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# Plasma-assisted dry reforming of CH<sub>4</sub>: How small amounts of O<sub>2</sub> addition can drastically enhance the oxygenates production - Experiments and insights from plasma chemical kinetics modeling

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ABSTRACT: Plasma-based dry reforming of methane (DRM) into high value-added oxygenates is an appealing approach to enable otherwise thermodynamically unfavorable chemical reactions at ambient pressure and near room temperature. However, it suffers from coke deposition due to the deep decomposition of CH4. In this work, we assess the DRM performance upon



 $O_2$  addition, as well as varying temperature,  $CO_2/CH_4$  ratio, discharge power and gas residence time, for optimizing oxygenates production. By adding  $O_2$ , the main products can be shifted from syngas ( $CO + H_2$ ) towards oxygenates. Chemical kinetics modelling shows that the improved oxygenates production is due to the increased concentration of oxygen-containing radicals, e.g., O, OH and  $HO_2$ , formed by electron impact dissociation ( $e + O_2 \rightarrow e + O + O/O(^{1}D)$ ) and subsequent reactions with H atoms. Our study reveals the crucial role of oxygen-coupling in DRM aimed at oxygenates, providing practical solutions to suppress carbon deposition, and at the same time enhance the oxygenates production in plasma-assisted DRM.

KEYWORD: Dry reforming of methane, oxygenates, plasma, chemical kinetics modeling

#### **1. INTRODUCTION**

The amounts of two important greenhouse gases, i.e., CO2 and CH4, are growing continuously in the atmosphere due to the high production and consumption of fossil fuels to satisfy the rapid energy demands. Dry reforming of methane (DRM) with carbon dioxide into value-added chemicals is promising for a carbon-neutral ecosystem, and is therefore one of utmost tasks of sustainable chemistry. Great efforts have been done in the chemical transformation of CO2 and CH4 into syngas, the mixture of CO and  $H_2$ , which can be commercially converted into bulk chemicals and fuels by the thermocatalytic Fischer-Tropsch (FT) synthesis.<sup>1,2</sup> However, due to the high bond energy of  $C=O(5.5 \text{ eV}, \text{ in } CO_2)$  and C-H (4.5 eV, in  $CH_4$ ), this two-step route generally starts with a highly endothermic process, requiring high temperature (> 700 •¢ for syngas production, and proceeds at high pressure (tens of atm) in the FT process. These conditions are very energy-demanding, and rely heavily on fossil fuels. In order to comply with the decarbonization of the chemical industry, the development of alternative, milder DRM approaches into high value-added liquid fuels and chemicals is very sought-after.

Non-thermal plasma provides a facile way to activate molecules by energetic electrons instead of heat, triggering chemical reactions near room temperature.<sup>3-5</sup> Plasma is a partially ionized gas, consisting of electrons, ions, photons, excited states, atoms, radicals, besides neutral gas molecules. Plasma-enabled processes have two main advantages: (i) they can be quickly switched on and off, compared to the long-time heating and cooling processes in thermal catalytic systems; (ii) they can be powered by intermittent renewable electricity (e.g., wind and solar energy) to reduce fossil fuel consumption and greenhouse gas emissions, and to comply with the goal of electrification of the chemical industry.

Dielectric barrier discharge (DBD) plasmas are frequently used for DRM.5,6 Early studies have shown that plasma-assisted DRM can realize the appealing gas-to-liquid (GtL) process, in which major liquid oxygenates include alcohols and acids, by optimizing the reactor geometry, plasma parameters and reaction conditions, although the total liquid selectivity was less than 15%.7,8 Rahmani et al. investigated the influence of steam on DRM and the distribution of products with specific energy input. The selectivity to liquid hydrocarbons was 3% by weight, with methanol, ethanol, isopropanol, and acetone as the most abundant liquid oxygenates at room temperature.<sup>9</sup> Interestingly, additional oxygen in the  $CO_2/CH_4$  feed gas has positive effects on the

yield of  $CH_3OH$ , HCHO and CO and reduces the total consumed energy.<sup>10</sup> Recently, Wang *et al.* studied the influence of process parameters (i.e., discharge power, reaction temperature, and residence time) on oxygenates production by using a water-cooled DBD reactor, with  $CH_3OH$  (43% relative selectivity) being the main liquid product.<sup>11</sup> By artificial neural network (ANN) models, discharge power was identified as the most critical process parameter for plasma-driven DRM to oxygenates.<sup>11</sup>



Figure 1. Schematic overview of the experimental set-up. Electrical connections are represented by full black lines, gas and liquid connections by full blue lines, water-cooling connections by dashed blue lines.

The development of chemical processes requires a detailed understanding of the underlying chemical reaction pathways. For this purpose, chemical kinetics modeling has been applied for DRM in DBD reactors.<sup>12-14</sup> Snoeckx *et al.* simulated the filamentary behavior of a DBD reactor and the main products were syngas in a H<sub>2</sub>/CO ratio of ca. 1.5, with low amounts of CH<sub>3</sub>OH and HCHO.<sup>12</sup> De Bie *et al.* developed a 1D fluid model for a  $CO_2/CH_4$  mixture in a DBD and compared the densities of the various plasma species as a function of residence time and gas mixing ratio.<sup>13</sup> The density of various plasma species showed different trends as a function of residence time, indicating that some targeted molecules could be selectively produced by optimizing the residence time (and thus flow rate).

DBD plasmas are highly non-equilibrium, i.e., the temperature of the electrons is much

higher than that of the gas.<sup>15,16</sup> The low temperature of the gas allows incorporating a catalyst into the DBD discharge region, which can improve the system efficiency. Various packing materials with both non-catalytic and catalytic properties have been used for plasma-catalytic DRM, including glass beads,<sup>17</sup> metal oxides,<sup>18</sup> supported catalysts with both transition and noble metals, 19,20 zeolites<sup>21</sup> and metal-organic frameworks (MOF).<sup>22</sup> However, the negative issue of coke deposition due to the fast rate of CH4 dissociation induced by plasma imposes the restriction on the stability of catalysts, and hinders further understanding of the mutual interaction between plasma and catalysts.<sup>23</sup>

Previously, we have studied the selective oxidation of methane to methanol by molecular oxygen (O2), and chemical kinetics modeling showed the reaction pathways for the formation of CH<sub>3</sub>OH and other oxygenates in the  $CH_4/O_2$  plasma.<sup>3</sup> In this work, we expand on DBD plasma – DRM studies, by introducing oxygen to tackle the problem of the inevitable carbon deposition, in an in-house developed temperature-controlled DBD reactor. On one hand, coke deposition might result in unstable plasma discharge and catalyst deactivation in plasma catalysis, which makes it challenging to find cost-effective and stable catalysts for this reaction, thus limiting the use of this process on a commercial scale. On the other hand, O2 addition could improve the concentration of oxygen-rich radicals in  $CO_2/CH_4$  plasma, which might increase the oxygenates production.<sup>3,10</sup> Therefore, we only focus on the catalyst-free process to obtain a fundamental understanding of  $CO_2/CH_4$ plasma behavior by introducing  $O_2$  in this work. In addition, we investigated the influence of various process parameters, i.e., the  $CO_2/CH_4$  molar ratio, temperature, plasma discharge power and residence time, on the reaction performance and the optimal  $O_2$ fraction. Finally, to support our experimental results, we performed computational plasma chemical kinetics modeling to unveil the possible chemical pathways for plasma-assisted DRM to oxygenates.

#### 2. EXPERIMENT AND MODELING

#### 2.1 Description of the experimental set-up

Plasma experiments (Figure 1) were carried out in a temperature-controlled coaxial DBD reactor with a water electrode (ground electrode) operated at atmospheric pressure. The DBD reactor consists of a pair of coaxial guartz cylinders (inner and outer guartz tubes) in which a stainless-steel (2 mm outer diameter) electrode was placed in the center, and circulating water was pumped into the space between the inner and outer cylinder. A tungsten rod was installed in the space between both cylinders to connect this circulating water (flowing between this inner and outer wall) with a ground wire (outside of the reactor wall), so that the circulating water acts as a ground electrode of our DBD. The water flow rate (5 L/min) and temperature (10-85 °C) was controlled by thermostatic baths with a circulation pump and external temperature controller (Huber KISS 104A),

which can effectively remove the heat generated by the discharge and maintain a constant reaction temperature. The discharge length is 60 mm (defined by the length of the ground electrode, i.e., region of circulating water) and the inner diameter of the inner quartz cylinder is 10 mm, yielding a discharge gap of 4 mm.

The feed gas flow  $(CO_2, CH_4 \text{ and } O_2)$  was supplied using mass flow controllers (MFC, Bronkhorst) connected to the gas cylinders (both 99.999%, Praxair). The feed gases were mixed using a T-connector, and subsequently introduced into the water-cooling DBD plasma reactor. O2 was introduced with concentration of 0-16%, which is in the safe range at the present experimental conditions. The detailed ternary flammability diagram for  $CO_2$ - $CH_4$ - $O_2$  mixtures is shown in Figure S1 of the Supporting Information (SI, section S.1). A cooling trap was placed at the exit of the DBD reactor to condense the liquid products. The gas flow rate was measured before and after the plasma reaction using a soapfilm flow meter, to account for gas expansion or contraction due to the chemical reaction, and thus, to correctly determine the gas conversion and product selectivity. In this study, the DBD reactor was connected to a high frequency power supply unit (PSU) AFS G10S-V (AFS GmbH) with a transformer. The electrical characteristics were monitored with a digital oscilloscope (Pico Technology Pico-Scope 6402D) using a high voltage probe (Tektronix P6015A), and a current monitor

(Pearson Electronics 4100). The PSU was operated at a frequency of 23.5 kHz. An additional low voltage probe was connected to an external capacitor (10 nF) to obtain the Lissajous figures, which were used to calculate the plasma power and monitor the discharge properties.

#### 2.2 Chromatographic analysis methods

Gas samples were analyzed by a micro gas chromatograph ( $\mu GC$ ; Agilent 990) equipped with thermal conductivity detectors (TCD) to quantify the production of gaseous products in two channels. The first channel was equipped with MoleSieve 5A and CP-PoraBOND Q columns used to analyze the permanent gases, including CO, H2, O2, N2 and CH4, while the second channel with  $Al_2O_3/KCI$  column was used to separate  $CO_2$ and hydrocarbons  $(C_2-C_4)$ . Samples were injected into the column from the reactor's outlet after passing through the cold trap. The total duration of the analysis was 5 min in the  $\mu$ GC. Ar and He were used as the carrier gases in channel one and channel two, respectively.

Liquid products condensed by the cold trap were first analyzed by GC (Thermo Focus SSL) with a flame ionization detector (FID) and a Restek Stabilwax column, which allowed efficient separation of all liquid products (e.g.,  $CH_3OH$ ,  $C_2H_5OH$ ,  $HCOOCH_3$ ). The same sample was also analysed by HPLC (Waters 2695) containing a Shodex RSpak KC-811 column, a photo-diode array (PDA) 2996 detector and a refractive index (RI) 2414 detector (Figure S2 in SI, section S.2). The mobile phase was 0.1% HClO4 in Milli-Q water, flowing at 1 mL/min. Formaldehyde, formic acid and acetic acid could be detected.

In this study, the gas flow rate ( $V_{intlet/outlet}$ ) before and after the reaction was detected by a bubble flow meter, to account for gas expansion or contraction due to the reaction, which is crucial for correct determination of the conversion, as mentioned above. The conversion of  $CO_2$ ,  $CH_4$  and  $O_2$ , as well as the selectivity of the main gaseous products (i.e., CO,  $H_2$ , hydrocarbons ( $C_xH_y$ )) and liquid products ( $C_xH_yO_z$ , including  $CH_3OH$ , HCHO, HCOOH and other oxygenates) was calculated as shown in SI, section S.3, equations (S1) – (S13).

Neutral molecules	Charged species	Radicals	Excited species
H <sub>2</sub> , O <sub>2</sub> , O <sub>3</sub> , H <sub>2</sub> O,	$H^{+}, H_{2}^{+}, H_{3}^{+}, O^{+}, O_{2}^{+}, O_{4}^{+},$	О, Н, ОН, НО₂, С, СН,	CO(E1).
H₂O₂, CH₄, CO,	OH⁺, H₂O⁺, H₃O⁺, C⁺,	СН2, СН3, С2, С2Н, С2Н3,	CO(E2),
CO <sub>2</sub> , C <sub>2</sub> H <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> ,	CH <sup>+</sup> , CH <sub>2</sub> <sup>+</sup> , CH <sub>3</sub> <sup>+</sup> , CH <sub>4</sub> <sup>+</sup> ,	С₂Н₅, С₃Н₅, С₃Н₁, СНО,	СО(ЕЗ),
C2H6, C3H6, C3H8,	СН <sub>5</sub> +, СНО+, СО+, СО <sub>2</sub> +,	СН₂ОН, СН₂СО, СН₃О,	CO(E4),
СН₂О, СН₃ОН,	C <sub>2</sub> <sup>+</sup> , C <sub>2</sub> H <sup>+</sup> , C <sub>2</sub> H <sub>2</sub> <sup>+</sup> , C <sub>2</sub> H <sub>3</sub> <sup>+</sup> ,	CH <sub>3</sub> CO, C <sub>2</sub> HO, CH <sub>3</sub> O <sub>2</sub> ,	O <sub>2</sub> (E1),
СН₃ООН,	C <sub>2</sub> H <sub>4</sub> <sup>+</sup> , C <sub>2</sub> H <sub>5</sub> <sup>+</sup> , C <sub>2</sub> H <sub>6</sub> <sup>+</sup> ,	C2H5O2, C2H5O, C2O,	O <sub>2</sub> (E <b>2</b> ),
C₂H₅OOH,	C <sub>2</sub> O <sub>2</sub> <sup>+</sup> , C <sub>2</sub> O <sub>3</sub> <sup>+</sup> , C <sub>2</sub> O <sub>4</sub> <sup>+</sup> , H <sup>-</sup> ,	СН₃СНОН, СООН, НСОО,	O <sub>2</sub> (E3),
CH₃CHO, C₂H₅OH,	0 <sup>-</sup> , 0 <sub>2</sub> <sup>-</sup> , 0 <sub>3</sub> <sup>-</sup> , 0 <sub>4</sub> <sup>-</sup> , 0H <sup>-</sup> ,	СН₃СО₂, СН₂СООН,	0(1D), 0(1S)
НСООН, НОСН₂О,	CH2 <sup>-</sup> , CO3 <sup>-</sup> , CO4 <sup>-</sup> , e <sup>-</sup>	CH <sub>2</sub> OO, CH <sub>2</sub> (S), CH <sub>2</sub> CHO,	
СН₃СООН		CH <sub>2</sub> CH <sub>2</sub> OH	

Table 1. Species taken into account in the OD chemical kinetics model

#### 2.3 Description of the chemical kinetics model

A zero-dimensional (OD) plasma kinetic model comprising various atoms, radicals, excited species, neutral molecules and ions, was developed to obtain insights into the underlying mechanism of plasma-assisted CH<sub>4</sub>/CO<sub>2</sub> reforming. The plasma kinetics solver ZDPlasKin<sup>24</sup>, which incorporates a Boltzmann equation solver BOLSIG+<sup>25</sup> was used to obtain the time evolution of the species densities generated in the reaction chamber. It solves the continuity equations for the various species densities,

$$\frac{dn_i}{dt} = \sum_j \left[ \left( a_{ij}^R - a_{ij}^L \right) k_j \prod_l n_l^L \right]$$
(1)

where  $n_i$  stands for the density of species *i*,  $a_{ij}^{R}$  and  $a_{ij}^{L}$  are the stoichiometric coefficients of the species *i* on the right and left hand side of the reaction j, respectively.  $n_i$  is the density of species i on the left side of the reaction, and  $k_j$  is the rate coefficient of reaction j. More information about the model can be found in SI, section S.4.

We developed a detailed kinetic mechanism consisting of electron impact reactions, neutral-neutral, neutral-ion, electron-ion recombination reactions and reactions involving excited species for atmospheric pressure AC plasma-assisted CH4/CO2 reforming. The main body of the chemistry set was adopted from works of our group PLASMANT for its excellent prediction ability for experimental results under different conditions.<sup>26,27</sup> Furthermore, other reactions were integrated to describe the formation and consumption pathways of liquid oxygenates and related intermediates from the NIST Chemical Kinetics Database<sup>28</sup> and HP-Mech.<sup>29,30</sup> For electron impact reactions, most of the cross sections were obtained from the online LXCat database<sup>31</sup> and Wanten *et al.*<sup>26</sup>. It is worth noting that three channels were considered regarding the dissociation of  $CO_2$  based on the  $CO_2$ electronic and vibrational levels,  $e + CO_2 \rightarrow e$ + CO + O, e +  $CO_2 \rightarrow e$  + CO +  $O(^{1}D)$ , and e+  $CO_2 \rightarrow e + CO + O(^{1}S).^{4}$  For the cross sections of the dissociation reaction  $e + CO_2 \rightarrow e$ +  $CO + O(^{1}S)$ , we used the recommended values by Itikawa.<sup>32</sup> The highly reactive intermediates,  $O(^{1}D)$  and  $O(^{1}S)$ , can easily react with hydrocarbon molecules to stimulate the chain branching reactions, and thus accelerate the fuel pyrolysis and oxidation.<sup>33,34</sup> Accordingly, reactions involving  $O(^{1}D)$  and

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 $O(^{1}S)$  were added and their corresponding kinetic parameters were available in Sun *et*  $a/.^{35,36}$  It is worth noting that the excited species were not detected due to the limitation of experimental measurements in this work. However, Lin *et al.*<sup>37</sup> and Slanger *et*  $al.^{38}$  have experimentally proven that the dissociation of  $O_2$  and  $CO_2$  can result in the production of excited O atom,  $O(^{1}D)$  and  $O(^{1}S)$ , respectively. As a result, a total of 1874 reactions with 1O2 species was described here for plasma-assisted DRM. The species considered in the kinetic mechanism are listed in Table 1, and the reactions are listed in the SI, section S.9.

#### 3. RESULTS AND DISCUSSION

#### 3.1 Effect of $O_2$ addition

First, we compare the performance of DRM in our experimental setup with and without  $O_2$  addition. As shown in Figure 2a - 2b, there is a negligible liquid formation (4% selectivity, products unidentified) without  $O_2$ addition. After introducing  $O_2$  in the range from 4% to 16% (in percentage of the total feed gas volume) while keeping the  $CH_4/CO_2$ ratio constant (1:1), the liquid selectivity gradually increases and reaches ca. 22%, with formic acid as the main product for  $12\% O_2$ added. More  $O_2$  (16%) results in less liquid formed, which suggests possible overoxidation of the oxygenates. Therefore, we select 12% as the optimal  $O_2$  percentage for further DRM experiments. The Lissajous figures (Figure 2c) were collected to better understand

the influence of  $O_2$  addition on the DRM reaction. The effective voltage dropped by adding O2 (12%), indicating that less energetic electrons were produced in  $CO_2/CH_4/O_2$ plasma at the same applied voltage. Consequently, at the same supplied PSU power (40 W), the power deposited into the plasma reduced from ca. 17 W to 15 W (i.e., by ca. 10%) after O<sub>2</sub> addition. Besides this, the total conversion increased substantially, thus significantly reducing the energy cost from 271.9 kJ/L to 144.9 kJ/L after the addition

of 12 %  $O_2$  (see equation S11, the weighted average of the conversion for each reactant, weighted over their concentration in the inlet gas mixture). In addition, we estimate the  $H_2O$  selectivity based on the hydrogen balance.  $H_2O$  selectivity increased from 29.8 % to 48.0% after 12%  $O_2$  addition, indicating more oxygenates can be formed at higher  $H_2O$  selectivity after  $O_2$  addition on plasmaassisted DRM reaction.



Figure 2. Plasma-driven DRM performance for different  $O_2$  percentages: (a) conversion and energy cost (above) and total selectivity distribution (below), (b) selectivity of various gas and liquid products. (c) Lissajous figures with and without  $O_2$  (12%) addition. (d). Off-gas volume change (V<sub>c</sub>) with and without  $O_2$  (12%) detected by the bubble flow meter. (PSU power 40 W, discharge power 15 - 17 W, discharge frequency 23.5 kHz, total flow rate 40 mL/min,  $CO_2/CH_4$  = 1:1, 35 °C circulating water, 6.78 s residence time, 1 atm pressure).

To reveal the effects of  $O_2$  addition on the plasma-driven DRM reaction, we calculated the outlet contraction factor (cf. Eq. (S10) in SI) both for the  $CO_2/CH_4$  plasma and the  $CO_2/CH_4/O_2$  plasma process. As shown in Figure 2d, the value of the contraction factor is negative in the CO<sub>2</sub>/CH<sub>4</sub> plasma, indicating the plasma ignition results in a rise in the outlet gas volume, while the contraction factor in the outlet of  $CO_2/CH_4/O_2$  plasma shows a reverse trend. This means that  $O_2$ addition shifts the reaction from expansion to contraction – but not directly in the gas phase. When the products of DRM are dominated by syngas  $(CH_4 + CO_2 \rightarrow 2CO + 2H_2)$ , the gas expands. However, in the presence of  $O_2$ , not only the product distribution shifts to oxygenates - but these oxygenates are condensed inside the cold trap, which leads to the observed apparent gas volume contraction. Therefore, the product distribution and the reaction pathways clearly change by adding 02.

#### 3.2 Effect of temperature and CO<sub>2</sub>/CH<sub>4</sub> ratio

We used circulating water as the ground electrode and for reactor cooling, with temperature between 10 and 85 °C, controlled by the water temperature. we performed experiments to test the temperature just near the outlet of our DBD reactor. In general, the water temperature and DBD outlet temperature are almost the same in our study. As shown in Figure 3a - 3b, the conversion of the feed gases  $(CO_2 + CH_4 + O_2)$  exhibits an increasing trend by imposing higher temperature, while the total liquid selectivity (21.5%) reaches its peak at the temperature of 35 °C with 12% O2 addition. At a lower temperature (10 °C), more hydrocarbons  $C_{x}H_{y}$  (i.e.,  $C_{2}H_{2}$ ,  $C_{2}H_{4}$ ,  $C_{2}H_{6}$ ,  $C_{3}H_{8}$ ) are formed, with a total selectivity of 24.4%, which might inhibit the formation of oxygenates in our present reactor.



Figure 3. Plasma-driven DRM performance for different reaction temperatures: (a) conversion and energy cost (above) and total selectivity distribution (below), (b) selectivity of various gas and liquid products. (PSU power 40 W, discharge power 15–17 W, discharge frequency 23.5 kHz, total flow rate 40 mL/min, 12%  $O_2$ ,  $CO_2/CH_4 = 1:1$ , 6.78 s residence time, 1 atm pressure). Both the reactor outlet temperature (upper x-axes) and the water temperature (lower x-axes) are given. Plasma-driven DRM performance for different  $CO_2/CH_4$  ratios; (c) conversion and energy cost (above) and total selectivity distribution (below), (d) selectivity of various gas and liquid products. (PSU power 40 W, discharge frequency 23.5 kHz, total flow rate 3.5 eV, discharge power 15–17 W, discharge frequency 23.5 kHz, total flow rate 4.0 mL/min, 12% O\_2, 3.5 eV, discharge frequency 23.5 kHz, total flow rate 4.0 mL/min, 12% O\_2, 3.5 eV, discharge frequency 23.5 kHz, total flow rate 4.0 mL/min, 12% O\_2, 3.5 eV, discharge frequency 23.5 kHz, total flow rate 4.0 mL/min, 12% O\_2, 3.5 eV, discharge power 1.5–1.7 W, discharge frequency 23.5 kHz, total flow rate 4.0 mL/min, 12% O\_2, 3.5 eV, circulating water, 6.78 s residence time, 1 atm pressure).

At a lower temperature (10 °C), more hydrocarbons  $C_xH_y$  (i.e.,  $C_2H_2$ ,  $C_2H_4$ ,  $C_2H_6$ ,  $C_3H_8$ ) are formed, with a total selectivity of 24.4%, which might inhibit the formation of oxygenates in our present reactor. Although we would expect a higher selectivity towards liquid oxygenates at lower temperature, also based on literature results,<sup>[11]</sup> we did not measure this, even in several repeat experiments. A possible reason might be that liquid products condensed at the walls inside the reactor, and cannot be removed immediately. However, we would need more dedicated experiments to test this hypothesis. By increasing the temperature from 10 to 85 °C, the  $C_xH_y$  selectivity gradually decreases, but the CO selectivity increases rapidly from 60% to 87%. Therefore, in order to maximize the oxygenates production, we continue our further experiments based on the optimal empirical temperature ( $35 \circ C$ ).

