CO<sub>2</sub>/CH<sub>4</sub> ratios (70/30, 50/50, 30/70) at  $\tau_{\text{mix}} = 10$  ms.

| T <sub>plasma</sub> | CH <sub>4</sub> conversion (%) |           |                          |        |           |                          |        |           |                          |
|---------------------|--------------------------------|-----------|--------------------------|--------|-----------|--------------------------|--------|-----------|--------------------------|
|                     | 70/30                          |           |                          | 50/50  |           |                          | 30/70  |           |                          |
|                     | Plasma                         | Afterglow | Additional (Relative, %) | Plasma | Afterglow | Additional (Relative, %) | Plasma | Afterglow | Additional (Relative, %) |
| 2000                | 97                             | 9.7       | 0.18                     | 96     | 9.6       | 0.21                     | 97     | 9.8       | 0.33                     |
| 2100                | 99                             | 10        | 1.1                      | 98     | 9.9       | 1.2                      | 99     | 10        | 1.6                      |
| 2200                | 100                            | 10        | 3.4                      | 99     | 10        | 3.1                      | 100    | 10        | 4.0                      |
| 2300                | 100                            | 11        | 7.3                      | 100    | 11        | 5.9                      | 100    | 11        | 7.3                      |
| 2400                | 100                            | 11        | 12                       | 100    | 11        | 9.9                      | 100    | 11        | 11                       |
| 2500                | 100                            | 12        | 17                       | 100    | 11        | 14                       | 100    | 12        | 16                       |
| 2600                | 100                            | 12        | 22                       | 100    | 12        | 20                       | 100    | 12        | 20                       |
| 2700                | 100                            | 13        | 28                       | 100    | 13        | 26                       | 100    | 13        | 26                       |
| 2800                | 100                            | 13        | 34                       | 100    | 13        | 32                       | 100    | 13        | 32                       |
| 2900                | 100                            | 14        | 42                       | 100    | 14        | 40                       | 100    | 14        | 39                       |
| 3000                | 100                            | 15        | 51                       | 100    | 15        | 48                       | 100    | 15        | 48                       |
| 3100                | 100                            | 16        | 63                       | 100    | 16        | 58                       | 100    | 16        | 58                       |
| 3200                | 100                            | 18        | 77                       | 100    | 17        | 69                       | 100    | 17        | 69                       |
| 3300                | 100                            | 19        | 94                       | 100    | 18        | 82                       | 100    | 18        | 82                       |
| 3400                | 100                            | 21        | 114                      | 100    | 20        | 96                       | 100    | 20        | 98                       |
| 3500                | 100                            | 24        | 138                      | 100    | 21        | 111                      | 100    | 21        | 115                      |
| 3600                | 100                            | 27        | 165                      | 100    | 23        | 127                      | 100    | 23        | 134                      |
| 3700                | 100                            | 29        | 194                      | 100    | 24        | 144                      | 100    | 26        | 155                      |
| 3800                | 100                            | 32        | 223                      | 100    | 26        | 162                      | 100    | 28        | 179                      |
| 3900                | 100                            | 35        | 251                      | 100    | 28        | 180                      | 100    | 30        | 203                      |
| 4000                | 100                            | 37        | 275                      | 100    | 30        | 197                      | 100    | 33        | 230                      |

Table S3: List of reactions with the rate coefficients (third column) expressed in  $cm^3 s^{-1}$  for two-body reactions, and in  $cm^6 s^{-1}$  for three-body reactions and references (fourth column). In the rate equations,  $N_A$  is Avogadro's constant,  $k_B$  is the Boltzmann constant,  $R$  is the ideal gas constant,  $T_g$  is the gas temperature in  $K$  and  $n_M$  is the total number density of neutral species in  $cm^{-3}$ .

| #  | Reaction                               | Rate equation  | Ref.             |
|----|--|--|------------------|
| 1  | $CH_4 + H \rightarrow CH_3 + H_2$      | $6.4 \times 10^{-18} \cdot T_g^{2.11} \cdot \exp\left(\frac{-3.9 \times 10^3}{T_g}\right)$   | [7]              |
| 2  | $CH_3 + H_2 \rightarrow CH_4 + H$      | $6.62 \times 10^{-20} \cdot T_g^{2.24} \cdot \exp\left(\frac{-3.22 \times 10^3}{T_g}\right)$   | [7]              |
| 3  | $CH_3 + H \rightarrow CH_2 + H_2$      | $2.1 \times 10^{-8} \cdot T_g^{-0.56} \cdot \exp\left(\frac{-8.0 \times 10^3}{T_g}\right)$   | [8]              |
| 4  | $CH_3 + H \rightarrow CH_4$            | $k_0 = 1.7 \times 10^{-24} \cdot T_g^{-1.8}$<br>$k_\infty = 3.5 \times 10^{-10}$<br>$F_c = 0.63 \cdot \exp\left(\frac{-T_g}{3.3150 \times 10^3}\right)$<br>$+ 0.37 \cdot \exp\left(\frac{-T_g}{6.10 \times 10^1}\right)$   | [8] <sup>a</sup> |
| 5  | $CH_2 + H_2 \rightarrow CH_3 + H$      | $7.32 \times 10^{-19} \cdot T_g^{2.3} \cdot \exp\left(\frac{-3.6990 \times 10^3}{T_g}\right)$  | [9]              |
| 6  | $CH_2 + H \rightarrow CH + H_2$        | $2 \times 10^{-10}$  | [8]              |
| 7  | $CH + H_2 \rightarrow CH_2 + H$        | $2.9 \times 10^{-10} \cdot \exp\left(\frac{-1.670 \times 10^3}{T_g}\right)$  | [8]              |
| 8  | $CH + H_2 \rightarrow CH_3$            | $k_0 = 4.7 \times 10^{-26} \cdot T_g^{-1.6}$<br>$k_\infty = 8.5 \times 10^{-11} \cdot T_g^{0.15}$<br>$F_c = 0.48$<br>$+ 0.25 \cdot \exp\left(\frac{-T_g}{3.0 \times 10^2}\right)$  | [8] <sup>a</sup> |
| 9  | $CH + H \rightarrow C + H_2$           | $2 \times 10^{-10}$  | [8]              |
| 10 | $C + CH_4 \rightarrow C_2H_4$          | $5 \times 10^{-15}$  | [10]             |
| 11 | $C + CH_3 \rightarrow C_2H_2 + H$      | $8.3 \times 10^{-11}$  | [11]             |
| 12 | $C + CH_2 \rightarrow C_2H + H$        | $8.3 \times 10^{-11}$  | [11]             |
| 13 | $CH_3 + CH_4 \rightarrow C_2H_6 + H$   | $\frac{8 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-1.6736 \times 10^5}{R \cdot T_g}\right)$  | [12]             |
| 14 | $CH_3 + CH_4 \rightarrow C_2H_5 + H_2$ | $\frac{1 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-9.6232 \times 10^4}{R \cdot T_g}\right)$  | [12]             |
| 15 | $CH_2 + CH_4 \rightarrow CH_3 + CH_3$  | $7.14 \times 10^{-12} \cdot \exp\left(\frac{-4.199 \times 10^4}{R \cdot T_g}\right)$   | [13]             |
| 16 | $CH + CH_4 \rightarrow C_2H_4 + H$     | $2.2 \times 10^{-8} \cdot T_g^{-0.94} \cdot \exp\left(\frac{-2.9 \times 10^1}{T_g}\right)$   | [8]              |
| 17 | $CH_3 + CH_3 \rightarrow C_2H_6$       | $k_0 = 3.5 \times 10^{-7} \cdot T_g^{-7} \cdot \exp\left(\frac{-1.39 \times 10^3}{T_g}\right)$<br>$k_\infty = 6 \times 10^{-11}$<br>$F_c = 0.38 \cdot \exp\left(\frac{-T_g}{7.3 \times 10^1}\right)$<br>$+ 0.62 \cdot \exp\left(\frac{-T_g}{1.18 \times 10^3}\right)$                        | [8] <sup>a</sup> |
| 18 | $CH_3 + CH_3 \rightarrow C_2H_5 + H$   | $9 \times 10^{-11} \cdot \exp\left(\frac{-8.08 \times 10^3}{T_g}\right)$   | [8]              |
| 19 | $CH_3 + CH_3 \rightarrow CH_2 + CH_4$  | $5.6 \times 10^{-17} \cdot T_g^{1.34} \cdot \exp\left(\frac{-6.791 \times 10^4}{R \cdot T_g}\right)$   | [14]             |
| 20 | $CH_2 + CH_3 \rightarrow C_2H_4 + H$   | $1.2 \times 10^{-10}$  | [8]              |
| 21 | $CH_2 + CH_2 \rightarrow C_2H_2 + H_2$ | $\frac{10^{1.52 \times 10^1}}{N_A} \cdot \exp\left(\frac{-5 \times 10^4}{R \cdot T_g}\right)$  | [15]             |
| 22 | $CH + CH \rightarrow C_2H_2$           | $\frac{1.2 \times 10^{14}}{N_A}$   | [16]             |
| 23 | $CH_4 \rightarrow CH_3 + H$            | $k_0 = 7.5 \times 10^{-7} \cdot \exp\left(\frac{-4.570 \times 10^4}{T_g}\right)$<br>$k_\infty = 2.4 \times 10^{16} \cdot \exp\left(\frac{-5.280 \times 10^4}{T_g}\right)$<br>$F_c = \exp\left(\frac{-T_g}{1.350 \times 10^3}\right)$<br>$+ \exp\left(\frac{-7.8340 \times 10^3}{T_g}\right)$ | [8] <sup>a</sup> |
| 24 | $CH_3 \rightarrow CH + H_2$            | $1.1 \times 10^{-8} \cdot \exp\left(\frac{-4.280 \times 10^4}{T_g}\right) \cdot n_M$   | [8]              |
| 25 | $CH_3 \rightarrow CH_2 + H$            | $1.7 \times 10^{-8} \cdot \exp\left(\frac{-4.560 \times 10^4}{T_g}\right) \cdot n_M$   | [8]              |
| 26 | $CH_2 \rightarrow CH + H$              | $1.56 \times 10^{-8} \cdot \exp\left(\frac{-4.488 \times 10^4}{T_g}\right) \cdot n_M$  | [8]              |

| #  | Reaction                                  | Rate equation  | Ref.             |
|----|---|--|------------------|
| 27 | $CH_2 \rightarrow C + H_2$                | $5 \times 10^{-10} \cdot \exp\left(\frac{-3.26 \times 10^4}{T_g}\right) \cdot n_M$   | [8]              |
| 28 | $CH \rightarrow C + H$                    | $\frac{1.9 \times 10^{14}}{N_A} \cdot \exp\left(\frac{-3.37 \times 10^4}{T_g}\right) \cdot n_M$  | [11]             |
| 29 | $C_2H_6 + H \rightarrow C_2H_5 + H_2$     | $1.63 \times 10^{-10} \cdot \exp\left(\frac{-4.640 \times 10^3}{T_g}\right)$   | [8]              |
| 30 | $C_2H_5 + H_2 \rightarrow C_2H_6 + H$     | $5.1 \times 10^{-24} \cdot T_g^{3.6} \cdot \exp\left(\frac{-4.253 \times 10^3}{T_g}\right)$  | [8]              |
| 31 | $C_2H_5 + H \rightarrow CH_3 + CH_3$      | $7 \times 10^{-11}$  | [8]              |
| 32 | $C_2H_5 + H \rightarrow C_2H_6$           | $\frac{6 \times 10^{-11}}{1 + 10^{-1.915 + 2.69 \times 10^{-3} \cdot T_g - 2.35 \times 10^{-7} \cdot T_g^2}}$  | [17]             |
| 33 | $C_2H_5 + H \rightarrow C_2H_4 + H_2$     | $3 \times 10^{-12}$  | [17]             |
| 34 | $C_2H_4 + H_2 \rightarrow C_2H_5 + H$     | $1.7 \times 10^{-11} \cdot \exp\left(\frac{-3.43 \times 10^4}{T_g}\right)$   | [17]             |
| 35 | $C_2H_4 + H \rightarrow C_2H_3 + H_2$     | $3.9 \times 10^{-22} \cdot T_g^{3.62} \cdot \exp\left(\frac{-5.67 \times 10^3}{T_g}\right)$  | [8]              |
| 36 | $C_2H_4 + H \rightarrow C_2H_5$           | $k_0 = 1.3 \times 10^{-29} \cdot \exp\left(\frac{-3.8 \times 10^2}{T_g}\right)$<br>$k_\infty = 6.6 \times 10^{-15} \cdot T_g^{1.28} \cdot \exp\left(\frac{-6.5 \times 10^2}{T_g}\right)$<br>$F_c = 0.24 \cdot \exp\left(\frac{-T_g}{4 \times 10^4}\right)$<br>$+ 0.76 \cdot \exp\left(\frac{-T_g}{1.025 \times 10^3}\right)$ | [8] <sup>a</sup> |
| 37 | $C_2H_3 + H_2 \rightarrow C_2H_4 + H$     | $1.57 \times 10^{-20} \cdot T_g^{2.56} \cdot \exp\left(\frac{-2.529 \times 10^3}{T_g}\right)$  | [18]             |
| 38 | $C_2H_3 + H \rightarrow C_2H_2 + H_2$     | $7 \times 10^{-11}$  | [8]              |
| 39 | $C_2H_3 + H \rightarrow C_2H_4$           | $k_0 = 3.5 \times 10^{-27}$<br>$k_\infty = 1.6 \times 10^{-10}$<br>$F_c = 0.5$   | [8] <sup>a</sup> |
| 40 | $C_2H_2 + H_2 \rightarrow C_2H_3 + H$     | $4 \times 10^{-12} \cdot \exp\left(\frac{-3.27 \times 10^4}{T_g}\right)$   | [17]             |
| 41 | $C_2H_2 + H_2 \rightarrow C_2H_4$         | $5 \times 10^{-13} \cdot \exp\left(\frac{-1.96 \times 10^4}{T_g}\right)$   | [17]             |
| 42 | $C_2H_2 + H \rightarrow C_2H_3$           | $k_0 = 1 \times 10^{-20} \cdot T_g^{-3.38} \cdot \exp\left(\frac{-4.26 \times 10^2}{T_g}\right)$<br>$k_\infty = 9.2 \times 10^{-16} \cdot T_g^{1.64} \cdot \exp\left(\frac{-1.055 \times 10^3}{T_g}\right)$<br>$F_c = 7.37 \times 10^{-4} \cdot T_g^{0.8}$   | [8] <sup>a</sup> |
| 43 | $C_2H_2 + H \rightarrow C_2H + H_2$       | $1.67 \times 10^{-14} \cdot T_g^{1.64} \cdot \exp\left(\frac{-1.525 \times 10^4}{T_g}\right)$  | [8]              |
| 44 | $C_2H + H_2 \rightarrow C_2H_2 + H$       | $3.5 \times 10^{-18} \cdot T_g^{2.32} \cdot \exp\left(\frac{-4.44 \times 10^2}{T_g}\right)$  | [8]              |
| 45 | $C_2H + H \rightarrow C_2H_2$             | $3 \times 10^{-10}$  | [17]             |
| 46 | $C + C_2H_4 \rightarrow C_2H_2 + CH_2$    | $1.239 \times 10^{-11}$  | [19, 20]         |
| 47 | $C_2H_6 + CH_3 \rightarrow C_2H_5 + CH_4$ | $9.3 \times 10^{-14} \cdot \exp\left(\frac{-4.740 \times 10^3}{T_g}\right)$<br>$+ 1.4 \times 10^{-9} \cdot \exp\left(\frac{-1.120 \times 10^4}{T_g}\right)$  | [8]              |
| 48 | $C_2H_6 + CH_2 \rightarrow C_2H_5 + CH_3$ | $\frac{6.5 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-3.31 \times 10^4}{R \cdot T_g}\right)$  | [13]             |
| 49 | $C_2H_6 + CH \rightarrow C_2H_4 + CH_3$   | $1.3 \times 10^{-10}$  | [21]             |
| 50 | $C_2H_5 + CH_4 \rightarrow C_2H_6 + CH_3$ | $1.43 \times 10^{-25} \cdot T_g^{4.14} \cdot \exp\left(\frac{-6.322 \times 10^3}{T_g}\right)$  | [17]             |
| 51 | $C_2H_5 + CH_3 \rightarrow C_2H_4 + CH_4$ | $1.5 \times 10^{-12}$  | [8]              |
| 52 | $C_2H_5 + CH_3 \rightarrow C_2H_6 + CH_2$ | $3 \times 10^{-44} \cdot T_g^{9.0956}$   | [22]             |
| 53 | $C_2H_5 + CH_2 \rightarrow C_2H_4 + CH_3$ | $3 \times 10^{-11}$  | [17]             |
| 54 | $C_2H_4 + CH_3 \rightarrow C_2H_3 + CH_4$ | $1 \times 10^{-16} \cdot T_g^{1.56} \cdot \exp\left(\frac{-8.37 \times 10^3}{T_g}\right)$  | [8]              |
| 55 | $C_2H_3 + CH_4 \rightarrow C_2H_4 + CH_3$ | $2.4 \times 10^{-24} \cdot T_g^{4.02} \cdot \exp\left(\frac{-2.754 \times 10^3}{T_g}\right)$   | [17]             |
| 56 | $C_2H_3 + CH_3 \rightarrow C_2H_2 + CH_4$ | $1.5 \times 10^{-11} \cdot \exp\left(\frac{3.850 \times 10^2}{T_g}\right)$   | [23]             |
| 57 | $C_2H_3 + CH_2 \rightarrow C_2H_2 + CH_3$ | $3 \times 10^{-11}$  | [17]             |
| 58 | $C_2H_2 + CH_3 \rightarrow C_2H + CH_4$   | $3 \times 10^{-13} \cdot \exp\left(\frac{-8.7 \times 10^3}{T_g}\right)$  | [17]             |