The conversion and products distribution for different CO<sub>2</sub>/CH<sub>4</sub> ratios are depicted in Figure 3c – 3d. When the  $CO_2/CH_4$  ratio in the feed gas is changed from 3:1 to 1:3, the CO<sub>2</sub> and CH<sub>4</sub> conversion both decrease gradually from 5.7% to 2.1% and from 26.5% to 13.6%, respectively. At the same time, the  $O_2$ conversion increases significantly from 49.3% to 74.7%. This clearly demonstrates that larger  $CH_4$  fractions speed up the  $O_2$  consumption compared to larger CO<sub>2</sub> fractions, which is expected. Besides, the total selectivity of liquid products also increases when changing the  $CO_2/CH_4$  ratio from 3:1 to 1:3, and the selectivity towards hydrocarbons  $(C_{x}H_{y})$  follows the same tendency as the liquid products, with a maximum of 14.1% at the  $CO_2/CH_4$  molar ratio of 1:3, while the CO selectivity exhibits the opposite trend, and clearly drops upon higher CH4 fraction (Figure 3d).

#### 3.3 Effect of power and residence time

Figure 4a – 4b shows the effect of different discharge powers on the plasma-driven DRM process. The conversion of  $CH_4$ ,  $CO_2$  and  $O_2$ significantly rises by applying higher PSU power in the range of 30 W to 60 W (corresponding to a discharge power range of 9 W ~ 32 W), while the total liquid selectivity drops from 26.0% to 5.7%. The selectivity of gaseous products, i.e., CO, H<sub>2</sub> and C<sub>x</sub>H<sub>y</sub>, increases by 25.7%, 65.7% and 41.2% upon raising the power. The selectivity of formic acid as the major liquid oxygenate drops to 1.9%. These results show that higher power generates more gaseous products and fewer oxygenates, which is consistent with previous work.<sup>11</sup>

Residence time is one of the crucial operating parameters for CH<sub>4</sub> oxidation to CH3OH by plasma catalysis.3 We applied different residence times (6.78 s - 0.84 s) by varying the feed gas flow rate (40 mL/min -320 mL/min). The effect of the different residence times on the plasma-assisted DRM process is shown in Figure 4c - 4d. By reducing the residence time from 6.78 s to 0.84 s, the reactant conversion  $(CO_2 + CH_4 +$  $O_2$ ) drops rapidly, as expected, while the liquid selectivity gradually rises from 21.5% to as high as 50.0%. The CH3OH and HCHO selectivity evolve similarly to the total liquid selectivity. Notably, the maximum selectivity of HCOOH (22.7%) was achieved at 0.84 s residence time.

#### 3.4 Plasma chemical kinetics modeling results

We performed plasma chemical kinetics modeling to obtain insights into how the effect of  $O_2$  addition shifts the formation pathways of syngas ( $CO + H_2$ ) to oxygenates near room temperature and atmospheric pressure for the plasma-assisted DRM reaction. As shown in Figure 5, we performed model validation by comparing the steady state experimental results with the predicted values from the model for the reactants conversion and the products selectivity under exactly the same conditions, with or without  $O_2$  addition (12%). The detailed plasma parameters are listed in Table S1. A good agreement between model and experiments is reached for the  $CH_4$ ,  $CO_2$  and  $O_2$  conversion (Figure 5a), indicating that the underlying chemistry of the conversion is well described in our model. As for the products selectivity, we consider the changes of syngas and hydrocarbons ( $C_xH_y$ ) after introducing  $O_2$  in the model, with the possible oxygenates production. Evidently, the simulation can effectively predict the decreasing trends of  $H_2$  and  $C_xH_y$  selectivity observed in the experiment upon  $O_2$  addition. However, a clear underestimation is observed for the calculated  $H_2$  selectivity without  $O_2$ addition and for the hydrocarbons selectivity with  $O_2$  addition.

As far as the oxygenates are concerned, our kinetic model predicts the selectivity towards HCOOH, CH3OH, CH3COOH, C2H5OH, and total oxygenates with good accuracy upon 12%  $O_2$  addition; only for  $CH_2O$ , there is a large discrepancy between our model and the experiments. Without O2 addition, our model predicts 2~3% selectivity for various oxygenates, such as HCOOH, CH<sub>3</sub>OH and CH<sub>2</sub>O, while the concentration of these species was too little to be detected by GC and HPLC in the experiment. Notably, the total selectivity towards oxygenates rapidly increases with O2 addition, both in our model and in the experiment. Altogether, there are some differences in the calculated and measured product selectivities, but these are not unexpected, in view of the large number of chemical reactions that can occur, and the fact that the rate coefficients of several of these reactions are subject to large uncertainties. However,

we prefer not to "tune" our model to reach better agreement with the experiments, without real scientific basis. Indeed, now, all assumptions made in our model (e.g., related to the number of microdischarge filaments) are based on logical and plausible physics. Overall, we believe our model is sufficiently realistic to reveal the underlying plasma chemistry for the improved oxygenates production upon  $O_2$  addition in the DRM reaction, as described below.

#### 3.5 Reaction pathway analysis

The reduced electric field (i.e., the ratio of electric field over total gas number density, E/N) is one of the most important parameters in controlling the distribution of the electron energy deposition to different excitation modes and the formation of active species in a non-equilibrium plasma. As shown in Figure S3, we compared the fraction of electron energy deposited into different excitation channels in a (a) 1:1  $CH_4/CO_2$  mixture and (b) 1:1  $CH_4/CO_2$  mixture with 12%  $O_2$  addition, as a function of E/N. The most efficient mechanism for electron energy loss is the elastic collision with  $CH_4$  and  $CO_2$  molecules and the dissociation of CH4 at a relatively low reduced electric field (< 20 Td) in a 1:1  $CH_4/CO_2$  mixture. However, the change of mixture ratio upon 12% O2 addition dramatically alters the energy branching, and the plasma energy is now primarily transferred to the dissociation modes of  $CH_4$  and  $O_2$  (Figure S 3b), indicating the addition of  $O_2$  to the CH4/CO2 mixture promotes the dissociation of  $O_2$  to produce O and  $O(^1D)$  radicals,

which facilitates the oxidation of CH4 to oxygenates.



Figure 4. Plasma-driven DRM performance for different power: (a) conversion and energy cost (above) and total selectivity distribution (below), (b) selectivity of various gas and liquid products. (discharge frequency 23.5 kHz, total flow rate 40 mL/min, 12%  $O_2$ ,  $CO_2/CH_4 = 1:1$ , 6.78 s residence time, 1 atm pressure). Plasma-driven DRM performance for different residence time: (c) conversion and energy cost (above) and total selectivity distribution (below), (d) selectivity of various gas and liquid products. (PSU power 40 W, discharge power 15-17 W, discharge frequency 23.5 kHz,  $12\% O_2$ ,  $35 \circ C$  circulating water,  $CO_2/CH_4 = 1:1$ , 1 atm pressure).

In order to elucidate the formation pathways of oxygenates, including HCOOH,  $CH_3OH$  and  $CH_2O$ , we present the reaction pathway analysis for selected species for the 1:1  $CH_4/CO_2$  mixture with 12%  $O_2$  addition in Figure 6. The corresponding analysis for the same mixture but without  $O_2$  addition is presented in Figure S4 of the SI, for comparison. The thickest arrows represent the contribution of reactions to the species formation or consumption in the order of 10<sup>-6</sup> mol cm<sup>-3</sup> <sup>3</sup> while the thinnest arrows represent the contribution of reactions in the order of 10<sup>-9</sup> <sup>9</sup> mol cm<sup>-3</sup>, and dashed lines represent the contribution of reactions less than 10<sup>-9</sup> mol cm<sup>-3</sup>. Note that these orders of magnitude represent the integral of the reaction rate over the entire residence time. The arrows pointing inward indicate formation reactions, while the arrows pointing outward represent consumption reactions. The blue arrows indicate reactions that occur both with and without  $O_2$  addition, while the green arrows indicate reactions that are only important upon 12%  $O_2$  addition. The numbers attached to the arrows denote the relative contributions of formation or consumption to the selected species, as calculated using Eq. (2)

$$f_{ij} = \frac{\left(a_{ij}^{R} - a_{ij}^{L}\right) \int_{0}^{t_{r}} r_{j} dt}{\sum \left(a_{ij}^{R} - a_{ij}^{L}\right) \int_{0}^{t_{r}} r_{j} dt}$$
(2)

where  $f_{ij}$  stands for the relative contribution of reaction j to the formation of species i.  $t_r$ represents the residence time, and  $r_j$  is the reaction rate of reaction j. The same formula applies to the relative contribution for consumption.

As shown in Figure 6 and Figure S4, the main oxygenated compound, formic acid (HCOOH), is primarily formed through the chain termination reaction H + COOH  $\rightarrow$  HCOOH, which is responsible for 96.1% and 84.1% of HCOOH formation with or without

O2 addition, respectively. As a primary intermediate, the carboxyl radical COOH is critical for the formation of HCOOH. COOH itself is mainly created upon recombination of CO with OH, which contributes for 75.6% and 87.8% to COOH formation with or without  $O_2$  addition. At the same time, the main HCOOH formation path (H + COOH  $\rightarrow$ HCOOH) plays a significant role in the consumption of COOH without  $O_2$  addition (see Figure S4). Upon  $O_2$  addition, the main formation pathway for COOH has not changed, as mentioned above, however, the main consumption pathway is changed from H +  $COOH \rightarrow HCOOH$  (without  $O_2$  addition) to  $COOH + CO \rightarrow CO_2 + CHO$  (with  $O_2$  addition); cf. Figure 6 and Figure S4. This is because electron impact dissociation (e +  $O_2 \rightarrow e + O$ +  $O/O(^{1}D)$ ) enhances the formation of O and  $O(^{1}D)$ , which further promotes the formation of OH and H2O2. Accordingly, the concentration of COOH with  $12\% O_2$  in the mixture is about 2 orders of magnitude higher than without  $O_2$  addition. Although the reaction H + COOH  $\rightarrow$  HCOOH contributes only for 12% of COOH consumption in the mixture with 12% O2, its reaction rate is still one order of magnitude higher compared with no O2 addition.



Figure 5. Comparison between steady state measurements and model predictions with and without  $O_2$  addition (12%) in plasma-assisted DRM: (a) gas conversion and main products selectivity, (b) various oxygenates selectivity at a PSU power of 40 W, residence time of 6.78 s, and temperature of 35 °C(exp: experiment; sim: simulation)

For the generation of methanol ( $CH_3OH$ ), the dominant pathways without  $O_2$  addition are the reactions of CH3O with H, CH3O,  $HO_2$ , and CHO radicals, in total accounting for 68.0% of the total CH3OH formation, as shown in Figure S4. In addition, 16.2% and 10.8% of CH<sub>3</sub>OH formation comes from the reactions of CH3 with OH and OH-, as well as from the reaction of  $CH_2OH$  with H and  $HO_2$ , respectively. However, upon 12% O2 addition, the main pathway for CH<sub>3</sub>OH formation has become the chain termination reaction,  $CH_3O_2 + HO_2 \rightarrow CH_3OH + O_3$  (contribution of 66.5%, see Figure 6). The main precursor, CH<sub>3</sub>O<sub>2</sub>, is mainly formed through the reaction  $CH_3 + O_2 \rightarrow CH_3O_2$ , regardless of whether there is O2 addition or not (see Figure 6 and Figure S4). However, the rate of this reaction is two orders of magnitude higher upon 12% O2 addition than without  $O_2$  addition, due to the high concentration of

tions  $CH_2OH + O_2 \rightarrow CH_2O + HO_2$  and  $CH_3OH + OH \rightarrow CH_2O + H_2O + H$ , which are responsible for 45.9% and 31.8% of  $CH_2O$  formation, respectively. Without  $O_2$  addition, the dominant pathways for  $CH_2O$  formation are the reactions  $CH_2 + CO_2 \rightarrow CH_2O + CO$ ,

are the reactions  $CH_2 + CO_2 \rightarrow CH_2O + CO$ ,  $CH_3 + O \rightarrow CH_2O + H$ , and  $CH_3O + H/CH_3 \rightarrow$   $CH_2O + H_2/CH_4$ . The significant increase in  $O_2$  concentration in the discharge mixture upon  $O_2$  addition can enhance the reaction rates of  $CH_2OH + O_2 \rightarrow CH_2O + HO_2$  and  $CH_3O + O_2 \rightarrow CH_2O + HO_2$  to promote the

 $O_2$ . At the same time, the reaction rate of

the major  $CH_3O_2$  consumption reaction

 $(CH_3O_2 + HO_2 \rightarrow CH_3OH + O_3)$  upon 12%  $O_2$ 

addition is 2 orders of magnitude higher than

without  $O_2$  addition. This explains the signif-

icant rise in CH3OH formation upon O2 ad-

formed upon O2 addition through the reac-

is

dominantly

dition, as observed in our experiments.

Formaldehyde (CH<sub>2</sub>O)

formation of  $CH_2O$ . Meanwhile, the dissociation of  $O_2$  strongly enhances the OH formation, significantly promoting the  $CH_2O$  formation through the reaction  $CH_3OH + OH$  $\rightarrow CH_2O + H_2O + H.$ 



Figure 6. Reaction pathway analysis for HCOOH, COOH, CH<sub>3</sub>OH, CH<sub>3</sub>O, CH<sub>3</sub>O<sub>2</sub>, CH<sub>2</sub>O, CH<sub>2</sub>OH and OH for a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture with 12% O<sub>2</sub> addition at atmospheric pressure, at a PSU power of 40 W, a residence time of 6.78 s, and temperature of 35 °C Note that for OH, for the sake of clarity, the analysis is split in formation reactions and consumption reactions, due to the many reactions taking place.

By analyzing the pathway of  $CH_2OH$ , as shown in Figure 6, we find that the consumption of  $CH_3OH$  to form  $CH_2OH$  via the reactions  $CH_3OH + OH \rightarrow CH_2OH + H_2O$  and  $CH_3OH + O \rightarrow CH_2OH + OH$  are the major source of  $CH_2OH$ . In addition, the chain branching reaction stimulated by excited  $O(^{1}D)$ , via  $O(^{1}D) + CH_4 \rightarrow CH_2OH + H$ , is also responsible for 15.8% of  $CH_2OH$  formation. Obviously, the major consumption pathways of  $CH_2OH$  are the reactions with  $O_2$  and O to form  $CH_2O$ , which are responsible for 84.8%and 7.3% of  $CH_2OH$  consumption, respectively.

As discussed above, OH is an important oxidizer in promoting the formation of oxygenates or their related intermediates. Therefore, we also compare the formation and consumption pathways of OH with and without O2 addition. The pathways of OH formation and consumption are very complicated, so we have plotted separate maps illustrating the production pathway and consumption pathway, respectively. As shown in Figure S4, the dominant formation pathways without  $O_2$  addition are the reactions  $HO_2$  +  $H \rightarrow OH + OH$  and  $CH_4 + O(^1D)/O(^1S) \rightarrow CH_3$ + OH, accounting for 31.4% and 25.0% of the total OH formation, respectively. In addition, 9.2% and 8.2% of OH formation comes from the reaction  $CH_2OH + H \rightarrow CH_3 + OH$  and  $CH_3 + HO_2 \rightarrow CH_3O + OH$ , respectively. However, upon 12%  $O_2$  addition, the dominant pathways for OH formation have become the chain branching reactions,  $O_3 + H \rightarrow OH + O_2$ (30.0% contribution),  $HO_2 + O \rightarrow OH + O_2$ 

(29.3% contribution) and  $CO + H_2O_2 \rightarrow OH + COOH$  (12.8% contribution), due to the significant rise in  $O_2$  and O concentration, further stimulating the oxygenated components formation. As shown in Figure S4 and Figure 6, upon  $O_2$  addition, the dominant pathways for OH consumption are changed from  $OH + CH_2O \rightarrow H_2O + CHO$ , and  $OH + CH_4 \rightarrow H_2O + CH_3$ , to  $OH + CO \rightarrow COOH$ , which promotes the formation of HCOOH.

In order to elucidate whether nonnegligible competing reactions between  $CO_2$  and  $O_2$  are responsible for the formation of important intermediates or oxygenates in the system, the consumption pathways of  $CO_2$  and  $O_2$  for the 1:1 mixture with or without O<sub>2</sub> addition are listed in Table R1-R4 in the SI. The main competing reactions between  $CO_2$  and  $O_2$  for the plasma energy are the electron impact reactions. In addition to the electron impact reactions, there is another competing reaction between  $CO_2$  and  $O_2$  based on the reaction pathway analysis, that is,  $CH_2 + CO_2 \rightarrow$  $CH_2O + CO$  and  $CH_2 + O_2 \rightarrow CO + H_2O$ ,  $CH_2$ +  $O_2 \rightarrow COOH$  + H. However, this competing reaction has negligible influence on the formation of oxygenates.

In summary, our plasma chemical kinetics modeling results show that two types of reactions are responsible for the production enhancement of oxygenated compounds upon  $O_2$  addition. Firstly, the direct promotion effect of  $O_2$  addition on the formation of important intermediates and oxygenates, such as the reactions  $CH_3 + O_2 \rightarrow CH_3O_2$  and  $CH_2OH + O_2 \rightarrow CH_2O + HO_2$  are responsible for 92.2% of CH3O2 formation and 45.9% of CH<sub>2</sub>O formation, respectively. Secondly, the rise in concentration of oxygen-containing radicals, such as O, OH, HO<sub>2</sub>, due to electron impact dissociation,  $e + O_2 \rightarrow e + O +$  $O/O(^{1}D)$ , and subsequent reactions of these O atoms into OH and HO<sub>2</sub>, will further enhance the formation of HCOOH via the pathways  $CO + OH \rightarrow COOH$ ,  $COOH + H \rightarrow HCOOH$ ; the formation of  $CH_3OH$  via the pathways  $CH_3O_2$ +  $HO_2 \rightarrow CH_3OH + O_3$  and  $CH_3O + HO_2 \rightarrow$  $CH_3OH + O_2$ ; and the formation of  $CH_2O$  via the pathways  $CH_3OH + OH \rightarrow CH_2O + H_2O +$ H and  $CH_3OH + O/OH \rightarrow CH_2OH + OH/H_2O$ , and  $CH_2OH + O_2 \rightarrow CH_2O + HO_2$ . Additional computational studies may aid in determining ways to increase the oxygenates yield, but were outside the scope of this work.

#### 4. CONCLUSION

In this paper, we demonstrate for the first time that the plasma-driven DRM can be shifted from the production of mainly syngas to the production of significant amounts of oxygenates by introducing moderate amounts of O<sub>2</sub> (12%), even without using catalysts. On the one hand,  $O_2$  addition can reduce carbon deposition resulting from the rapid decomposition of CH4 induced by non-thermal plasma, hence making the plasma-based DRM process more stable and allowing to operate it at higher CH4 fractions. This is also relevant when catalysts would be introduced in the plasma, as catalyst deactivation by carbon deposition would be reduced. On the other hand, oxygen-containing species upon  $O_2$  addition can improve the oxygenates production. We evaluated multiple parameters in order to optimize the formation of oxygenates in our experiments. We show that lower power and shorter residence time enhance the liquid production, leading to a maximal oxygenates selectivity of 50%.

We also developed a plasma chemical kinetics model to investigate how the effect of  $O_2$  addition shifts the formation pathways of syngas to oxygenates near room temperature and atmospheric pressure for the plasma-assisted DRM reaction. Two types of reactions are responsible for the improvement of the oxygenates production upon  $O_2$  addition. The first is the direct promotion effect of O2 addition on the formation of important intermediates and oxygenates. In addition, the increasing concentration of oxygen-containing radicals, such as, O, OH, HO2, due to electron impact dissociation,  $e + O_2 \rightarrow e + O +$  $O/O(^{1}D)$ , and the subsequent reaction of O atoms into OH and HO<sub>2</sub>, can further enhance the formation of oxygenates.

Our results not only yield a better fundamental understanding of the gas-to-liquid conversion by the plasma-driven DRM process, but also provide a novel strategy for reducing carbon deposition to improve the DRM reaction stability.

#### ASSOCIATED CONTENT

Supporting Information.

The Supporting Information is available free of charge on the ACS Publications website. Ternary flammability diagram for  $CO_2$ - $CH_4$ - $O_2$ mixtures; results of qualitative analysis of liquid products by HPLC; calculation of conversion, selectivity, and the contraction factor; description of the chemical kinetics model; fraction of electron energy into different excitation channels; reaction pathway analysis for the oxygenates in a 1:1  $CO_2/CH_4$  mixture; the consumption pathways of  $CO_2$  and  $O_2$  for the 1:1  $CH_4/CO_2$  mixture with or without  $O_2$  addition; reaction pathway analysis of singlet oxygen  $O_2(e1)$ ; overview of the reactions included in our model.

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A brief (~ 20 word) synopsis, describing the graphic and explaining how the paper relates to sustainability:

Plasma-assisted dry reforming of methane (DRM) into high value-added fuels by introducing small amounts of  $O_2$  is an appealing approach under room temperature and atmosphere pressure.

## **Supporting information**

# Plasma-assisted dry reforming of $CH_4$ : How small amounts of $O_2$ addition can drastically enhance the oxygenates production - Experiments and insights from plasma chemical kinetics modelling

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#### S.1. Ternary flammability diagram for CO<sub>2</sub>-CH<sub>4</sub>-O<sub>2</sub> mixtures



Figure S1: Ternary flammability diagram for  $CO_2$ -CH<sub>4</sub>-O<sub>2</sub> mixtures, experimentally obtained by Janes et al. at 1 bar.<sup>1</sup> The yellow area represents flammable mixtures. The orange points label the compositions where an explosion was observed, whereas the white points represent the compositions for which no explosion took place. The right straight line indicates stoichiometric CH<sub>4</sub>/O<sub>2</sub> mixtures. The large orange stars indicate the compositions used in our experiments.

As shown on Figure S1, the feed gas of  $CO_2/CH_4/O_2$  was operated in the safe range, which is important to make sure it is safe without plasma. After plasma ignition, H<sub>2</sub> can be produced but the concentration of produced H<sub>2</sub> in the DBD plasma is less than 2 %, while the H<sub>2</sub> explosion limit in the air is 4% - 74%. We put the DBD reactor inside a Faraday cage within the fume hood in case of a leak.

#### S.2. Results of qualitative analysis of liquid products by HPLC



Figure S2. Results of qualitative analysis of liquid products by HPLC. (A) Photo-diode array (PDA) detector, indicating the presence of HCOOH and  $CH_3COOH$ . (B). Refractive index (RI) detector, indicating the presence of HCHO, HCOOH and  $CH_3OH$ 

#### S.3. Calculation of conversion, selectivity, and the contraction factor

In this study, the gas flow rate ( $V_{intlet/outlet}$ ) before and after the reaction was detected by a bubble flow meter, to account for gas expansion or contraction due to the reaction, which is crucial for correct determination of the conversion, as mentioned in the main paper. The conversion of CO<sub>2</sub>, CH<sub>4</sub> and O<sub>2</sub>, as well as the selectivity of the main gaseous products (i.e., CO, H<sub>2</sub>, hydrocarbons (C<sub>x</sub>H<sub>y</sub>) and liquid products (C<sub>x</sub>H<sub>y</sub>O<sub>z</sub>, including CH<sub>3</sub>OH, HCHO, HCOOH and other oxygenates) was calculated by equations (S1) - (S8).

$$X_{\text{CO}_2} = \frac{\text{C}_{\text{outlet}_{\text{CO}_2}} \times \text{V}_{\text{outlet}}}{\text{C}_{\text{inlet}_{\text{CO}_2}} \times \text{V}_{\text{inlet}}} \times 100\%$$
(S1)

$$X_{CH_4} = \frac{C_{outlet}}{C_{CH_4} \times V_{outlet}} \times 100\%$$
(S2)

$$X_{O_2} = \frac{C_{outlet_{O_2}} \times V_{outlet}}{C_{inlet_{O_2}} \times V_{inlet}} \times 100\%$$
(S3)

$$S_{CO} = \frac{C_{outlet_{CO}} \times V_{outlet}}{\left(C_{inlet_{CO_{2}}} + C_{inlet_{CH_{4}}}\right) \times V_{inlet} - \left(C_{outlet_{CO_{2}}} + C_{outlet_{CH_{4}}}\right) \times V_{outlet}} \times 100\%$$
(S4)

$$S_{H_2} = \frac{C_{outlet_{H_2}} \times V_{outlet}}{2 \times \left(C_{inlet_{CH_4}} \times V_{inlet} - C_{outlet_{CH_4}} \times V_{outlet}\right)} \times 100\%$$
(S5)

$$S_{C_xH_y} = \frac{x \times C_{outlet_{C_xH_y}} \times V_{outlet}}{\left(C_{inlet_{CO_2}} + C_{inlet_{CH_4}}\right) \times V_{inlet} - \left(C_{outlet_{CO_2}} + C_{outlet_{CH_4}}\right) \times V_{outlet}} \times 100\%$$
(S6)

$$S_{C_xH_yO_z,total} = 100\% - (S_{CO} + S_{C_xH_y})$$
 (S7)

$$S_{C_xH_yO_z} = \frac{x \times \text{mol of } C_xH_yO_z \text{ produced}}{\sum x \times C_xH_yO_z \text{ produced}} \times S_{C_xH_yO_z,\text{total}}$$
(S8)

Note that equation (S7) is only valid when the amount of coking is negligible, which is the case in our experiments (certainly when adding  $O_2$ ).