| #  | Reaction                                      | Rate equation  | Ref.              |
|----|---|--|-------------------|
| 59 | $C_2H + CH_4 \rightarrow C_2H_2 + CH_3$       | $3.6 \times 10^{-14} \cdot T_g^{0.94} \cdot \exp\left(\frac{-3.28 \times 10^2}{T_g}\right)$  | [8]               |
| 60 | $C_2H + CH_2 \rightarrow C_2H_2 + CH$         | $3 \times 10^{-11}$  | [17]              |
| 61 | $C_2H_3 + C_2H_6 \rightarrow C_2H_4 + C_2H_5$ | $1 \times 10^{-21} \cdot T_g^{3.3} \cdot \exp\left(\frac{-5.285 \times 10^3}{T_g}\right)$  | [17]              |
| 62 | $C_2H + C_2H_6 \rightarrow C_2H_2 + C_2H_5$   | $6.75 \times 10^{-12} \cdot T_g^{0.28} \cdot \exp\left(\frac{6.2 \times 10^1}{T_g}\right)$   | [8]               |
| 63 | $C_2H_5 + C_2H_5 \rightarrow C_2H_4 + C_2H_6$ | $2.3 \times 10^{-12}$  | [8]               |
| 64 | $C_2H_4 + C_2H_5 \rightarrow C_2H_3 + C_2H_6$ | $8.1 \times 10^{-31} \cdot T_g^{5.82} \cdot \exp\left(\frac{-6 \times 10^3}{T_g}\right)$   | [8]               |
| 65 | $C_2H_3 + C_2H_5 \rightarrow C_2H_2 + C_2H_6$ | $2.3985 \times 10^{-11}$   | [24, 25]          |
| 66 | $C_2H_3 + C_2H_5 \rightarrow C_2H_4 + C_2H_4$ | $4.42 \times 10^{-11}$   | [24, 25]          |
| 67 | $C_2H_2 + C_2H_5 \rightarrow C_2H + C_2H_6$   | $4.5 \times 10^{-13} \cdot \exp\left(\frac{-1.18 \times 10^4}{T_g}\right)$   | [17]              |
| 68 | $C_2H + C_2H_5 \rightarrow C_2H_2 + C_2H_4$   | $3 \times 10^{-12}$  | [17]              |
| 69 | $C_2H_4 + C_2H_4 \rightarrow C_2H_3 + C_2H_5$ | $8 \times 10^{-10} \cdot \exp\left(\frac{-3.6 \times 10^4}{T_g}\right)$  | [17]              |
| 70 | $C_2H_2 + C_2H_4 \rightarrow C_2H_3 + C_2H_3$ | $4 \times 10^{-11} \cdot \exp\left(\frac{-3.44 \times 10^4}{T_g}\right)$   | [17]              |
| 71 | $C_2H + C_2H_4 \rightarrow C_2H_2 + C_2H_3$   | $3.35 \times 10^{-18} \cdot T_g^{2.24}$  | [26]              |
| 72 | $C_2H_3 + C_2H_3 \rightarrow C_2H_2 + C_2H_4$ | $1.6 \times 10^{-12}$  | [17]              |
| 73 | $C_2H + C_2H_3 \rightarrow C_2H_2 + C_2H_2$   | $1.6 \times 10^{-12}$  | [17]              |
| 74 | $C_2H_2 + C_2H_2 \rightarrow C_2H + C_2H_3$   | $1.6 \times 10^{-11} \cdot \exp\left(\frac{-4.25 \times 10^4}{T_g}\right)$   | [17]              |
| 75 | $C_2H_6 \rightarrow CH_3 + CH_3$              | $k_0 = 2.6 \times 10^{25} \cdot T_g^{-8.37} \cdot \exp\left(\frac{-4.729 \times 10^4}{T_g}\right)$<br>$k_\infty = 4.5 \times 10^{21} \cdot T_g^{-1.37} \cdot \exp\left(\frac{-4.59 \times 10^4}{T_g}\right)$<br>$F_c = 0.38 \cdot \exp\left(\frac{-T_g}{7.3 \times 10^1}\right)$<br>$+ 0.62 \cdot \exp\left(\frac{-T_g}{1.18 \times 10^3}\right)$                                  | [8] <sup>a</sup>  |
| 76 | $C_2H_6 \rightarrow C_2H_5 + H$               | $k_0 = \frac{10^{4.2839 \times 10^1}}{n_M} \cdot T_g^{-6.431} \cdot \exp\left(\frac{-5.3938 \times 10^4}{T_g}\right)$<br>$k_\infty = 10^{2.0947 \times 10^1} \cdot T_g^{-1.228} \cdot \exp\left(\frac{-5.1439 \times 10^4}{T_g}\right)$<br>$F_c = 4.761 \times 10^1 \cdot \exp\left(\frac{-1.6182 \times 10^4}{T_g}\right)$<br>$+ \exp\left(\frac{-T_g}{3.371 \times 10^3}\right)$ | [27] <sup>a</sup> |
| 77 | $C_2H_5 \rightarrow C_2H_4 + H$               | $k_0 = 1.7 \times 10^{-6} \cdot \exp\left(\frac{-1.68 \times 10^4}{T_g}\right)$<br>$k_\infty = 8.2 \times 10^{13} \cdot \exp\left(\frac{-2.007 \times 10^4}{T_g}\right)$<br>$F_c = 0.25 \cdot \exp\left(\frac{-T_g}{9.7 \times 10^1}\right)$<br>$+ 0.75 \cdot \exp\left(\frac{-T_g}{1.379 \times 10^3}\right)$   | [8] <sup>a</sup>  |
| 78 | $C_2H_4 \rightarrow C_2H_3 + H$               | $10^{1.63 \times 10^1} \cdot \exp\left(\frac{-4.6 \times 10^5}{R \cdot T_g}\right)$  | [28]              |
| 79 | $C_2H_4 \rightarrow C_2H_2 + H_2$             | $10^{1.29 \times 10^1} \cdot T_g^{0.44} \cdot \exp\left(\frac{-4.467 \times 10^4}{T_g}\right)$   | [17]              |
| 80 | $C_2H_3 \rightarrow C_2H_2 + H$               | $k_0 = 4.3 \times 10^3 \cdot T_g^{-3.4} \cdot \exp\left(\frac{-1.802 \times 10^4}{T_g}\right)$<br>$k_\infty = 3.9 \times 10^8 \cdot T_g^{1.62} \cdot \exp\left(\frac{-1.865 \times 10^4}{T_g}\right)$<br>$F_c = 7.37 \times 10^{-4} \cdot T_g^{0.8}$   | [8] <sup>a</sup>  |
| 81 | $C_2H_2 \rightarrow C_2H + H$                 | $10^{1.542 \times 10^1} \cdot \exp\left(\frac{-6.2445 \times 10^4}{T_g}\right)$  | [17]              |
| 82 | $O + OH \rightarrow H + O_2$                  | $4.33 \times 10^{-11} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{-0.5} \cdot \exp\left(\frac{-3.0 \times 10^1}{T_g}\right)$   | [17]              |
| 83 | $H + OH \rightarrow H_2 + O$                  | $4.1 \times 10^{-12} \cdot \frac{T_g}{3.0 \times 10^2} \cdot \exp\left(\frac{-3.50 \times 10^3}{T_g}\right)$   | [29]              |
| 84 | $OH + OH \rightarrow H_2O + O$                | $1.02 \times 10^{-12} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{1.4} \cdot \exp\left(\frac{2.0 \times 10^2}{T_g}\right)$   | [17]              |
| 85 | $OH + OH \rightarrow H + HO_2$                | $2 \times 10^{-11} \cdot \exp\left(\frac{-2.020 \times 10^4}{T_g}\right)$  | [29]              |
| 86 | $OH + OH \rightarrow H_2 + O_2$               | $1.82 \times 10^{-13} \cdot T_g^{0.51} \cdot \exp\left(\frac{-2.54 \times 10^4}{T_g}\right)$   | [30]              |

| #   | Reaction                               | Rate equation   | Ref.             |
|-----|--|---|------------------|
| 87  | $M + OH \rightarrow M + H + O$         | $4.7 \times 10^{-8} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{-1.0} \cdot \exp\left(\frac{-5.0830 \times 10^4}{T_g}\right)$   | [29]             |
| 88  | $H_2 + OH \rightarrow H + H_2O$        | $3.6 \times 10^{-16} \cdot T_g^{1.52} \cdot \exp\left(\frac{-1.74 \times 10^3}{T_g}\right)$   | [8]              |
| 89  | $O_2 + OH \rightarrow H + O_3$         | $2.7 \times 10^{-13} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{1.44} \cdot \exp\left(\frac{-3.860 \times 10^4}{T_g}\right)$   | [29]             |
| 90  | $O_2 + OH \rightarrow HO_2 + O$        | $2.2 \times 10^{-11} \cdot \exp\left(\frac{-2.820 \times 10^4}{T_g}\right)$   | [29]             |
| 91  | $O_3 + OH \rightarrow HO_2 + O_2$      | $1.69 \times 10^{-12} \cdot \exp\left(\frac{-9.410 \times 10^2}{T_g}\right)$  | [31]             |
| 92  | $H_2O + OH \rightarrow H + H_2O_2$     | $4 \times 10^{-10} \cdot \exp\left(\frac{-4.050 \times 10^4}{T_g}\right)$   | [29]             |
| 93  | $HO_2 + OH \rightarrow H_2O + O_2$     | $8.05 \times 10^{-11} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{-1.0}$  | [17]             |
| 94  | $HO_2 + OH \rightarrow H_2O_2 + O$     | $1.5 \times 10^{-12} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{0.5} \cdot \exp\left(\frac{-1.060 \times 10^4}{T_g}\right)$  | [29]             |
| 95  | $H_2O_2 + OH \rightarrow H_2O + HO_2$  | $2.9 \times 10^{-12} \cdot \exp\left(\frac{-1.60 \times 10^2}{T_g}\right)$  | [17]             |
| 96  | $H + HO_2 \rightarrow H_2 + O_2$       | $1.1 \times 10^{-10} \cdot \exp\left(\frac{-1.070 \times 10^3}{T_g}\right)$   | [17]             |
| 97  | $H + HO_2 \rightarrow OH + OH$         | $2.8 \times 10^{-10} \cdot \exp\left(\frac{-4.40 \times 10^2}{T_g}\right)$  | [17]             |
| 98  | $H + HO_2 \rightarrow H_2O + O$        | $5 \times 10^{-11} \cdot \exp\left(\frac{-8.660 \times 10^2}{T_g}\right)$   | [32]             |
| 99  | $H_2O + HO_2 \rightarrow H_2O_2 + OH$  | $3 \times 10^{-11} \cdot \exp\left(\frac{-1.510 \times 10^4}{T_g}\right)$   | [29]             |
| 100 | $H_2 + HO_2 \rightarrow H_2O + OH$     | $1.1 \times 10^{-12} \cdot \exp\left(\frac{-9.40 \times 10^3}{T_g}\right)$  | [29]             |
| 101 | $H_2 + HO_2 \rightarrow H + H_2O_2$    | $1 \times 10^{-12} \cdot \exp\left(\frac{-9.30 \times 10^3}{T_g}\right)$  | [29]             |
| 102 | $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$ | $2.2 \times 10^{-13} \cdot \exp\left(\frac{6.0 \times 10^2}{T_g}\right)$  | [33]             |
| 103 | $HO_2 + O \rightarrow O_2 + OH$        | $2.9 \times 10^{-11} \cdot \exp\left(\frac{2.0 \times 10^2}{T_g}\right)$  | [17]             |
| 104 | $HO_2 + O_2 \rightarrow O_3 + OH$      | $1.5 \times 10^{-15}$   | [29]             |
| 105 | $H + H_2O_2 \rightarrow H_2 + HO_2$    | $8 \times 10^{-11} \cdot \exp\left(\frac{-4.0 \times 10^3}{T_g}\right)$   | [17]             |
| 106 | $H + H_2O_2 \rightarrow H_2O + OH$     | $4 \times 10^{-11} \cdot \exp\left(\frac{-2.0 \times 10^3}{T_g}\right)$   | [17]             |
| 107 | $H_2O_2 + O \rightarrow HO_2 + OH$     | $1.44 \times 10^{-12} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{2.0} \cdot \exp\left(\frac{-2.0 \times 10^3}{T_g}\right)$   | [17]             |
| 108 | $H_2O_2 \rightarrow OH + OH$           | $k_0 = 3.8 \times 10^{-8} \cdot \exp\left(\frac{-2.196 \times 10^4}{T_g}\right)$<br>$k_\infty = 3 \times 10^{14} \cdot \exp\left(\frac{-2.44 \times 10^4}{T_g}\right)$<br>$F_c = 0.5$ | [8] <sup>a</sup> |
| 109 | $H_2O_2 + O_2 \rightarrow HO_2 + HO_2$ | $5 \times 10^{-11} \cdot \exp\left(\frac{-2.160 \times 10^4}{T_g}\right)$   | [29]             |
| 110 | $H_2O + O \rightarrow OH + OH$         | $7.6 \times 10^{-15} \cdot T_g^{1.3} \cdot \exp\left(\frac{-8.6 \times 10^3}{T_g}\right)$   | [17]             |
| 111 | $M + H_2O \rightarrow M + H + OH$      | $5.9 \times 10^{-7} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{-2.2} \cdot \exp\left(\frac{-5.90 \times 10^4}{T_g}\right)$   | [29]             |
| 112 | $H + H_2O \rightarrow H_2 + OH$        | $7.5 \times 10^{-16} \cdot T_g^{1.6} \cdot \exp\left(\frac{-9.03 \times 10^3}{T_g}\right)$  | [8]              |
| 113 | $H_2O + OH \rightarrow H_2 + HO_2$     | $1.4 \times 10^{-13} \cdot \exp\left(\frac{-3.610 \times 10^4}{T_g}\right)$   | [29]             |
| 114 | $H_2O + O \rightarrow H + HO_2$        | $2.8 \times 10^{-12} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{0.37} \cdot \exp\left(\frac{-2.87430 \times 10^4}{T_g}\right)$   | [29]             |
| 115 | $H_2O + O_2 \rightarrow H_2O_2 + O$    | $9.8 \times 10^{-8} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{0.5} \cdot \exp\left(\frac{-4.480 \times 10^4}{T_g}\right)$   | [29]             |
| 116 | $H_2O + O_2 \rightarrow HO_2 + OH$     | $4.3 \times 10^{-12} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{0.5} \cdot \exp\left(\frac{-3.660 \times 10^4}{T_g}\right)$  | [29]             |
| 117 | $M + H + O \rightarrow M + OH$         | $4.33 \times 10^{-32} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{-1}$  | [17]             |
| 118 | $H + O_2 \rightarrow O + OH$           | $1.62 \times 10^{-10} \cdot \exp\left(\frac{-7.4740 \times 10^3}{T_g}\right)$   | [32]             |
| 119 | $M + H + O_2 \rightarrow M + HO_2$     | $3.33 \times 10^{-31} \cdot \left(\frac{T_g}{3.0 \times 10^2}\right)^{-1}$  | [8]              |
| 120 | $H + O_3 \rightarrow HO_2 + O$         | $7.76 \times 10^{-13}$  | [34]             |
| 121 | $H + O_3 \rightarrow O_2 + OH$         | $2.36 \times 10^{-11}$  | [34]             |
| 122 | $H_2 + O_3 \rightarrow HO_2 + OH$      | $1 \times 10^{-13} \cdot \exp\left(\frac{-1.0 \times 10^4}{T_g}\right)$   | [29]             |

| #   | Reaction                                | Rate equation   | Ref.             |
|-----|---|---|------------------|
| 123 | $H_2 + O_2 \rightarrow H + HO_2$        | $3.2 \times 10^{-11} \cdot \exp\left(\frac{-2.410 \times 10^4}{T_g}\right)$   | [29]             |
| 124 | $H_2 + O \rightarrow H + OH$            | $9 \times 10^{-12} \cdot \frac{T_g}{3.0 \times 10^2} \cdot \exp\left(\frac{-4.480 \times 10^3}{T_g}\right)$   | [29]             |
| 125 | $C + OH \rightarrow CO + H$             | $\frac{5 \times 10^{13}}{N_A}$  | [35]             |
| 126 | $CO_2 + H \rightarrow CO + OH$          | $4.7 \times 10^{-10} \cdot \exp\left(\frac{-1.3915 \times 10^4}{T_g}\right)$  | [8]              |
| 127 | $CO + H \rightarrow HCO$                | $2 \times 10^{-35} \cdot T_g^{0.2} \cdot n_M$   | [8]              |
| 128 | $CO + OH \rightarrow CO_2 + H$          | $\frac{3.3 \times 10^6}{N_A} \cdot T_g^{1.55} \cdot \exp\left(\frac{4.02 \times 10^2}{T_g}\right)$  | [36]             |
| 129 | $CO + HO_2 \rightarrow CO_2 + OH$       | $\frac{5.8 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-2.293 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$  | [37]             |
| 130 | $CO + H_2O_2 \rightarrow COOH + OH$     | $\frac{3.6 \times 10^4}{N_A} \cdot T_g^{2.5} \cdot \exp\left(\frac{-1.4425 \times 10^4}{T_g}\right)$  | [38]             |
| 131 | $CH_4 + O \rightarrow CH_3 + OH$        | $7.3 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-3.31 \times 10^3}{T_g}\right)$  | [8]              |
| 132 | $CH_4 + O_2 \rightarrow CH_3 + HO_2$    | $8.1 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-2.637 \times 10^4}{T_g}\right)$   | [8]              |
| 133 | $CH_4 + O_2 \rightarrow CH_3OO + H$     | $\frac{4.3 \times 10^{13}}{N_A} \cdot \left(\frac{T_g}{1 \times 10^3}\right)^{1.96} \cdot \exp\left(\frac{-8.73 \times 10^1 \cdot 4.184 \times 10^3}{R \cdot T_g}\right)$   | [39]             |
| 134 | $CH_3 + O \rightarrow H + HCHO$         | $1.12 \times 10^{-10}$  | [8]              |
| 135 | $CH_3 + O_2 \rightarrow HCHO + OH$      | $3.7 \times 10^{-12} \cdot \exp\left(\frac{-1.114 \times 10^4}{T_g}\right)$   | [8]              |
| 136 | $CH_3 + O_2 \rightarrow CH_3O + O$      | $3.5 \times 10^{-11} \cdot \exp\left(\frac{-1.634 \times 10^4}{T_g}\right)$   | [8]              |
| 137 | $CH_3 + O_2 \rightarrow CH_3OO$         | $1.3 \times 10^{-15} \cdot T_g^{1.2}$   | [8]              |
| 138 | $CH_2 + O \rightarrow CO + H_2$         | $0.4 \cdot 3.4 \times 10^{-10} \cdot \exp\left(\frac{-2.7 \times 10^2}{T_g}\right)$   | [8]              |
| 139 | $CH_2 + O_2 \rightarrow HCHO + O$       | $\frac{4 \times 10^{10}}{N_A}$  | [40]             |
| 140 | $CH_2 + O_2 \rightarrow CO + H_2O$      | $4.2 \times 10^{-13}$   | [17]             |
| 141 | $CH + O \rightarrow CO + H$             | $6.6 \times 10^{-11}$   | [8]              |
| 142 | $CH + O_2 \rightarrow CO_2 + H$         | $4.2 \times 10^{-11}$   | [8]              |
| 143 | $CH + O_2 \rightarrow CO + OH$          | $2.8 \times 10^{-11}$   | [8]              |
| 144 | $CH + O_2 \rightarrow HCO + O$          | $2.8 \times 10^{-11}$   | [8]              |
| 145 | $CH_3 + CO \rightarrow CH_3CO$          | $k_0 = 1.6 \times 10^{-37} \cdot T_g^{1.05} \cdot \exp\left(\frac{-1.3 \times 10^3}{T_g}\right)$<br>$k_\infty = 3.1 \times 10^{-16} \cdot T_g^{1.05} \cdot \exp\left(\frac{-2.85 \times 10^3}{T_g}\right)$<br>$F_c = 0.5$   | [8] <sup>a</sup> |
| 146 | $CH_2 + CO_2 \rightarrow CO + HCHO$     | $3.9 \times 10^{-14}$   | [17]             |
| 147 | $CH_2 + CO \rightarrow CH_2CO$          | $1 \times 10^{-15}$   | [17]             |
| 148 | $CH + CO_2 \rightarrow CO + HCO$        | $0.5 \cdot 1.06 \times 10^{-16} \cdot T_g^{1.51} \cdot \exp\left(\frac{3.6 \times 10^2}{T_g}\right)$  | [8]              |
| 149 | $CH + CO \rightarrow HCCO$              | $k_0 = 6.3 \times 10^{-24} \cdot T_g^{-2.5}$<br>$k_\infty = 1.7 \times 10^{-9} \cdot T_g^{-0.4}$<br>$F_c = 0.6$   | [8] <sup>a</sup> |
| 150 | $CH_4 + OH \rightarrow CH_3 + H_2O$     | $1.66 \times 10^{-18} \cdot T_g^{2.182} \cdot \exp\left(\frac{-1.231 \times 10^3}{T_g}\right)$  | [41]             |
| 151 | $CH_4 + HO_2 \rightarrow CH_3 + H_2O_2$ | $7.8 \times 10^{-20} \cdot T_g^{2.5} \cdot \exp\left(\frac{-1.057 \times 10^4}{T_g}\right)$   | [8]              |
| 152 | $CH_3 + OH \rightarrow CH_3OH$          | $k_0 = 1.06 \times 10^{-10} \cdot T_g^{-6.21} \cdot \exp\left(\frac{-6.71 \times 10^2}{T_g}\right)$<br>$k_\infty = 7.2 \times 10^{-9} \cdot T_g^{-0.79}$<br>$F_c = 0.75 \cdot \exp\left(\frac{-T_g}{2.1 \times 10^2}\right)$<br>$+0.25 \cdot \exp\left(\frac{-T_g}{1.434 \times 10^3}\right)$ | [8] <sup>a</sup> |