Additionally, we estimate the H<sub>2</sub>O formation based on the hydrogen balance (S9):  $S_{H_2O} = 100\% - (S_{C_xH_y} + S_{C_xH_yO_z} + S_{H_2})$ (S9)

The specific energy input (SEI) is defined as:

$$SEI(kJ/L) = \frac{\text{discharge power}(J/s)}{\text{feed gas flow rate}(L/\min)} \times \frac{60(s/\min)}{1000(J/kJ)}$$
(S10)

The total conversion is defined as the weighted average of the conversion for each reactant, weighted over their concentration in the inlet gas mixture:

$$X^{total} = \sum_{i} c_i X_i \tag{S11}$$

The total energy cost (S12) is expressed in terms of the total conversion and the specific

energy input (SEI, kJ/L). Note that equation (S12) can also be expressed in terms of eV/molecule (S13):

$$EC(kJ/L) = \frac{SEI(kJ/L)}{X^{total}(\%)} \times 100\%$$
 (S12)

Finally, as mentioned above, the stoichiometry of chemical reactions leads to a change of the total volume of the gas exiting the reactor, indicated by the bubble flow meter. Therefore, in order to evaluate the volume change of the outlet gas flow, i.e., expansion/contraction, we define the contraction factor ( $V_c$ ) based on volume change before and after plasma ignition.

$$V_{\rm C} = \left(1 - \frac{V_{\rm outlet}}{V_{\rm inlet}}\right) \times 100\%$$
(S13)

#### S.4. Description of the chemical kinetics model

Unlike the rate coefficients for reactions between heavy particles, which can be directly obtained from literature, the rate coefficients for electron impact reactions are usually calculated by solving the Boltzmann equation with BOLSIG+, based on the cross-section data, as shown in Eq. (S11)

 $k_{k} = r \int_{0}^{\infty} \varepsilon \sigma_{k} f_{0} d\varepsilon$  (S14) where  $\gamma = (2e/m_{e})^{1/2}$  is constant (in C<sup>1/2</sup> kg<sup>-1/2</sup>), *e* and *m<sub>e</sub>* are the elementary charge (1.6021766208×10<sup>-19</sup> C) and electron mass (9.10956×10<sup>-31</sup> kg), respectively.  $\varepsilon$  is the electron energy,  $\sigma_{k}$  is the cross section of the various electron-neutral collision processes *k*, and *f*<sub>0</sub> is the electron energy distribution function (EEDF).

The AC power supply activates the DBD, which typically exhibits filamentary behavior at atmospheric pressure in our experiments and other work.<sup>2</sup> An improved and detailed method that more systematically translates the experimental conditions and observations to an equivalent 0D model was used in our study, and the detailed description of the model can be found in previous works from our group.<sup>3,4</sup>

The electric field E, at which BOLSIG+ solves the Boltzmann equation, is calculated using the differential from of the Joule heating equation

$$\frac{\mathrm{d}P}{\mathrm{d}V} = \mathbf{Jg}\mathbf{E} = \sigma E^2 \tag{S15}$$

where *P* is the power and d*V* a volume element,  $\mathbf{J} = \sigma \mathbf{E}$  is the current density and  $\sigma$  is the electron conductivity. Assuming no spatial dependence, the reduced electric field (*E*/*N*) can be calculated from the power density  $p \equiv P/V$  as

$$\left(\frac{E}{N}\right) = \frac{1}{N}\sqrt{\frac{p}{\sigma}}$$
(S16)

where *N* is the number density of neutral species. The electron conductivity  $\sigma$  is calculated by

 $\sigma = en_e \mu_e$  (S17) where  $n_e$  is the electron number density and  $\mu_e$  the electron mobility, calculated by BOLSIG+.

#### S.5. Fraction of electron energy into different excitation channels

The detailed plasma parameters of our model are listed in the Table S1. The reduced electric field (i.e., the ratio of electric field over total gas number density, E/N) is one of the most important parameters in controlling the distribution of the electron energy deposition to different excitation modes and to the formation of active species in a non-equilibrium plasma. It is expressed in Td, where 1 Td =  $10^{-17}$  V cm<sup>2</sup>. Figure S3 shows the fraction of electron energy deposited into different excitation channels in a (a) 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture and (b) 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture with 12% O<sub>2</sub> addition, as a function of E/N. The electron energy loss fractions were calculated by the BOLSIG+ solver.<sup>5</sup> The regions in blue indicate the range of E/N values of the discharge conditions solved in our chemical kinetics model. As shown in Figure S3(a), the most efficient mechanism for electron energy loss is the elastic collision with CH<sub>4</sub> and CO<sub>2</sub> molecules and the dissociation of CH<sub>4</sub> at a relatively low reduced electric field (< 20 Td). In our model, the E/N ranges from several 100 Td (during the microdischarges) to a few Td (during the afterglows in between the microdischarges), so if we take a timeaverage, we get a range of 20-100 Td, for which the dissociation channel of CH<sub>4</sub> dominates the plasma discharge. The change of mixture ratio upon 12% O<sub>2</sub> addition dramatically alters the energy branching, and the plasma energy is now primarily transferred to the dissociation modes of CH<sub>4</sub> and O<sub>2</sub>, as shown in Figure S3(b). As a result, the addition of O<sub>2</sub> to the CH<sub>4</sub>/CO<sub>2</sub> mixture promotes the dissociation of O<sub>2</sub> to produce O and O(<sup>1</sup>D) radicals, which facilitates the oxidation of CH<sub>4</sub> to oxygenates.

Condition	peak power	duration	n <sub>e,max</sub>	$T_{\rm e,max}$	E/N, <sub>max</sub>
Condition	density (W/cm <sup>3</sup> )	(ns)	(cm <sup>-3</sup> )	(eV)	(Td)
0.50 CH <sub>4</sub> /0.50 CO <sub>2</sub>	2.13×10⁵	200	2.40×10 <sup>13</sup>	4.32	242
0.44 CH <sub>4</sub> /0.44 CO <sub>2</sub> /0.12 O <sub>2</sub>	2.78×10⁵	200	1.05×10 <sup>13</sup>	6.29	571

Table S1. Plasma parameters in the model

(n<sub>e,max</sub>: maximum electron density; T<sub>e,max</sub>: maximum electron temperature; E/N<sub>,max</sub>: maximum electron

temperature)



Figure S3. Fractions of electron energy deposited into different excitation modes in a (a) 1:1 CH<sub>4</sub>/CO<sub>2</sub>, and (b) 1:1 CH<sub>4</sub>/CO<sub>2</sub>/ mixture with 12% O<sub>2</sub>, as a function of E/N (att: attachment; ela: elastic; ele: electronic excitation; dis: dissociation; ion: ionization).

# S.6. Reaction pathway analysis for the most important oxygenates in a 1:1 $CO_2$ -CH<sub>4</sub> mixture



Figure S4. Reaction pathway analysis for HCOOH, COOH,  $CH_3OH$ ,  $CH_3O$ ,  $CH_3O_2$ ,  $CH_2O$ ,  $CH_2OH$  and OH for a 1:1  $CH_4/CO_2$  discharge mixture without  $O_2$ , at atmospheric pressure, at a PSU power of 40 W, a residence time of 6.78 s, and temperature of 35 °C. Note that for OH, for the sake of clarity, the analysis is split in formation reactions and consumption reactions, due to the many reactions taking place.

# S.7. The consumption pathways of $CO_2$ and $O_2$ for the 1:1 $CH_4/CO_2$ mixture with or without $O_2$ addition (Table R1-R4)

The consumption pathways of CO<sub>2</sub> and O<sub>2</sub> for the 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture with or without O<sub>2</sub> addition are listed in Table R1-R4. As can be seen, the main competing reaction of CO<sub>2</sub> and O<sub>2</sub> is the electron impact reaction for plasma energy. In addition to the electron impact reaction, there is another competing reaction of CO<sub>2</sub> or O<sub>2</sub> based on the path flux analysis, that is,  $CH_2 + CO_2 \rightarrow CH_2O + CO$  and  $CH_2 + O_2 \rightarrow CO + H_2O$  (COOH + H). However, this competing reaction has negligible influence on the formation of oxygenates. This further enhances the conclusion presented in the manuscript that two types of reactions are responsible for the production enhancement of oxygenated compounds upon O<sub>2</sub> addition.

Reaction	(mol/cm <sup>3</sup> )	Contribution ratio
$e + CO_2 \rightarrow e + CO + O/O(^1D)/O(^1S)$	1.05×10 <sup>-6</sup>	52.4%
$e + CO_2 \rightarrow CO + O^-$	3.14×10 <sup>-7</sup>	15.6%
$O(^{1}D) + CO_{2} \rightarrow CO + O_{2}$	3.06×10 <sup>-7</sup>	15.2%
$CH_2 + CO_2 \rightarrow CH_2O + CO$	2.76×10 <sup>-7</sup>	13.7%
$O(^{1}S) + CO_{2} \rightarrow CO + O_{2}$	4.45×10⁻ <sup>8</sup>	2.2%
$\mathrm{CO}_2{}^+ + \mathrm{CO}_2 + \mathrm{M} \to \mathrm{C}_2\mathrm{O}_4{}^+ + \mathrm{M}$	6.68×10 <sup>-9</sup>	0.3%
$e + CO_2 \rightarrow CO_2^+ + 2e$	4.20×10 <sup>-9</sup>	0.2%

Table R1. CO<sub>2</sub> consumption pathways in a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture.

Table R2. O<sub>2</sub> consumption pathways in a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture.

Reaction	(mol/cm <sup>3</sup> )	Contribution ratio
$CHO + O_2 \rightarrow CO + HO_2$	<b>3.17</b> ×10-7	59.1%
$C_2H_5 + O_2 \rightarrow C_2H_5O_2$	6.28×10 <sup>-8</sup>	11.7%
$H + O_2 + M \rightarrow HO_2 + M$	4.83×10 <sup>−8</sup>	9.0%
$CH_2(S) + O_2 \rightarrow CO + OH + H$	3.15×10⁻ <sup>8</sup>	5.9%
$C_2H_3 + O_2 \rightarrow CH_2O + CHO$	1.62×10 <sup>-8</sup>	3.0%
$CH_2(S) + O_2 \rightarrow CO + H_2O$	1.35×10 <sup>-8</sup>	2.5%

$CH_3 + O_2 \rightarrow CH_3O_2$	1.25×10 <sup>-8</sup>	2.3%
$e + O_2 \rightarrow e + O_2(e1)$	9.44×10 <sup>-9</sup>	1.8%
$CH_{3}CHOH + O_{2} \rightarrow CH_{3}CHO + HO_{2}$	7.93×10 <sup>-9</sup>	1.5%
$CH_2OH + O_2 \rightarrow CH_2O + HO_2$	5.20×10 <sup>-9</sup>	1.0%

Table R3. CO<sub>2</sub> consumption pathways in a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture with 12% O<sub>2</sub> addition.

Reaction	(mol/cm <sup>3</sup> )	Contribution ratio
$e + CO_2 \rightarrow e + CO + O/O(^1D)/O(^1S)$	6.77×10 <sup>-6</sup>	86.8%
$O(^{1}D) + CO_{2} \rightarrow CO + O_{2}$	7.63×10 <sup>-7</sup>	9.8%
$O_3^- + CO_2 \rightarrow CO_3^- + O_2$	8.08×10 <sup>-8</sup>	1.0%
$O(^{1}S) + CO_{2} \rightarrow CO + O_{2}$	6.45×10 <sup>-8</sup>	0.8%
$O_4^- + CO_2 \rightarrow CO_4^- + O_2$	3.75×10 <sup>-8</sup>	0.5%
$e + CO_2 \rightarrow CO + O^-$	3.17×10 <sup>-8</sup>	0.4%
$CH_2 + CO_2 \rightarrow CH_2O + CO$	1.75×10 <sup>-8</sup>	0.2%

Table R4.  $O_2$  consumption pathways in a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture with 12% O<sub>2</sub> addition.

Reaction	(mol/cm <sup>3</sup> )	Contribution ratio
$CHO + O_2 \rightarrow CO + HO_2$	6.99×10 <sup>-6</sup>	43.2%
$O + O_2 + M \to O_3 + M$	2.64×10 <sup>-6</sup>	16.3%
$e + O_2 \rightarrow e + O + O/O(^1D)$	1.45×10 <sup>-6</sup>	9.0%
$e + O_2 \rightarrow e + O_2(e)$	1.40×10 <sup>-6</sup>	8.6%
$CH_3 + O_2 \rightarrow CH_3O_2$	1.25×10 <sup>-6</sup>	7.8%
$\rm H + O_2 + M \rightarrow \rm HO_2 + M$	1.14×10 <sup>-6</sup>	7.0%
$CH_2OH + O_2 \rightarrow CH_2O + HO_2$	6.12×10 <sup>-7</sup>	3.8%
$O_2^+ + O_2 + M \rightarrow O_4^+ + M$	1.20×10 <sup>-7</sup>	0.7%
$CH_2 + O_2 \rightarrow CO + H_2O$	1.04×10 <sup>-7</sup>	0.6%
$CH_2 + O_2 \rightarrow COOH + H$	3.94×10 <sup>-8</sup>	0.2%

### S.8. Reaction pathway analysis of singlet oxygen O<sub>2</sub>( $a^{1}\Delta_{g}$ )\*.

As can be seen in Figure S5,  $O_2(a^1\Delta_g)$  is primarily formed via electron impact electronic excitation,  $e + O_2 \rightarrow e + O_2(a^1\Delta_g)$ , which is responsible for 99.9% and 100.0% for  $O_2(a^1\Delta_g)$ formation, with or without  $O_2$  addition, respectively. However, the consumption way shows that most of the  $O_2(a^1\Delta_g)$  are consumed via the relaxation reactions. Only 1.8% of  $O_2(a^1\Delta_g)$ react with  $CH_3CHOH$  to form  $HO_2$  without  $O_2$  addition. Upon  $O_2$  addition, 0.3% of  $O_2(a^1\Delta_g)$ participate in the chain reaction to form  $O_3$ . The reaction pathway analysis demonstrates that the effects of  $O_2(a^1\Delta_g)$  are negligible in this work.

\*:  $O_2(a^1\Delta_g)$  represents  $O_2(e1)$ .



Figure S5. Reaction pathway analysis for  $O_2(a^1\Delta_g)$  for a 1:1 CH<sub>4</sub>/CO<sub>2</sub> mixture (a) with and (b) without 12% O<sub>2</sub> addition respectively. at atmospheric pressure, at a PSU power of 40 W, a residence time of 6.78 s, and temperature of 35 °C.
## S.9. Overview of the reactions included in our model (Table S2 – S12).

The units of the rate coefficients are in s<sup>-1</sup>, cm<sup>3</sup> s<sup>-1</sup> and cm<sup>6</sup> s<sup>-1</sup> for first, second and third reactions, respectively. In the expressions of the rate constants,  $T_g$  denotes the gas temperature in K,  $T_e$  denotes the average electron temperature in K, and R denotes the ideal gas constant, 8.3145 J mol<sup>-1</sup> K<sup>-1</sup>.

Reaction	Rate coefficients	Ref
$e + O + M \rightarrow O^- + M$	1.00×10 <sup>-31</sup>	6,7
$e + O_2 + M \rightarrow O_2^- + M$	f(σ, EEDF) <sup>[1]</sup>	8
$e + O_2 + H_2 \rightarrow O_2^- + H_2$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + CO \rightarrow O_2^- + CO$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + CO(e1) \rightarrow O_2^- + CO(e1)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + CO(e2) \rightarrow O_2^- + CO(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + CO(e3) \rightarrow O_2^- + CO(e3)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + CO(e4) \rightarrow O_2^- + CO(e4)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + O_2(e1) \rightarrow O_2^- + O_2(e1)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 + O_2(e2) \rightarrow O_2^- + O_2(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2 \rightarrow O^- + O$	f(σ, EEDF)	8
$e + O_3 \rightarrow O^- + O_2$	f(σ, EEDF)	8
$e + O_3 \rightarrow O_2^- + O$	f(σ, EEDF)	8
$e + H_2O \rightarrow O^- + H_2$	f(σ, EEDF)	8
$e + H_2O \rightarrow OH^- + H$	f(σ, EEDF)	8
$e + CO \rightarrow O^- + C$	f(σ, EEDF)	8
$e + CO_2 \rightarrow O^- + CO$	f(σ, EEDF)	8

Table S2. Electron impact attachment and dissociative attachment reactions

<sup>[1]</sup>: the rate coefficients for electron impact reactions depend on the cross sections and electron energy distribution function (EEDF), and is calculated by means of a Boltzmann solver, integrated in ZDPlasKin.

Table S3.	Electron	impact	excitation	reactions
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Reaction	Rate coefficients	Ref
$e + O \rightarrow e + O(^{1}D)$	f(σ, EEDF)	8

$e + O_2 \rightarrow e + O_2(e1)$	f(σ, EEDF)	8
$e + O_2 \rightarrow e + O_2(e2)$	f(σ, EEDF)	8
$e + O_2 \rightarrow e + O_2(e3)$	f(σ, EEDF)	8
$e + CO \rightarrow e + CO(e1)$	f(σ, EEDF)	8
$e + CO \rightarrow e + CO(e2)$	f(σ, EEDF)	8
$e + CO \rightarrow e + CO(e3)$	f(σ, EEDF)	8
$e + CO \rightarrow e + CO(e4)$	f(σ, EEDF)	8

## Table S4. Electron impact dissociation reactions

Reaction	Rate coefficients	Ref
$e + H_2 \rightarrow e + H + H$	f(σ, EEDF)	8,9
$e + O_2 \rightarrow e + O + O$	f(σ, EEDF)	8
$e + O_2 \rightarrow e + O + O(^1D)$	f(σ, EEDF)	8
$e + O_3 \rightarrow e + O_2 + O$	f(σ, EEDF)	6,7
$e + H_2O \rightarrow e + OH + H$	f(σ, EEDF)	8
$e + H_2O \rightarrow e + O(^1D) + H_2$	f(σ, EEDF)	8
$e + H_2O \rightarrow e + O + H + H$	f(σ, EEDF)	8
$e + CO \rightarrow e + C + O$	f(σ, EEDF)	8
$e + CO_2 \rightarrow e + CO + O$	f(σ, EEDF)	8,10
$e + CO_2 \rightarrow e + CO + O(^1D)$	f(σ, EEDF)	8,10
$e + CO_2 \rightarrow e + CO + O(^1S)$	f(σ, EEDF)	8,10,11
$e + CH \rightarrow e + C + H$	f(σ, EEDF)	12
$e + CH_2 \rightarrow e + CH + H$	f(σ, EEDF)	12
$e + CH_2 \rightarrow e + C + H_2$	f(σ, EEDF)	12
$e + CH_2 \rightarrow e + C + H + H$	f(σ, EEDF)	12
$e + CH_3 \rightarrow e + CH_2 + H$	f(σ, EEDF)	12
$e + CH_3 \rightarrow e + CH + H_2$	f(σ, EEDF)	12
$e + CH_3 \rightarrow e + C + H_2 + H$	f(σ, EEDF)	12
$e + CH_4 \rightarrow e + CH_3 + H$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow e + CH_2 + H_2$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow e + CH + H_2 + H$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow e + C + H_2 + H_2$	f(σ, EEDF)	6,7
$e + C_2 H \rightarrow e + C_2 + H$	f(σ, EEDF)	13
$e + C_2 H \rightarrow e + C + CH$	f(σ, EEDF)	13

$e + C_2 H_2 \rightarrow e + C_2 H + H$	f(σ, EEDF)	13
$e + C_2 H_2 \rightarrow e + C_2 + H_2$	f(σ, EEDF)	13
$e + C_2H_2 \rightarrow e + C_2 + H + H$	f(σ, EEDF)	13
$e + C_2H_2 \rightarrow e + CH_2 + C$	f(σ, EEDF)	13
$e + C_2 H_2 \rightarrow e + CH + CH$	f(σ, EEDF)	13
$e + C_2 H_3 \rightarrow e + C_2 H_2 + H$	f(σ, EEDF)	13
$e + C_2 H_3 \rightarrow e + C_2 H + H_2$	f(σ, EEDF)	13
$e + C_2 H_3 \rightarrow e + C_2 H + H + H$	f(σ, EEDF)	13
$e + C_2H_3 \rightarrow e + C_2 + H_2 + H$	f(σ, EEDF)	13
$e + C_2H_3 \rightarrow e + CH_3 + C$	f(σ, EEDF)	13
$e + C_2H_3 \rightarrow e + CH_2 + CH$	f(σ, EEDF)	13
$e + C_2H_4 \rightarrow e + C_2H_3 + H$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + C_2H_2 + H_2$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + C_2H_2 + H + H$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + C_2H + H_2 + H$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + CH_4 + C$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + CH_3 + CH$	f(σ, EEDF)	8,14
$e + C_2H_4 \rightarrow e + CH_2 + CH_2$	f(σ, EEDF)	8,14
$e + C_2 H_5 \rightarrow e + C_2 H_4 + H$	f(σ, EEDF)	13
$e + C_2 H_5 \rightarrow e + C_2 H_3 + H_2$	f(σ, EEDF)	13
$e + C_2H_5 \rightarrow e + C_2H_3 + H + H$	f(σ, EEDF)	13
$e + C_2H_5 \rightarrow e + C_2H_2 + H_2 + H$	f(σ, EEDF)	13
$e + C_2H_5 \rightarrow e + C_2H + H_2 + H_2$	f(σ, EEDF)	13
$e + C_2 H_5 \rightarrow e + C H_4 + C H$	f(σ, EEDF)	13
$e + C_2 H_5 \rightarrow e + C H_3 + C H_2$	f(σ, EEDF)	13
$e + C_2 H_6 \rightarrow e + C_2 H_5 + H$	f(σ, EEDF)	8,15
$e + C_2 H_6 \rightarrow e + C_2 H_4 + H_2$	f(σ, EEDF)	8,15
$e + C_2H_6 \rightarrow e + C_2H_3 + H_2 + H$	f(σ, EEDF)	8,15
$e + C_2H_6 \rightarrow e + C_2H_2 + H_2 + H_2$	f(σ, EEDF)	8,15
$e + C_2 H_6 \rightarrow e + C H_4 + C H_2$	f(σ, EEDF)	8,15
$e + C_2H_6 \rightarrow e + CH_3 + CH_3$	f(σ, EEDF)	8,15
$e + C_3H_5 \rightarrow e + C_2H_2 + CH_3$	f(σ, EEDF)	13
$e + C_3H_5 \rightarrow e + C_2H + CH_4$	f(σ, EEDF)	13
$e + C_3H_6 \rightarrow e + C_3H_5 + H$	f(σ, EEDF)	8,16

$e + C_3H_6 \rightarrow e + C_2H_4 + CH_2$	f(σ, EEDF)	8,16
$e + C_3H_6 \rightarrow e + C_2H_3 + CH_3$	f(σ, EEDF)	8,16
$e + C_3H_6 \rightarrow e + C_2H_2 + CH_4$	f(σ, EEDF)	8,16
$e + C_3H_7 \rightarrow e + C_3H_6 + H$	f(σ, EEDF)	13
$e + C_3H_7 \rightarrow e + C_3H_5 + H_2$	f(σ, EEDF)	13
$e + C_3H_7 \rightarrow e + C_2H_4 + CH_3$	f(σ, EEDF)	13
$e + C_3H_7 \rightarrow e + C_2H_3 + CH_4$	f(σ, EEDF)	13
$e + C_3 H_8 \rightarrow e + C_3 H_7 + H$	f(σ, EEDF)	8
$e + C_3 H_8 \rightarrow e + C_3 H_6 + H_2$	f(σ, EEDF)	8
$e + C_3 H_8 \rightarrow e + C_2 H_6 + C H_2$	f(σ, EEDF)	8
$e + C_3H_8 \rightarrow e + C_2H_5 + CH_3$	f(σ, EEDF)	8
$e + C_3 H_8 \rightarrow e + C_2 H_4 + C H_4$	f(σ, EEDF)	8

## Table S5. Electron impact ionization reactions

Reaction	Rate coefficients	Ref
$e + H \rightarrow 2e + H^+$	f(σ, EEDF)	8
e + O →2e + O <sup>+</sup>	f(σ, EEDF)	8
$e + H_2 \rightarrow 2e + H_2^+$	f(σ, EEDF)	8
$e + OH \rightarrow 2e + OH^+$	f(σ, EEDF)	6,7
$e + O_2 \rightarrow 2e + O_2^+$	f(σ, EEDF)	8
$e + O_2 \rightarrow 2e + O^+ + O$	f(σ, EEDF)	8
$e + O_3 \rightarrow 2e + O_2^+ + O$	f(σ, EEDF)	8
$e + O_3 \rightarrow e + O^+ + O^- + O$	f(σ, EEDF)	8
$e + C \rightarrow 2e + C^+$	f(σ, EEDF)	8
$e + CO \rightarrow 2e + CO^+$	f(σ, EEDF)	8
$e + CO \rightarrow 2e + C^+ + O$	f(σ, EEDF)	8
$e + CO \rightarrow 2e + O^+ + C$	f(σ, EEDF)	8
$e + CO_2 \rightarrow 2e + CO_2^+$	f(σ, EEDF)	8
$e + CO_2 \rightarrow 2e + O^+ + CO$	f(σ, EEDF)	8
$e + CO_2 \rightarrow 2e + C^+ + O_2$	f(σ, EEDF)	8
$e + CO_2 \rightarrow 2e + CO^+ + O$	f(σ, EEDF)	8
$e + CO_2 \rightarrow 2e + O_2^+ + C$	f(σ, EEDF)	8
$e + CH \rightarrow 2e + CH^+$	f(σ, EEDF)	6,7
$e + CH_2 \rightarrow 2e + CH_2^+$	f(σ, EEDF)	6,7

$e + CH_3 \rightarrow 2e + CH_3^+$	f(σ, EEDF)	6,7
$e + CH_3 \rightarrow 2e + CH_2^+ + H$	f(σ, EEDF)	6,7
$e + CH_3 \rightarrow 2e + CH^+ + H_2$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow 2e + CH_4^+$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow 2e + CH_3^+ + H$	f(σ, EEDF)	6,7
$e + CH_4 \rightarrow 2e + CH_2^+ + H_2$	f(σ, EEDF)	6,7
$e + C_2 H_2 \rightarrow 2e + C_2 H_2^+$	f(σ, EEDF)	6,7
$e + C_2 H_3 \rightarrow 2e + C_2 H_3^+$	f(σ, EEDF)	6,7
$e + C_2H_3 \rightarrow 2e + C_2H_2^+ + H$	f(σ, EEDF)	6,7
$e + C_2 H_4 \rightarrow 2e + C_2 H_4^+$	f(σ, EEDF)	6,7
$e + C_2H_4 \rightarrow 2e + C_2H_3^+ + H$	f(σ, EEDF)	6,7
$e + C_2H_4 \rightarrow 2e + C_2H_2^+ + H_2$	f(σ, EEDF)	6,7
$e + C_2 H_5 \rightarrow 2e + C_2 H_5^+$	f(σ, EEDF)	6,7
$e + C_2H_5 \rightarrow 2e + C_2H_4^+ + H$	f(σ, EEDF)	6,7
$e + C_2H_5 \rightarrow 2e + C_2H_3^+ + H_2$	f(σ, EEDF)	6,7
$e + C_2H_5 \rightarrow 2e + C_2H_2^+ + H_2 + H_3$	f(σ, EEDF)	6,7
$e + C_2 H_6 \rightarrow 2e + C_2 H_6^+$	f(σ, EEDF)	6,7
$e + C_2H_6 \rightarrow 2e + C_2H_5^+ + H$	f(σ, EEDF)	6,7
$e + C_2 H_6 \rightarrow 2e + C_2 H_4^+ + H_2$	f(σ, EEDF)	6,7
$e + C_2H_6 \rightarrow 2e + C_2H_3^+ + H_2 + H_3^+$	f(σ, EEDF)	6,7
$e + C_2H_6 \rightarrow 2e + C_2H_2^+ + H_2 + H_2$	f(σ, EEDF)	6,7
$e + C_2H_6 \rightarrow 2e + CH_3^+ + CH_3$	f(σ, EEDF)	6,7
$e + C_3H_5 \rightarrow 2e + C_2H_3^+ + CH_2$	f(σ, EEDF)	6,7
$e + C_3H_5 \rightarrow 2e + C_2H_2^+ + CH_3$	f(σ, EEDF)	6,7
$e + C_3H_5 \rightarrow 2e + CH_3^+ + C_2H_2$	f(σ, EEDF)	6,7
$e + C_3H_6 \rightarrow 2e + C_2H_5^+ + CH$	f(σ, EEDF)	6,7
$e + C_3H_6 \rightarrow 2e + C_2H_4^+ + CH_2$	f(σ, EEDF)	6,7
$e + C_3H_6 \rightarrow 2e + C_2H_3^+ + CH_3$	f(σ, EEDF)	6,7
$e + C_3H_6 \rightarrow 2e + C_2H_2^+ + CH_4$	f(σ, EEDF)	6,7
$e + C_3H_6 \rightarrow 2e + CH_3^+ + C_2H_3$	f(σ, EEDF)	6,7
$e + C_3H_7 \rightarrow 2e + C_2H_5^+ + CH_2$	f(σ, EEDF)	6,7
$e + C_3H_7 \rightarrow 2e + C_2H_4^+ + CH_3$	f(σ, EEDF)	6,7
$e + C_3H_7 \rightarrow 2e + C_2H_3^+ + CH_4$	f(σ, EEDF)	6,7
$e + C_3H_7 \rightarrow 2e + \overline{CH_3^+ + C_2H_4}$	f(σ, EEDF)	6,7

$e + C_3H_8 \rightarrow 2e + C_2H_5^+ + CH_3$	f(σ, EEDF)	6,7
$e + C_3H_8 \rightarrow 2e + C_2H_4^+ + CH_4$	f(σ, EEDF)	6,7

Table S6. Electron	impact excited	species at	tachment o	r ionization
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Reaction	Rate coefficients	Ref
$e + O_2(e1) + CH_4 \rightarrow O_2^- + CH_4$	3.00×10 <sup>-30</sup>	6,7
$e + O_2(e2) + CH_4 \rightarrow O_2^- + CH_4$	3.00×10 <sup>-30</sup>	6,7
$e + O_2(e1) + H_2 \rightarrow O_2^- + H_2$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + H_2 \rightarrow O_2^- + H_2$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + CO_2 \rightarrow O_2^- + CO_2$	3.00×10 <sup>-30</sup>	6,7
$e + O_2(e2) + CO_2 \rightarrow O_2^- + CO_2$	3.00×10 <sup>-30</sup>	6,7
$e + O_2(e1) + CO \rightarrow O_2^- + CO$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + CO \rightarrow O_2^- + CO$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + CO(e1) \rightarrow O_2^- + CO(e1)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + CO(e1) \rightarrow O_2^- + CO(e1)$	3.00×1 <sup>0-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + CO(e2) \rightarrow O_2^- + CO(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + CO(e2) \rightarrow O_2^- + CO(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + CO(e3) \rightarrow O_2^- + CO(e3)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + CO(e3) \rightarrow O_2^- + CO(e3)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + CO(e4) \rightarrow O_2^- + CO(e4)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + CO(e4) \rightarrow O_2^- + CO(e4)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + O_2 \rightarrow O_2^- + O_2$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + O_2(e1) \rightarrow O_2^- + O_2(e1)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e1) + O_2(e2) \rightarrow O_2^- + O_2(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + O_2 \rightarrow O_2^- + O_2$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + O_2(e1) \rightarrow O_2^- + O_2(e1)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
$e + O_2(e2) + O_2(e2) \rightarrow O_2^- + O_2(e2)$	3.00×10 <sup>-30</sup> ×(2.0/3.0)	6,7
e + O <sub>2</sub> (e1) →2e + O <sub>2</sub> <sup>+</sup>	f(σ, EEDF)	6,7
$e + O_2(e1) \rightarrow 2e + O^+ + O$	f(σ, EEDF)	6,7
$e + O_2(e2) \rightarrow 2e + O_2^+$	f(σ, EEDF)	6,7
$e + O_2(e2) \rightarrow 2e + O^+ + O$	f(σ, EEDF)	6,7
$e + O_2(e3) \rightarrow 2e + O_2^+$	f(σ, EEDF)	6,7
$e + O_2(e3) \rightarrow 2e + O^+ + O$	f(σ, EEDF)	6,7
$e + CO(e1) \rightarrow 2e + CO^+$	f(σ, EEDF)	6,7

$e + CO(e1) \rightarrow 2e + C^+ + O$	f(σ, EEDF)	6,7
$e + CO(e1) \rightarrow 2e + O^+ + C$	f(σ, EEDF)	6,7
$e + CO(e2) \rightarrow 2e + CO^+$	f(σ, EEDF)	6,7
$e + CO(e2) \rightarrow 2e + C^+ + O$	f(σ, EEDF)	6,7
$e + CO(e2) \rightarrow 2e + O^+ + C$	f(σ, EEDF)	6,7
$e + CO(e3) \rightarrow 2e + CO^+$	f(σ, EEDF)	6,7
$e + CO(e3) \rightarrow 2e + C^+ + O$	f(σ, EEDF)	6,7
$e + CO(e3) \rightarrow 2e + O^+ + C$	f(σ, EEDF)	6,7
$e + CO(e4) \rightarrow 2e + CO^+$	f(σ, EEDF)	6,7
$e + CO(e4) \rightarrow 2e + C^+ + O$	f(σ, EEDF)	6,7
$e + CO(e4) \rightarrow 2e + O^+ + C$	f(σ, EEDF)	6,7

# Table S7. Electron impact de-excitation reactions

Reaction	Rate coefficients	Ref
$e + O_2(e1) \rightarrow e + O_2$	f(σ, EEDF)	6,7
$e + O_2(e2) \rightarrow e + O_2$	f(σ, EEDF)	6,7
$e + O_2(e3) \rightarrow e + O_2$	f(σ, EEDF)	6,7
$e + CO(e1) \rightarrow CO + e$	f(σ, EEDF)	6,7
$e + CO(e2) \rightarrow CO + e$	f(σ, EEDF)	6,7
$e + CO(e3) \rightarrow CO + e$	f(σ, EEDF)	6,7
$e + CO(e4) \rightarrow CO + e$	f(σ, EEDF)	6,7

# Table S8. Reactions stimulated by excited species

Reaction	Rate coefficients	Ref
$O(^{1}D) + H \rightarrow OH$	4.36×10 <sup>-32</sup> ×(298/ <i>T</i> <sub>g</sub> ) <sup>1.0</sup>	17
$O(^{1}D) + O \rightarrow O + O$	8.00×10 <sup>-12</sup>	17
$O(^{1}D) + O_{2} \rightarrow O + O_{2}$	$6.40 \times 10^{-12} \times \exp(67.0/T_g)$	17
$O(^{1}D) + O_{3} \rightarrow O_{2} + O + O$	1.20×10 <sup>-10</sup>	17
$O(^{1}D) + O_{3} \rightarrow O_{2} + O_{2}$	1.20×10 <sup>-10</sup>	17
$O(^{1}D) + H_{2} \rightarrow OH + H$	$1.38 \times 10^{-10} \times \exp(21.0/T_g)$	17
$O(^{1}D) + H_{2} \rightarrow H_{2} + O$	$2.37 \times 10^{-10} \times \exp(120.7/T_g)$	17
$O(^{1}D) + OH \rightarrow H + O_{2}$	$6.00 \times 10^{-11} \times T_g^{-0.186} \times \exp(-154.0/T_g)$	17
$O(^{1}D) + HO_{2} \rightarrow OH + O_{2}$	$2.90 \times 10^{-11} \times \exp(200.0/T_g)$	17
$O(^{1}D) + H_{2}O \rightarrow OH + OH$	1.69×10 <sup>-10</sup> ×exp(36.0/ <i>T</i> <sub>g</sub> )	17

$O(^1D) + H_2O \rightarrow H_2 + O_2$	2.20×10 <sup>-12</sup>	17
$O(^1D) + H_2O \rightarrow H_2O + O$	1.20×10 <sup>-11</sup>	17
$O(^{1}D) + H_{2}O_{2} \rightarrow H_{2}O + O_{2}$	5.20×10 <sup>-10</sup>	17
$O(^{1}D) + H_{2}O_{2} \rightarrow HO_{2} + OH$	5.20×10 <sup>-10</sup>	17
$O(^{1}D) + CO \rightarrow O + CO$	4.70×10 <sup>-11</sup> ×exp(-62.4/T <sub>g</sub> )	17
$O(^{1}D) + CO \rightarrow CO_{2}$	5.00×10 <sup>-11</sup>	23
$O(^{1}D) + CO_{2} \rightarrow CO + O_{2}$	2.01×10 <sup>-10</sup>	17
$O(^{1}D) + CO_{2} \rightarrow O + CO_{2}$	7.40×10 <sup>-11</sup>	17
$O(^{1}D) + CH_{4} \rightarrow CH_{4} + O$	$1.79 \times 10^{-13} \times \exp(107.0/T_g)$	17
$O(^{1}D) + CH_{4} \rightarrow CH_{3} + OH$	1.13×10 <sup>-10</sup>	17
$O(^{1}D) + CH_{4} \rightarrow CH_{2}O + H_{2}$	7.50×10 <sup>-12</sup>	17
$O(^{1}D) + CH_{4} \rightarrow CH_{2}OH + H$	3.00×10 <sup>-11</sup>	17
$O(^{1}D) + CH_{2}O \rightarrow CO + H_{2}O$	1.66×10 <sup>-10</sup>	17
$O(^{1}D) + CH_{3}OH \rightarrow CH_{2}OH + OH$	2.99×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{2} \rightarrow C_{2}H + OH$	2.20×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{2} \rightarrow CH_{2}(S)^{[2]} + CO$	2.66×10 <sup>-10</sup>	18
$O(^{1}D) + C_{2}H_{2} \rightarrow C_{2}HO + H$	1.00×10 <sup>-10</sup>	18
$O(^1D) + C_2H_4 \rightarrow C_2H_3 + OH$	2.20×10 <sup>-10</sup>	17
$O(^1D) + C_2H_4 \rightarrow CH_2O + CH_2$	2.20×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{4} \rightarrow CHO + CH_{3}$	1.19×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{6} \rightarrow C_{2}H_{6} + O$	7.31×10 <sup>-10</sup>	17
$O(^1D) + C_2H_6 \rightarrow C_2H_5 + OH$	6.29×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{6} \rightarrow CH_{2}OH + CH_{3}$	3.49×10 <sup>-10</sup>	18
$O(^{1}D) + C_{2}H_{6} \rightarrow CH_{3}O + CH_{3}$	1.60×10 <sup>-10</sup>	17
$O(^1D) + C_2H_6 \rightarrow C_2H_5O + H$	1.60×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{6} \rightarrow CH_{3}CHOH + H$	1.60×10 <sup>-10</sup>	17
$O(^{1}D) + C_{2}H_{6} \rightarrow CH_{3}CHO + H_{2}$	9.96×10 <sup>-12</sup>	18
$O(^{1}D) + C_{3}H_{8} \rightarrow C_{3}H_{8} + O$	9.51×10 <sup>-10</sup>	17
$O(^{1}D) + C_{3}H_{8} \rightarrow C_{3}H_{7} + OH$	2.20×10 <sup>-10</sup>	17
$O(^{1}S) \rightarrow O(^{1}D)$	1.34	19
$O(^{1}S) + H \rightarrow OH$	$4.36 \times 10^{-32} \times (298/T_g)^{1.0}$	17
$O(^{1}S) + O \rightarrow O(^{1}D) + O$	$5.00 \times 10^{-11} \times \exp(-301.0/T_g)$	17
$O(^{1}S) + O \rightarrow O + O$	$3.33 \times 10^{-11} \times \exp(-300.0/T_g)$	17
$O(^{1}S) + O_{2} \rightarrow O + O_{2}$	$4.30 \times 10^{-12} \times \exp(-850.0/T_g)$	20

$O(^1S) + O_2 \rightarrow O(^1D) + O_2$	1.30×10 <sup>-12</sup> ×exp(-850.0/ <i>T</i> <sub>g</sub> )	21,23
$O(^1S) + O_2 \rightarrow O + O + O$	$3.00 \times 10^{-12} \times \exp(-850.0/T_g)$	17
$O(^1S) + O_3 \rightarrow O_2 + O_2$	2.90×10 <sup>-10</sup>	17
$O(^1S) + O_3 \rightarrow O(^1D) + O_2 + O$	2.90×10 <sup>-10</sup>	17
$O(^1S) + H_2 \rightarrow H_2 + O$	1.00×10 <sup>-10</sup>	17
$O(^1S) + H_2 \rightarrow OH + H$	2.60×10 <sup>-16</sup>	17
$O(^1S) + OH \rightarrow H + O_2$	$6.00 \times 10^{-11} \times T_g^{-0.186} \times \exp(-154.0/T_g)$	17
$O(^1S) + HO_2 \rightarrow OH + O_2$	$2.90 \times 10^{-11} \times \exp(200.0/T_g)$	17
$O(^1S) + H_2O \rightarrow H_2O + O(^1D)$	1.50×10 <sup>-10</sup>	17
$O(^1S) + H_2O \rightarrow H_2O + O$	4.50×10 <sup>-11</sup>	17
$O(^1S) + H_2O \rightarrow OH + OH$	3.00×10 <sup>-10</sup>	17
$O(^1S) + CO_2 \rightarrow CO + O_2$	2.00×10 <sup>-10</sup>	17
$O(^1S) + CO_2 \rightarrow CO_2 + O$	2.00×10 <sup>-10</sup>	17
$O(^1S) + CH_4 \rightarrow CH_3 + OH$	2.20×10 <sup>-10</sup>	17
$O(^1S) + CH_4 \rightarrow CH_2O + H_2$	2.40×10 <sup>-11</sup>	17
$O(^1S) + C_2H_2 \rightarrow C_2H + OH$	2.20×10 <sup>-10</sup>	17
$O(^1S) + C_2H_4 \rightarrow C_2H_3 + OH$	2.20×10 <sup>-10</sup>	17
$O(^1S) + C_2H_6 \rightarrow C_2H_5 + OH$	1.60×10 <sup>-10</sup>	17
$O(^1S) + C_2H_6 \rightarrow CH_3 + CH_3O$	1.60×10 <sup>-10</sup>	17
$O(^1S) + C_3H_8 \rightarrow C_3H_7 + OH$	2.20×10 <sup>-10</sup>	17
$O_2(e1) \rightarrow O_2$	2.60×10 <sup>-4</sup>	6,7
$O_2(e2) \rightarrow O_2$	1.10×10	6,7
$O_2(e1) + M \rightarrow O_2 + M$	$3.80 \times 10^{-18} \times \exp(-205.0/T_g)$	6,7
$O_2(e2) + M \rightarrow O_2 + M$	3.00×10 <sup>-13</sup>	6,7
$O_2(e1) + H_2 \rightarrow HO_2 + H$	$2.41 \times 10^{-10} \times \exp(-237.0 \times 10^3/(R \times T_g))$	6,7
$O_2(e2) + H_2 \rightarrow HO_2 + H$	$2.41 \times 10^{-10} \times \exp(-237.0 \times 10^3/(R \times T_g))$	6,7
$O_2(e1) + O \rightarrow O_2 + O$	7.00×10 <sup>-16</sup>	6,7
$O_2(e2) + O \rightarrow O_2(e1) + O$	$1.00 \times 10^{-11} \times \exp(-2300/T_g)$	6,7
$O_2(e1) + O + M \rightarrow O_3 + M$	$5.51 \times 10^{-34} \times (T_g/298)^{-2.6}$	6,7
$O_2(e2) + O + M \rightarrow O_3 + M$	$5.51 \times 10^{-34} \times (T_g/298)^{-2.6}$	6,7
$O_2(e1) + O_2 \rightarrow O_2 + O_2$	3.80×10 <sup>-18</sup> ×exp(-205.0×100/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + O_2 \rightarrow O_2(e1) + O_2$	$4.30 \times 10^{-22} \times T_g^{2.4} \times \exp(-281/T_g)$	6,7
$O_2(e1) + O_3 \rightarrow O + O_2 + O_2(e1)$	2.29×10 <sup>-26</sup>	6,7
$O_2(e2) + O_3 \rightarrow O + O_2 + O_2(e2)$	2.29×10 <sup>-26</sup>	6,7

$O_2(e1) + OH \rightarrow HO_2 + O$	$3.70 \times 10^{-11} \times \exp(-220000.0/(R \times T_g))$	6,7
$O_2(e2) + OH \rightarrow HO_2 + O$	$3.70 \times 10^{-11} \times \exp(-220000.0/(R \times T_g))$	6,7
$H_2O + O_2(e1) \rightarrow HO_2 + OH$	$7.72 \times 10^{-12} \times \exp(-310000.0/(R \times T_g))$	6,7
$H_2O + O_2(e2) \rightarrow HO_2 + OH$	$7.72 \times 10^{-12} \times \exp(-310000.0/(R \times T_g))$	6,7
$H_2O_2 + O_2(e1) \rightarrow HO_2 + HO_2$	$9.00 \times 10^{-11} \times \exp(-166000.0/(R \times T_g))$	6,7
$H_2O_2 + O_2(e2) \rightarrow HO_2 + HO_2$	$9.00 \times 10^{-11} \times \exp(-166000.0/(R \times T_g))$	6,7
$O_2(e1) + C \rightarrow CO + O$	3.00×10 <sup>-11</sup>	6,7
$O_2(e2) + C \rightarrow CO + O$	3.00×10 <sup>-11</sup>	6,7
$O_2(e1) + CH_3 \rightarrow CH_3O + O$	1.25×10 <sup>-11</sup> ×exp(-118000.0/(R× <i>T</i> <sub>g</sub> ))	6,7
$O_2(e2) + CH_3 \rightarrow CH_3O + O$	1.25×10 <sup>-11</sup> ×exp(-118000.0/(R× <i>T</i> <sub>g</sub> ))	6,7
$O_2(e1) + CH_4 \rightarrow CH_3 + HO_2$	6.59×10 <sup>-11</sup> ×exp(-238000.0/(R× <i>T</i> <sub>g</sub> ))	6,7
$O_2(e2) + CH_4 \rightarrow CH_3 + HO_2$	6.59×10 <sup>-11</sup> ×exp(-238000.0/(R×T <sub>g</sub> ))	6,7
$O_2(e1) + C_2H_2 \rightarrow C_2H + HO_2$	2.01×10 <sup>-11</sup> ×exp(-312000.0/(R×T <sub>g</sub> ))	6,7
$O_2(e2) + C_2H_2 \rightarrow C_2H + HO_2$	2.01×10 <sup>-11</sup> ×exp(-312000.0/(R×T <sub>g</sub> ))	6,7
$O_2(e1) + C_2H_3 \rightarrow C_2H_2 + HO_2$	$2.14 \times 10^{-14} \times (T_g/298)^{1.61} \times \exp(1.60 \times 10^{3}/(R \times T_g))$	6,7
$O_2(e2) + C_2H_3 \rightarrow C_2H_2 + HO_2$	$2.14 \times 10^{-14} \times (T_g/298)^{1.61} \times \exp(1.60 \times 10^3/(R \times T_g))$	6,7
$O_2(e1) + C_2H_5 \rightarrow C_2H_5O + O$	$6.14 \times 10^{-12} \times (T_g/298)^{-0.20} \times \exp(-1.17 \times 10^{5/(R \times T_g)})$	6,7
$O_2(e2) + C_2H_5 \rightarrow C_2H_5O + O$	$6.14 \times 10^{-12} \times (T_g/298)^{-0.20} \times \exp(-1.17 \times 10^{5}/(\mathbb{R} \times T_g))$	6,7
$O_2(e1) + C_2H_6 \rightarrow C_2H_5 + HO_2$	1.00×10 <sup>-10</sup> ×exp(-217000.0/(R× <i>T</i> <sub>g</sub> ))	6,7
$O_2(e2) + C_2H_6 \rightarrow C_2H_5 + HO_2$	$1.00 \times 10^{-10} \times \exp(-217000.0/(R \times T_g))$	6,7
$O_2(e1) + C_3H_6 \rightarrow C_3H_5 + HO_2$	9.00×10 <sup>-11</sup> ×exp(-166000.0/(R×T <sub>g</sub> ))	6,7
$O_2(e2) + C_3H_6 \rightarrow C_3H_5 + HO_2$	9.00×10 <sup>-11</sup> ×exp(-166000.0/(R×T <sub>g</sub> ))	6,7
$O_2(e1) + CO \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + CO \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e1) + C_2O \rightarrow CO_2 + CO$	3.30×10 <sup>-13</sup>	6,7
$O_2(e2) + C_2O \rightarrow CO_2 + CO$	3.30×10 <sup>-13</sup>	6,7
$O_2(e1) + CH_3CHOH \rightarrow CH_3CHO + HO_2$	1.90×10 <sup>-11</sup>	6,7
$O_2(e2) + CH_3CHOH \rightarrow CH_3CHO + HO_2$	1.90×10 <sup>-11</sup>	6,7
$CO(e1) + M \rightarrow CO + M$	1.20×10 <sup>-11</sup>	6,7
$CO(e2) + M \rightarrow CO + M$	1.20×10 <sup>-11</sup>	6,7
$CO(e3) + M \rightarrow CO + M$	1.20×10 <sup>-11</sup>	6,7
$CO(e4) + M \rightarrow CO + M$	1.20×10 <sup>-11</sup>	6,7
$CO(e1) + O + M \rightarrow CO_2 + M$	8.20×10 <sup>-34</sup> ×exp(-1510.0/ <i>T</i> g)×2.000	6,7
$CO(e2) + O + M \rightarrow CO_2 + M$	8.20×10 <sup>-34</sup> ×exp(-1510.0/ <i>T</i> <sub>g</sub> )×2.000	6,7