| #   | Reaction                                | Rate equation  | Ref.             |
|-----|---|--|------------------|
| 153 | $CH_3 + OH \rightarrow CH_2 + H_2O$     | $\frac{k}{n_M}$<br>$k_0 = 1.8 \times 10^{-8} \cdot T_g^{-0.91} \cdot \exp\left(\frac{-2.75 \times 10^2}{T_g}\right)$<br>$k_\infty = 6.4 \times 10^{-8} \cdot T_g^{5.8} \cdot \exp\left(\frac{4.85 \times 10^2}{T_g}\right)$<br>$F_c = 0.664 \cdot \exp\left(\frac{-T_g}{3.569 \times 10^3}\right)$<br>$+ 0.336 \cdot \exp\left(\frac{-T_g}{1.08 \times 10^2}\right)$<br>$+ \exp\left(\frac{-3.24 \times 10^3}{T_g}\right)$ | [8] <sup>a</sup> |
| 154 | $CH_3 + OH \rightarrow CH_2OH + H$      | $1.2 \times 10^{-12} \cdot \exp\left(\frac{-2.76 \times 10^3}{T_g}\right)$   | [8]              |
| 155 | $CH_3 + OH \rightarrow CH_3O + H$       | $2 \times 10^{-14} \cdot \exp\left(\frac{-6.99 \times 10^3}{T_g}\right)$   | [8]              |
| 156 | $CH_3 + OH \rightarrow H_2 + HCHO$      | $5.3 \times 10^{-15} \cdot \exp\left(\frac{-2.53 \times 10^3}{T_g}\right)$   | [8]              |
| 157 | $CH_3 + OH \rightarrow CH_4 + O$        | $1.16 \times 10^{-19} \cdot T_g^{2.2} \cdot \exp\left(\frac{-2.24 \times 10^3}{T_g}\right)$  | [42]             |
| 158 | $CH_3 + H_2O \rightarrow CH_4 + OH$     | $8 \times 10^{-22} \cdot T_g^{2.9} \cdot \exp\left(\frac{-7.48 \times 10^3}{T_g}\right)$   | [43]             |
| 159 | $CH_3 + HO_2 \rightarrow CH_3O + OH$    | $3 \times 10^{-11}$  | [8]              |
| 160 | $CH_3 + HO_2 \rightarrow CH_4 + O_2$    | $6 \times 10^{-12}$  | [17]             |
| 161 | $CH_3 + H_2O_2 \rightarrow CH_4 + HO_2$ | $2 \times 10^{-14} \cdot \exp\left(\frac{3.0 \times 10^2}{T_g}\right)$   | [17]             |
| 162 | $CH_2 + OH \rightarrow H + HCHO$        | $5 \times 10^{-11}$  | [17]             |
| 163 | $CH_2 + H_2O \rightarrow CH_3 + OH$     | $1 \times 10^{-16}$  | [17]             |
| 164 | $CH_2 + HO_2 \rightarrow HCHO + OH$     | $3 \times 10^{-11}$  | [17]             |
| 165 | $CH_2 + H_2O_2 \rightarrow CH_3 + HO_2$ | $1 \times 10^{-14}$  | [17]             |
| 166 | $CH + OH \rightarrow C + H_2O$          | $\frac{4 \times 10^7}{N_A} \cdot T_g^2 \cdot \exp\left(\frac{-3 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$  | [37]             |
| 167 | $CH + OH \rightarrow H + HCO$           | $\frac{3 \times 10^{13}}{N_A}$   | [37]             |
| 168 | $CH + H_2O \rightarrow H + HCHO$        | $\frac{8.5 \times 10^8}{N_A} \cdot T_g^{1.144} \cdot \exp\left(\frac{2.051 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$   | [35]             |
| 169 | $CO + COOH \rightarrow CO_2 + HCO$      | $1 \times 10^{-14}$  | [44]             |
| 170 | $CH_3O + CO \rightarrow CH_3 + CO_2$    | $2.6 \times 10^{-11} \cdot \exp\left(\frac{-5.94 \times 10^3}{T_g}\right)$   | [17]             |
| 171 | $CH_3O + CO \rightarrow HCHO + HCO$     | $5.23 \times 10^{-15}$   | [45]             |
| 172 | $CH_3OO + CO \rightarrow CH_3O + CO_2$  | $7 \times 10^{-18}$  | [46]             |
| 173 | $H + HCO \rightarrow CO + H_2$          | $1.5 \times 10^{-10}$  | [8]              |
| 174 | $H + HCO \rightarrow CH_2 + O$          | $\frac{3.98107171 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-4.29 \times 10^5}{R \cdot T_g}\right)$   | [47]             |
| 175 | $H + HCHO \rightarrow H_2 + HCO$        | $3.34 \times 10^{-23} \cdot T_g^{-3.81} \cdot \exp\left(\frac{-2.02 \times 10^2}{T_g}\right)$  | [8]              |
| 176 | $H + HCHO \rightarrow CH_3O$            | $\frac{2.4 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-4.11 \times 10^3 \cdot 4.184}{T_g}\right)$  | [48]             |
| 177 | $CH_3O + H \rightarrow H_2 + HCHO$      | $3.3 \times 10^{-11}$  | [17]             |
| 178 | $CH_3O + H \rightarrow CH_3OH$          | $3.4 \times 10^{-10} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{0.33}$  | [49]             |
| 179 | $CH_3O + H_2 \rightarrow CH_3OH + H$    | $1.7 \times 10^{-15} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^4 \cdot \exp\left(\frac{-2.47 \times 10^3}{T_g}\right)$  | [50]             |
| 180 | $CH_2OH + H \rightarrow H_2 + HCHO$     | $1 \times 10^{-11}$  | [51]             |
| 181 | $CH_2OH + H \rightarrow CH_3 + OH$      | $1.6 \times 10^{-10}$  | [51]             |
| 182 | $CH_2OH + H_2 \rightarrow CH_3OH + H$   | $1.12 \times 10^{-18} \cdot T_g^2 \cdot \exp\left(\frac{-6.722 \times 10^3}{T_g}\right)$   | [51]             |
| 183 | $CH_3OH + H \rightarrow CH_2OH + H_2$   | $5.7 \times 10^{-15} \cdot T_g^{1.24} \cdot \exp\left(\frac{-2.26 \times 10^3}{T_g}\right)$  | [8]              |
| 184 | $CH_3OH + H \rightarrow CH_3 + H_2O$    | $\frac{2 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-5.3 \cdot 4.184 \times 10^3}{R \cdot T_g}\right)$   | [52]             |
| 185 | $CH_3OO + H \rightarrow CH_4 + O_2$     | $\frac{4.02 \times 10^{13}}{N_A} \cdot \left(\frac{T_g}{1 \times 10^3}\right)^{1.02} \cdot \exp\left(\frac{-1.66 \times 10^4 \cdot 4.184 \times 10^3}{R \cdot T_g}\right)$   | [39]             |
| 186 | $CH_3OO + H \rightarrow CH_3O + OH$     | $1.6 \times 10^{-10}$  | [17]             |

| #   | Reaction                                     | Rate equation   | Ref. |
|-----|--|---|------|
| 187 | $CH_3OO + H_2 \rightarrow CH_3OOH + H$       | $5 \times 10^{-11} \cdot \exp\left(\frac{-1.31 \times 10^4}{T_g}\right)$  | [17] |
| 188 | $HCO + OH \rightarrow CO + H_2O$             | $1.8 \times 10^{-10}$   | [8]  |
| 189 | $H_2O + HCO \rightarrow HCHO + OH$           | $3.9 \times 10^{-16} \cdot T_g^{1.35} \cdot \exp\left(\frac{-1.3146 \times 10^4}{T_g}\right)$   | [17] |
| 190 | $H_2O_2 + HCO \rightarrow HCHO + HO_2$       | $1.7 \times 10^{-13} \cdot \exp\left(\frac{-3.486 \times 10^3}{T_g}\right)$   | [17] |
| 191 | $HCHO + OH \rightarrow H_2O + HCO$           | $2.31 \times 10^{-11} \cdot \exp\left(\frac{-3.04 \times 10^2}{T_g}\right)$   | [8]  |
| 192 | $HCHO + OH \rightarrow H + HCOOH$            | $2 \times 10^{-13}$   | [53] |
| 193 | $HCHO + HO_2 \rightarrow H_2O_2 + HCO$       | $6.8 \times 10^{-20} \cdot T_g^{2.5} \cdot \exp\left(\frac{-5.14 \times 10^3}{T_g}\right)$  | [8]  |
| 194 | $HCHO + HO_2 \rightarrow CH_2OH + O_2$       | $\frac{3.38844156 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-8 \times 10^4}{R \cdot T_g}\right)$   | [47] |
| 195 | $HCOOH + OH \rightarrow COOH + H_2O$         | $\frac{5.93 \times 10^8 \cdot 1 \times 10^3}{N_A} \cdot \exp\left(\frac{-1.036 \times 10^3}{T_g}\right)$  | [54] |
| 196 | $CH_3O + OH \rightarrow H_2O + HCHO$         | $3 \times 10^{-11}$   | [17] |
| 197 | $CH_3O + HO_2 \rightarrow H_2O_2 + HCHO$     | $5 \times 10^{-13}$   | [17] |
| 198 | $CH_3O + HO_2 \rightarrow CH_3OH + O_2$      | $4.7 \times 10^{-11}$   | [55] |
| 199 | $CH_2OH + OH \rightarrow H_2O + HCHO$        | $4 \times 10^{-11}$   | [51] |
| 200 | $CH_2OH + H_2O \rightarrow CH_3OH + OH$      | $\frac{1.54881662 \times 10^{14}}{N_A} \cdot \exp\left(\frac{-1.1 \times 10^5}{R \cdot T_g}\right)$   | [47] |
| 201 | $CH_2OH + HO_2 \rightarrow H_2O_2 + HCHO$    | $\frac{1.3 \times 10^6 \cdot 1 \times 10^3}{N_A} \cdot \left(\frac{T_g}{2.98 \times 10^2}\right)^{5.31} \cdot \exp\left(\frac{-6.01 \times 10^4}{R \cdot T_g}\right)$ | [56] |
| 202 | $CH_2OH + HO_2 \rightarrow CH_3OH + O_2$     | $\frac{5.7 \times 10^4 \cdot 1 \times 10^3}{N_A} \cdot \left(\frac{T_g}{2.98 \times 10^2}\right)^{3.2} \cdot \exp\left(\frac{-6.8 \times 10^3}{R \cdot T_g}\right)$   | [56] |
| 203 | $CH_2OH + HO_2 \rightarrow H_2O + HCOOH$     | $\frac{3.6 \times 10^9 \cdot 1 \times 10^3}{N_A} \cdot T_g^{0.12} \cdot \exp\left(\frac{-1.9 \times 10^3}{R \cdot T_g}\right)$  | [56] |
| 204 | $CH_2OH + H_2O_2 \rightarrow CH_3OH + HO_2$  | $5 \times 10^{-15} \cdot \exp\left(\frac{-1.3 \times 10^3}{T_g}\right)$   | [51] |
| 205 | $CH_3OH + HO_2 \rightarrow CH_2OH + H_2O_2$  | $5.41 \times 10^{-11} \cdot \exp\left(\frac{-9.2 \times 10^3}{T_g}\right)$  | [57] |
| 206 | $CH_3OH + HO_2 \rightarrow CH_3O + H_2O_2$   | $2.02 \times 10^{-12} \cdot \exp\left(\frac{-1.01 \times 10^4}{T_g}\right)$   | [57] |
| 207 | $CH_3OOH + OH \rightarrow CH_3OO + H_2O$     | $1.8 \times 10^{-12} \cdot \exp\left(\frac{2.2 \times 10^2}{T_g}\right)$  | [8]  |
| 208 | $CH_3OO + OH \rightarrow CH_3OH + O_2$       | $1 \times 10^{-10}$   | [17] |
| 209 | $CH_3OO + HO_2 \rightarrow CH_3OOH + O_2$    | $0.9 \cdot 4.2 \times 10^{-13} \cdot \exp\left(\frac{7.5 \times 10^2}{T_g}\right)$  | [8]  |
| 210 | $CH_3OO + H_2O_2 \rightarrow CH_3OOH + HO_2$ | $4 \times 10^{-12} \cdot \exp\left(\frac{-5 \times 10^3}{T_g}\right)$   | [17] |
| 211 | $HCO + O \rightarrow CO + OH$                | $5 \times 10^{-11}$   | [17] |
| 212 | $HCO + O \rightarrow CO_2 + H$               | $5 \times 10^{-11}$   | [17] |
| 213 | $HCO + O_2 \rightarrow CO + HO_2$            | $4.5 \times 10^{-14} \cdot T_g^{0.68} \cdot \exp\left(\frac{2.36 \times 10^2}{T_g}\right)$  | [8]  |
| 214 | $HCHO + O \rightarrow HCO + OH$              | $6.9 \times 10^{-13} \cdot T_g^{0.57} \cdot \exp\left(\frac{-1.39 \times 10^3}{T_g}\right)$   | [8]  |
| 215 | $HCHO + O_2 \rightarrow HCO + HO_2$          | $4.05 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-1.835 \times 10^4}{T_g}\right)$  | [8]  |
| 216 | $CH_3O + O \rightarrow CH_3 + O_2$           | $1.875 \times 10^{-11}$   | [8]  |
| 217 | $CH_3O + O \rightarrow HCHO + OH$            | $6.25 \times 10^{-12}$  | [8]  |
| 218 | $CH_3O + O_2 \rightarrow HCHO + HO_2$        | $3.6 \times 10^{-14} \cdot \exp\left(\frac{-8.8 \times 10^2}{T_g}\right)$   | [8]  |
| 219 | $CH_2OH + O_2 \rightarrow HCHO + HO_2$       | $4.8 \times 10^{-8} \cdot T_g^{-1.5} + 1.2 \times 10^{-10} \cdot \exp\left(\frac{-1.88 \times 10^3}{T_g}\right)$  | [8]  |
| 220 | $CH_3OH + O \rightarrow CH_2OH + OH$         | $4.1 \times 10^{-11} \cdot \exp\left(\frac{-2.67 \times 10^3}{T_g}\right)$  | [8]  |
| 221 | $CH_3OH + O_2 \rightarrow CH_2OH + HO_2$     | $3.4 \times 10^{-11} \cdot \exp\left(\frac{-2.26 \times 10^4}{T_g}\right)$  | [51] |
| 222 | $CH_3OO + O \rightarrow CH_3O + O_2$         | $6 \times 10^{-11}$   | [17] |
| 223 | $CH_4 + HCO \rightarrow CH_3 + HCHO$         | $1.21 \times 10^{-20} \cdot T_g^{2.85} \cdot \exp\left(\frac{-1.133 \times 10^4}{T_g}\right)$   | [17] |
| 224 | $CH_3 + HCO \rightarrow CH_4 + CO$           | $2 \times 10^{-10}$   | [17] |