$CO(e3) + O + M \rightarrow CO_2 + M$	$8.20 \times 10^{-34} \times \exp(-1510.0/T_g) \times 2.000$	6,7
$CO(e4) + O + M \rightarrow CO_2 + M$	$8.20 \times 10^{-34} \times \exp(-1510.0/T_g) \times 2.000$	6,7
$CO(e1) + O_2 \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$CO(e2) + O_2 \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$CO(e3) + O_2 \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$CO(e4) + O_2 \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$CO(e1) + O_3 \rightarrow CO_2 + O_2$	4.00×10 <sup>-25</sup>	6,7
$CO(e2) + O_3 \rightarrow CO_2 + O_2$	4.00×10 <sup>-25</sup>	6,7
$CO(e3) + O_3 \rightarrow CO_2 + O_2$	4.00×10 <sup>-25</sup>	6,7
$CO(e4) + O_3 \rightarrow CO_2 + O_2$	4.00×10 <sup>-25</sup>	6,7
$CO(e1) + OH \rightarrow CO_2 + H$	$5.40 \times 10^{-14} \times (T_g/298)^{1.50} \times \exp(2080/(R \times T_g))$	6,7
$CO(e2) + OH \rightarrow CO_2 + H$	$5.40 \times 10^{-14} \times (T_g/298)^{1.50} \times \exp(2080/(R \times T_g))$	6,7
$CO(e3) + OH \rightarrow CO_2 + H$	$5.40 \times 10^{-14} \times (T_g/298)^{1.50} \times \exp(2080/(R \times T_g))$	6,7
$CO(e4) + OH \rightarrow CO_2 + H$	$5.40 \times 10^{-14} \times (T_g/298)^{1.50} \times \exp(2080/(R \times T_g))$	6,7
$CO(e1) + HO_2 \rightarrow CO_2 + OH$	2.51×10 <sup>-10</sup> ×exp(-98940/(R×T <sub>g</sub> ))	6,7
$CO(e2) + HO_2 \rightarrow CO_2 + OH$	2.51×10 <sup>-10</sup> ×exp(-98940/(R×T <sub>g</sub> ))	6,7
$CO(e3) + HO_2 \rightarrow CO_2 + OH$	2.51×10 <sup>-10</sup> ×exp(-98940/(R×T <sub>g</sub> ))	6,7
$CO(e4) + HO_2 \rightarrow CO_2 + OH$	2.51×10 <sup>-10</sup> ×exp(-98940/(R×T <sub>g</sub> ))	6,7
$CO(e1) + C + M \rightarrow C_2O + M$	6.31×10 <sup>-32</sup>	6,7
$CO(e2) + C + M \rightarrow C_2O + M$	6.31×10 <sup>-32</sup>	6,7
$CO(e3) + C + M \rightarrow C_2O + M$	6.31×10 <sup>-32</sup>	6,7
$CO(e4) + C + M \rightarrow C_2O + M$	6.31×10 <sup>-32</sup>	6,7
$CO(e1) + CH_3 \rightarrow C_2H_2 + OH$	6.31×10 <sup>-11</sup> ×exp(-253×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CO(e2) + CH_3 \rightarrow C_2H_2 + OH$	6.31×10 <sup>-11</sup> ×exp(-253×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CO(e3) + CH_3 \rightarrow C_2H_2 + OH$	6.31×10 <sup>-11</sup> ×exp(-253×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CO(e4) + CH_3 \rightarrow C_2H_2 + OH$	6.31×10 <sup>-11</sup> ×exp(-253×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CO(e1) + CH_3O \rightarrow CO_2 + CH_3$	2.61×10 <sup>-11</sup> ×exp(-49390/(R×T <sub>g</sub> ))	6,7
$CO(e2) + CH_3O \rightarrow CO_2 + CH_3$	2.61×10 <sup>-11</sup> ×exp(-49390/(R×T <sub>g</sub> ))	6,7
$CO(e3) + CH_3O \rightarrow CO_2 + CH_3$	2.61×10 <sup>-11</sup> ×exp(-49390/(R×T <sub>g</sub> ))	6,7
$CO(e4) + CH_3O \rightarrow CO_2 + CH_3$	2.61×10 <sup>-11</sup> ×exp(-49390/(R×T <sub>g</sub> ))	6,7
$CO(e1) + C_2H_2 \rightarrow C_2H + CHO$	$8.00 \times 10^{-10} \times \exp(-446.0 \times 10^{3}/(R \times T_g))$	6,7
$CO(e2) + C_2H_2 \rightarrow C_2H + CHO$	$8.00 \times 10^{-10} \times \exp(-446.0 \times 10^{3}/(R \times T_g))$	6,7
$CO(e3) + C_2H_2 \rightarrow C_2H + CHO$	8.00×10 <sup>-10</sup> ×exp(-446.0×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
$CO(e4) + C_2H_2 \rightarrow C_2H + CHO$	8.00×10 <sup>-10</sup> ×exp(-446.0×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
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$CO(e1) + C_2H_4 \rightarrow CHO + C_2H_3$	$2.51 \times 10^{-10} \times \exp(-379000.0/(R \times T_g))$	6,7
$CO(e2) + C_2H_4 \rightarrow CHO + C_2H_3$	$2.51 \times 10^{-10} \times \exp(-379000.0/(R \times T_g))$	6,7
$CO(e3) + C_2H_4 \rightarrow CHO + C_2H_3$	$2.51 \times 10^{-10} \times \exp(-379000.0/(R \times T_g))$	6,7
$CO(e4) + C_2H_4 \rightarrow CHO + C_2H_3$	$2.51 \times 10^{-10} \times \exp(-379000.0/(R \times T_g))$	6,7
$O_2(e1) + CO(e1) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + CO(e1) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e1) + CO(e2) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + CO(e2) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e1) + CO(e3) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + CO(e3) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e1) + CO(e4) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$O_2(e2) + CO(e4) \rightarrow CO_2 + O$	4.20×10 <sup>-12</sup> ×exp(-24000.0/ <i>T</i> <sub>g</sub> )	6,7
$C + OH \rightarrow CO(e1) + H$	1.15×10 <sup>-10</sup> ×( <i>T</i> <sub>g</sub> /298) <sup>-0.34</sup>	6,7

<sup>[2]</sup>: CH<sub>2</sub>(S) is an isomer of CH<sub>2</sub>.

## Table S9. Ion-neutral reactions

Reaction	Rate constants	Ref
$C_2O_3^+ + CO \rightarrow C_2O_2^+ + CO_2$	1.10×10 <sup>-9</sup>	6,7
$H^+ + O_2 \rightarrow O_2^+ + H$	2.00×10 <sup>-9</sup>	24
$H_2^+ + O_2 \rightarrow O_2^+ + H_2$	8.00×10 <sup>-10</sup>	24
$O_2^+ + CHO \rightarrow CHO^+ + O_2$	$3.60 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$O_2^+ + CH \rightarrow CHO^+ + O$	$3.10 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$O_2^+ + CH_2O \rightarrow CHO^+ + O_2 + H$	$2.30 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$O_2^+ + C_2H_2 \rightarrow CHO^+ + H + CO$	6.50×10 <sup>-11</sup>	24
$O_2^+ + C_2H_4 \rightarrow C_2H_4^+ + O_2$	6.80×10 <sup>-10</sup>	24
$O_2^+ + C_2 H_2 \rightarrow C_2 H_2^+ + O_2$	1.11×10 <sup>-9</sup>	24
$CH_4^+ + O_2 \rightarrow O_2^+ + CH_4$	3.90×10 <sup>-10</sup>	24
$O_2^+ + CH_2 \rightarrow CH_2^+ + O_2$	4.30×10 <sup>-10</sup>	24
$O_2^+ + CH \rightarrow CH^+ + O_2$	3.10×10 <sup>-10</sup>	6,7
$H_2O^+ + O \rightarrow O_2^+ + H_2$	4.00×10 <sup>-11</sup>	24
$O^+ + OH \rightarrow O_2^+ + H$	$3.60 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$OH^{+} + O \rightarrow O_{2}^{+} + H$	7.10×10 <sup>-10</sup>	24
$O^+ + CO_2 \rightarrow O_2^+ + CO$	8.10×10 <sup>-10</sup>	6,7
$\mathrm{CO}_{2^{+}} + \mathrm{O}_{2} \rightarrow \mathrm{O}_{2^{+}} + \mathrm{CO}_{2}$	5.30×10 <sup>-11</sup>	24

$\mathrm{CO_2}^+ + \mathrm{O_2}(\mathrm{e1}) \to \mathrm{O_2}^+ + \mathrm{CO_2}$	1.19×5.30×10 <sup>-11</sup>	6,7
$\mathrm{CO}_2^+ + \mathrm{O}_2(\mathrm{e2}) \to \mathrm{O}_2^+ + \mathrm{CO}_2$	1.33×5.30×10 <sup>-11</sup>	6,7
$\mathrm{CO}_2^+ + \mathrm{O} \rightarrow \mathrm{O}_2^+ + \mathrm{CO}$	1.64×10 <sup>-10</sup>	24
$\mathrm{CO}^{+} + \mathrm{O}_2 \rightarrow \mathrm{O}_2^{+} + \mathrm{CO}$	1.20×10 <sup>-10</sup>	24
$CO^{+} + O_2(e1) \rightarrow O_2^{+} + CO$	1.19×1.20×10 <sup>-10</sup>	6,7
$\mathrm{CO^{+}+O_{2}(e2)}\rightarrow\mathrm{O_{2}^{+}+CO}$	1.33×1.20×10 <sup>-10</sup>	6,7
$O_2^+ + C \rightarrow CO^+ + O$	5.20×10 <sup>-11</sup>	24
$O^+ + O_3 \rightarrow O_2^+ + O_2$	1.00×10 <sup>-10</sup>	6,7
$O_2^+ + C \rightarrow C^+ + O_2$	5.20×10 <sup>-11</sup>	24
$C_2O_2^+ + O_2 \rightarrow O_2^+ + CO + CO$	5.00×10 <sup>-12</sup>	6,7
$C_2O_2^+ + O_2(e1) \rightarrow O_2^+ + CO + CO$	5.00×10 <sup>-12</sup>	6,7
$C_2O_2^+ + O_2(e2) \rightarrow O_2^+ + CO + CO$	5.00×10 <sup>-12</sup>	6,7
$C_2O_2^+ + M \rightarrow CO^+ + CO + M$	1.00×10 <sup>-12</sup>	6,7
$C_2O_4{}^+ + CO \rightarrow C_2O_3{}^+ + CO_2$	9.00×10 <sup>-10</sup>	6,7
$C_2O_4{}^+ + CO(e1) \rightarrow C_2O_3{}^+ + CO_2$	9.00×10 <sup>-10</sup>	6,7
$C_2O_4{}^+ + CO(e2) \rightarrow C_2O_3{}^+ + CO_2$	9.00×10 <sup>-10</sup>	6,7
$C_2O_4{}^+ + CO(e3) \rightarrow C_2O_3{}^+ + CO_2$	9.00×10 <sup>-10</sup>	6,7
$C_2O_4{}^+ + CO(e4) \rightarrow C_2O_3{}^+ + CO_2$	9.00×10 <sup>-10</sup>	6,7
$C_2O_3^+ + CO(e1) \rightarrow C_2O_2^+ + CO_2$	1.10×10 <sup>-9</sup>	6,7
$C_2O_3^+ + CO(e2) \rightarrow C_2O_2^+ + CO_2$	1.10×10 <sup>-9</sup>	6,7
$C_2O_3^+ + CO(e3) \rightarrow C_2O_2^+ + CO_2$	1.10×10 <sup>-9</sup>	6,7
$C_2O_3^+ + CO(e4) \rightarrow C_2O_2^+ + CO_2$	1.10×10 <sup>-9</sup>	6,7
$\mathrm{CO}_2^+ + \mathrm{CO}_2 + \mathrm{M} \to \mathrm{C}_2\mathrm{O}_4^+ + \mathrm{M}$	3.00×10 <sup>-28</sup>	6,7
$C_2O_4{}^+ + M \rightarrow CO_2{}^+ + CO_2 + M$	1.00×10 <sup>-14</sup>	6,7
$O_4^+ + O \rightarrow O_2^+ + O_3$	3.00×10 <sup>-10</sup>	6,7
$O_4{}^+ + M \rightarrow O_2{}^+ + O_2 + M$	$3.30 \times 10^{-6} \times (300/T_g)^{4.0} \times \exp(-5030.0/T_g)$	6,7
$O_2^+ + O_2 + M \rightarrow O_4^+ + M$	$2.40 \times 10^{-30} \times (T_g/300)^{-3.2}$	6,7
$O_2^+ + O_2(e1) + M \rightarrow O_4^+ + M$	$2.40 \times 10^{-30} \times (T_g/300)^{-3.2}$	6,7
$O_2^+ + O_2(e2) + M \rightarrow O_4^+ + M$	$2.40 \times 10^{-30} \times (T_g/300)^{-3.2}$	6,7
$O_2^+ + C_2 \to C_2^+ + O_2$	4.10×10 <sup>-10</sup>	24
$O^+ + O_2 \rightarrow O_2^+ + O$	1.90×10 <sup>-11</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	6,7
$O^+ + O_2(e1) \rightarrow O_2^+ + O$	1.19×1.90×10 <sup>-11</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.5</sup>	6,7
$O^+ + O_2(e2) \rightarrow O_2^+ + O$	1.33×1.90×10 <sup>-11</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.5</sup>	6,7
$O^+ + O + M \rightarrow O_2^+ + M$	1.00×10 <sup>-29</sup>	6,7

$H_2O^+ + O_2 \rightarrow O_2^+ + H_2O$	4.60×10 <sup>-10</sup>	24
$OH^+ + O_2 \rightarrow O_2^+ + OH$	5.90×10 <sup>-10</sup>	24
$O^+ + CHO \rightarrow CHO^+ + O$	$4.30 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$O^+ + CH_2O \rightarrow CHO^+ + OH$	1.40×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$O^+ + C_2H_4 \rightarrow C_2H_4^+ + O$	7.00×10 <sup>-11</sup>	24
$O^+ + C_2 H_4 \rightarrow C_2 H_3^+ + OH$	2.10×10 <sup>-10</sup>	24
$O^+ + C_2H_4 \rightarrow C_2H_2^+ + H2O$	1.12×10 <sup>-9</sup>	24
$O^+ + C_2 H_2 \rightarrow C_2 H_2^+ + O$	3.90×10 <sup>-11</sup>	24
$O^+ + C_2 H \rightarrow C_2 H^+ + O$	4.60×10 <sup>-10</sup>	24
$O^{+} + C_{2}H \rightarrow CO^{+} + CH$	4.60×10 <sup>-10</sup>	24
$O^{+} + CH_4 \rightarrow CH_4^{+} + O$	8.90×10 <sup>-10</sup>	24
$O^{+} + CH_4 \rightarrow CH_3^{+} + OH$	1.10×10 <sup>-10</sup>	24
$O^{+} + CH_2 \rightarrow CH_2^{+} + O$	9.70×10 <sup>-10</sup>	24
$O^+ + CH \rightarrow CH^+ + O$	3.50×10 <sup>-10</sup>	6,7
$O^+ + C_2 \rightarrow C_2^+ + O$	4.80×10 <sup>-10</sup>	24
$O^+ + OH \rightarrow OH^+ + O$	3.60×10 <sup>-10</sup>	6,7
$O^+ + H_2 O \rightarrow H_2 O^+ + O$	3.20×10 <sup>-9</sup>	6,7
$O^+ + H_2 \rightarrow OH^+ + H$	1.70×10 <sup>-9</sup>	24
$CH^+ + O_2 \rightarrow O^+ + CHO$	1.00×10 <sup>-11</sup>	24
$O^+ + H \rightarrow H^+ + O$	5.82×10 <sup>-10</sup>	6,7
$H^+ + O \rightarrow O^+ + H$	3.44×10 <sup>-10</sup>	6,7
$O^+ + CO_2 \rightarrow CO_2^+ + O$	9.00×10 <sup>-11</sup>	6,7
$CO_2^+ + O \rightarrow O^+ + CO_2$	9.62×10 <sup>-11</sup>	24
$O^+ + CO \rightarrow CO^+ + O$	$4.90 \times 10^{-12} \times (T_g/300)^{0.5} \times \exp(-4580.0/T_g)$	24
$C^+ + O_2 \rightarrow O^+ + CO$	4.54×10 <sup>-10</sup>	24
$C^+ + O_2(e1) \rightarrow O^+ + CO$	4.54×10 <sup>-10</sup>	6,7
$C^+ + O_2(e2) \rightarrow O^+ + CO$	4.54×10 <sup>-10</sup>	6,7
$CO^+ + O \rightarrow O^+ + CO$	1.40×10 <sup>-10</sup>	24
$O^+ + CO(e1) \rightarrow CO^+ + O$	$1.58 \times 10^{-11} \times (T_g/300)^{0.5} \times \exp(-4580.0/T_g)$	6,7
$O^+ + CO(e2) \rightarrow CO^+ + O$	$2.59 \times 10^{-11} \times (T_g/300)^{0.5} \times \exp(-4580.0/T_g)$	6,7
$O^+ + CO(e3) \rightarrow CO^+ + O$	$1.23 \times 10^{-10} \times (T_g/300)^{0.5} \times \exp(-4580.0/T_g)$	6,7
$O^+ + CO(e4) \rightarrow CO^+ + O$	$7.81 \times 10^{-10} \times (T_g/300)^{0.5} \times \exp(-4580.0/T_g)$	6,7
$O^+ + C_2 \rightarrow CO^+ + C$	4.80×10 <sup>-10</sup>	24
$C^{+} + C_{3}H_{6} \rightarrow C_{2}H_{2}^{+} + C_{2}H_{4}$	3.00×10 <sup>-10</sup>	24

$C^+ + C_3H_6 \to C_2H_3^+ + C_2H_3$	6.00×10 <sup>-10</sup>	24
$C^+ + CH_3OH \rightarrow CH_3^+ + CHO$	2.08×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C^+ + CHO \rightarrow CHO^+ + C$	$4.80 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C^+ + CH_2O \rightarrow CHO^+ + CH$	$7.80 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C^+ + H_2O \rightarrow CHO^+ + H$	$9.00 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C^+ + CO_2 \rightarrow CO^+ + CO$	1.10×10 <sup>-9</sup>	24
$C^+ + CO \rightarrow CO^+ + C$	5.00×10 <sup>-13</sup>	6,7
$CO^+ + C \rightarrow C^+ + CO$	1.10×10 <sup>-10</sup>	24
$C^+ + CO(e1) \rightarrow CO^+ + C$	3.23×5.00×10 <sup>-13</sup>	6,7
$C^+ + CO(e2) \rightarrow CO^+ + C$	5.28×5.00×10 <sup>-13</sup>	6,7
$C^+ + CO(e3) \rightarrow CO^+ + C$	23.18×5.00×10 <sup>-13</sup>	6,7
$C^+ + CO(e4) \rightarrow CO^+ + C$	159.31×5.00×10 <sup>-13</sup>	6,7
$C^+ + O_2 \rightarrow CO^+ + O$	3.80×10 <sup>-10</sup>	6,7
$C^+ + O_2(e1) \rightarrow CO^+ + O$	3.80×10 <sup>-10</sup>	6,7
$C^+ + O_2(e2) \rightarrow CO^+ + O$	3.80×10 <sup>-10</sup>	6,7
$C^+ + C_2 H_6 \rightarrow C_2 H_5^+ + CH$	2.31×10 <sup>-10</sup>	24
$C^+ + C_2 H_6 \rightarrow C_2 H_4^+ + C H_2$	1.16×10 <sup>-10</sup>	24
$C^+ + C_2H_6 \rightarrow C_2H_3^+ + CH_3$	4.95×10 <sup>-10</sup>	24
$C^+ + C_2 H_6 \rightarrow C_2 H_2^+ + C H_4$	8.25×10 <sup>-11</sup>	24
$C^+ + CH \rightarrow CH^+ + C$	3.80×10 <sup>-10</sup>	6,7
$C^{+} + CH \rightarrow C_{2}^{+} + H$	3.80×10 <sup>-10</sup>	6,7
$C^+ + C_2 H_5 \rightarrow C_2 H_5^+ + C$	5.00×10 <sup>-10</sup>	24
$C^+ + C_2 H_4 \rightarrow C_2 H_4^+ + C$	1.70×10 <sup>-11</sup>	24
$C^+ + C_2H_4 \rightarrow C_2H_3^+ + CH$	8.50×10 <sup>-11</sup>	24
$C^+ + CH_4 \rightarrow C_2H_3^+ + H$	1.10×10 <sup>-9</sup>	24
$C^+ + CH_4 \rightarrow C_2H_2^+ + H_2$	4.00×10 <sup>-10</sup>	6,7
$C^{++CH_{3}\rightarrow C_{2}H_{2}^{+}+H}$	1.30×10 <sup>-9</sup>	24
$C^{++CH_{3}\rightarrow C_{2}H^{+}+H_{2}}$	1.00×10 <sup>-9</sup>	24
$C^+ + CH_2 \rightarrow C_2H^+ + H$	5.20×10 <sup>-10</sup>	24
$C^{++CH_{2}\rightarrow CH_{2}^{+}+C}$	5.20×10 <sup>-10</sup>	24
$C_2^+ + C \rightarrow C^+ + C_2$	1.10×10 <sup>-10</sup>	24
$CH^+ + H \rightarrow C^+ + H_2$	7.50×10 <sup>-10</sup>	6,7
$C_2^+ + CHO \rightarrow CHO^+ + C_2$	$3.80 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C_2^+ + H_2O \rightarrow C_2H^+ + OH$	4.40×10 <sup>-10</sup>	24

$C_2^+ + O_2 \rightarrow CO^+ + CO$	8.00×10 <sup>-10</sup>	24	
$O_2^+ + C_2 \rightarrow CO^+ + CO$	4.10×10 <sup>-10</sup>	6,7	
$CO^+ + C_2 \rightarrow C_2^+ + CO$	8.40×10 <sup>-10</sup>	24	
$C_2^+ + O \rightarrow CO^+ + C$	3.10×10 <sup>-10</sup>	24	
$H_2O^+ + C_2 \rightarrow C_2^+ + H_2O$	4.70×10 <sup>-10</sup>	6,7	
$C_2^+ + OH \rightarrow OH^+ + C_2$	6.50×10 <sup>-10</sup>	6,7	
$OH^{+} + C_2 \rightarrow C_2^{+} + OH$	4.80×10 <sup>-10</sup>	24	
$C_2^+ + CH_4 \rightarrow C_2H_2^+ + CH_2$	1.82×10 <sup>-10</sup>	24	
$C_2^+ + CH_4 \rightarrow C_2H^+ + CH_3$	2.38×10 <sup>-10</sup>	24	
$C_2^+ + H_2 \rightarrow C_2 H^+ + H$	1.10×10 <sup>-9</sup>	24	
$C_2^+ + CH_2 \rightarrow CH_2^+ + C_2$	4.50×10 <sup>-10</sup>	24	
$C_2^+ + CH \rightarrow CH^+ + C_2$	3.20×10 <sup>-10</sup>	6,7	
$CH^{+} + CH \rightarrow C_{2}^{+} + H_{2}$	7.40×10 <sup>-10</sup>	6,7	
$H^{*} + C_{2}H \to C_{2}^{*} + H_{2}$	1.50×10 <sup>-9</sup>	24	
$CH^{*}+C\toC_{2^{*}}+H$	1.20×10 <sup>-9</sup>	24	
$H_2^+ + C_2 \rightarrow C_2^+ + H_2$	1.10×10 <sup>-9</sup>	24	
$H^{*} + C_{2} \to C_{2}^{*} + H$	3.10×10 <sup>-9</sup>	24	
$\rm H_2O^+ + CHO \rightarrow CHO^+ + H_2O$	$2.80 \times 10^{-10} \times (T_g/300)^{-0.50}$	24	
$H_2O^+ + CO \rightarrow CHO^+ + OH$	5.00×10 <sup>-10</sup>	24	
$H_2O^+ + CO(e1) \rightarrow CHO^+ + OH$	5.00×10 <sup>-10</sup>	6,7	
$H_2O^+ + CO(e2) \rightarrow CHO^+ + OH$	5.00×10 <sup>-10</sup>	6,7	
$H_2O^+ + CO(e3) \rightarrow CHO^+ + OH$	5.00×10 <sup>-10</sup>	6,7	
$H_2O+ + CO(e4) \rightarrow CHO^+ + OH$	5.00×10 <sup>-10</sup>	6,7	
$CHO^{+} + OH \rightarrow H_2O^{+} + CO$	$6.20 \times 10^{-10} \times (T_g/300)^{-0.50}$	24	
$H_2O^+ + C_2 \rightarrow C_2H^+ + OH$	4.70×10 <sup>-10</sup>	24	
$CH_5^+ + OH \rightarrow H_2O^+ + CH_4$	7.00×10 <sup>-10</sup>	6,7	
$H_3^+ + O \rightarrow H_2O^+ + H$	3.60×10 <sup>-10</sup>	6,7	
$H_3^+ + OH \rightarrow H_2O^+ + H_2$	1.30×10 <sup>-9</sup>	6,7	
$H_2^+ + OH \rightarrow H_2O^+ + H$	7.60×10 <sup>-10</sup>	6,7	
$H_2^+ + H_2O \rightarrow H_2O^+ + H_2$	3.90×10 <sup>-9</sup>	6,7	
$H^{+} + H_2O \rightarrow H_2O^{+} + H$	6.90×10 <sup>-9</sup>	6,7	
$CO_2^+ + H_2O \rightarrow H_2O^+ + CO_2$	2.04×10 <sup>-9</sup>	6,7	
$CO^+ + H_2O \rightarrow H_2O^+ + CO$	1.72×10-9	6,7	
$H_2O^+ + CH_4 \rightarrow H_3O^+ + CH_3$	1.40×10 <sup>-9</sup>	24	