| #   | Reaction                                       | Rate equation  | Ref. |
|-----|--|--|------|
| 225 | $CH_3 + HCO \rightarrow CH_3CHO$               | $3 \times 10^{-11}$  | [17] |
| 226 | $CH_2 + HCO \rightarrow CH_3 + CO$             | $3 \times 10^{-11}$  | [17] |
| 227 | $CH_3 + COOH \rightarrow CH_2CO + H_2O$        | $(1.52 + 1.95 \times 10^{-4} \cdot T_g) \cdot 3.24 \times 10^{-11} \cdot T_g^{0.1024}$                   | [58] |
| 228 | $CH_3 + COOH \rightarrow CH_4 + CO_2$          | $3.24 \times 10^{-11} \cdot T_g^{0.1024}$  | [58] |
| 229 | $CH_3 + HCHO \rightarrow CH_3CH_2O$            | $\frac{3 \times 10^{11}}{N_A} \cdot \exp\left(\frac{-6.336 \times 10^3 \cdot 4.186}{R \cdot T_g}\right)$ | [48] |
| 230 | $CH_3 + HCHO \rightarrow CH_4 + HCO$           | $5.3 \times 10^{-23} \cdot T_g^{3.36} \cdot \exp\left(\frac{-2.17 \times 10^3}{T_g}\right)$              | [8]  |
| 231 | $CH_2 + HCHO \rightarrow CH_3 + HCO$           | $1 \times 10^{-14}$  | [17] |
| 232 | $CH + HCHO \rightarrow CH_2CO + H$             | $7.62 \times 10^{-10} \cdot T_g^{-0.32} \cdot \exp\left(\frac{3.86 \times 10^2}{T_g}\right)$             | [59] |
| 233 | $CH_3O + CH_4 \rightarrow CH_3 + CH_3OH$       | $2.6 \times 10^{-13} \cdot \exp\left(\frac{-4.45 \times 10^3}{T_g}\right)$                               | [17] |
| 234 | $CH_3 + CH_3O \rightarrow CH_4 + HCHO$         | $4 \times 10^{-11}$  | [17] |
| 235 | $CH_2 + CH_3O \rightarrow CH_3 + HCHO$         | $3 \times 10^{-11}$  | [17] |
| 236 | $CH_2OH + CH_4 \rightarrow CH_3 + CH_3OH$      | $3.6 \times 10^{-23} \cdot T_g^{3.1} \cdot \exp\left(\frac{-8.166 \times 10^3}{T_g}\right)$              | [51] |
| 237 | $CH_2OH + CH_3 \rightarrow CH_3CH_2OH$         | $2 \times 10^{-11}$  | [51] |
| 238 | $CH_2OH + CH_3 \rightarrow CH_4 + HCHO$        | $4 \times 10^{-12}$  | [51] |
| 239 | $CH_2 + CH_2OH \rightarrow C_2H_4 + OH$        | $4 \times 10^{-11}$  | [51] |
| 240 | $CH_2 + CH_2OH \rightarrow CH_3 + HCHO$        | $2 \times 10^{-12}$  | [51] |
| 241 | $CH_3 + CH_3OH \rightarrow CH_2OH + CH_4$      | $0.33 \cdot 5 \times 10^{-23} \cdot T_g^{3.45} \cdot \exp\left(\frac{-4.02 \times 10^3}{T_g}\right)$     | [8]  |
| 242 | $CH_3 + CH_3OH \rightarrow CH_3O + CH_4$       | $0.67 \cdot 5 \times 10^{-23} \cdot T_g^{3.45} \cdot \exp\left(\frac{-4.02 \times 10^3}{T_g}\right)$     | [8]  |
| 243 | $CH_2 + CH_3OH \rightarrow CH_2OH + CH_3$      | $5.3 \times 10^{-23} \cdot T_g^{3.2} \cdot \exp\left(\frac{-3.609 \times 10^3}{T_g}\right)$              | [51] |
| 244 | $CH_2 + CH_3OH \rightarrow CH_3 + CH_3O$       | $2.4 \times 10^{-23} \cdot T_g^{3.1} \cdot \exp\left(\frac{-3.49 \times 10^3}{T_g}\right)$               | [51] |
| 245 | $CH_3OO + CH_4 \rightarrow CH_3 + CH_3OOH$     | $3 \times 10^{-13} \cdot \exp\left(\frac{-9.3 \times 10^3}{T_g}\right)$                                  | [17] |
| 246 | $CH_3 + CH_3OO \rightarrow CH_3O + CH_3O$      | $4 \times 10^{-11}$  | [17] |
| 247 | $CH_2 + CH_3OO \rightarrow CH_3O + HCHO$       | $3 \times 10^{-11}$  | [17] |
| 248 | $CH_2 + CH_3OO \rightarrow C_2H_5 + O_2$       | $3 \times 10^{-11}$  | [17] |
| 249 | $HCO + HCO \rightarrow CO + HCHO$              | $4.265 \times 10^{-11}$  | [8]  |
| 250 | $CH_3O + HCO \rightarrow CH_3OH + CO$          | $1.5 \times 10^{-10}$  | [17] |
| 251 | $CH_2OH + HCO \rightarrow CH_3OH + CO$         | $2 \times 10^{-10}$  | [51] |
| 252 | $CH_2OH + HCO \rightarrow HCHO + HCHO$         | $3 \times 10^{-10}$  | [51] |
| 253 | $CH_3OH + HCO \rightarrow CH_2OH + HCHO$       | $1.6 \times 10^{-20} \cdot T_g^{2.9} \cdot \exp\left(\frac{-6.596 \times 10^3}{T_g}\right)$              | [51] |
| 254 | $CH_3OH + HCO \rightarrow CH_3O + HCHO$        | $1.6 \times 10^{-22} \cdot T_g^{2.9} \cdot \exp\left(\frac{-6.596 \times 10^3}{T_g}\right)$              | [51] |
| 255 | $CH_3O + HCHO \rightarrow CH_3OH + HCO$        | $1.7 \times 10^{-13} \cdot \exp\left(\frac{-1.5 \times 10^3}{T_g}\right)$                                | [17] |
| 256 | $CH_2OH + HCHO \rightarrow CH_3OH + HCO$       | $9.1 \times 10^{-21} \cdot T_g^{2.8} \cdot \exp\left(\frac{-2.95 \times 10^3}{T_g}\right)$               | [51] |
| 257 | $CH_3O + CH_3O \rightarrow CH_3OH + HCHO$      | $1 \times 10^{-10}$  | [17] |
| 258 | $CH_2OH + CH_3O \rightarrow CH_3OH + HCHO$     | $4 \times 10^{-11}$  | [51] |
| 259 | $CH_3O + CH_3OH \rightarrow CH_2OH + CH_3OH$   | $5 \times 10^{-13} \cdot \exp\left(\frac{-2.05 \times 10^3}{T_g}\right)$                                 | [51] |
| 260 | $CH_2OH + CH_2OH \rightarrow CH_3OH + HCHO$    | $8 \times 10^{-12}$  | [51] |
| 261 | $CH_2OH + CH_3OH \rightarrow CH_3O + CH_3OH$   | $1.3 \times 10^{-14} \cdot \exp\left(\frac{-6.07 \times 10^3}{T_g}\right)$                               | [51] |
| 262 | $CH_3O + CH_3OO \rightarrow CH_3OOH + HCHO$    | $5 \times 10^{-13}$  | [17] |
| 263 | $CH_3OH + CH_3OO \rightarrow CH_2OH + CH_3OOH$ | $3.421 \times 10^{-33} \cdot T_g^{6.2} \cdot \exp\left(\frac{-2.9826 \times 10^4}{R \cdot T_g}\right)$   | [60] |

| #   | Reaction                                      | Rate equation   | Ref. |
|-----|---|---|------|
| 264 | $CH_3OH + CH_3OO \rightarrow CH_3O + CH_3OOH$ | $1.318 \times 10^{-27} \cdot T_g^{4.71} \cdot \exp\left(\frac{-5.6739 \times 10^4}{R \cdot T_g}\right)$ | [60] |
| 265 | $CH_2OH + CH_3OO \rightarrow CH_3OOH + HCHO$  | $1.047 \times 10^{-24} \cdot T_g^{2.69} \cdot \exp\left(\frac{1.4344 \times 10^4}{R \cdot T_g}\right)$  | [60] |
| 266 | $CH_2OH + CH_3OO \rightarrow CH_3OH + HCOOH$  | $3.89 \times 10^{-24} \cdot T_g^{2.74} \cdot \exp\left(\frac{1.4922 \times 10^4}{R \cdot T_g}\right)$   | [60] |
| 267 | $CH_3OO + HCHO \rightarrow CH_3OOH + HCO$     | $3.3 \times 10^{-12} \cdot \exp\left(\frac{-5.87 \times 10^3}{T_g}\right)$                              | [17] |
| 268 | $C_2H_6 + OH \rightarrow C_2H_5 + H_2O$       | $1.52 \times 10^{-17} \cdot T_g^2 \cdot \exp\left(\frac{-5 \times 10^2}{T_g}\right)$                    | [8]  |
| 269 | $C_2H_6 + HO_2 \rightarrow C_2H_5 + H_2O_2$   | $1.83 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-8.48 \times 10^3}{T_g}\right)$             | [8]  |
| 270 | $C_2H_5 + OH \rightarrow C_2H_6 + O$          | $1.7 \times 10^{-40} \cdot T_g^{8.8} \cdot \exp\left(\frac{-2.5 \times 10^2}{T_g}\right)$               | [42] |
| 271 | $C_2H_5 + OH \rightarrow C_2H_4 + H_2O$       | $4 \times 10^{-11}$   | [17] |
| 272 | $C_2H_5 + H_2O \rightarrow C_2H_6 + OH$       | $5.6 \times 10^{-18} \cdot T_g^{1.44} \cdot \exp\left(\frac{-1.015 \times 10^4}{T_g}\right)$            | [17] |
| 273 | $C_2H_5 + HO_2 \rightarrow C_2H_6 + O_2$      | $5 \times 10^{-13}$   | [17] |
| 274 | $C_2H_5 + HO_2 \rightarrow C_2H_4 + H_2O_2$   | $5 \times 10^{-13}$   | [17] |
| 275 | $C_2H_5 + H_2O_2 \rightarrow C_2H_6 + HO_2$   | $1.45 \times 10^{-14} \cdot \exp\left(\frac{-4.9 \times 10^2}{T_g}\right)$                              | [17] |
| 276 | $C_2H_4 + OH \rightarrow CH_3 + HCHO$         | $\frac{1}{3} \cdot 3.4 \times 10^{-11} \cdot \exp\left(\frac{-2.99 \times 10^3}{T_g}\right)$            | [8]  |
| 277 | $C_2H_4 + OH \rightarrow CH_3CHO + H$         | $\frac{1}{3} \cdot 3.4 \times 10^{-11} \cdot \exp\left(\frac{-2.99 \times 10^3}{T_g}\right)$            | [8]  |
| 278 | $C_2H_4 + OH \rightarrow CH_2CH_2OH$          | $1.92 \times 10^{-18} \cdot T_g^{2.03} \cdot \exp\left(\frac{7.97 \times 10^3}{R \cdot T_g}\right)$     | [61] |
| 279 | $C_2H_4 + HO_2 \rightarrow C_2H_5 + O_2$      | $1 \times 10^{-13} \cdot T_g^{0.07} \cdot \exp\left(\frac{-6.58 \times 10^3}{T_g}\right)$               | [8]  |
| 280 | $C_2H_3 + OH \rightarrow CH_3 + HCO$          | $1.09 \times 10^{-5} \cdot T_g^{-1.85} \cdot \exp\left(\frac{-5.01 \times 10^2}{T_g}\right)$            | [62] |
| 281 | $C_2H_3 + OH \rightarrow CH_3CO + H$          | $9.42 \times 10^{-9} \cdot T_g^{-1.014} \cdot \exp\left(\frac{-1.95 \times 10^2}{T_g}\right)$           | [62] |
| 282 | $C_2H_3 + OH \rightarrow C_2H_2 + H_2O$       | $3.96 \times 10^{-13} \cdot T_g^{0.081} \cdot \exp\left(\frac{1.91 \times 10^2}{T_g}\right)$            | [62] |
| 283 | $C_2H_3 + OH \rightarrow CH_2CO + H_2$        | $1.26 \times 10^{-8} \cdot T_g^{-1.517} \cdot \exp\left(\frac{-3.63 \times 10^2}{T_g}\right)$           | [62] |
| 284 | $C_2H_3 + OH \rightarrow CH_4 + CO$           | $1.32 \times 10^{-8} \cdot T_g^{-1.328} \cdot \exp\left(\frac{-2.98 \times 10^2}{T_g}\right)$           | [62] |
| 285 | $C_2H_3 + H_2O \rightarrow C_2H_4 + OH$       | $8 \times 10^{-22} \cdot T_g^{2.9} \cdot \exp\left(\frac{-7.48 \times 10^3}{T_g}\right)$                | [17] |
| 286 | $C_2H_3 + H_2O_2 \rightarrow C_2H_4 + HO_2$   | $2 \times 10^{-14} \cdot \exp\left(\frac{3 \times 10^2}{T_g}\right)$                                    | [17] |
| 287 | $C_2H_2 + OH \rightarrow CH_2CO + H$          | $0.5 \cdot 1.3 \times 10^{-10} \cdot \exp\left(\frac{-6.8 \times 10^3}{T_g}\right)$                     | [8]  |
| 288 | $C_2H_2 + OH \rightarrow C_2H + H_2O$         | $0.5 \cdot 1.3 \times 10^{-10} \cdot \exp\left(\frac{-6.8 \times 10^3}{T_g}\right)$                     | [8]  |
| 289 | $C_2H_2 + HO_2 \rightarrow C_2H_3 + O_2$      | $5.18 \times 10^{-18} \cdot T_g^{1.61} \cdot \exp\left(\frac{-7.1309 \times 10^3}{T_g}\right)$          | [63] |
| 290 | $C_2H + OH \rightarrow C_2H_2 + O$            | $3 \times 10^{-11}$   | [17] |
| 291 | $C_2H + OH \rightarrow CH_2 + CO$             | $3 \times 10^{-11}$   | [17] |
| 292 | $C_2H + H_2O \rightarrow C_2H_2 + OH$         | $2.2 \times 10^{-21} \cdot T_g^{3.05} \cdot \exp\left(\frac{-3.76 \times 10^2}{T_g}\right)$             | [64] |
| 293 | $C_2H + HO_2 \rightarrow C_2H_2 + O_2$        | $3 \times 10^{-11}$   | [17] |
| 294 | $C_2H + HO_2 \rightarrow HCCO + OH$           | $3 \times 10^{-11}$   | [17] |
| 295 | $C_2H_6 + O \rightarrow C_2H_5 + OH$          | $3 \times 10^{-19} \cdot T_g^{2.8} \cdot \exp\left(\frac{-2.92 \times 10^3}{T_g}\right)$                | [8]  |
| 296 | $C_2H_6 + O_2 \rightarrow C_2H_5 + HO_2$      | $1.21 \times 10^{-18} \cdot T_g^{2.5} \cdot \exp\left(\frac{-2.474 \times 10^4}{T_g}\right)$            | [8]  |
| 297 | $C_2H_5 + O \rightarrow CH_3CHO + H$          | $8.8 \times 10^{-11}$   | [8]  |
| 298 | $C_2H_5 + O \rightarrow CH_3 + HCHO$          | $6.6 \times 10^{-11}$   | [8]  |
| 299 | $C_2H_5 + O \rightarrow C_2H_4 + OH$          | $4.4 \times 10^{-11}$   | [8]  |
| 300 | $C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$      | $1 \times 10^{-13}$   | [8]  |
| 301 | $C_2H_4 + O \rightarrow CH_3 + HCO$           | $0.6 \cdot 2.25 \times 10^{-17} \cdot T_g^{1.88} \cdot \exp\left(\frac{-9.2 \times 10^1}{T_g}\right)$   | [8]  |

| #   | Reaction  | Rate equation   | Ref. |
|-----|---|---|------|
| 302 | $C_2H_4 + O \rightarrow CH_2CO + H_2$           | $0.05 \cdot 2.25 \times 10^{-17} \cdot T_g^{1.88} \cdot \exp\left(\frac{-9.2 \times 10^1}{T_g}\right)$  | [8]  |
| 303 | $C_2H_4 + O_2 \rightarrow C_2H_3 + HO_2$        | $7 \times 10^{-11} \cdot \exp\left(\frac{-2.9 \times 10^4}{T_g}\right)$   | [17] |
| 304 | $C_2H_3 + O \rightarrow C_2H_2 + OH$            | $1.6666667 \times 10^{-11}$   | [8]  |
| 305 | $C_2H_3 + O \rightarrow CH_3 + CO$              | $1.6666667 \times 10^{-11}$   | [8]  |
| 306 | $C_2H_3 + O \rightarrow CH_2 + HCO$             | $1.6666667 \times 10^{-11}$   | [8]  |
| 307 | $C_2H_3 + O_2 \rightarrow C_2H_2 + HO_2$        | $\frac{6.6 \times 10^{21}}{N_A} \cdot T_g^{-3.3} \cdot \exp\left(\frac{-5.41 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$  | [65] |
| 308 | $C_2H_3 + O_2 \rightarrow HCHO + HCO$           | $\frac{4 \times 10^{21}}{N_A} \cdot T_g^{-3} \cdot \exp\left(\frac{-2.4 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$   | [65] |
| 309 | $C_2H_2 + O \rightarrow CH_2 + CO$              | $0.2 \cdot 1.95 \times 10^{-15} \cdot T_g^{1.4} \cdot \exp\left(\frac{-1.11 \times 10^3}{T_g}\right)$   | [8]  |
| 310 | $C_2H_2 + O \rightarrow H + HCCO$               | $0.8 \cdot 1.95 \times 10^{-15} \cdot T_g^{1.4} \cdot \exp\left(\frac{-1.11 \times 10^3}{T_g}\right)$   | [8]  |
| 311 | $C_2H_2 + O_2 \rightarrow HCO + HCO$            | $\frac{6.1 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-5.325 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$  | [66] |
| 312 | $C_2H + O \rightarrow CH + CO$                  | $9.9 \times 10^{-11}$   | [8]  |
| 313 | $C_2H + O_2 \rightarrow CO + HCO$               | $0.45 \cdot 2.7 \times 10^{-10} \cdot T_g^{-0.35}$  | [8]  |
| 314 | $C_2H + O_2 \rightarrow CH + CO_2$              | $0.1 \cdot 2.7 \times 10^{-10} \cdot T_g^{-0.35}$   | [8]  |
| 315 | $C_2H_4 + CO \rightarrow C_2H_3 + HCO$          | $2.5 \times 10^{-10} \cdot \exp\left(\frac{-4.56 \times 10^4}{T_g}\right)$  | [17] |
| 316 | $C_2H_2 + CO \rightarrow C_2H + HCO$            | $8 \times 10^{-10} \cdot \exp\left(\frac{-5.37 \times 10^4}{T_g}\right)$  | [17] |
| 317 | $C_2H_6 + HCO \rightarrow C_2H_5 + HCHO$        | $7.8 \times 10^{-20} \cdot T_g^{2.72} \cdot \exp\left(\frac{-9.176 \times 10^3}{T_g}\right)$  | [17] |
| 318 | $C_2H_6 + CH_3O \rightarrow C_2H_5 + CH_3OH$    | $4 \times 10^{-13} \cdot \exp\left(\frac{-3.57 \times 10^3}{T_g}\right)$  | [17] |
| 319 | $C_2H_6 + CH_2OH \rightarrow C_2H_5 + CH_3OH$   | $3.3 \times 10^{-22} \cdot T_g^{2.95} \cdot \exp\left(\frac{-7.033 \times 10^3}{T_g}\right)$  | [51] |
| 320 | $C_2H_6 + CH_3OO \rightarrow C_2H_5 + CH_3OOH$  | $4.9 \times 10^{-13} \cdot \exp\left(\frac{-7.52 \times 10^3}{T_g}\right)$  | [17] |
| 321 | $C_2H_5 + HCO \rightarrow C_2H_6 + CO$          | $2 \times 10^{-10}$   | [17] |
| 322 | $C_2H_5 + HCHO \rightarrow C_2H_6 + HCO$        | $9.2 \times 10^{-21} \cdot T_g^{2.81} \cdot \exp\left(\frac{-2.95 \times 10^3}{T_g}\right)$   | [17] |
| 323 | $C_2H_5 + CH_3O \rightarrow C_2H_6 + HCHO$      | $4 \times 10^{-11}$   | [17] |
| 324 | $C_2H_5 + CH_2OH \rightarrow C_2H_4 + CH_3OH$   | $4 \times 10^{-12}$   | [51] |
| 325 | $C_2H_5 + CH_2OH \rightarrow C_2H_6 + HCHO$     | $4 \times 10^{-12}$   | [51] |
| 326 | $C_2H_5 + CH_3OH \rightarrow C_2H_6 + CH_2OH$   | $5.3 \times 10^{-23} \cdot T_g^{3.2} \cdot \exp\left(\frac{-4.61 \times 10^3}{T_g}\right)$  | [51] |
| 327 | $C_2H_5 + CH_3OH \rightarrow C_2H_6 + CH_3O$    | $2.4 \times 10^{-23} \cdot T_g^{3.1} \cdot \exp\left(\frac{-4.5 \times 10^3}{T_g}\right)$   | [51] |
| 328 | $C_2H_5 + CH_3OO \rightarrow CH_3CH_2O + CH_3O$ | $4 \times 10^{-11}$   | [17] |
| 329 | $C_2H_4 + COOH \rightarrow C_2H_5 + CO_2$       | $1 \times 10^{-14}$   | [44] |
| 330 | $C_2H_4 + CH_2OH \rightarrow C_2H_5 + HCHO$     | $\frac{8 \times 10^{-14} \cdot \exp\left(\frac{-3.5 \times 10^3}{T_g}\right) \cdot \exp\left(\frac{-2 \times 10^3}{T_g}\right)}{1.0 + \exp\left(\frac{-2 \times 10^3}{T_g}\right)}$ | [51] |
| 331 | $C_2H_3 + HCO \rightarrow C_2H_4 + CO$          | $1.5 \times 10^{-10}$   | [17] |
| 332 | $C_2H_3 + HCHO \rightarrow C_2H_4 + HCO$        | $9 \times 10^{-21} \cdot T_g^{2.81} \cdot \exp\left(\frac{-2.95 \times 10^3}{T_g}\right)$   | [17] |
| 333 | $C_2H_3 + CH_3O \rightarrow C_2H_4 + HCHO$      | $4 \times 10^{-11}$   | [17] |
| 334 | $C_2H_3 + CH_2OH \rightarrow C_2H_4 + HCHO$     | $5 \times 10^{-11}$   | [51] |
| 335 | $C_2H_3 + CH_3OH \rightarrow C_2H_4 + CH_2OH$   | $5.3 \times 10^{-23} \cdot T_g^{3.2} \cdot \exp\left(\frac{-3.609 \times 10^3}{T_g}\right)$   | [51] |
| 336 | $C_2H_3 + CH_3OH \rightarrow C_2H_4 + CH_3O$    | $2.4 \times 10^{-23} \cdot T_g^{3.1} \cdot \exp\left(\frac{-3.49 \times 10^3}{T_g}\right)$  | [51] |
| 337 | $C_2H_2 + COOH \rightarrow C_2H_3 + CO_2$       | $3 \times 10^{-14}$   | [44] |
| 338 | $C_2H_2 + CH_2OH \rightarrow C_2H_3 + HCHO$     | $1.2 \times 10^{-12} \cdot \exp\left(\frac{-4.531 \times 10^3}{T_g}\right)$   | [51] |
| 339 | $C_2H + HCO \rightarrow C_2H_2 + CO$            | $1 \times 10^{-10}$   | [17] |