$H_2O^+ + CH_2 \rightarrow CH_3^+ + OH$	4.70×10 <sup>-10</sup>	24
$H_2O^+ + CH_2 \rightarrow CH_2^+ + H_2O$	4.70×10 <sup>-10</sup>	24
$H_2O^+ + CH \rightarrow CH_2^+ + OH$	3.40×10 <sup>-10</sup>	6,7
$\rm H_2O^+ + CH \rightarrow CH^+ + H_2O$	3.40×10 <sup>-10</sup>	6,7
$H_2O^+ + C \rightarrow CH^+ + OH$	1.10×10 <sup>-9</sup>	24
$H_2O^+ + C_2H_6 \rightarrow H_3O^+ + C_2H_5$	1.33×10 <sup>-9</sup>	24
$H_2O^+ + C_2H_6 \rightarrow C_2H_6^+ + H_2O$	6.40×10 <sup>-11</sup>	24
$H_2O^+ + C_2H_6 \to C_2H_4^+ + H_2O + H_2$	1.92×10 <sup>-10</sup>	24
$H_2O^+ + C_2H_4 \rightarrow C_2H_4^+ + H_2O$	1.50×10 <sup>-9</sup>	24
$H_2O^+ + C_2H_2 \rightarrow C_2H_2^+ + H_2O$	1.90×10 <sup>-9</sup>	24
$H_2O^+ + C_2H \rightarrow C_2H_2^+ + OH$	4.40×10 <sup>-10</sup>	24
$H_2O^+ + C_2H \rightarrow C_2H^+ + H_2O$	4.40×10 <sup>-10</sup>	24
$H_2O^+ + H_2 \rightarrow H_3O^+ + H_3O^+$	6.40×10 <sup>-10</sup>	24
$H_2O^+ + H_2O \rightarrow H_3O^+ + OH$	2.10×10 <sup>-9</sup>	6,7
$H_2O^+ + OH \rightarrow H_3O^+ + O$	6.90×10 <sup>-10</sup>	6,7
$OH^+ + H_2 \rightarrow H_2O^+ + H$	1.01×10 <sup>-9</sup>	24
$OH^{+} + H_2O \rightarrow H_2O^{+} + OH$	1.59×10 <sup>-9</sup>	6,7
$OH^{+} + OH \rightarrow H_{2}O^{+} + O$	7.00×10 <sup>-10</sup>	6,7
$OH^+ + CHO \rightarrow CHO^+ + OH$	$2.80 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$OH^+ + CO \rightarrow CHO^+ + O$	1.05×10 <sup>-9</sup>	24
$OH^+ + CO(e1) \rightarrow CHO^+ + O$	1.05×10 <sup>-9</sup>	6,7
$OH^+ + CO(e2) \rightarrow CHO^+ + O$	1.05×10 <sup>-9</sup>	6,7
$OH^+ + CO(e3) \rightarrow CHO^+ + O$	1.05×10 <sup>-9</sup>	6,7
$OH^+ + CO(e4) \rightarrow CHO^+ + O$	1.05×10 <sup>-9</sup>	6,7
$OH^{*} + C_{2} \rightarrow C_{2}H^{*} + O$	4.80×10 <sup>-10</sup>	24
$H_3^+ + O \rightarrow OH^+ + H_2$	8.40×10 <sup>-10</sup>	6,7
$H_2^+ + O \rightarrow OH^+ + H$	1.50×10 <sup>-9</sup>	24
$H_2^+ + OH \rightarrow OH^+ + H_2$	7.60×10 <sup>-10</sup>	6,7
$H^{+} + OH \rightarrow OH^{+} + H$	2.10×10 <sup>-9</sup>	6,7
$CO^+ + OH \rightarrow OH^+ + CO$	3.10×10 <sup>-10</sup>	6,7
$OH^+ + CH_4 \rightarrow CH_5^+ + O$	1.95×10 <sup>-10</sup>	24
$OH^+ + CH_4 \rightarrow H_3O^+ + CH_2$	1.31×10 <sup>-9</sup>	24
$OH^+ + CH_2 \rightarrow CH_{3^+} + O$	4.80×10 <sup>-10</sup>	24
$OH^+ + CH_2 \rightarrow CH_2^+ + OH$	4.80×10 <sup>-10</sup>	24

$OH^+ + CH \rightarrow CH_2^+ + O$	3.50×10 <sup>-10</sup>	6,7
$OH^{+} + CH \rightarrow CH^{+} + OH$	3.50×10 <sup>-10</sup>	6,7
$OH^+ + C \rightarrow CH^+ + O$	1.20×10 <sup>-9</sup>	24
$OH^{*} + C_{2}H_{6} \rightarrow H_{3}O^{*} + C_{2}H_{4}$	1.60×10 <sup>-10</sup>	24
$OH^{*} + C_{2}H_{6} \rightarrow C_{2}H_{6}^{*} + OH$	4.80×10 <sup>-11</sup>	24
$OH^{+} + C_2H_6 \rightarrow C_2H_5^{+} + H_2 + O$	3.20×10 <sup>-10</sup>	24
$OH^{+} + C_2H_6 \rightarrow C_2H_4^{+} + H_2 + OH$	1.04×10 <sup>-9</sup>	24
$OH^{*} + C_{2}H \rightarrow C_{2}H_{2}^{+} + O$	4.50×10 <sup>-10</sup>	24
$OH^+ + C_2H \rightarrow C_2H^+ + OH$	4.50×10 <sup>-10</sup>	24
$OH^{+} + H_2O \rightarrow H_3O^{+} + O$	1.30×10 <sup>-9</sup>	24
$H_3O^+ + C \rightarrow CHO^+ + H_2$	1.00×10 <sup>-11</sup>	24
$CHO^{+} + H_2O \rightarrow H_3O^{+} + CO$	2.50×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$H_3O^+ + C_2 \rightarrow C_2H^+ + H_2O$	9.20×10 <sup>-10</sup>	24
$CH_5^+ + O \rightarrow H_3O^+ + CH_2$	2.20×10 <sup>-10</sup>	24
$CH_5^+ + H_2O \rightarrow H_3O^+ + CH_4$	3.70×10 <sup>-9</sup>	24
$CH_4^+ + H_2O \rightarrow H_3O^+ + CH_3$	2.60×10 <sup>-9</sup>	6,7
$CH^{+} + H_2O \rightarrow H_3O^{+} + C$	5.50×10 <sup>-10</sup>	6,7
$C_2H_6^+ + H_2O \rightarrow H_3O^+ + C_2H_5$	2.95×10 <sup>-9</sup>	24
$C_2H_5^+ + H_2O \rightarrow H_3O^+ + C_2H_4$	1.40×10 <sup>-9</sup>	6,7
$C_2H_3^+ + H_2O \rightarrow H_3O^+ + C_2H_2$	1.11×10 <sup>-9</sup>	6,7
$C_2H_2^+ + H_2O \rightarrow H_3O^+ + C_2H$	2.20×10 <sup>-10</sup>	6,7
$H_3^+ + H_2O \rightarrow H_3O^+ + H_2$	5.90×10 <sup>-9</sup>	6,7
$H_2^+ + H_2O \rightarrow H_3O^+ + H$	3.40×10 <sup>-9</sup>	6,7
$H_3O^+ + CH_2 \rightarrow CH_3^+ + H_2O$	9.40×10 <sup>-10</sup>	24
$H_3O^+ + CH \rightarrow CH_2^+ + H_2O$	6.80×10 <sup>-10</sup>	6,7
$H_3O^+ + C_2H_3 \rightarrow C_2H_4^+ + H_2O$	2.00×10 <sup>-9</sup>	6,7
$H_3^+ + C_2 H_5 OH \rightarrow C_2 H_3^+ + H_2 O + H_2 + H_2$	$4.00 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$H_{3}^{+} + C_{3}H_{6} \rightarrow C_{2}H_{3}^{+} + CH_{4} + H_{2}$	9.00×10 <sup>-10</sup>	24
$H_{3}^{+} + CH_{3}CHO \rightarrow C_{2}H_{3}^{+} + H_{2} + H_{2}O$	$8.97 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$H_3^+ + C_2H_5OH \rightarrow CH_3^+ + CH_4 + H_2O$	1.50×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$H_3^+ + CH_3CHO \rightarrow CH_3^+ + CH_3OH$	1.45×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$\mathrm{H_{3}^{+}+CH_{3}OH}\rightarrow\mathrm{CH_{3}^{+}+H_{2}O+H_{2}}$	$3.71 \times 10^{-9} \times (T_g/300)^{-0.50}$	24
$H_{3}{}^{+} + CO \rightarrow CHO^{+} + H_{2}$	$1.36 \times 10^{-9} \times (T_g/300)^{-0.14} \times \exp(3.40/T_g)$	24
$H_3^+$ + CO(e1) $\rightarrow$ CHO <sup>+</sup> + $H_2$	$1.36 \times 10^{-9} \times (T_g/300)^{-0.14} \times \exp(3.40/T_g)$	6,7

$H_3^+ + CO(e2) \rightarrow CHO^+ + H_2$	1.36×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.14</sup> ×exp(3.40/ <i>T</i> <sub>g</sub> )	6,7
$\rm H_{3^{+}} + \rm CO(e3) \rightarrow \rm CHO^{+} + \rm H_{2}$	$1.36 \times 10^{-9} \times (T_g/300)^{-0.14} \times \exp(3.40/T_g)$	6,7
$H_{3}^{+}$ + CO(e4) $\rightarrow$ CHO <sup>+</sup> + $H_{2}$	$1.36 \times 10^{-9} \times (T_g/300)^{-0.14} \times \exp(3.40/T_g)$	6,7
$H_3^+ + C_2 \rightarrow C_2 H^+ + H_2$	1.80×10 <sup>-9</sup>	24
$H_2^+ + H_2 \rightarrow H_3^+ + H + H$	2.11×10 <sup>-9</sup>	6,7
$H^{+} + H_{2} + H_{2} \rightarrow H_{3}^{+} + H_{2}$	3.10×10 <sup>-29</sup> ×(300/ <i>T</i> g) <sup>0.5</sup>	6,7
$H_3^+ + CH_4 \rightarrow CH_5^+ + H_2$	2.40×10 <sup>-9</sup>	24
$H_3^+ + CH_3 \rightarrow CH_4^+ + H_2$	2.10×10 <sup>-9</sup>	24
$H_3^+ + CH_2 \rightarrow CH_3^+ + H_2$	1.70×10 <sup>-9</sup>	24
$H_3^+ + CH \rightarrow CH_2^+ + H_2$	1.20×10 <sup>-9</sup>	6,7
$H_3^+ + C \rightarrow CH^+ + H_2$	2.00×10 <sup>-9</sup>	24
$H_{3}{}^{+} + C_{2}H_{6} \rightarrow C_{2}H_{5}{}^{+} + H_{2} + H_{2}$	2.40×10 <sup>-9</sup>	24
$H_{3}^{+} + C_{2}H_{5} \rightarrow C_{2}H_{6}^{+} + H_{2}$	1.40×10 <sup>-9</sup>	24
$H_{3}^{+} + C_{2}H_{4} \rightarrow C_{2}H_{5}^{+} + H_{2}$	1.15×10 <sup>-9</sup>	24
$H_{3}^{+} + C_{2}H_{4} \rightarrow C_{2}H_{3}^{+} + H_{2} + H_{2}$	1.15×10 <sup>-9</sup>	24
$H_{3}^{+} + C_{2}H_{3} \rightarrow C_{2}H_{4}^{+} + H_{2}$	2.00×10 <sup>-9</sup>	6,7
$H_{3}^{+} + C_{2}H_{2} \rightarrow C_{2}H_{3}^{+} + H_{2}$	3.50×10 <sup>-9</sup>	24
$H_2^+ + H \rightarrow H_3^+$	2.10×10 <sup>-9</sup>	6,7
$H^{*} + H_{2} + M \to H_{3}^{+} + M$	1.50×10 <sup>-29</sup>	6,7
$H_3^+ + C_2 H \rightarrow C_2 H_2^+ + H_2$	1.70×10 <sup>-9</sup>	24
$H_2^+ + CHO \rightarrow CHO^+ + H_2$	1.00×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$\rm H_{2}{}^{+} + \rm CO \rightarrow \rm CHO^{+} + \rm H$	2.16×10 <sup>-9</sup>	24
$H_2^+$ + CO(e1) $\rightarrow$ CHO <sup>+</sup> + H	2.16×10 <sup>-9</sup>	6,7
$H_2^+$ + CO(e2) $\rightarrow$ CHO <sup>+</sup> + H	2.16×10 <sup>-9</sup>	6,7
$\mathrm{H_{2}^{+}+CO(e3)}\rightarrow\mathrm{CHO^{+}+H}$	2.16×10 <sup>-9</sup>	6,7
$H_2^+$ + CO(e4) $\rightarrow$ CHO <sup>+</sup> + H	2.16×10 <sup>-9</sup>	6,7
$H_2^+ + CH_2O \rightarrow CHO^+ + H_2 + H$	1.40×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$H_2^+ + C_2 \rightarrow C_2 H^+ + H$	1.10×10 <sup>-9</sup>	24
$H_2^+ + CH_4 \rightarrow CH_5^+ + H$	1.14×10 <sup>-10</sup>	24
$H_{2^{+}+CH_{4}\rightarrow CH_{4}^{+}+H_{2}}$	1.40×10 <sup>-9</sup>	24
$\mathrm{H_{2}^{+}+CH_{4}\rightarrow CH_{3}^{+}+H_{2}+H}$	2.30×10 <sup>-9</sup>	24
$H_2^+ + CH_2 \rightarrow CH_3^+ + H$	1.00×10 <sup>-9</sup>	24
$H_2^+ + CH_2 \rightarrow CH_2^+ + H_2$	1.00×10 <sup>-9</sup>	24
$H_2^+ + CH \rightarrow CH_2^+ + H$	7.10×10 <sup>-10</sup>	6,7

$H_2^+ + CH \rightarrow CH^+ + H_2$	7.10×10 <sup>-10</sup>	6,7
$H_2^+ + C \rightarrow CH^+ + H$	2.40×10 <sup>-9</sup>	24
$H_2^+ + C_2 H_6 \rightarrow C_2 H_6^+ + H_2$	2.94×10 <sup>-10</sup>	24
$H_2^+ + C_2 H_6 \rightarrow C_2 H_5^+ + H_2 + H$	1.37×10 <sup>-9</sup>	24
$H_2^+ + C_2 H_6 \rightarrow C_2 H_4^+ + H_2 + H_2$	2.35×10 <sup>-9</sup>	24
$H_2^+ + C_2 H_6 \rightarrow C_2 H_3^+ + H_2 + H_2 + H$	6.86×10 <sup>-10</sup>	6,7
$H_2^+ + C_2 H_6 \rightarrow C_2 H_2^+ + H_2 + H_2 + H_2$	1.96×10 <sup>-10</sup>	6,7
$H_2^+ + C_2 H_4 \rightarrow C_2 H_4^+ + H_2$	2.21×10 <sup>-9</sup>	24
$H_2^+ + C_2 H_4 \rightarrow C_2 H_3^+ + H_2 + H$	1.81×10 <sup>-9</sup>	24
$H_2^+ + C_2 H_4 \rightarrow C_2 H_2^+ + H_2 + H_2$	8.82×10 <sup>-10</sup>	24
$H_2^+ + C_2 H_2 \rightarrow C_2 H_3^+ + H$	4.80×10 <sup>-10</sup>	24
$H_2^+ + C_2 H_2 \rightarrow C_2 H_2^+ + H_2$	4.82×10 <sup>-9</sup>	24
$H_2^+ + C_2 H \rightarrow C_2 H_2^+ + H$	1.00×10 <sup>-9</sup>	24
$H_2^+ + C_2 H \rightarrow C_2 H^+ + H_2$	1.00×10 <sup>-9</sup>	24
$H_2^+ + H_2 \rightarrow H^+ + H_2 + H$	1.00×10 <sup>-8</sup> ×exp(-84100/ <i>T</i> <sub>g</sub> )	6,7
$H_2^+ + H \rightarrow H^+ + H_2$	6.39×10 <sup>-10</sup>	24
$H^+ + H + M \rightarrow H_2^+ + M$	1.00×10 <sup>-34</sup>	6,7
$H^+ + CH_3OH \rightarrow CH_3^+ + H_2O$	$5.90 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$H^+$ + CHO $\rightarrow$ CHO <sup>+</sup> + H	9.40×10 <sup>-10</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$H^+ + CH_3OH \rightarrow CHO^+ + H_2 + H_2$	$8.85 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$H^+ + CO_2 \rightarrow CHO^+ + O$	3.50×10 <sup>-9</sup>	24
$H^{+} + CH_{2}O \rightarrow CHO^{+} + H_{2}$	3.57×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$H^{++CH_{4}\rightarrow CH_{4}^{+}+H}$	1.50×10 <sup>-9</sup>	24
$H^{++CH_{4}\rightarrow CH_{3}^{+}+H_{2}}$	2.30×10 <sup>-9</sup>	24
$H^{++CH_{3}\rightarrow CH_{3}^{+}+H}$	3.40×10 <sup>-9</sup>	24
$H^+ + CH_2 \rightarrow CH_2^+ + H$	1.40×10 <sup>-9</sup>	24
$H^+ + CH_2 \rightarrow CH^+ + H_2$	1.40×10 <sup>-9</sup>	24
$H^+ + CH \rightarrow CH^+ + H$	1.90×10 <sup>-9</sup>	6,7
$H^+ + C_2 H_6 \rightarrow C_2 H_5^+ + H_2$	1.30×10 <sup>-9</sup>	6,7
$H^+ + C_2 H_6 \rightarrow C_2 H_4^+ + H_2 + H$	1.40×10 <sup>-9</sup>	24
$H^+ + C_2 H_6 \rightarrow C_2 H_3^+ + H_2 + H_2$	2.80×10 <sup>-9</sup>	24
$H^+ + C_2H_5 \rightarrow C_2H_4^+ + H_2$	1.65×10 <sup>-9</sup>	24
$H^{++C_{2}H_{5}\rightarrow C_{2}H_{3}^{+}+H_{2}+H}$	3.06×10 <sup>-9</sup>	24
$H^{++C_{2}H_{4}\rightarrow C_{2}H_{4}^{+}+H}$	1.00×10 <sup>-9</sup>	24
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$H^{++C_{2}H_{4}\rightarrow C_{2}H_{3}^{+}+H_{2}}$	3.00×10 <sup>-9</sup>	24
$H^+ + C_2H_4 \rightarrow C_2H_2^+ + H_2 + H$	1.00×10 <sup>-9</sup>	24
$H^{+} + C_2H_3 \to C_2H_3^{+} + H$	2.00×10 <sup>-9</sup>	6,7
$H^{+} + C_2H_3 \to C_2H_2^{+} + H_2$	2.00×10 <sup>-9</sup>	6,7
$H^+ + C_2 H_2 \rightarrow C_2 H_2^+ + H$	5.40×10 <sup>-10</sup>	24
$H^+ + C_2 H \rightarrow C_2 H^+ + H$	1.50×10 <sup>-9</sup>	24
$CO^+ + CHO \rightarrow CHO^+ + CO$	$7.40 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CO^{+} + C_{2}H \rightarrow CHO^{+} + C_{2}$	3.90×10 <sup>-10</sup>	24
$CO^+ + CH_2 \rightarrow CHO^+ + CH$	4.30×10 <sup>-10</sup>	24
$CO^+ + CH_4 \rightarrow CHO^+ + CH_3$	4.55×10 <sup>-10</sup>	24
$CO^+ + CH \rightarrow CHO^+ + C$	$3.20 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CO^{+} + CH_{2}O \rightarrow CHO^{+} + CHO$	1.65×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CO^+ + H_2 \rightarrow CHO^+ + H$	7.50×10 <sup>-10</sup>	24
$CO^+ + H_2O \rightarrow CHO^+ + OH$	8.84×10 <sup>-10</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CO^+ + OH \rightarrow CHO^+ + O$	$3.10 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CO^+ + CO_2 \rightarrow CO_2^+ + CO$	1.00×10 <sup>-9</sup>	24
$CH^+ + O \rightarrow CO^+ + H$	3.50×10 <sup>-10</sup>	24
$CH^+ + O_2 \rightarrow CO^+ + OH$	1.00×10 <sup>-11</sup>	24
$H_2^+ + CO \rightarrow CO^+ + H_2$	6.44×10 <sup>-10</sup>	24
$CO^+ + CH_4 \rightarrow CH_4^+ + CO$	7.93×10 <sup>-10</sup>	24
$CO^+ + CH_2 \rightarrow CH_2^+ + CO$	4.30×10 <sup>-10</sup>	24
$CO^+ + CH \rightarrow CH^+ + CO$	3.20×10 <sup>-10</sup>	6,7
$CO^+ + C_2H \rightarrow C_2H^+ + CO$	3.90×10 <sup>-10</sup>	24
$CO^+ + H \rightarrow H^+ + CO$	7.50×10 <sup>-10</sup>	24
$CO_2^+ + H \rightarrow CHO^+ + O$	2.90×10 <sup>-10</sup>	24
$\boxed{\operatorname{CO}_2^+ + \operatorname{CH}_4 \to \operatorname{CH}_4^+ + \operatorname{CO}_2}$	5.50×10 <sup>-10</sup>	24
$CO_2^+ + C_2H_4 \rightarrow C_2H_4^+ + CO_2$	1.50×10 <sup>-10</sup>	24
$CO_2^+ + C_2H_2 \rightarrow C_2H_2^+ + CO_2$	7.30×10 <sup>-10</sup>	24
$CH^+ + CH_3OH \rightarrow CH_3^+ + CH_2O$	1.45×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH^+ + CH_2O \rightarrow CH_3^+ + CO$	$9.60 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CH^+ + CHO \rightarrow CHO^+ + CH$	$4.60 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CH^{+} + CO_{2} \rightarrow CHO^{+} + CO$	1.60×10 <sup>-9</sup>	24
$CH^{+} + CH_2O \rightarrow CHO^{+} + CH_2$	$9.60 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CH^+ + H_2O \rightarrow CHO^+ + H_2$	2.90×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24