| #   | Reaction                                      | Rate equation  | Ref.     |
|-----|---|--|----------|
| 340 | $C_2H + CH_3O \rightarrow C_2H_2 + HCHO$      | $4 \times 10^{-11}$  | [17]     |
| 341 | $C_2H + CH_2OH \rightarrow C_2H_2 + HCHO$     | $6 \times 10^{-11}$  | [51]     |
| 342 | $C_2H + CH_3OH \rightarrow C_2H_2 + CH_2OH$   | $1 \times 10^{-11}$  | [51]     |
| 343 | $C_2H + CH_3OH \rightarrow C_2H_2 + CH_3O$    | $2 \times 10^{-12}$  | [51]     |
| 344 | $C_2H + CH_3OO \rightarrow CH_3O + HCCO$      | $4 \times 10^{-11}$  | [17]     |
| 345 | $H + HCCO \rightarrow CH_2 + CO$              | $9.92 \times 10^{-13} \cdot T_g^{0.76} \cdot \exp\left(\frac{4.38 \times 10^2}{T_g}\right)$  | [67]     |
| 346 | $CH_2CO + H \rightarrow CH_3 + CO$            | $\frac{1.11 \times 10^7}{N_A} \cdot T_g^2 \cdot \exp\left(\frac{-2 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$   | [68]     |
| 347 | $CH_2CO + H \rightarrow H_2 + HCCO$           | $\frac{1.8 \times 10^{14}}{N_A} \cdot \exp\left(\frac{-8.6 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$   | [68]     |
| 348 | $CH_2CO + H \rightarrow CH_3CO$               | $\frac{1.63 \times 10^9}{N_A} \cdot T_g^{1.3766} \cdot \exp\left(\frac{-1.664 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$  | [69]     |
| 349 | $CH_3CO + H \rightarrow CH_3 + HCO$           | $\frac{0.65 \cdot 2 \times 10^{13}}{N_A}$  | [70, 71] |
| 350 | $CH_3CO + H \rightarrow CH_2CO + H_2$         | $\frac{0.35 \cdot 2 \times 10^{13}}{N_A}$  | [70, 71] |
| 351 | $CH_3CO + H \rightarrow CH_3CHO$              | $6.02 \times 10^{-11} \cdot T_g^{0.16}$  | [62]     |
| 352 | $CH_3CO + H_2 \rightarrow CH_3CHO + H$        | $6.8 \times 10^{-18} \cdot T_g^{1.82} \cdot \exp\left(\frac{-8.862 \times 10^3}{T_g}\right)$   | [17]     |
| 353 | $CH_3CHO + H \rightarrow CH_3CO + H_2$        | $2.18 \times 10^{-19} \cdot T_g^{2.58} \cdot \exp\left(\frac{-6.14 \times 10^2}{T_g}\right)$   | [72]     |
| 354 | $CH_3CHO + H \rightarrow CH_3CH_2O$           | $7.66 \times 10^{-17} \cdot T_g^{1.71} \cdot \exp\left(\frac{-3.57 \times 10^3}{T_g}\right)$   | [72]     |
| 355 | $CH_3CHO + H \rightarrow CH_3CHOH$            | $2.89 \times 10^{-18} \cdot T_g^{2.2} \cdot \exp\left(\frac{-3.78 \times 10^3}{T_g}\right)$  | [72]     |
| 356 | $CH_3CH_2O + H \rightarrow CH_2OH + CH_3$     | $2.26 \times 10^{-12} \cdot T_g^{0.701} \cdot \exp\left(\frac{-1.74 \times 10^2}{T_g}\right)$  | [73]     |
| 357 | $CH_3CH_2O + H \rightarrow CH_3CH_2OH$        | $5.11 \times 10^{-13} \cdot T_g^{0.894} \cdot \exp\left(\frac{-6.5}{T_g}\right)$   | [73]     |
| 358 | $CH_3CH_2O + H \rightarrow C_2H_5 + OH$       | $9.04 \times 10^{-16} \cdot T_g^{1.27} \cdot \exp\left(\frac{-1.57 \times 10^2}{T_g}\right)$   | [73]     |
| 359 | $CH_3CH_2O + H \rightarrow CH_3CHOH + H$      | $1.33 \times 10^{-22} \cdot T_g^{3.1} \cdot \exp\left(\frac{-1.42 \times 10^2}{T_g}\right)$  | [73]     |
| 360 | $CH_3CH_2O + H \rightarrow C_2H_4 + H_2O$     | $9.95 \times 10^{-10} \cdot T_g^{-0.813} \cdot \exp\left(\frac{-3.59 \times 10^2}{T_g}\right)$   | [73]     |
| 361 | $CH_3CH_2O + H \rightarrow CH_3CHO + H_2$     | $1.25 \times 10^{-20} \cdot T_g^{1.78} \cdot \exp\left(\frac{-4.07 \times 10^1}{T_g}\right)$<br>$+ 1.24 \times 10^{-14} \cdot T_g^{1.15} \cdot \exp\left(\frac{-3.39 \times 10^2}{T_g}\right)$ | [73]     |
| 362 | $CH_3CH_2O + H \rightarrow CH_4 + HCHO$       | $1.32 \times 10^{-21} \cdot T_g^{2.21} \cdot \exp\left(\frac{9.05 \times 10^1}{T_g}\right)$  | [73]     |
| 363 | $CH_3CHOH + H \rightarrow CH_3CH_2OH$         | $5.99 \times 10^{-11} \cdot T_g^{0.06} \cdot \exp\left(\frac{-2.2 \times 10^2}{T_g}\right)$  | [73]     |
| 364 | $CH_3CHOH + H \rightarrow CH_2OH + CH_3$      | $1.44 \times 10^{-7} \cdot T_g^{-0.891} \cdot \exp\left(\frac{-1.461 \times 10^3}{T_g}\right)$   | [73]     |
| 365 | $CH_3CHOH + H \rightarrow C_2H_5 + OH$        | $4.02 \times 10^{-9} \cdot T_g^{-0.83} \cdot \exp\left(\frac{-2.414 \times 10^3}{T_g}\right)$  | [73]     |
| 366 | $CH_3CHOH + H \rightarrow CH_3CH_2O + H$      | $4.95 \times 10^{-23} \cdot T_g^{2.94} \cdot \exp\left(\frac{-4.266 \times 10^3}{T_g}\right)$  | [73]     |
| 367 | $CH_3CHOH + H \rightarrow C_2H_4 + H_2O$      | $7.81 \times 10^{-3} \cdot T_g^{-3.02} \cdot \exp\left(\frac{-1.432 \times 10^3}{T_g}\right)$  | [73]     |
| 368 | $CH_3CHOH + H \rightarrow CH_3CHO + H_2$      | $7.42 \times 10^{-21} \cdot T_g^{1.62} \cdot \exp\left(\frac{5.4}{T_g}\right)$<br>$+ 2.26 \times 10^{-15} \cdot T_g^{1.29} \cdot \exp\left(\frac{-1.421 \times 10^3}{T_g}\right)$              | [73]     |
| 369 | $CH_3CHOH + H \rightarrow CH_4 + HCHO$        | $5.56 \times 10^{-22} \cdot T_g^{2.1} \cdot \exp\left(\frac{-1.07 \times 10^2}{T_g}\right)$  | [73]     |
| 370 | $CH_3CH_2OH + H \rightarrow C_2H_5 + H_2O$    | $\frac{5.9 \times 10^{11}}{N_A} \cdot \exp\left(\frac{-3.45 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$  | [74]     |
| 371 | $CH_3CH_2OH + H \rightarrow CH_3CHOH + H_2$   | $1.46 \times 10^{-19} \cdot T_g^{2.68} \cdot \exp\left(\frac{-1.467 \times 10^3}{T_g}\right)$  | [75]     |
| 372 | $CH_3CH_2OH + H \rightarrow CH_2CH_2OH + H_2$ | $8.82 \times 10^{-20} \cdot T_g^{2.81} \cdot \exp\left(\frac{-3.772 \times 10^3}{T_g}\right)$  | [75]     |
| 373 | $CH_3CH_2OH + H \rightarrow CH_3CH_2O + H_2$  | $1.57 \times 10^{-21} \cdot T_g^{3.14} \cdot \exp\left(\frac{-4.379 \times 10^3}{T_g}\right)$  | [75]     |
| 374 | $HCCO + OH \rightarrow CH_2CO + O$            | $2.1 \times 10^{-18} \cdot T_g^{1.99} \cdot \exp\left(\frac{-1.128 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$   | [76]     |
| 375 | $CH_2CO + OH \rightarrow CH_2OH + CO$         | $0.6 \cdot 2.8 \times 10^{-12} \cdot \exp\left(\frac{5.1 \times 10^2}{T_g}\right)$   | [8]      |

| #   | Reaction  | Rate equation  | Ref.    |
|-----|---|--|---------|
| 376 | $CH_2CO + OH \rightarrow H_2O + HCCO$             | $0.01 \cdot 2.8 \times 10^{-12} \cdot \exp\left(\frac{5.1 \times 10^2}{T_g}\right)$  | [8]     |
| 377 | $CH_2CO + OH \rightarrow HCHO + HCO$              | $0.02 \cdot 2.8 \times 10^{-12} \cdot \exp\left(\frac{5.1 \times 10^2}{T_g}\right)$  | [8]     |
| 378 | $CH_2CO + OH \rightarrow CH_3 + CO_2$             | $0.37 \cdot 2.8 \times 10^{-12} \cdot \exp\left(\frac{5.1 \times 10^2}{T_g}\right)$  | [8]     |
| 379 | $CH_3CO + OH \rightarrow CH_2CO + H_2O$           | $2 \times 10^{-11}$  | [17]    |
| 380 | $CH_3CO + H_2O_2 \rightarrow CH_3CHO + HO_2$      | $3 \times 10^{-13} \cdot \exp\left(\frac{-4.14 \times 10^3}{T_g}\right)$   | [17]    |
| 381 | $CH_3CHO + OH \rightarrow CH_3CO + H_2O$          | $0.93 \cdot 4.8 \times 10^{-16} \cdot T_g^{1.35} \cdot \exp\left(\frac{7.92 \times 10^2}{T_g}\right)$                          | [8]     |
| 382 | $CH_3CHO + OH \rightarrow CH_3 + HCOOH$           | $0.03 \cdot 4.8 \times 10^{-16} \cdot T_g^{1.35} \cdot \exp\left(\frac{7.92 \times 10^2}{T_g}\right)$                          | [8, 77] |
| 383 | $CH_3CHO + OH \rightarrow CH_3COOH + H$           | $0.02 \cdot 4.8 \times 10^{-16} \cdot T_g^{1.35} \cdot \exp\left(\frac{7.92 \times 10^2}{T_g}\right)$                          | [8, 77] |
| 384 | $CH_3CHO + HO_2 \rightarrow CH_3CO + H_2O_2$      | $6.8 \times 10^{-20} \cdot T_g^{2.5} \cdot \exp\left(\frac{-5.135 \times 10^3}{T_g}\right)$                                    | [8]     |
| 385 | $CH_3CH_2OH + OH \rightarrow CH_2CH_2OH + H_2O$   | $\frac{1.74 \times 10^{11}}{N_A} \cdot T_g^{0.27} \cdot \exp\left(\frac{-6 \times 10^2 \cdot 4.184}{R \cdot T_g}\right)$       | [78]    |
| 386 | $CH_3CH_2OH + OH \rightarrow CH_3CHOH + H_2O$     | $\frac{4.64 \times 10^{11}}{N_A} \cdot T_g^{0.15}$   | [78]    |
| 387 | $CH_3CH_2OH + OH \rightarrow CH_3CH_2O + H_2O$    | $\frac{7.46 \times 10^{11}}{N_A} \cdot T_g^{0.3} \cdot \exp\left(\frac{-1.634 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$    | [78]    |
| 388 | $CH_3CH_2OH + HO_2 \rightarrow CH_3CHOH + H_2O_2$ | $\frac{5.544 \times 10^{18}}{N_A} \cdot T_g^{-1.808} \cdot \exp\left(\frac{-8.29197 \times 10^3}{T_g}\right)$                  | [79]    |
| 389 | $HCCO + O \rightarrow CH + CO_2$                  | $4.9 \times 10^{-11} \cdot \exp\left(\frac{-5.6 \times 10^2}{T_g}\right)$  | [8]     |
| 390 | $CH_2CO + O \rightarrow HCCO + OH$                | $3.11 \times 10^{-10} \cdot \exp\left(\frac{-1.669 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$                               | [76]    |
| 391 | $CH_2CO + O \rightarrow CO + HCHO$                | $0.2 \cdot 3 \times 10^{-12} \cdot \exp\left(\frac{-6.8 \times 10^2}{T_g}\right)$  | [8]     |
| 392 | $CH_2CO + O \rightarrow HCO + HCO$                | $0.1 \cdot 3 \times 10^{-12} \cdot \exp\left(\frac{-6.8 \times 10^2}{T_g}\right)$  | [8]     |
| 393 | $CH_2CO + O \rightarrow CH_2 + CO_2$              | $0.6 \cdot 3 \times 10^{-12} \cdot \exp\left(\frac{-6.8 \times 10^2}{T_g}\right)$  | [8]     |
| 394 | $CH_3CO + O \rightarrow CH_2CO + OH$              | $8.75 \times 10^{-11}$   | [8]     |
| 395 | $CH_3CO + O \rightarrow CH_3 + CO_2$              | $2.625 \times 10^{-10}$  | [8]     |
| 396 | $CH_3CHO + O \rightarrow CH_3CO + OH$             | $\frac{5 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-7.5 \times 10^3}{R \cdot T_g}\right)$                                     | [71]    |
| 397 | $CH_3CHO + O_2 \rightarrow CH_3CO + HO_2$         | $2 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-1.89 \times 10^4}{T_g}\right)$                                       | [8]     |
| 398 | $CH_3CH_2O + O_2 \rightarrow CH_3CHO + HO_2$      | $3.8 \times 10^{-14} \cdot \exp\left(\frac{-4.4 \times 10^2}{T_g}\right)$  | [8]     |
| 399 | $CH_3CHOH + O \rightarrow CH_3 + HCOOH$           | $3.9 \times 10^{-10} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{0.18} \cdot \exp\left(\frac{-0.49}{T_g}\right)$             | [80]    |
| 400 | $CH_3CHOH + O \rightarrow CH_3CHO + OH$           | $4.8 \times 10^{-11} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{0.19} \cdot \exp\left(\frac{-0.39}{T_g}\right)$             | [80]    |
| 401 | $CH_3CHOH + O \rightarrow CH_3COOH + H$           | $2.2 \times 10^{-10} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{0.16} \cdot \exp\left(\frac{-0.59}{T_g}\right)$             | [80]    |
| 402 | $CH_3CHOH + O_2 \rightarrow CH_3CHO + HO_2$       | $\frac{5.28 \times 10^{17}}{N_A} \cdot T_g^{-1.638} \cdot \exp\left(\frac{-0.839 \cdot 4.184 \times 10^3}{R \cdot T_g}\right)$ | [81]    |
| 403 | $CH_2CH_2OH + O \rightarrow CH_2OH + HCHO$        | $4.6 \times 10^{-10} \cdot \left(\frac{T_g}{3 \times 10^2}\right)^{0.17} \cdot \exp\left(\frac{-0.51}{T_g}\right)$             | [80]    |
| 404 | $CH_3CH_2OH + O \rightarrow CH_3CHOH + OH$        | $0.99 \cdot 1 \times 10^{-18} \cdot T_g^{2.5} \cdot \exp\left(\frac{-9.3 \times 10^2}{T_g}\right)$                             | [8]     |
| 405 | $CH_3CH_2OH + O \rightarrow CH_2CH_2OH + OH$      | $0.005 \cdot 1 \times 10^{-18} \cdot T_g^{2.5} \cdot \exp\left(\frac{-9.3 \times 10^2}{T_g}\right)$                            | [8]     |
| 406 | $CH_3CH_2OH + O \rightarrow CH_3CH_2O + OH$       | $0.005 \cdot 1 \times 10^{-18} \cdot T_g^{2.5} \cdot \exp\left(\frac{-9.3 \times 10^2}{T_g}\right)$                            | [8]     |
| 407 | $CH_3CH_2OH + O_2 \rightarrow CH_3CHOH + HO_2$    | $4 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-2.217 \times 10^4}{T_g}\right)$                                      | [8]     |
| 408 | $CH_3CH_2OH + O_2 \rightarrow CH_2CH_2OH + HO_2$  | $6 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-2.403 \times 10^4}{T_g}\right)$                                      | [8]     |
| 409 | $CH_3CH_2OH + O_2 \rightarrow CH_3CH_2O + HO_2$   | $2 \times 10^{-19} \cdot T_g^{2.5} \cdot \exp\left(\frac{-2.653 \times 10^4}{T_g}\right)$                                      | [8]     |
| 410 | $CH_2CO + CH_3 \rightarrow C_2H_5 + CO$           | $\frac{1.24 \times 10^5}{N_A} \cdot T_g^{2.29} \cdot \exp\left(\frac{-1.0642 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$     | [82]    |
| 411 | $CH_2CO + CH_3 \rightarrow CH_4 + HCCO$           | $\frac{1.55 \times 10^2}{N_A} \cdot T_g^{3.38} \cdot \exp\left(\frac{-1.0512 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$     | [82]    |
| 412 | $CH_2 + CH_2CO \rightarrow C_2H_4 + CO$           | $\frac{1 \times 10^{12}}{N_A}$   | [83]    |
| 413 | $CH_2 + CH_2CO \rightarrow CH_3 + HCCO$           | $\frac{3.6 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-1.1 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$                       | [68]    |