$CH^+ + O_2 \rightarrow CHO^+ + O$	9.70×10 <sup>-10</sup>	24
$CH^+ + O_2(e1) \rightarrow CHO^+ + O$	9.70×10 <sup>-10</sup>	6,7
$CH^+ + O_2(e2) \rightarrow CHO^+ + O$	9.70×10 <sup>-10</sup>	6,7
$CHO^+ + C \rightarrow CH^+ + CO$	1.10×10 <sup>-9</sup>	24
$CH_5^+ + C \rightarrow CH^+ + CH_4$	1.20×10 <sup>-9</sup>	24
$CH^+ + CH_4 \rightarrow C_2H_4^+ + H$	6.50×10 <sup>-11</sup>	24
$CH^+ + CH_4 \rightarrow C_2H_3^+ + H_2$	1.09×10 <sup>-9</sup>	24
$CH^+ + CH_4 \rightarrow C_2H_2^+ + H_2 + H$	1.43×10 <sup>-10</sup>	24
$CH^+ + CH_2 \rightarrow C_2H^+ + H_2$	1.00×10 <sup>-9</sup>	24
$CH^{+} + H_{2} \rightarrow CH_{2}^{+} + H$	1.20×10 <sup>-9</sup>	24
$CH_2^+ + CHO \rightarrow CH_3^+ + CO$	$4.50 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$CH_2^+ + CH_2O \rightarrow CHO^+ + CH_3$	2.81×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_2^+ + O_2 \rightarrow CHO^+ + OH$	9.10×10 <sup>-10</sup>	24
$CH_2^+ + O_2(e1) \rightarrow CHO^+ + OH$	9.10×10 <sup>-10</sup>	6,7
$CH_2^+ + O_2(e2) \rightarrow CHO^+ + OH$	9.10×10 <sup>-10</sup>	6,7
$CH_2^+ + O \rightarrow CHO^+ + H$	7.50×10 <sup>-10</sup>	24
$CHO^{++CH} \to CH_{2^{+}+CO}$	$6.30 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C_2H^+ + CH \rightarrow CH_2^+ + C_2$	3.20×10 <sup>-10</sup>	6,7
$CH_{5}^{+} + CH \to CH_{2}^{+} + CH_{4}$	6.90×10 <sup>-10</sup>	6,7
$CH_2^+ + CH_4 \rightarrow CH_3^+ + CH_3$	1.38×10 <sup>-10</sup>	6,7
$CH_2^+ + CH_4 \rightarrow C_2H_5^+ + H$	3.60×10 <sup>-10</sup>	24
$CH_2^+ + CH_4 \rightarrow C_2H_4^+ + H_2$	8.40×10 <sup>-10</sup>	24
$CH_2^+ + CH_4 \rightarrow C_2H_3^+ + H_2 + H$	2.31×10 <sup>-10</sup>	6,7
$CH_2^+ + CH_4 \rightarrow C_2H_2^+ + H_2 + H_2$	3.97×10 <sup>-10</sup>	6,7
$CH_2^+ + H_2 \rightarrow CH_3^+ + H$	1.60×10 <sup>-9</sup>	24
$CH_2{}^+ + C \rightarrow C_2H^+ + H$	1.20×10 <sup>-9</sup>	24
$CH_3^+ + CHO \rightarrow CHO^+ + CH_3$	4.40×10 <sup>-10</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + CH_2O \rightarrow CHO^+ + CH_4$	1.60×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + O \rightarrow CHO^+ + H_2$	4.00×10 <sup>-10</sup>	24
$CHO^+ + CH_2 \rightarrow CH_3^+ + CO$	8.60×10 <sup>-10</sup>	24
$C_2H^+ + CH_2 \rightarrow CH_3^+ + C_2$	4.40×10 <sup>-10</sup>	24
$CH_5^+ + CH_2 \rightarrow CH_3^+ + CH_4$	9.60×10 <sup>-10</sup>	24
$CH_4{}^+ + H \rightarrow CH_3{}^+ + H_2$	1.00×10 <sup>-11</sup>	24
$CH_3^+ + CH_4 \rightarrow CH_4^+ + CH_3$	1.36×10 <sup>-10</sup>	6,7
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$CH_3{}^+ + CH_4 \rightarrow C_2H_5{}^+ + H_2$	1.20×10 <sup>-9</sup>	24
$CH_3^+ + CH_2 \rightarrow C_2H_3^+ + H_2$	9.90×10 <sup>-10</sup>	24
$CH_3^+ + CH \rightarrow C_2H_2^+ + H_2$	7.10×10 <sup>-10</sup>	6,7
$CH_3^+ + C \to C_2H^+ + H_2$	1.20×10 <sup>-9</sup>	24
$CH_3^+ + C_2H_6 \rightarrow C_2H_5^+ + CH_4$	1.48×10 <sup>-9</sup>	24
$CH_3^+ + C_2H_4 \rightarrow C_2H_3^+ + CH_4$	3.50×10 <sup>-10</sup>	24
$CH_3^+ + C_2H_3 \rightarrow C_2H_3^+ + CH_3$	3.00×10 <sup>-10</sup>	6,7
$CH_4{}^+ + O \rightarrow CH_3{}^+ + OH$	1.00×10 <sup>-9</sup>	24
$C_2H_4^+ + O \rightarrow CH_3^+ + CHO$	1.08×10 <sup>-10</sup>	24
$CH_4^+ + CO \rightarrow CHO^+ + CH_3$	1.40×10 <sup>-9</sup>	24
$CH_4^+ + CO(e1) \rightarrow CHO^+ + CH_3$	1.40×10 <sup>-9</sup>	6,7
$CH_4^+ + CO(e2) \rightarrow CHO^+ + CH_3$	1.40×10 <sup>-9</sup>	6,7
$CH_4^+ + CO(e3) \rightarrow CHO^+ + CH_3$	1.40×10 <sup>-9</sup>	6,7
$CH_4^+ + CO(e4) \rightarrow CHO^+ + CH_3$	1.40×10 <sup>-9</sup>	6,7
$CH_5^+ + H \to CH_4^+ + H_2$	1.50×10 <sup>-10</sup>	24
$CH_4{}^+ + CH_4 \to CH_5{}^+ + CH_3$	1.50×10 <sup>-9</sup>	24
$CH_4^+ + C_2H_6 \rightarrow C_2H_4^+ + CH_4 + H_2$	1.91×10 <sup>-9</sup>	6,7
$CH_4{}^+ + C_2H_4 \rightarrow C_2H_5{}^+ + CH_3$	4.23×10 <sup>-10</sup>	24
$CH_4{}^+ + C_2H_4 \rightarrow C_2H_4{}^+ + CH_4$	1.38×10 <sup>-9</sup>	24
$CH_4^+ + C_2H_2 \rightarrow C_2H_3^+ + CH_3$	1.23×10 <sup>-9</sup>	24
$CH_4^+ + C_2H_2 \to C_2H_2^+ + CH_4$	1.13×10 <sup>-9</sup>	24
$CH_4{}^+ + H_2 \rightarrow CH_5{}^+ + H$	3.30×10 <sup>-11</sup>	6,7
$CH_5^+ + CO \rightarrow CHO^+ + CH_4$	1.00×10 <sup>-9</sup>	24
$CH_{5}^{+}$ + $CO(e1) \rightarrow CHO^{+}$ + $CH_{4}$	1.00×10 <sup>-9</sup>	6,7
$CH_5^+ + CO(e2) \rightarrow CHO^+ + CH_4$	1.00×10 <sup>-9</sup>	6,7
$CH_{5}{}^{+} + CO(e3) \rightarrow CHO^{+} + CH_{4}$	1.00×10 <sup>-9</sup>	6,7
$CH_5^+ + CO(e4) \rightarrow CHO^+ + CH_4$	1.00×10 <sup>-9</sup>	6,7
$CH_{5}^{+} + C_2 \to C_2H^{+} + CH_4$	9.50×10 <sup>-10</sup>	24
$CH_5^+ + C_2H_6 \rightarrow C_2H_5^+ + H_2 + CH_4$	2.25×10 <sup>-10</sup>	6,7
$CH_5^+ + C_2H_4 \rightarrow C_2H_5^+ + CH_4$	1.50×10 <sup>-9</sup>	24
$CH_5^+ + C_2H_2 \rightarrow C_2H_3^+ + CH_4$	1.60×10 <sup>-9</sup>	24
$CH_5^+ + C_2H \rightarrow C_2H_2^+ + CH_4$	9.00×10 <sup>-10</sup>	24
$C_2H^+ + O \rightarrow CHO^+ + C$	3.30×10 <sup>-10</sup>	24
$CHO^+ + C_2 \rightarrow C_2H^+ + CO$	8.30×10 <sup>-10</sup>	24

$C_2H^+ + CH_4 \rightarrow C_2H_2^+ + CH_3$	3.74×10 <sup>-10</sup>	24
$C_2H^+ + H_2 \rightarrow C_2H_2^+ + H$	1.10×10 <sup>-9</sup>	24
$C_2H_2^+ + CHO \rightarrow CHO^+ + C_2H_2$	$5.00 \times 10^{-10} \times (T_g/300)^{-0.50}$	24
$C_2H_2^+ + O \rightarrow CHO^+ + CH$	8.50×10 <sup>-11</sup>	24
$CHO^{+} + C_2H \to C_2H_2^{+} + CO$	7.80×10 <sup>-10</sup>	24
$C_2H_3^+ + C_2H \rightarrow C_2H_2^+ + C_2H_2$	3.30×10 <sup>-10</sup>	24
$C_2H_3^+ + H \rightarrow C_2H_2^+ + H_2$	6.80×10 <sup>-11</sup>	24
$C_2H_2^+ + CH_4 \rightarrow C_2H_3^+ + CH_3$	4.10×10 <sup>-9</sup>	6,7
$C_2H_2^+ + C_2H_6 \rightarrow C_2H_5^+ + C_2H_3$	1.31×10 <sup>-10</sup>	6,7
$C_2H_2^+ + C_2H_6 \rightarrow C_2H_4^+ + C_2H_4$	2.48×10 <sup>-10</sup>	24
$C_2H_2^+ + C_2H_4 \rightarrow C_2H_4^+ + C_2H_2$	4.14×10 <sup>-10</sup>	24
$C_2H_2^+ + C_2H_3 \rightarrow C_2H_3^+ + C_2H_2$	3.30×10 <sup>-10</sup>	24
$C_2H_2^+ + H_2 \rightarrow C_2H_3^+ + H$	1.00×10 <sup>-11</sup>	24
$CHO^{+} + C_2H_2 \rightarrow C_2H_3^{+} + CO$	1.40×10 <sup>-9</sup>	24
$C_2H_4^+ + C_2H_3 \rightarrow C_2H_3^+ + C_2H_4$	5.00×10 <sup>-10</sup>	6,7
$C_2H_4^+ + H \rightarrow C_2H_3^+ + H_2$	3.00×10 <sup>-10</sup>	24
$C_2H_3^+ + C_2H_6 \rightarrow C_2H_5^+ + C_2H_4$	2.91×10 <sup>-10</sup>	24
$C_2H_3^+ + C_2H_4 \rightarrow C_2H_5^+ + C_2H_2$	8.90×10 <sup>-10</sup>	24
$C_2H_3^+ + C_2H_3 \rightarrow C_2H_5^+ + C_2H$	5.00×10 <sup>-10</sup>	24
$C_2H_4^+ + O \rightarrow CHO^+ + CH_3$	8.40×10 <sup>-11</sup>	24
$CHO^+ + C_2H_3 \rightarrow C_2H_4^+ + CO$	1.40×10 <sup>-9</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_6^+ + C_2H_4 \rightarrow C_2H_4^+ + C_2H_6$	1.15×10 <sup>-9</sup>	24
$C_2H_5^+ + H \rightarrow C_2H_4^+ + H_2$	1.00×10 <sup>-11</sup>	24
$C_2H_4^+ + C_2H_3 \rightarrow C_2H_5^+ + C_2H_2$	5.00×10 <sup>-10</sup>	6,7
$CHO^+ + C_2H_4 \rightarrow C_2H_5^+ + CO$	1.40×10 <sup>-9</sup>	24
$C_2H_6^+ + C_2H_2 \rightarrow C_2H_5^+ + C_2H_3$	2.47×10 <sup>-10</sup>	24
$C_2H_6^+ + H \rightarrow C_2H_5^+ + H_2$	1.00×10 <sup>-10</sup>	24
$CHO^{+} + C_2H_5 \rightarrow C_2H_6^{+} + CO$	1.40×10 <sup>-9</sup>	24
$H^- + H \rightarrow H_2 + e$	$2.37 \times 10^{-9} \times T_g^{-0.146} \times \exp(-815/T_g)$	6,7
$H^{-}$ + H $\rightarrow$ H + H + e	$7.47 \times 10^{-16} \times T_g^{1.5} \times \exp(-698/T_g)$	6,7
$H^- + M \rightarrow H + e + M$	$2.70 \times 10^{-10} \times (T_g/300)^{0.50} \times \exp(-5590.0/T_g)$	6,7
$H^- + O \rightarrow OH + e$	1.00×10 <sup>-9</sup>	24
$H^-$ + $OH \rightarrow H_2O$ + e	1.00×10 <sup>-10</sup>	24
$H^{-} + H_2O \rightarrow OH^{-} + H_2$	3.80×10-9	6,7

$H^- + C \rightarrow CH + e$	1.00×10 <sup>-9</sup>	24
$H^{-} + CH \rightarrow CH_{2} + e$	1.00×10 <sup>-10</sup>	24
$H^-$ + $CH_2 \rightarrow CH_3$ + e	1.00×10 <sup>-9</sup>	24
$H^-$ + $CH_3 \rightarrow CH_4$ + e	1.00×10 <sup>-9</sup>	24
$H^{-} + C_2 \rightarrow C_2 H + e$	1.00×10 <sup>-9</sup>	24
$H^{-} + C_2 H \rightarrow C_2 H_2 + e$	1.00×10 <sup>-9</sup>	24
$H^-$ + CO $\rightarrow$ CHO + e	2.00×10 <sup>-11</sup>	24
$O^-$ + H $\rightarrow$ OH + e	5.00×10 <sup>-10</sup>	24
$O^-$ + $H_2 \rightarrow H_2O$ + e	7.00×10 <sup>-10</sup>	24
$O^- + H_2 \rightarrow OH^- + H$	3.00×10 <sup>-11</sup>	24
$O^- + M \rightarrow O + M + e$	2.30×10 <sup>-9</sup> ×exp(-26000.0/ <i>T</i> <sub>g</sub> )	6,7
$O^- + O \rightarrow O_2 + e$	2.30×10 <sup>-10</sup>	6,7
$O^- + O_2 \rightarrow O_2^- + O$	7.30×10 <sup>-10</sup>	24
$O^- + O_2 \rightarrow O_3 + e$	1.00×10 <sup>-12</sup>	6,7
$O^- + O_2 + M \rightarrow O_3^- + M$	1.10×10 <sup>-30</sup> ×(300/ <i>T</i> <sub>g</sub> )	6,7
$O^- + O_2(e1) + M \rightarrow O_3^- + M$	1.10×10 <sup>-30</sup> ×(300/ <i>T</i> <sub>g</sub> )	6,7
$O^- + O_2(e2) + M \rightarrow O_3^- + M$	1.10×10 <sup>-30</sup> ×(300/ <i>T</i> <sub>g</sub> )	6,7
$O^- + O_2(e1) \rightarrow O_3 + e$	1.00×10 <sup>-12</sup>	6,7
$O^- + O_2(e2) \rightarrow O_3 + e$	1.00×10 <sup>-12</sup>	6,7
$O^- + O_2(e1) \rightarrow O_2^- + O$	1.00×10 <sup>-10</sup>	6,7
$O^- + O_3 \rightarrow O_2 + O_2 + e$	3.00×10 <sup>-10</sup>	6,7
$O^- + O_3 \rightarrow O_3^- + O$	5.30×10 <sup>-10</sup>	6,7
$O^- + C \rightarrow CO + e$	5.00×10 <sup>-10</sup>	24
$O^-$ + CH $\rightarrow$ CHO + e	5.00×10 <sup>-10</sup>	24
$O^- + CH_2 \rightarrow CH_2O + e$	5.00×10 <sup>-10</sup>	24
$O^- + CH_4 \rightarrow OH^- + CH_3$	1.00×10 <sup>-10</sup>	24
$O^- + CO \rightarrow CO_2 + e$	5.50×10 <sup>-10</sup>	6,7
$O^- + CO(e1) \rightarrow CO_2 + e$	5.50×10 <sup>-10</sup>	6,7
$O^- + CO(e2) \rightarrow CO_2 + e$	5.50×10 <sup>-10</sup>	6,7
$O^- + CO(e3) \rightarrow CO_2 + e$	5.50×10 <sup>-10</sup>	6,7
$O^- + CO(e4) \rightarrow CO_2 + e$	5.50×10 <sup>-10</sup>	6,7
$OH^- + CH_3 \rightarrow CH_3OH + e$	1.00×10 <sup>-9</sup>	24
$OH^- + CH \rightarrow CH_2O + e$	5.00×10 <sup>-10</sup>	24
$OH^- + C \rightarrow CHO + e$	5.00×10 <sup>-10</sup>	24

$OH^- + H \rightarrow H_2O + e$	1.40×10 <sup>-9</sup>	24
$O_2^- + M \rightarrow O_2 + M + e$	$2.70 \times 10^{-10} \times (T_g/300)^{0.50} \times \exp(-5590.0/T_g)$	6,7
$O_2^- + O \rightarrow O^- + O_2$	1.50×10 <sup>-10</sup>	6,7
$O_2^- + O \rightarrow O_3 + e$	1.50×10 <sup>-10</sup>	6,7
$O_2^- + O_2 \rightarrow O_2 + O_2 + e$	2.18×10 <sup>-18</sup>	6,7
$O_2^- + O_2(e1) \rightarrow O_2(e1) + O_2 + e$	2.18×10 <sup>-18</sup>	6,7
$O_2^- + O_2(e2) \rightarrow O_2(e2) + O_2 + e$	2.18×10 <sup>-18</sup>	6,7
$O_2^- + O_2 + M \rightarrow O_4^- + M$	$3.50 \times 10^{-31} \times (T_g/300)^{-1.0}$	6,7
$O_2^- + O_2(e1) + M \rightarrow O_4^- + M$	$3.50 \times 10^{-31} \times (T_g/300)^{-1.0}$	6,7
$O_2^- + O_2(e2) + M \rightarrow O_4^- + M$	$3.50 \times 10^{-31} \times (T_g/300)^{-1.0}$	6,7
$O_2^- + O_3 \rightarrow O_3^- + O_2$	4.00×10 <sup>-10</sup>	6,7
$O_3^- + CO_2 \rightarrow CO_3^- + O_2$	5.50×10- <sup>10</sup>	6,7
$O_3^- + O \rightarrow O^- + O_3$	1.00×10 <sup>-13</sup>	6,7
$O_3^- + O \rightarrow O_2 + O_2 + e$	1.00×10 <sup>-13</sup>	6,7
$O_3^- + O \rightarrow O_2^- + O_2$	2.50×10 <sup>-10</sup>	6,7
$O_3^- + M \rightarrow O_3 + M + e$	2.30×10 <sup>-11</sup>	6,7
$O_3^- + O_2 \rightarrow O_2 + O_3 + e$	2.30×10 <sup>-11</sup>	6,7
$O_3^- + O_2(e1) \rightarrow O_2(e1) + O_3 + e$	2.30×10 <sup>-11</sup>	6,7
$O_3^- + O_2(e2) \rightarrow O_2(e2) + O_3 + e$	2.30×10 <sup>-11</sup>	6,7
$O_3^- + O_3 \rightarrow O_2 + O_2 + O_2 + e$	3.00×10 <sup>-10</sup>	6,7
$O_4^- + O \rightarrow O_3^- + O_2$	4.00×10 <sup>-10</sup>	6,7
$O_4^- + O \rightarrow O^- + O_2 + O_2$	3.00×10 <sup>-10</sup>	6,7
$O_4^- + M \rightarrow O_2^- + O_2 + M$	$1.00 \times 10^{-10} \times \exp(-1044.0/T_g)$	6,7
$O_4^- + CO_2 \rightarrow CO_4^- + O_2$	4.80×10 <sup>-10</sup>	6,7
$CH_2^- + M \rightarrow CH_2 + e + M$	$2.70 \times 10^{-10} \times (T_g/300)^{0.50} \times \exp(-5590.0/T_g)$	6,7
$\mathrm{CO}_3^- + \mathrm{O} \to \mathrm{O}_2^- + \mathrm{CO}_2$	8.00×10 <sup>-11</sup>	6,7
$CO_3^- + CO \rightarrow CO_2 + CO_2 + e$	5.00×10 <sup>-13</sup>	6,7
$CO_3^- + CO(e1) \rightarrow CO_2 + CO_2 + e$	5.00×10 <sup>-13</sup>	6,7
$CO_3^- + CO(e2) \rightarrow CO_2 + CO_2 + e$	5.00×10 <sup>-13</sup>	6,7
$CO_3^- + CO(e3) \rightarrow CO_2 + CO_2 + e$	5.00×10 <sup>-13</sup>	6,7
$CO_3^- + CO(e4) \rightarrow CO_2 + CO_2 + e$	5.00×10 <sup>-13</sup>	6,7
$\mathrm{CO}_4^- + \mathrm{O} \to \mathrm{CO}_2 + \mathrm{O}_2 + \mathrm{O}^-$	1.40×10 <sup>-11</sup>	6,7
$\mathrm{CO}_4^- + \mathrm{O} \to \mathrm{CO}_3^- + \mathrm{O}_2$	0.8×1.40×10 <sup>-10</sup>	6,7
$\mathrm{CO}_4^- + \mathrm{O} \to \mathrm{O}_3^- + \mathrm{CO}_2$	1.40×10 <sup>-11</sup>	6,7

$\mathrm{CO}_4^- + \mathrm{O}_3 \rightarrow \mathrm{O}_3^- + \mathrm{CO}_2 + \mathrm{O}_2$	1.30×10 <sup>-10</sup>	6,7

#### Table S10. Ion-Ion reactions

Reaction	Rate coefficients	Ref
$H^+ + H^- \rightarrow H + H$	2.00×10 <sup>-7</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	6,7
$H^{+} + H^{-} + M \to H + H + M$	$2.00 \times 10^{-25} \times (T_g/300)^{-2.50}$	6,7
$H^+ + O^- \rightarrow H + O$	1.93×10 <sup>-7</sup>	6,7
$H_2^+ + O^- \rightarrow H_2 + O$	1.93×10 <sup>-7</sup>	6,7
$H^{+} + O_{2^{-}} \rightarrow H + O_{2}$	1.93×10 <sup>-7</sup>	6,7
$H^+ + O_2^- \rightarrow H + O + O$	1.00×10 <sup>-7</sup>	6,7
$H^+ + OH^- \rightarrow OH + H$	1.93×10 <sup>-7</sup>	6,7
$H^+ + OH^- \rightarrow H + O + H$	1.00×10 <sup>-7</sup>	6,7
$H^+ + CO_3^- \rightarrow H + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$H^+ + CO_4^- \rightarrow H + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + H^- \rightarrow H + H + H$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + H^- \rightarrow H + H_2$	$2.00 \times 10^{-7} \times (300/T_g)^{0.5}$	6,7
$H_2^+ + H^- + M \rightarrow H + H_2 + M$	$2.00 \times 10^{-25} \times (T_g/300)^{-2.50}$	6,7
$H_2^+ + O^- \rightarrow H + H + O$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + O_2^- \rightarrow H_2 + O_2$	1.93×10 <sup>-7</sup>	6,7
$H_2^+ + O_2^- \rightarrow H + H + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + O_2^- \rightarrow H_2 + O + O$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + O_2^- \rightarrow H + H + O + O$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + OH^- \rightarrow H_2 + OH$	1.93×10 <sup>-7</sup>	6,7
$H_2^+ + OH^- \rightarrow OH + H + H$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + OH^- \rightarrow O + H + H_2$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + OH^- \rightarrow O + H + H + H$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + CO_3^- \rightarrow H_2 + CO_2 + O$	1.93×10 <sup>-7</sup>	6,7
$H_2^+ + CO_3^- \rightarrow H + H + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$H_2^+ + CO_4^- \rightarrow H_2 + CO_2 + O_2$	1.93×10 <sup>-7</sup>	6,7
$H_2^+ + CO_4^- \rightarrow H + H + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + H^- \rightarrow H_2 + H + H$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + H^- \rightarrow H_2 + H_2$	$2.00 \times 10^{-7} \times (300/T_g)^{0.5}$	6,7
$H_3^+ + O^- \rightarrow O + H_2 + H$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + O_2^- \rightarrow O_2 + H_2 + H$	1.00×10 <sup>-7</sup>	6,7