| #   | Reaction  | Rate equation   | Ref.                 |
|-----|---|---|----------------------|
| 414 | $CH_3CO + CH_4 \rightarrow CH_3 + CH_3CHO$        | $3.6 \times 10^{-21} \cdot T_g^{2.88} \cdot \exp\left(\frac{-1.08 \times 10^4}{T_g}\right)$   | [17]                 |
| 415 | $CH_3 + CH_3CO \rightarrow CH_2CO + CH_4$         | $\frac{6.1 \times 10^9 \cdot 1 \times 10^3}{N_A}$   | [84]                 |
| 416 | $CH_2 + CH_3CO \rightarrow CH_2CO + CH_3$         | $3 \times 10^{-11}$   | [17]                 |
| 417 | $CH_3 + CH_3CHO \rightarrow CH_3CO + CH_4$        | $0.993 \cdot 5.8 \times 10^{-32} \cdot T_g^{6.21} \cdot \exp\left(\frac{-8.2 \times 10^2}{T_g}\right)$  | [8]                  |
| 418 | $CH_3 + CH_3CH_2OH \rightarrow CH_3CHOH + CH_4$   | $\frac{2.476 \times 10^1}{N_A} \cdot T_g^{3.368} \cdot \exp\left(\frac{-3.95579 \times 10^3}{T_g}\right)$   | [79]                 |
| 419 | $CH_3 + CH_3CH_2OH \rightarrow CH_2CH_2OH + CH_4$ | $\frac{1.861 \times 10^2}{N_A} \cdot T_g^{3.45} \cdot \exp\left(\frac{-5.54285 \times 10^3}{T_g}\right)$  | [79]                 |
| 420 | $CH_3 + CH_3CH_2OH \rightarrow CH_3CH_2O + CH_4$  | $\frac{0.09533}{N_A} \cdot T_g^{4.159} \cdot \exp\left(\frac{-4.119 \times 10^3}{T_g}\right)$   | [79]                 |
| 421 | $C_2H_6 + CH_3CO \rightarrow C_2H_5 + CH_3CHO$    | $3 \times 10^{-20} \cdot T_g^{2.75} \cdot \exp\left(\frac{-8.82 \times 10^3}{T_g}\right)$   | [17]                 |
| 422 | $C_2H_5 + CH_3CHO \rightarrow C_2H_6 + CH_3CO$    | $\frac{1.25892541 \times 10^{12}}{N_A} \cdot \exp\left(\frac{-8.5 \cdot 4.184 \times 10^3}{R \cdot T_g}\right)$   | [85]                 |
| 423 | $CH_3CO + HCO \rightarrow CH_3CHO + CO$           | $1.5 \times 10^{-11}$   | [17]                 |
| 424 | $CH_3CO + HCHO \rightarrow CH_3CHO + HCO$         | $3 \times 10^{-13} \cdot \exp\left(\frac{-6.5 \times 10^3}{T_g}\right)$   | [17]                 |
| 425 | $CH_3CO + CH_3O \rightarrow CH_2CO + CH_3OH$      | $1 \times 10^{-11}$   | [17]                 |
| 426 | $CH_3CO + CH_3O \rightarrow CH_3CHO + HCHO$       | $1 \times 10^{-11}$   | [17]                 |
| 427 | $CH_3CO + CH_3OH \rightarrow CH_2OH + CH_3CHO$    | $8.06 \times 10^{-21} \cdot T_g^{2.99} \cdot \exp\left(\frac{-6.21 \times 10^3}{T_g}\right)$  | [51]                 |
| 428 | $CH_3CHO + CH_3O \rightarrow CH_3CO + CH_3OH$     | $\frac{1.69 \times 10^5}{N_A} \cdot T_g^{2.04} \cdot \exp\left(\frac{-2.353 \times 10^3 \cdot 4.184}{R \cdot T_g}\right) + \frac{9.62 \times 10^3}{N_A} \cdot T_g^{2.5} \cdot \exp\left(\frac{-1.59 \times 10^2 \cdot 4.184}{R \cdot T_g}\right)$   | [86]                 |
| 429 | $CH_3CHO + CH_3OO \rightarrow CH_3CO + CH_3OOH$   | $\frac{0.322}{N_A} \cdot T_g^{3.94} \cdot \exp\left(\frac{-9.503 \times 10^3 \cdot 4.184}{R \cdot T_g}\right) + \frac{4.99 \times 10^{-6}}{N_A} \cdot T_g^{4.98} \cdot \exp\left(\frac{-5.2682 \times 10^3 \cdot 4.184}{R \cdot T_g}\right)$  | [86]                 |
| 430 | $CH_3CO + CH_3CO \rightarrow CH_2CO + CH_3CHO$    | $\frac{9 \times 10^9 \cdot 1 \times 10^3}{N_A}$   | [84]                 |
| 431 | $COOH \rightarrow CO + OH$                        | $k_0 = \frac{10^{2.5137 \times 10^1}}{N_A} \cdot T_g^{-2.396} \cdot \exp\left(\frac{-1.8862 \times 10^4}{T_g}\right)$<br>$k_\infty = 10^{1.4074 \times 10^1} \cdot T_g^{0.132} \cdot \exp\left(\frac{-1.8349 \times 10^4}{T_g}\right)$<br>$F_c = 0.729 \cdot \exp\left(\frac{-5.13 \times 10^2}{T_g}\right) + \exp\left(\frac{-T_g}{5.4 \times 10^2}\right)$  | [87] <sup>a</sup>    |
| 432 | $COOH \rightarrow CO_2 + H$                       | $k_0 = \frac{10^{2.6775 \times 10^1}}{N_A} \cdot T_g^{-3.148} \cdot \exp\left(\frac{-1.8629 \times 10^4}{T_g}\right)$<br>$k_\infty = 10^{1.1915 \times 10^1} \cdot T_g^{0.413} \cdot \exp\left(\frac{-1.7783 \times 10^4}{T_g}\right)$<br>$F_c = 1.049 \cdot \exp\left(\frac{-2.407 \times 10^3}{T_g}\right) + \exp\left(\frac{-T_g}{8.23 \times 10^2}\right)$  | [87] <sup>a</sup>    |
| 433 | $HCHO \rightarrow H + HCO$                        | $8.09 \times 10^{-9} \cdot \exp\left(\frac{-3.805 \times 10^4}{T_g}\right) \cdot n_M$   | [8]                  |
| 434 | $CH_2OH \rightarrow H + HCHO$                     | $k_0 = \frac{6.01 \times 10^{33}}{N_A} \cdot T_g^{-5.39} \cdot \exp\left(\frac{-3.62 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$<br>$k_\infty = 2.8 \times 10^{14} \cdot T_g^{-0.73} \cdot \exp\left(\frac{-3.282 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$<br>$F_c = (1 - 0.96) \cdot \exp\left(\frac{-T_g}{6.76 \times 10^1}\right) + 0.96 \cdot \exp\left(\frac{-T_g}{1.855 \times 10^3}\right) + \exp\left(\frac{-7.543 \times 10^3}{T_g}\right)$ | [88] <sup>a</sup>    |
| 435 | $CH_3OH \rightarrow CH_3 + OH$                    | $0.8 \cdot k$<br>$k_0 = 1.1 \times 10^{-7} \cdot \exp\left(\frac{-3.308 \times 10^4}{T_g}\right)$<br>$k_\infty = 2.5 \times 10^{19} \cdot T_g^{-0.94} \cdot \exp\left(\frac{-4.703 \times 10^4}{T_g}\right)$<br>$F_c = 0.18 \cdot \exp\left(\frac{-T_g}{2 \times 10^2}\right) + 0.82 \cdot \exp\left(\frac{-T_g}{1.438 \times 10^3}\right)$   | [8, 89] <sup>a</sup> |

| #   | Reaction                               | Rate equation   | Ref.                 |
|-----|--|---|----------------------|
| 436 | $CH_3OH \rightarrow CH_2 + H_2O$       | $0.15 \cdot k$<br>$k_0 = 1.1 \times 10^{-7} \cdot \exp\left(\frac{-3.308 \times 10^4}{T_g}\right)$<br>$k_\infty = 2.5 \times 10^{19} \cdot T_g^{-0.94} \cdot \exp\left(\frac{-4.703 \times 10^4}{T_g}\right)$<br>$F_c = 0.18 \cdot \exp\left(\frac{-T_g}{2 \times 10^2}\right)$<br>$+ 0.82 \cdot \exp\left(\frac{-T_g}{1.438 \times 10^3}\right)$   | [8, 89] <sup>a</sup> |
| 437 | $CH_3OH \rightarrow CH_2OH + H$        | $0.05 \cdot k$<br>$k_0 = 1.1 \times 10^{-7} \cdot \exp\left(\frac{-3.308 \times 10^4}{T_g}\right)$<br>$k_\infty = 2.5 \times 10^{19} \cdot T_g^{-0.94} \cdot \exp\left(\frac{-4.703 \times 10^4}{T_g}\right)$<br>$F_c = 0.18 \cdot \exp\left(\frac{-T_g}{2 \times 10^2}\right)$<br>$+ 0.82 \cdot \exp\left(\frac{-T_g}{1.438 \times 10^3}\right)$   | [8, 89] <sup>a</sup> |
| 438 | $CH_3OOH \rightarrow CH_3O + OH$       | $6 \times 10^{14} \cdot \exp\left(\frac{-2.13 \times 10^4}{T_g}\right)$   | [8]                  |
| 439 | $HCCO \rightarrow CH + CO$             | $\frac{6 \times 10^{15}}{N_A} \cdot \exp\left(\frac{-2.96 \times 10^4}{T_g}\right) \cdot n_M$   | [90]                 |
| 440 | $CH_2CO \rightarrow CH_2 + CO$         | $\frac{2.3 \times 10^{15}}{N_A} \cdot \exp\left(\frac{-2.899 \times 10^4}{T_g}\right) \cdot n_M$  | [83]                 |
| 441 | $CH_3CO \rightarrow CH_3 + CO$         | $k_0 = 1 \times 10^{-8} \cdot \exp\left(\frac{-7.08 \times 10^3}{T_g}\right)$<br>$k_\infty = 2 \times 10^{13} \cdot \exp\left(\frac{-8.63 \times 10^3}{T_g}\right)$<br>$F_c = 0.5$  | [8] <sup>a</sup>     |
| 442 | $CH_3CO \rightarrow CH_2CO + H$        | $1.36 \times 10^8 \cdot T_g^{1.9433} \cdot \exp\left(\frac{-4.6005 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$  | [69]                 |
| 443 | $CH_3CHO \rightarrow CH_3CO + H$       | $5 \times 10^{14} \cdot \exp\left(\frac{-8.79 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$   | [91]                 |
| 444 | $CH_3CHO \rightarrow CH_3 + HCO$       | $2.1 \times 10^{16} \cdot \exp\left(\frac{-4.1135 \times 10^4}{T_g}\right)$   | [8]                  |
| 445 | $CH_3COOH \rightarrow CH_3 + COOH$     | $10^{5.7 \times 10^1} \cdot T_g^{-1.204 \times 10^1} \cdot \exp\left(\frac{-1.1313 \times 10^5 \cdot 4.182}{R \cdot T_g}\right)$  | [92]                 |
| 446 | $CH_3CH_2O \rightarrow CH_3CHO + H$    | $\frac{5.43 \times 10^{15}}{N_A} \cdot T_g^{-0.69} \cdot \exp\left(\frac{-2.223 \times 10^4 \cdot 4.184}{R \cdot T_g}\right)$   | [48]                 |
| 447 | $CH_3CH_2O \rightarrow CH_3 + HCHO$    | $k_0 = \frac{4.7 \times 10^{25}}{N_A} \cdot T_g^{-3} \cdot \exp\left(\frac{-8.32 \times 10^3}{T_g}\right)$<br>$k_\infty = 6.31 \times 10^{10} \cdot T_g^{0.93} \cdot \exp\left(\frac{-8.605 \times 10^3}{T_g}\right)$<br>$F_c = (1 - 0.426) \cdot \exp\left(\frac{-T_g}{0.3}\right)$<br>$+ 0.426 \cdot \exp\left(\frac{-T_g}{2.278 \times 10^3}\right)$<br>$+ \exp\left(\frac{-1 \times 10^5}{T_g}\right)$                    | [93] <sup>a</sup>    |
| 448 | $CH_3CHOH \rightarrow CH_3CHO + H$     | $k_0 = \frac{1.77 \times 10^{16}}{N_A} \cdot \exp\left(\frac{-1.0458 \times 10^4}{T_g}\right)$<br>$k_\infty = 6.17 \times 10^9 \cdot T_g^{1.31} \cdot \exp\left(\frac{-1.6998 \times 10^4}{T_g}\right)$<br>$F_c = (1 - 0.187) \cdot \exp\left(\frac{-T_g}{6.52 \times 10^1}\right)$<br>$+ 0.187 \cdot \exp\left(\frac{-T_g}{2.568 \times 10^3}\right)$<br>$+ \exp\left(\frac{-4.1226 \times 10^4}{T_g}\right)$                | [93] <sup>a</sup>    |
| 449 | $CH_3CHOH \rightarrow CH_3 + HCHO$     | $k_0 = \frac{5.86 \times 10^{15}}{N_A} \cdot \exp\left(\frac{-1.0735 \times 10^4}{T_g}\right)$<br>$k_\infty = 2.22 \times 10^9 \cdot T_g^{1.18} \cdot \exp\left(\frac{-1.7103 \times 10^4}{T_g}\right)$<br>$F_c = (1 - 0.124) \cdot \exp\left(\frac{-T_g}{1}\right)$<br>$+ 0.124 \cdot \exp\left(\frac{-T_g}{1.729 \times 10^3}\right)$<br>$+ \exp\left(\frac{-5 \times 10^4}{T_g}\right)$                                    | [93] <sup>a</sup>    |
| 450 | $CH_3CH_2OH \rightarrow CH_2OH + CH_3$ | $k_0 = \frac{2.88 \times 10^{85}}{N_A} \cdot T_g^{-1.89 \times 10^1} \cdot \exp\left(\frac{-5.5317 \times 10^4}{T_g}\right)$<br>$k_\infty = 5.94 \times 10^{23} \cdot T_g^{-1.68} \cdot \exp\left(\frac{-4.588 \times 10^4}{T_g}\right)$<br>$F_c = 0.5 \cdot \exp\left(\frac{-T_g}{2 \times 10^2}\right)$<br>$+ 0.5 \cdot \exp\left(\frac{-T_g}{8.9 \times 10^2}\right)$<br>$+ \exp\left(\frac{-4.6 \times 10^3}{T_g}\right)$ | [78] <sup>a</sup>    |

| #   | Reaction                                      | Rate equation   | Ref. |
|-----|---|---|------|
| 451 | $M + O + O \rightarrow M + O_2$               | $5.2 \times 10^{-35} \cdot \exp\left(\frac{9 \times 10^2}{T_g}\right)$                                  | [17] |
| 452 | $O + O_3 \rightarrow O_2 + O_2$               | $8 \times 10^{-12} \cdot \exp\left(\frac{-2.060 \times 10^3}{T_g}\right)$                               | [31] |
| 453 | $M + O + O_2 \rightarrow M + O_3$             | $5.4 \times 10^{-34} \cdot \left(\frac{3 \times 10^2}{T_g}\right)^{1.9}$                                | [29] |
| 454 | $O_2 + O_2 \rightarrow O + O_3$               | $2 \times 10^{-11} \cdot \exp\left(\frac{-4.980 \times 10^4}{T_g}\right)$                               | [29] |
| 455 | $M + O_2 \rightarrow M + O + O$               | $3 \times 10^{-6} \cdot T_g^{-1} \cdot \exp\left(\frac{-5.938 \times 10^4}{T_g}\right)$                 | [17] |
| 456 | $M + O_3 \rightarrow M + O + O_2$             | $6.6 \times 10^{-10} \cdot \exp\left(\frac{-1.160 \times 10^4}{T_g}\right)$                             | [29] |
| 457 | $M + C + O \rightarrow M + CO$                | $9.1 \times 10^{-22} \cdot T_g^{-3.08} \cdot \exp\left(\frac{-2.114 \times 10^3}{T_g}\right)$           | [94] |
| 458 | $C + O_2 \rightarrow CO + O$                  | $\frac{1.2 \times 10^{14}}{N_A} \cdot \exp\left(\frac{-2.01 \times 10^3}{T_g}\right)$                   | [95] |
| 459 | $CO_2 + O \rightarrow CO + O_2$               | $\frac{1.7 \times 10^{13}}{N_A} \cdot \exp\left(\frac{-2.65 \times 10^4}{T_g}\right)$                   | [94] |
| 460 | $M + CO + O \rightarrow M + CO_2$             | $8.3 \times 10^{-34} \cdot \exp\left(\frac{-1.51 \times 10^3}{T_g}\right)$                              | [17] |
| 461 | $CO + O_2 \rightarrow CO_2 + O$               | $4.2 \times 10^{-12} \cdot \exp\left(\frac{-2.4 \times 10^4}{T_g}\right)$                               | [17] |
| 462 | $CO + O_3 \rightarrow CO_2 + O_2$             | $4 \times 10^{-25}$   | [96] |
| 463 | $C + CO_2 \rightarrow CO + CO$                | $1 \times 10^{-15}$   | [97] |
| 464 | $M + CO_2 \rightarrow M + CO + O$             | $\frac{3.65 \times 10^{14}}{N_A} \cdot \exp\left(\frac{-5.2525 \times 10^4}{T_g}\right)$                | [98] |
| 465 | $M + CO \rightarrow M + C + O$                | $1.46 \times 10^6 \cdot T_g^{-3.52} \cdot \exp\left(\frac{-1.287 \times 10^5}{T_g}\right)$              | [94] |
| 466 | $M + H + H \rightarrow M + H_2$               | $\frac{1.5 \times 10^{-29}}{N_A} \cdot T_g^{-1.3}$  | [17] |
| 467 | $M + H_2 \rightarrow M + H + H$               | $\frac{7.6 \times 10^{-5}}{N_A} \cdot T_g^{-1.4} \cdot \exp\left(\frac{-5.253 \times 10^4}{T_g}\right)$ | [17] |
| 468 | $C + H_2 \rightarrow CH + H$                  | $k_{rev} \cdot K_{eq}$  | b    |
| 469 | $C_2H_4 \rightarrow C + CH_4$                 | $k_{rev} \cdot K_{eq}$  | b    |
| 470 | $C_2H_2 + H \rightarrow C + CH_3$             | $k_{rev} \cdot K_{eq}$  | b    |
| 471 | $C_2H + H \rightarrow C + CH_2$               | $k_{rev} \cdot K_{eq}$  | b    |
| 472 | $C_2H_6 + H \rightarrow CH_3 + CH_4$          | $k_{rev} \cdot K_{eq}$  | b    |
| 473 | $C_2H_5 + H_2 \rightarrow CH_3 + CH_4$        | $k_{rev} \cdot K_{eq}$  | b    |
| 474 | $C_2H_4 + H \rightarrow CH + CH_4$            | $k_{rev} \cdot K_{eq}$  | b    |
| 475 | $C_2H_4 + H \rightarrow CH_2 + CH_3$          | $k_{rev} \cdot K_{eq}$  | b    |
| 476 | $C_2H_2 + H_2 \rightarrow CH_2 + CH_2$        | $k_{rev} \cdot K_{eq}$  | b    |
| 477 | $C_2H_2 \rightarrow CH + CH$                  | $k_{rev} \cdot K_{eq}$  | b    |
| 478 | $CH_2 + H \rightarrow CH_3$                   | $k_{rev} \cdot K_{eq}$  | b    |
| 479 | $CH + H \rightarrow CH_2$                     | $k_{rev} \cdot K_{eq}$  | b    |
| 480 | $C + H_2 \rightarrow CH_2$                    | $k_{rev} \cdot K_{eq}$  | b    |
| 481 | $C + H \rightarrow CH$                        | $k_{rev} \cdot K_{eq}$  | b    |
| 482 | $C_2H_2 + CH_2 \rightarrow C + C_2H_4$        | $k_{rev} \cdot K_{eq}$  | b    |
| 483 | $C_2H_4 + CH_3 \rightarrow C_2H_6 + CH$       | $k_{rev} \cdot K_{eq}$  | b    |
| 484 | $C_2H_4 + CH_4 \rightarrow C_2H_5 + CH_3$     | $k_{rev} \cdot K_{eq}$  | b    |
| 485 | $C_2H_4 + CH_3 \rightarrow C_2H_5 + CH_2$     | $k_{rev} \cdot K_{eq}$  | b    |
| 486 | $C_2H_2 + CH_4 \rightarrow C_2H_3 + CH_3$     | $k_{rev} \cdot K_{eq}$  | b    |
| 487 | $C_2H_2 + CH_3 \rightarrow C_2H_3 + CH_2$     | $k_{rev} \cdot K_{eq}$  | b    |
| 488 | $C_2H_2 + CH \rightarrow C_2H + CH_2$         | $k_{rev} \cdot K_{eq}$  | b    |
| 489 | $C_2H_4 + C_2H_6 \rightarrow C_2H_5 + C_2H_5$ | $k_{rev} \cdot K_{eq}$  | b    |



| #   | Reaction                                      | Rate equation          | Ref. |
|-----|---|------------------------|------|
| 490 | $C_2H_2 + C_2H_6 \rightarrow C_2H_3 + C_2H_5$ | $k_{rev} \cdot K_{eq}$ | b    |
| 491 | $C_2H_2 + C_2H_4 \rightarrow C_2H + C_2H_5$   | $k_{rev} \cdot K_{eq}$ | b    |
| 492 | $C_2H_2 + C_2H_3 \rightarrow C_2H + C_2H_4$   | $k_{rev} \cdot K_{eq}$ | b    |
| 493 | $H_2 + O_2 \rightarrow OH + OH$               | $k_{rev} \cdot K_{eq}$ | b    |
| 494 | $OH + OH \rightarrow H_2O_2$                  | $k_{rev} \cdot K_{eq}$ | b    |
| 495 | $M + H + OH \rightarrow M + H_2O$             | $k_{rev} \cdot K_{eq}$ | b    |
| 496 | $H_2O_2 + O \rightarrow H_2O + O_2$           | $k_{rev} \cdot K_{eq}$ | b    |
| 497 | $M + HO_2 \rightarrow M + H + O_2$            | $k_{rev} \cdot K_{eq}$ | b    |
| 498 | $HO_2 + O \rightarrow H + O_3$                | $k_{rev} \cdot K_{eq}$ | b    |
| 499 | $HO_2 + OH \rightarrow H_2 + O_3$             | $k_{rev} \cdot K_{eq}$ | b    |
| 500 | $CO + H \rightarrow C + OH$                   | $k_{rev} \cdot K_{eq}$ | b    |
| 501 | $HCO \rightarrow CO + H$                      | $k_{rev} \cdot K_{eq}$ | b    |
| 502 | $CO_2 + OH \rightarrow CO + HO_2$             | $k_{rev} \cdot K_{eq}$ | b    |
| 503 | $COOH + OH \rightarrow CO + H_2O_2$           | $k_{rev} \cdot K_{eq}$ | b    |
| 504 | $H + HCHO \rightarrow CH_3 + O$               | $k_{rev} \cdot K_{eq}$ | b    |
| 505 | $HCHO + OH \rightarrow CH_3 + O_2$            | $k_{rev} \cdot K_{eq}$ | b    |
| 506 | $CH_3OO \rightarrow CH_3 + O_2$               | $k_{rev} \cdot K_{eq}$ | b    |
| 507 | $CO + H_2 \rightarrow CH_2 + O$               | $k_{rev} \cdot K_{eq}$ | b    |
| 508 | $HCHO + O \rightarrow CH_2 + O_2$             | $k_{rev} \cdot K_{eq}$ | b    |
| 509 | $CO + H_2O \rightarrow CH_2 + O_2$            | $k_{rev} \cdot K_{eq}$ | b    |
| 510 | $CO + H \rightarrow CH + O$                   | $k_{rev} \cdot K_{eq}$ | b    |
| 511 | $CO_2 + H \rightarrow CH + O_2$               | $k_{rev} \cdot K_{eq}$ | b    |
| 512 | $CO + OH \rightarrow CH + O_2$                | $k_{rev} \cdot K_{eq}$ | b    |
| 513 | $HCO + O \rightarrow CH + O_2$                | $k_{rev} \cdot K_{eq}$ | b    |
| 514 | $CO + HCHO \rightarrow CH_2 + CO_2$           | $k_{rev} \cdot K_{eq}$ | b    |
| 515 | $CO + HCO \rightarrow CH + CO_2$              | $k_{rev} \cdot K_{eq}$ | b    |
| 516 | $CH_3O + H \rightarrow CH_3 + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 517 | $H_2 + HCHO \rightarrow CH_3 + OH$            | $k_{rev} \cdot K_{eq}$ | b    |
| 518 | $CH_3O + OH \rightarrow CH_3 + HO_2$          | $k_{rev} \cdot K_{eq}$ | b    |
| 519 | $H + HCHO \rightarrow CH_2 + OH$              | $k_{rev} \cdot K_{eq}$ | b    |
| 520 | $HCHO + OH \rightarrow CH_2 + HO_2$           | $k_{rev} \cdot K_{eq}$ | b    |
| 521 | $CH_3 + HO_2 \rightarrow CH_2 + H_2O_2$       | $k_{rev} \cdot K_{eq}$ | b    |
| 522 | $C + H_2O \rightarrow CH + OH$                | $k_{rev} \cdot K_{eq}$ | b    |
| 523 | $H + HCO \rightarrow CH + OH$                 | $k_{rev} \cdot K_{eq}$ | b    |
| 524 | $H + HCHO \rightarrow CH + H_2O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 525 | $CO_2 + HCO \rightarrow CO + COOH$            | $k_{rev} \cdot K_{eq}$ | b    |
| 526 | $CH_3 + CO_2 \rightarrow CH_3O + CO$          | $k_{rev} \cdot K_{eq}$ | b    |
| 527 | $HCHO + HCO \rightarrow CH_3O + CO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 528 | $CH_3O + CO_2 \rightarrow CH_3OO + CO$        | $k_{rev} \cdot K_{eq}$ | b    |
| 529 | $CO + H_2 \rightarrow H + HCO$                | $k_{rev} \cdot K_{eq}$ | b    |

| #   | Reaction                                     | Rate equation          | Ref. |
|-----|--|------------------------|------|
| 530 | $CH_2 + O \rightarrow H + HCO$               | $k_{rev} \cdot K_{eq}$ | b    |
| 531 | $H_2 + HCO \rightarrow H + HCHO$             | $k_{rev} \cdot K_{eq}$ | b    |
| 532 | $CH_3O \rightarrow H + HCHO$                 | $k_{rev} \cdot K_{eq}$ | b    |
| 533 | $H_2 + HCHO \rightarrow CH_3O + H$           | $k_{rev} \cdot K_{eq}$ | b    |
| 534 | $CH_3OH \rightarrow CH_3O + H$               | $k_{rev} \cdot K_{eq}$ | b    |
| 535 | $CH_3OH + H \rightarrow CH_3O + H_2$         | $k_{rev} \cdot K_{eq}$ | b    |
| 536 | $H_2 + HCHO \rightarrow CH_2OH + H$          | $k_{rev} \cdot K_{eq}$ | b    |
| 537 | $CH_3 + H_2O \rightarrow CH_3OH + H$         | $k_{rev} \cdot K_{eq}$ | b    |
| 538 | $CH_3O + OH \rightarrow CH_3OO + H$          | $k_{rev} \cdot K_{eq}$ | b    |
| 539 | $CH_3OOH + H \rightarrow CH_3OO + H_2$       | $k_{rev} \cdot K_{eq}$ | b    |
| 540 | $CO + H_2O \rightarrow HCO + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 541 | $H + HCOOH \rightarrow HCHO + OH$            | $k_{rev} \cdot K_{eq}$ | b    |
| 542 | $COOH + H_2O \rightarrow HCOOH + OH$         | $k_{rev} \cdot K_{eq}$ | b    |
| 543 | $H_2O + HCHO \rightarrow CH_3O + OH$         | $k_{rev} \cdot K_{eq}$ | b    |
| 544 | $H_2O_2 + HCHO \rightarrow CH_3O + HO_2$     | $k_{rev} \cdot K_{eq}$ | b    |
| 545 | $CH_3OH + O_2 \rightarrow CH_3O + HO_2$      | $k_{rev} \cdot K_{eq}$ | b    |
| 546 | $H_2O + HCHO \rightarrow CH_2OH + OH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 547 | $CH_3OH + OH \rightarrow CH_2OH + H_2O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 548 | $H_2O_2 + HCHO \rightarrow CH_2OH + HO_2$    | $k_{rev} \cdot K_{eq}$ | b    |
| 549 | $H_2O + HCOOH \rightarrow CH_2OH + HO_2$     | $k_{rev} \cdot K_{eq}$ | b    |
| 550 | $CH_3O + H_2O_2 \rightarrow CH_3OH + HO_2$   | $k_{rev} \cdot K_{eq}$ | b    |
| 551 | $CH_3OO + H_2O \rightarrow CH_3OOH + OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 552 | $CH_3OH + O_2 \rightarrow CH_3OO + OH$       | $k_{rev} \cdot K_{eq}$ | b    |
| 553 | $CH_3OOH + O_2 \rightarrow CH_3OO + HO_2$    | $k_{rev} \cdot K_{eq}$ | b    |
| 554 | $CH_3OOH + HO_2 \rightarrow CH_3OO + H_2O_2$ | $k_{rev} \cdot K_{eq}$ | b    |
| 555 | $CO + OH \rightarrow HCO + O$                | $k_{rev} \cdot K_{eq}$ | b    |
| 556 | $CO_2 + H \rightarrow HCO + O$               | $k_{rev} \cdot K_{eq}$ | b    |
| 557 | $CO + HO_2 \rightarrow HCO + O_2$            | $k_{rev} \cdot K_{eq}$ | b    |
| 558 | $HCO + OH \rightarrow HCHO + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 559 | $HCO + HO_2 \rightarrow HCHO + O_2$          | $k_{rev} \cdot K_{eq}$ | b    |
| 560 | $HCHO + OH \rightarrow CH_3O + O$            | $k_{rev} \cdot K_{eq}$ | b    |
| 561 | $HCHO + HO_2 \rightarrow CH_3O + O_2$        | $k_{rev} \cdot K_{eq}$ | b    |
| 562 | $CH_2OH + OH \rightarrow CH_3OH + O$         | $k_{rev} \cdot K_{eq}$ | b    |
| 563 | $CH_3O + O_2 \rightarrow CH_3OO + O$         | $k_{rev} \cdot K_{eq}$ | b    |
| 564 | $CH_4 + CO \rightarrow CH_3 + HCO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 565 | $CH_3 + CO \rightarrow CH_2 + HCO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 566 | $CH_2CO + H_2O \rightarrow CH_3 + COOH$      | $k_{rev} \cdot K_{eq}$ | b    |
| 567 | $CH_4 + CO_2 \rightarrow CH_3 + COOH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 568 | $CH_3 + HCO \rightarrow CH_2 + HCHO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 569 | $CH_2CO + H \rightarrow CH + HCHO$           | $k_{rev} \cdot K_{eq}$ | b    |

| #   | Reaction                                       | Rate equation          | Ref. |
|-----|--|------------------------|------|
| 570 | $CH_4 + HCHO \rightarrow CH_3 + CH_3O$         | $k_{rev} \cdot K_{eq}$ | b    |
| 571 | $CH_3 + HCHO \rightarrow CH_2 + CH_3O$         | $k_{rev} \cdot K_{eq}$ | b    |
| 572 | $CH_4 + HCHO \rightarrow CH_2OH + CH_3$        | $k_{rev} \cdot K_{eq}$ | b    |
| 573 | $C_2H_4 + OH \rightarrow CH_2 + CH_2OH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 574 | $CH_3 + HCHO \rightarrow CH_2 + CH_2OH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 575 | $CH_2OH + CH_3 \rightarrow CH_2 + CH_3OH$      | $k_{rev} \cdot K_{eq}$ | b    |
| 576 | $CH_3 + CH_3O \rightarrow CH_2 + CH_3OH$       | $k_{rev} \cdot K_{eq}$ | b    |
| 577 | $CH_3 + CH_3OOH \rightarrow CH_3OO + CH_4$     | $k_{rev} \cdot K_{eq}$ | b    |
| 578 | $CH_3O + CH_3O \rightarrow CH_3 + CH_3OO$      | $k_{rev} \cdot K_{eq}$ | b    |
| 579 | $CH_3O + HCHO \rightarrow CH_2 + CH_3OO$       | $k_{rev} \cdot K_{eq}$ | b    |
| 580 | $C_2H_5 + O_2 \rightarrow CH_2 + CH_3OO$       | $k_{rev} \cdot K_{eq}$ | b    |
| 581 | $CO + HCHO \rightarrow HCO + HCO$              | $k_{rev} \cdot K_{eq}$ | b    |
| 582 | $CH_3OH + CO \rightarrow CH_3O + HCO$          | $k_{rev} \cdot K_{eq}$ | b    |
| 583 | $CH_3OH + CO \rightarrow CH_2OH + HCO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 584 | $HCHO + HCHO \rightarrow CH_2OH + HCO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 585 | $CH_3OH + HCHO \rightarrow CH_3O + CH_3O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 586 | $CH_3OH + HCHO \rightarrow CH_2OH + CH_3O$     | $k_{rev} \cdot K_{eq}$ | b    |
| 587 | $CH_3OH + HCHO \rightarrow CH_2OH + CH_2OH$    | $k_{rev} \cdot K_{eq}$ | b    |
| 588 | $CH_3OOH + HCHO \rightarrow CH_3O + CH_3OO$    | $k_{rev} \cdot K_{eq}$ | b    |
| 589 | $CH_2OH + CH_3OOH \rightarrow CH_3OH + CH_3OO$ | $k_{rev} \cdot K_{eq}$ | b    |
| 590 | $CH_3O + CH_3OOH \rightarrow CH_3OH + CH_3OO$  | $k_{rev} \cdot K_{eq}$ | b    |
| 591 | $CH_3OOH + HCHO \rightarrow CH_2OH + CH_3OO$   | $k_{rev} \cdot K_{eq}$ | b    |
| 592 | $CH_3OH + HCOOH \rightarrow CH_2OH + CH_3OO$   | $k_{rev} \cdot K_{eq}$ | b    |
| 593 | $CH_3OOH + HCO \rightarrow CH_3OO + HCHO$      | $k_{rev} \cdot K_{eq}$ | b    |
| 594 | $C_2H_4 + H_2O \rightarrow C_2H_5 + OH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 595 | $C_2H_4 + H_2O_2 \rightarrow C_2H_5 + HO_2$    | $k_{rev} \cdot K_{eq}$ | b    |
| 596 | $CH_3 + HCHO \rightarrow C_2H_4 + OH$          | $k_{rev} \cdot K_{eq}$ | b    |
| 597 | $CH_3CHO + H \rightarrow C_2H_4 + OH$          | $k_{rev} \cdot K_{eq}$ | b    |
| 598 | $CH_2CH_2OH \rightarrow C_2H_4 + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 599 | $CH_3 + HCO \rightarrow C_2H_3 + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 600 | $CH_3CO + H \rightarrow C_2H_3 + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 601 | $C_2H_2 + H_2O \rightarrow C_2H_3 + OH$        | $k_{rev} \cdot K_{eq}$ | b    |
| 602 | $CH_2CO + H_2 \rightarrow C_2H_3 + OH$         | $k_{rev} \cdot K_{eq}$ | b    |
| 603 | $CH_4 + CO \rightarrow C_2H_3 + OH$            | $k_{rev} \cdot K_{eq}$ | b    |
| 604 | $C_2H_4 + OH \rightarrow C_2H_3 + H_2O$        | $k_{rev} \cdot K_{eq}$ | b    |
| 605 | $C_2H_4 + HO_2 \rightarrow C_2H_3 + H_2O_2$    | $k_{rev} \cdot K_{eq}$ | b    |
| 606 | $CH_2CO + H \rightarrow C_2H_2 + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 607 | $C_2H_2 + O \rightarrow C_2H + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 608 | $CH_2 + CO \rightarrow C_2H + OH$              | $k_{rev} \cdot K_{eq}$ | b    |
| 609 | $C_2H_2 + O_2 \rightarrow C_2H + HO_2$         | $k_{rev} \cdot K_{eq}$ | b    |

| #   | Reaction  | Rate equation          | Ref. |
|-----|---|------------------------|------|
| 610 | $HCCO + OH \rightarrow C_2H + HO_2$             | $k_{rev} \cdot K_{eq}$ | b    |
| 611 | $CH_3CHO + H \rightarrow C_2H_5 + O$            | $k_{rev} \cdot K_{eq}$ | b    |
| 612 | $CH_3 + HCHO \rightarrow C_2H_5 + O$            | $k_{rev} \cdot K_{eq}$ | b    |
| 613 | $C_2H_4 + OH \rightarrow C_2H_5 + O$            | $k_{rev} \cdot K_{eq}$ | b    |
| 614 | $CH_3 + HCO \rightarrow C_2H_4 + O$             | $k_{rev} \cdot K_{eq}$ | b    |
| 615 | $CH_2CO + H_2 \rightarrow C_2H_4 + O$           | $k_{rev} \cdot K_{eq}$ | b    |
| 616 | $C_2H_3 + HO_2 \rightarrow C_2H_4 + O_2$        | $k_{rev} \cdot K_{eq}$ | b    |
| 617 | $C_2H_2 + OH \rightarrow C_2H_3 + O$            | $k_{rev} \cdot K_{eq}$ | b    |
| 618 | $CH_3 + CO \rightarrow C_2H_3 + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 619 | $CH_2 + HCO \rightarrow C_2H_3 + O$             | $k_{rev} \cdot K_{eq}$ | b    |
| 620 | $HCHO + HCO \rightarrow C_2H_3 + O_2$           | $k_{rev} \cdot K_{eq}$ | b    |
| 621 | $CH_2 + CO \rightarrow C_2H_2 + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 622 | $H + HCCO \rightarrow C_2H_2 + O$               | $k_{rev} \cdot K_{eq}$ | b    |
| 623 | $HCO + HCO \rightarrow C_2H_2 + O_2$            | $k_{rev} \cdot K_{eq}$ | b    |
| 624 | $CH + CO \rightarrow C_2H + O$                  | $k_{rev} \cdot K_{eq}$ | b    |
| 625 | $CO + HCO \rightarrow C_2H + O_2$               | $k_{rev} \cdot K_{eq}$ | b    |
| 626 | $CH + CO_2 \rightarrow C_2H + O_2$              | $k_{rev} \cdot K_{eq}$ | b    |
| 627 | $C_2H_5 + CH_3OOH \rightarrow C_2H_6 + CH_3OO$  | $k_{rev} \cdot K_{eq}$ | b    |
| 628 | $C_2H_6 + CO \rightarrow C_2H_5 + HCO$          | $k_{rev} \cdot K_{eq}$ | b    |
| 629 | $C_2H_6 + HCHO \rightarrow C_2H_5 + CH_3O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 630 | $C_2H_4 + CH_3OH \rightarrow C_2H_5 + CH_2OH$   | $k_{rev} \cdot K_{eq}$ | b    |
| 631 | $C_2H_6 + HCHO \rightarrow C_2H_5 + CH_2OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 632 | $CH_3CH_2O + CH_3O \rightarrow C_2H_5 + CH_3OO$ | $k_{rev} \cdot K_{eq}$ | b    |
| 633 | $C_2H_5 + CO_2 \rightarrow C_2H_4 + COOH$       | $k_{rev} \cdot K_{eq}$ | b    |
| 634 | $C_2H_5 + HCHO \rightarrow C_2H_4 + CH_2OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 635 | $C_2H_4 + HCO \rightarrow C_2H_3 + HCHO$        | $k_{rev} \cdot K_{eq}$ | b    |
| 636 | $C_2H_4 + HCHO \rightarrow C_2H_3 + CH_3O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 637 | $C_2H_4 + HCHO \rightarrow C_2H_3 + CH_2OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 638 | $C_2H_4 + CH_2OH \rightarrow C_2H_3 + CH_3OH$   | $k_{rev} \cdot K_{eq}$ | b    |
| 639 | $C_2H_4 + CH_3O \rightarrow C_2H_3 + CH_3OH$    | $k_{rev} \cdot K_{eq}$ | b    |
| 640 | $C_2H_3 + CO_2 \rightarrow C_2H_2 + COOH$       | $k_{rev} \cdot K_{eq}$ | b    |
| 641 | $C_2H_3 + HCHO \rightarrow C_2H_2 + CH_2OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 642 | $C_2H_2 + HCHO \rightarrow C_2H + CH_3O$        | $k_{rev} \cdot K_{eq}$ | b    |
| 643 | $C_2H_2 + HCHO \rightarrow C_2H + CH_2OH$       | $k_{rev} \cdot K_{eq}$ | b    |
| 644 | $C_2H_2 + CH_2OH \rightarrow C_2H + CH_3OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 645 | $C_2H_2 + CH_3O \rightarrow C_2H + CH_3OH$      | $k_{rev} \cdot K_{eq}$ | b    |
| 646 | $CH_3O + HCCO \rightarrow C_2H + CH_3OO$        | $k_{rev} \cdot K_{eq}$ | b    |
| 647 | $CH_2 + CO \rightarrow H + HCCO$                | $k_{rev} \cdot K_{eq}$ | b    |
| 648 | $CH_3 + CO \rightarrow CH_2CO + H$              | $k_{rev} \cdot K_{eq}$ | b    |
| 649 | $H_2 + HCCO \rightarrow CH_2CO + H$             | $k_{rev} \cdot K_{eq}$ | b    |

| #   | Reaction  | Rate equation          | Ref. |
|-----|---|------------------------|------|
| 650 | $CH_3 + HCO \rightarrow CH_3CO + H$               | $k_{rev} \cdot K_{eq}$ | b    |
| 651 | $CH_2CO + H_2 \rightarrow CH_3CO + H$             | $k_{rev} \cdot K_{eq}$ | b    |
| 652 | $CH_2OH + CH_3 \rightarrow CH_3CH_2O + H$         | $k_{rev} \cdot K_{eq}$ | b    |
| 653 | $CH_3CH_2OH \rightarrow CH_3CH_2O + H$            | $k_{rev} \cdot K_{eq}$ | b    |
| 654 | $C_2H_5 + OH \rightarrow CH_3CH_2O + H$           | $k_{rev} \cdot K_{eq}$ | b    |
| 655 | $C_2H_4 + H_2O \rightarrow CH_3CH_2O + H$         | $k_{rev} \cdot K_{eq}$ | b    |
| 656 | $CH_3CHO + H_2 \rightarrow CH_3CH_2O + H$         | $k_{rev} \cdot K_{eq}$ | b    |
| 657 | $CH_4 + HCHO \rightarrow CH_3CH_2O + H$           | $k_{rev} \cdot K_{eq}$ | b    |
| 658 | $CH_3CH_2OH \rightarrow CH_3CHOH + H$             | $k_{rev} \cdot K_{eq}$ | b    |
| 659 | $CH_2OH + CH_3 \rightarrow CH_3CHOH + H$          | $k_{rev} \cdot K_{eq}$ | b    |
| 660 | $C_2H_5 + OH \rightarrow CH_3CHOH + H$            | $k_{rev} \cdot K_{eq}$ | b    |
| 661 | $C_2H_4 + H_2O \rightarrow CH_3CHOH + H$          | $k_{rev} \cdot K_{eq}$ | b    |
| 662 | $CH_3CHO + H_2 \rightarrow CH_3CHOH + H$          | $k_{rev} \cdot K_{eq}$ | b    |
| 663 | $CH_4 + HCHO \rightarrow CH_3CHOH + H$            | $k_{rev} \cdot K_{eq}$ | b    |
| 664 | $C_2H_5 + H_2O \rightarrow CH_3CH_2OH + H$        | $k_{rev} \cdot K_{eq}$ | b    |
| 665 | $CH_3CHOH + H_2 \rightarrow CH_3CH_2OH + H$       | $k_{rev} \cdot K_{eq}$ | b    |
| 666 | $CH_2CH_2OH + H_2 \rightarrow CH_3CH_2OH + H$     | $k_{rev} \cdot K_{eq}$ | b    |
| 667 | $CH_3CH_2O + H_2 \rightarrow CH_3CH_2OH + H$      | $k_{rev} \cdot K_{eq}$ | b    |
| 668 | $CH_2OH + CO \rightarrow CH_2CO + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 669 | $H_2O + HCCO \rightarrow CH_2CO + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 670 | $HCHO + HCO \rightarrow CH_2CO + OH$              | $k_{rev} \cdot K_{eq}$ | b    |
| 671 | $CH_3 + CO_2 \rightarrow CH_2CO + OH$             | $k_{rev} \cdot K_{eq}$ | b    |
| 672 | $CH_2CO + H_2O \rightarrow CH_3CO + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 673 | $CH_3CO + H_2O \rightarrow CH_3CHO + OH$          | $k_{rev} \cdot K_{eq}$ | b    |
| 674 | $CH_3 + HCOOH \rightarrow CH_3CHO + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 675 | $CH_3COOH + H \rightarrow CH_3CHO + OH$           | $k_{rev} \cdot K_{eq}$ | b    |
| 676 | $CH_2CH_2OH + H_2O \rightarrow CH_3CH_2OH + OH$   | $k_{rev} \cdot K_{eq}$ | b    |
| 677 | $CH_3CHOH + H_2O \rightarrow CH_3CH_2OH + OH$     | $k_{rev} \cdot K_{eq}$ | b    |
| 678 | $CH_3CH_2O + H_2O \rightarrow CH_3CH_2OH + OH$    | $k_{rev} \cdot K_{eq}$ | b    |
| 679 | $CH_3CHOH + H_2O_2 \rightarrow CH_3CH_2OH + HO_2$ | $k_{rev} \cdot K_{eq}$ | b    |
| 680 | $CH + CO_2 \rightarrow HCCO + O$                  | $k_{rev} \cdot K_{eq}$ | b    |
| 681 | $CO + HCHO \rightarrow CH_2CO + O$                | $k_{rev} \cdot K_{eq}$ | b    |
| 682 | $HCO + HCO \rightarrow CH_2CO + O$                | $k_{rev} \cdot K_{eq}$ | b    |
| 683 | $CH_2 + CO_2 \rightarrow CH_2CO + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 684 | $CH_2CO + OH \rightarrow CH_3CO + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 685 | $CH_3 + CO_2 \rightarrow CH_3CO + O$              | $k_{rev} \cdot K_{eq}$ | b    |
| 686 | $CH_3CO + OH \rightarrow CH_3CHO + O$             | $k_{rev} \cdot K_{eq}$ | b    |
| 687 | $CH_3CO + HO_2 \rightarrow CH_3CHO + O_2$         | $k_{rev} \cdot K_{eq}$ | b    |
| 688 | $CH_3CHO + HO_2 \rightarrow CH_3CH_2O + O_2$      | $k_{rev} \cdot K_{eq}$ | b    |
| 689 | $CH_3 + HCOOH \rightarrow CH_3CHOH + O$           | $k_{rev} \cdot K_{eq}$ | b    |

| #   | Reaction  | Rate equation          | Ref. |
|-----|---|------------------------|------|
| 690 | $CH_3CHO + OH \rightarrow CH_3CHOH + O$           | $k_{rev} \cdot K_{eq}$ | b    |
| 691 | $CH_3COOH + H \rightarrow CH_3CHOH + O$           | $k_{rev} \cdot K_{eq}$ | b    |
| 692 | $CH_3CHO + HO_2 \rightarrow CH_3CHOH + O_2$       | $k_{rev} \cdot K_{eq}$ | b    |
| 693 | $CH_2OH + HCHO \rightarrow CH_2CH_2OH + O$        | $k_{rev} \cdot K_{eq}$ | b    |
| 694 | $CH_3CHOH + OH \rightarrow CH_3CH_2OH + O$        | $k_{rev} \cdot K_{eq}$ | b    |
| 695 | $CH_2CH_2OH + OH \rightarrow CH_3CH_2OH + O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 696 | $CH_3CH_2O + OH \rightarrow CH_3CH_2OH + O$       | $k_{rev} \cdot K_{eq}$ | b    |
| 697 | $CH_3CHOH + HO_2 \rightarrow CH_3CH_2OH + O_2$    | $k_{rev} \cdot K_{eq}$ | b    |
| 698 | $CH_2CH_2OH + HO_2 \rightarrow CH_3CH_2OH + O_2$  | $k_{rev} \cdot K_{eq}$ | b    |
| 699 | $CH_3CH_2O + HO_2 \rightarrow CH_3CH_2OH + O_2$   | $k_{rev} \cdot K_{eq}$ | b    |
| 700 | $C_2H_5 + CO \rightarrow CH_2CO + CH_3$           | $k_{rev} \cdot K_{eq}$ | b    |
| 701 | $CH_4 + HCCO \rightarrow CH_2CO + CH_3$           | $k_{rev} \cdot K_{eq}$ | b    |
| 702 | $C_2H_4 + CO \rightarrow CH_2 + CH_2CO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 703 | $CH_3 + HCCO \rightarrow CH_2 + CH_2CO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 704 | $CH_2CO + CH_4 \rightarrow CH_3 + CH_3CO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 705 | $CH_2CO + CH_3 \rightarrow CH_2 + CH_3CO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 706 | $CH_3CHOH + CH_4 \rightarrow CH_3 + CH_3CH_2OH$   | $k_{rev} \cdot K_{eq}$ | b    |
| 707 | $CH_2CH_2OH + CH_4 \rightarrow CH_3 + CH_3CH_2OH$ | $k_{rev} \cdot K_{eq}$ | b    |
| 708 | $CH_3CH_2O + CH_4 \rightarrow CH_3 + CH_3CH_2OH$  | $k_{rev} \cdot K_{eq}$ | b    |
| 709 | $CH_3CHO + CO \rightarrow CH_3CO + HCO$           | $k_{rev} \cdot K_{eq}$ | b    |
| 710 | $CH_3CHO + HCO \rightarrow CH_3CO + HCHO$         | $k_{rev} \cdot K_{eq}$ | b    |
| 711 | $CH_2CO + CH_3OH \rightarrow CH_3CO + CH_3O$      | $k_{rev} \cdot K_{eq}$ | b    |
| 712 | $CH_3CHO + HCHO \rightarrow CH_3CO + CH_3O$       | $k_{rev} \cdot K_{eq}$ | b    |
| 713 | $CH_2OH + CH_3CHO \rightarrow CH_3CO + CH_3OH$    | $k_{rev} \cdot K_{eq}$ | b    |
| 714 | $CH_3CO + CH_3OH \rightarrow CH_3CHO + CH_3O$     | $k_{rev} \cdot K_{eq}$ | b    |
| 715 | $CH_3CO + CH_3OOH \rightarrow CH_3CHO + CH_3OO$   | $k_{rev} \cdot K_{eq}$ | b    |
| 716 | $CH_2CO + CH_3CHO \rightarrow CH_3CO + CH_3CO$    | $k_{rev} \cdot K_{eq}$ | b    |
| 717 | $CO + OH \rightarrow COOH$                        | $k_{rev} \cdot K_{eq}$ | b    |
| 718 | $CO_2 + H \rightarrow COOH$                       | $k_{rev} \cdot K_{eq}$ | b    |
| 719 | $H + HCO \rightarrow HCHO$                        | $k_{rev} \cdot K_{eq}$ | b    |
| 720 | $H + HCHO \rightarrow CH_2OH$                     | $k_{rev} \cdot K_{eq}$ | b    |
| 721 | $CH_2 + H_2O \rightarrow CH_3OH$                  | $k_{rev} \cdot K_{eq}$ | b    |
| 722 | $CH_2OH + H \rightarrow CH_3OH$                   | $k_{rev} \cdot K_{eq}$ | b    |
| 723 | $CH_3O + OH \rightarrow CH_3OOH$                  | $k_{rev} \cdot K_{eq}$ | b    |
| 724 | $CH_3 + COOH \rightarrow CH_3COOH$                | $k_{rev} \cdot K_{eq}$ | b    |
| 725 | $CH_3 + HCHO \rightarrow CH_3CHOH$                | $k_{rev} \cdot K_{eq}$ | b    |
| 726 | $CO + O \rightarrow C + O_2$                      | $k_{rev} \cdot K_{eq}$ | b    |
| 727 | $CO_2 + O_2 \rightarrow CO + O_3$                 | $k_{rev} \cdot K_{eq}$ | b    |
| 728 | $CO + CO \rightarrow C + CO_2$                    | $k_{rev} \cdot K_{eq}$ | b    |

Constants:

$$N_A = 6.02214076 \times 10^{23} \text{ mol}^{-1}$$

$$k_B = 1.38064852 \times 10^{-23} \text{ J/K}$$

$$R = 8.31446261815324 \text{ JK}^{-1} \text{ mol}^{-1}$$

$$n_M = \text{total number density of neutral species (cm}^{-3}\text{)}$$

Notes:

<sup>a</sup> falloff expression, Lindemann-Hinshelwood expression with broadening factor:

$$k = \frac{k_0[M]k_\infty}{k_0[M] + k_\infty} F; \log F = \frac{\log F_c}{1 + \left[ \frac{\log(k_0[M]/k_\infty)}{N} \right]^2}; N = 0.75 - 1.27 \log F_c$$

<sup>b</sup> reaction rate expression calculated from equilibrium constant and reverse reaction rate:

$$K_{eq} = e^{\left( \frac{-\Delta G_r}{RT} \right)} \cdot \left( \frac{p}{R \cdot T} \right)^{\Delta v}; p = 1 \text{ bar}; \Delta v = \sum \mu_P - \sum \mu_R$$

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