$H_3^+ + O_3^- \rightarrow H_2 + H + O_3$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + O_3^- \rightarrow H_2 + H + O_2 + O$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + O_3^- + M \rightarrow H_2 + H + O_3 + M$	1.66×10 <sup>-25</sup>	6,7
$H_3^+ + OH^- \rightarrow OH + H + H_2$	1.00×10 <sup>-7</sup>	6,7
$H_3^+ + OH^- \rightarrow O + H + H + H_2$	1.00×10 <sup>-7</sup>	6,7
$O^+ + H^- \rightarrow H + O$	2.30×10 <sup>-7</sup>	6,7
$O^+ + O^- \rightarrow O + O$	4.00×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>0.43</sup>	6,7
$O^+ + O^- + M \rightarrow O_2 + M$	$1.00 \times 10^{-25} \times (300/T_g)^{2.5}$	6,7
$O^+ + O_2^- \rightarrow O + O_2$	2.70×10 <sup>-7</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>0.5</sup>	6,7
$O^+ + O_2^- + M \rightarrow O_3 + M$	$1.00 \times 10^{-25} \times (300/T_g)^{2.5}$	6,7
$O^+ + O_3^- \rightarrow O_3 + O$	$1.00 \times 10^{-7} \times (300/T_g)^{0.5}$	6,7
$O^+ + OH^- \rightarrow O + H + O$	1.00×10 <sup>-7</sup>	6,7
$O^+ + OH^- \rightarrow OH + O$	1.93×10 <sup>-7</sup>	6,7
$O_2^+ + H^- \rightarrow O_2 + H$	1.93×10 <sup>-7</sup>	6,7
$O_2^+ + H^- \rightarrow O + O + H$	1.00×10 <sup>-7</sup>	6,7
$O_2^+ + O^- \rightarrow O_2 + O$	2.60×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>0.44</sup>	6,7
$O_2^+ + O^- \to O + O + O$	4.20×10 <sup>-7</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>0.44</sup>	6,7
$O_2^+ + O^- + M \rightarrow O_3 + M$	$1.00 \times 10^{-25} \times (300/T_g)^{2.5}$	6,7
$O_2^+ + O_2^- \rightarrow O_2 + O_2$	2.01×10 <sup>-7</sup> ×(300/ <i>T</i> g) <sup>0.5</sup>	6,7
$O_2^+ + O_2^- \to O_2^- + O_2^- + O_2^-$	4.20×10 <sup>-7</sup>	6,7
$O_2^+ + O_2^- + M \to O_2 + O_2 + M$	1.00×10 <sup>-25</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>2.5</sup>	6,7
$O_2^+ + O_3^- \rightarrow O_2 + O_3$	$2.00 \times 10^{-7} \times (300/T_g)^{0.5}$	6,7
$O_2^+ + O_3^- \rightarrow O + O + O_3$	$1.00 \times 10^{-7} \times (300/T_g)^{0.5}$	6,7
$O_2^+ + OH^- \rightarrow O + H + O_2$	1.00×10 <sup>-7</sup>	6,7
$O_2^+ + OH^- \rightarrow O + H + O + O$	1.00×10 <sup>-7</sup>	6,7
$O_2^+ + OH^- \rightarrow OH + O_2$	1.93×10 <sup>-7</sup>	6,7
$O_2^+ + OH^- \rightarrow OH + O + O$	1.00×10 <sup>-7</sup>	6,7
$O_2^+ + CO_3^- \rightarrow CO_2 + O_2 + O_2$	3.00×10 <sup>-7</sup>	6,7
$O_2^+ + CO_4^- \rightarrow CO_2 + O_2 + O_2$	3.00×10 <sup>-7</sup>	6,7
$OH^+ + H^- \rightarrow H + OH$	1.93×10 <sup>-7</sup>	6,7
$OH^+ + H^- \rightarrow H + O + H$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + O^- \rightarrow O + OH$	1.93×10 <sup>-7</sup>	6,7
$OH^+ + O^- \rightarrow O + H + O$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + O_2^- \rightarrow OH + O_2$	1.93×10 <sup>-7</sup>	6,7
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$OH^+ + O_2^- \rightarrow O + H + O_2$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + O_2^- \rightarrow OH + O + O$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + O_2^- \rightarrow O + H + O + O$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + OH^- \rightarrow OH + OH$	1.93×10 <sup>-7</sup>	6,7
$OH^+ + OH^- \rightarrow OH + O + H$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + OH^- \rightarrow O + H + O + H$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + CO_3^- \rightarrow OH + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + CO_3^- \rightarrow O + H + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + CO_4^- \rightarrow OH + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$OH^+ + CO_4^- \rightarrow O + H + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + H^- \rightarrow H_2O + H$	1.93×10 <sup>-7</sup>	6,7
$H_2O^+ + H^- \rightarrow H + H + OH$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + O^- \rightarrow H_2O + O$	1.93×10 <sup>-7</sup>	6,7
$H_2O^+ + O^- \rightarrow OH + H + O$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + O_2^- \rightarrow H_2O + O_2$	1.93×10 <sup>-7</sup>	6,7
$H_2O^+ + O_2^- \rightarrow OH + H + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + O_2^- \rightarrow H_2O + O + O$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + O_2^- \rightarrow H + OH + O + O$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + OH^- \rightarrow OH + H_2O$	1.93×10 <sup>-7</sup>	6,7
$H_2O^+ + OH^- \rightarrow O + H + H_2O$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + OH^- \rightarrow OH + OH + H$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + OH^- \rightarrow O + H + OH + H$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + CO_3^- \rightarrow H_2O + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$\mathrm{H_2O^+} + \mathrm{CO_3^-} \rightarrow \mathrm{OH} + \mathrm{H} + \mathrm{CO_2} + \mathrm{O}$	1.00×10 <sup>-6</sup>	6,7
$H_2O^+ + CO_4^- \rightarrow H_2O + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$H_2O^+ + CO_4^- \rightarrow OH + H + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$\rm H_3O^+ + H^- \rightarrow H + H + H_2O$	7.51×10 <sup>-8</sup> ×( <i>T</i> g/300) <sup>-0.50</sup>	24
$\mathrm{H_3O^+} + \mathrm{H^-} \rightarrow \mathrm{H_2} + \mathrm{OH} + \mathrm{H}$	2.30×10 <sup>-7</sup>	6,7
$H_3O^+ + H^- \rightarrow H_2O + H_2$	2.30×10 <sup>-7</sup>	6,7
$\mathrm{H_{3}O^{+}+O^{-}}\rightarrow\mathrm{H_{2}O+H+O}$	1.00×10 <sup>-7</sup>	6,7
$H_3O^+ + O_2^- \rightarrow H_2O + H + O2$	1.00×10 <sup>-7</sup>	6,7
$H_3O^+ + O_2^- \rightarrow H_2O + H + O + O$	1.00×10 <sup>-7</sup>	6,7
$\rm H_3O^+ + OH^- \rightarrow OH + H_2O + H$	1.00×10 <sup>-7</sup>	6,7
$\rm H_3O^+ + OH^- \rightarrow O + H + H_2O + H$	1.00×10 <sup>-7</sup>	6,7

$H_3O^+ + CO_3^- \rightarrow H_2O + H + CO_2 + O$	1.00×10 <sup>-7</sup>	6,7
$H_3O^+ + CO_4^- \rightarrow H_2O + H + CO_2 + O_2$	1.00×10 <sup>-7</sup>	6,7
$C^+ + H^- \rightarrow C + H$	2.30×10 <sup>-7</sup>	6,7
$C^+ + O^- \rightarrow C + O$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C^+ + O_2^- \rightarrow C + O_2$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C^+ + OH^- \rightarrow C + OH$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + H^- \rightarrow H + CH_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + O^- \rightarrow O + CH_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + O_2^- \rightarrow O_2 + CH_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CH_3^+ + OH^- \rightarrow OH + CH_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_2^+ + H^- \rightarrow H + C_2H_2$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_2^+ + O^- \rightarrow O + C_2H_2$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_2^+ + O_2^- \rightarrow O_2 + C_2H_2$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_2^+ + OH^- \rightarrow OH + C_2H_2$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_3^+ + H^- \rightarrow H + C_2H_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_3^+ + O^- \rightarrow O + C_2H_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_3^+ + O_2^- \rightarrow O_2 + C_2H_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$C_2H_3^+ + OH^- \rightarrow OH + C_2H_3$	7.51×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + H^- \rightarrow H + H + CO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + H^- \rightarrow H + CHO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + O^- \rightarrow O + H + CO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + O^- \rightarrow O + CHO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + O_2^- \to O_2 + H + CO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + O_2^- \rightarrow O_2 + CHO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + OH^- \rightarrow OH + H + CO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CHO^+ + OH^- \rightarrow OH + CHO$	3.76×10 <sup>-8</sup> ×( <i>T</i> <sub>g</sub> /300) <sup>-0.50</sup>	24
$CO^+ + H^- \rightarrow CO + H$	1.93×10 <sup>-7</sup>	6,7
$CO^+ + OH^- \rightarrow CO + OH$	1.93×10 <sup>-7</sup>	6,7
$CO^+ + OH^- \rightarrow CO + O + H$	1.00×10 <sup>-7</sup>	6,7
$CO_2^+ + H^- \rightarrow CO_2 + H$	1.93×10 <sup>-7</sup>	6,7
$CO_2^+ + H^- \rightarrow CO + O + H$	1.00×10 <sup>-7</sup>	6,7
$CO_2^+ + OH^- \rightarrow CO_2 + OH$	1.93×10 <sup>-7</sup>	6,7
$CO_2^+ + OH^- \rightarrow CO_2 + O + H$	1.00×10 <sup>-7</sup>	6,7
$\mathrm{CO}_2^+ + \mathrm{OH}^- \rightarrow \mathrm{CO} + \mathrm{O} + \mathrm{OH}$	1.00×10 <sup>-7</sup>	6,7
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$\mathrm{CO}_2^+ + \mathrm{OH}^- \rightarrow \mathrm{CO} + \mathrm{O} + \mathrm{O} + \mathrm{H}$	1.00×10 <sup>-7</sup>	6,7
$C_2O_2^+ + O_2^- \rightarrow CO + CO + O_2$	6.00×10 <sup>-7</sup>	6,7
$C_2O_2^+ + CO_3^- \rightarrow CO_2 + CO + CO + O$	5.00×10 <sup>-7</sup>	6,7
$C_2O_2^+ + CO_4^- \rightarrow CO_2 + CO + CO + O_2$	5.00×10 <sup>-7</sup>	6,7
$C_2O_3^+ + O_2^- \rightarrow CO_2 + CO + O_2$	6.00×10 <sup>-7</sup>	6,7
$C_2O_3^+ + CO_3^- \rightarrow CO_2 + CO_2 + CO + O$	5.00×10 <sup>-7</sup>	6,7
$C_2O_3^+ + CO_4^- \rightarrow CO_2 + CO_2 + CO + O_2$	5.00×10 <sup>-7</sup>	6,7
$C_2O_4^+ + O_2^- \rightarrow CO_2 + CO_2 + O_2$	6.00×10 <sup>-7</sup>	6,7
$C_2O_4^+ + CO_3^- \rightarrow CO_2 + CO_2 + CO_2 + O_2$	5.00×10 <sup>-7</sup>	6,7
$C_2O_4^+ + CO_4^- \rightarrow CO_2 + CO_2 + CO_2 + O_2$	5.00×10 <sup>-7</sup>	6,7

## Table S11. Electron recombination reactions

Reaction	Rate coefficients	Ref
$H^+ + e \rightarrow H$	3.50×10 <sup>-12</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.75</sup>	24
$H_2^+ + e \rightarrow H + H$	5.33×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>0.40</sup>	6,7
$H_2^+ + e \rightarrow H^+ + H + e$	f(σ, EEDF)	6,7
$H_2^+ + e \rightarrow H^+ + H^-$	f(σ, EEDF)	6,7
$H_2^+ + e + e \rightarrow e + H + H$	$5.26 \times 10^{-3} \times T_{e}^{-4.5}$	6,7
$H_2^+ + e + e \rightarrow H_2 + e$	8.80×10 <sup>-27</sup> ×(300/ <i>T</i> <sub>g</sub> ) <sup>4.50</sup>	6,7
$H_3^+ + e \rightarrow H^+ + H_2 + e$	f(σ, EEDF)	6,7
$H_3^+ + e \rightarrow H^+ + H + H + e$	f(σ, EEDF)	6,7
$H_3^+ + e \rightarrow H_2 + H$	f(σ, EEDF)	6,7
$H_3^+ + e \rightarrow H + H + H$	f(σ, EEDF)	6,7
$H_3^+ + e + e \rightarrow e + H + H_2$	5.26×10 <sup>-3</sup> ×7 <sub>e</sub> <sup>-4.5</sup>	6,7
$O^+ + e + M \rightarrow O + M$	6.00×10 <sup>-27</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>1.5</sup>	6,7
$O^+ + e + e \rightarrow O + e$	7.00×10 <sup>-20</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>4.5</sup>	6,7
$O_2^+ + e + M \rightarrow O_2 + M$	1.00×10 <sup>-26</sup>	6,7
$O_2^+ + e \rightarrow O + O$	$6.46 \times 10^{-5} \times T_e^{-0.5} \times T_g^{-0.50}$	6,7
$O_4{}^+ + e \rightarrow O_2 + O_2$	2.42×10 <sup>-5</sup> ×7 <sub>e</sub> <sup>-0.50</sup>	6,7
$OH^+ + e \rightarrow O + H$	3.56×10 <sup>-9</sup>	6,7
$OH^+ + e + e \rightarrow OH + e$	7.92×10 <sup>-29</sup>	6,7
$OH^- + e \rightarrow e + e + H + O$	1.95×10 <sup>-8</sup>	6,7
$H_2O^+ + e \rightarrow O + H_2$	3.70×10 <sup>-9</sup>	6,7
$H_2O^+ + e \rightarrow O + H + H$	2.89×10 <sup>-8</sup>	6,7

$H_2O^+ + e \rightarrow OH + H$	8.14×10 <sup>-9</sup>	6,7
$H_2O^+$ + e + e $\rightarrow$ $H_2O$ + e	7.92×10 <sup>-29</sup>	6,7
$H_3O^+ + e \rightarrow H_2O + H$	2.45×10 <sup>-8</sup> ×( <i>T</i> <sub>e</sub> /300) <sup>-0.83</sup>	6,7
$H_3O^+ + e \rightarrow OH + H_2$	6.58×10 <sup>-9</sup> ×( <i>T</i> <sub>e</sub> /300) <sup>-0.83</sup>	6,7
$H_3O^+ + e \rightarrow OH + H + H$	$4.02 \times 10^{-9} \times (T_e/300)^{-0.83}$	6,7
$CH^+ + e \rightarrow C + H$	3.23×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.42</sup>	6,7
$CH_2^+ + e \rightarrow CH + H$	1.00×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_2^+ + e \rightarrow C + H_2$	4.82×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_2^+ + e \rightarrow C + H + H$	2.53×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_3^+ + e \rightarrow CH_2 + H$	2.25×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_3^+ + e \rightarrow CH + H_2$	7.88×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_3^+ + e \rightarrow CH + H + H$	9.00×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_3^+ + e \rightarrow C + H_2 + H$	1.69×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_4^+ + e \rightarrow CH_3 + H$	1.18×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_4^+ + e \rightarrow CH_2 + H + H$	2.42×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_4^+ + e \rightarrow CH + H_2 + H$	1.41×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.50</sup>	6,7
$CH_5^+ + e \rightarrow CH_3 + H + H$	2.57×10 <sup>-7</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.30</sup>	6,7
$CH_5^+ + e \rightarrow CH_2 + H_2 + H$	6.61×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.30</sup>	6,7
$CH_5^+ + e \rightarrow CH + H_2 + H_2$	8.40×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.52</sup>	24
$CH_5^+ + e \rightarrow CH_3 + H_2$	1.40×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.52</sup>	24
$CH_5^+ + e \rightarrow CH_4 + H$	1.40×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.52</sup>	24
$CHO^+ + e \rightarrow H + CO$	0.88×2.40×10 <sup>-7</sup> ×( <i>T</i> <sub>e</sub> /300) <sup>-0.69</sup>	25
$CHO^+ + e \rightarrow C + OH$	$0.06 \times 2.40 \times 10^{-7} \times (T_e/300)^{-0.69}$	25
$CHO^+ + e \rightarrow CH + O$	$0.06 \times 2.40 \times 10^{-7} \times (T_e/300)^{-0.69}$	25
$CO^+ + e \rightarrow C + O$	2.00×10 <sup>-7</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.48</sup>	24
$CO_2^+ + e \rightarrow C + O_2$	$1.07 \times 10^{-3} \times T_{e}^{-0.50}/T_{g}$	6,7
$C_2^+ + e \rightarrow C + C$	1.93×10 <sup>-6</sup> × <i>T</i> e <sup>-0.50</sup>	6,7
$C_2H_2^+ + e \rightarrow C_2H + H$	1.87×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_2^+$ + e $\rightarrow$ CH + CH	4.87×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_3^+ + e \rightarrow C_2H_2 + H$	1.34×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_3^+ + e \rightarrow C_2H + H + H$	$2.74 \times 10^{-8} \times (300/T_{\rm e})^{0.71}$	6,7
$C_2H_4^+ + e \rightarrow C_2H_3 + H$	$8.29 \times 10^{-9} \times (300/T_e)^{0.71}$	6,7
$C_2H_4^+ + e \rightarrow C_2H_2 + H + H$	$3.43 \times 10^{-8} \times (300/T_e)^{0.71}$	6,7
$C_2H_4^+ + e \rightarrow C_2H + H_2 + H$	5.53×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7

$C_2H_5^+ + e \rightarrow C_2H_4 + H$	7.70×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_5^+ + e \rightarrow C_2H_3 + H + H$	1.92×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_5^+ + e \rightarrow C_2H_2 + H_2 + H$	1.60×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_5^+ + e \rightarrow C_2H_2 + H + H + H$	8.98×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_5^+ + e \rightarrow CH_3 + CH_2$	9.62×10 <sup>-9</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_6^+ + e \rightarrow C_2H_5 + H$	2.19×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2H_6^+ + e \rightarrow C_2H_4 + H + H$	3.36×10 <sup>-8</sup> ×(300/ <i>T</i> <sub>e</sub> ) <sup>0.71</sup>	6,7
$C_2O_2^+ + e \rightarrow CO + CO$	$4.00 \times 10^{-7} \times T_e^{-0.34}$	6,7
$C_2O_3^+ + e \rightarrow CO_2 + CO$	$3.78 \times 10^{-5} \times T_e^{-0.70}$	6,7
$C_2O_4^+ + e \rightarrow CO_2 + CO_2$	$2.15 \times 10^{-3} \times T_e^{-0.50}/T_g$	6,7
$H^{-}$ + e $\rightarrow$ H + e + e	f(σ, EEDF)	6,7
$OH^- + e \rightarrow OH + e + e$	f(σ, EEDF)	6,7

## Table S12. Neutral-Neutral reactions

Reaction	Rate coefficients	Ref
$CH_3CHOH + O \rightarrow CH_3COOH + H$	$2.20 \times 10^{-10} \times (T_g/298)^{0.16} \times \exp(-4.91/(R \times T_g))$	23
$CH_3CHO + OH \rightarrow CH_3COOH + H$	$0.02 \times 2.49 \times 10^{-12} \times (T_g/298)^{0.73} \times \exp(4656/(R \times T_g))$	23
$CH_3CHO + HO_2 \rightarrow CH_3COOH + OH$	5.00×10 <sup>-12</sup> ×exp(-49890.0/(R× <i>T</i> <sub>g</sub> ))	23
$CH_3CO_2 + M \rightarrow CH_3 + CO_2 + M$	$7.31 \times 10^{-9} \times \exp(-10500.0/(0.2389 \times R \times T_g))$	26
$CH_3 + CO_2 + M \rightarrow CH_3CO_2 + M$	$1.25 \times 10^{-29} \times T_g^{1.378} \times \exp(-17520.0/(0.2389 \times R \times T_g))$	26
$CH_2COOH \rightarrow CH_2CO + OH$	$1.69 \times 10^{18} \times T_g^{-1.18} \times \exp(-53720.0/(0.2389 \times R \times T_g))$	26
$CH_2CO + OH \rightarrow CH_2COOH$	$4.32 \times 10^{-12} \times \exp(614.0/(0.2389 \times R \times T_g))$	26
$CH_3CO + OH \rightarrow CH_3COOH$	1.66×10 <sup>-10</sup>	27
$CH_2COOH + H_2 \rightarrow CH_3COOH + H$	$3.37 \times 10^{-21} \times T_g^{3.13} \times \exp(-37843.8/(R \times T_g))$	27
$CH_2COOH + OH \rightarrow CH_3COOH + O$	$2.04 \times 10^{-15} \times T_g^{1.03} \times \exp(-33241.4/(R \times T_g))$	27
$CH_2COOH + H_2O \rightarrow CH_3COOH + OH$	$3.11 \times 10^{-19} \times T_g^{2.50} \times \exp(-73294.3/(R \times T_g))$	27
$CH_2COOH + H_2O_2 \rightarrow CH_3COOH + HO_2$	$2.64 \times 10^{-13} \times T_g^{0.35} \times \exp(-21175.3/(R \times T_g))$	27
$CH_2COOH + CH_4 \rightarrow CH_3COOH + CH_3$	1.08×10 <sup>-14</sup> ×7 <sup>0.81</sup> ×exp(-25278.1/(R×7g))	27
$CH_2COOH + HO_2 \rightarrow CH_3COOH + O_2$	$6.27 \times 10^{-12} \times T_g^{-0.24} \times \exp(11718.9/(R \times T_g))$	27
$CH_3CO_2 + H_2 \rightarrow CH_3COOH + H$	$2.24 \times 10^{-50} \times T_g^{11.63} \times \exp(23665.5/(R \times T_g))$	27
$CH_3CO_2 + OH \rightarrow CH_3COOH + O$	$4.46 \times 10^{-31} \times T_g^{5.69} \times \exp(3392.3/(R \times T_g))$	27
$CH_3CO_2 + H_2O_2 \rightarrow CH_3COOH + HO_2$	$1.77 \times 10^{-13} \times T_g^{0.49} \times \exp(-27927.5/(R \times T_g))$	27
$CH_3CO_2 + CH_4 \rightarrow CH_3COOH + CH_3$	$3.72 \times 10^{-25} \times T_g^{4.41} \times \exp(-34391.2/(R \times T_g))$	27
$CH_3CO_2 + H_2O \rightarrow CH_3COOH + OH$	$2.06 \times 10^{-16} \times T_g^{1.14} \times \exp(-54713.2/(R \times T_g))$	27

$CH_2OH + HO_2 \rightarrow O_2(e1) + CH3OH$	$9.47 \times 10^{-17} \times (T_g/298)^{3.20} \times \exp(-6800.0/(R \times T_g))$	23
$CH_{3}O + CH_{3}CHO \rightarrow CH_{3}OH + CH_{3}CO$	8.30×10 <sup>-15</sup>	23
$CH_3 + OH \rightarrow CH_2(S) + H_2O$	$6.37 \times 10^{-11} \times (T_g/298)^{-1.27} \times \exp(-1549.0/(R \times T_g))$	23
$CO + CH \to C_2HO$	$1.70 \times 10^{-10} \times (T_g/298)^{-0.40}$	23
$C_2H_2 + OH \rightarrow C_2HO + H_2$	1.91×10 <sup>-13</sup>	23
$C_2HO + O \rightarrow CO_2 + CH$	$4.90 \times 10^{-11} \times \exp(-4656.0/(R \times T_g))$	23
$C_2HO + H \rightarrow CH_2(S) + CO$	$2.14 \times 10^{-10} \times (T_g/298)^{0.16} \times \exp(-166.0/(R \times T_g))$	23
$C_2H_2 + O \rightarrow C_2HO + H$	$1.50 \times 10^{-11} \times \exp(-19000.0/(R \times T_g))$	23
$C_2H_2 + OH \rightarrow CH_2CO + H$	5.31×10 <sup>-13</sup> ×exp(-840.0/(R× <i>T</i> <sub>g</sub> ))	23
$CH_2 + CO \rightarrow CH_2CO$	$1.35 \times 10^{-12} \times T_g^{0.50} \times \exp(-4510.0/(0.2389 \times R \times T_g))$	27
$C_2H + OH \rightarrow C_2HO + H$	3.32×10 <sup>-11</sup>	27
$C_2H_2 + O_2 \rightarrow C_2HO + OH$	$3.32 \times 10^{-16} \times T_g^{1.50} \times \exp(-30100.0/(0.2389 \times R \times T_g))$	27
$CH_2CO + H \rightarrow C_2HO + H_2$	$8.30 \times 10^{-11} \times \exp(-8000.0/(0.2389 \times R \times T_g))$	27
$CH_2CO + O \rightarrow C_2HO + OH$	$1.66 \times 10^{-11} \times \exp(-8000.0/(0.2389 \times R \times T_g))$	27
$CH_2CO + OH \rightarrow C_2HO + H_2O$	1.25×10 <sup>-11</sup> ×exp(-2000.0/(0.2389×R× <i>T</i> <sub>g</sub> ))	27
$CH_2O + CH \rightarrow CH_2CO + H$	$1.57 \times 10^{-10} \times \exp(515.0/(0.2389 \times R \times T_g))$	27
$CH_{3}O + H \rightarrow CH_{2}(s) + H_{2}O$	$4.35 \times 10^{-10} / T_g^{0.23} \times \exp(-1070.0 / (0.2389 \times \mathbb{R} \times T_g))$	27
$CH_2OH + H \rightarrow CH_2(s) + H_2O$	$5.45 \times 10^{-11}/T_g^{0.09} \times \exp(-610.0/(0.2389 \times R \times T_g))$	27
$C_2H_5O + H_2 \rightarrow C_2H_5OH + H$	$4.10 \times 10^{-21} \times T_g^{2.74} \times \exp(-4188.0/(0.2389 \times R \times T_g))$	28
$C_2H_5O + OH \rightarrow C_2H_5OH + O$	$5.79 \times 10^{-29} \times T_g^{4.924} \times \exp(-98.0/(0.2389 \times R \times T_g))$	28
$C_2H_5O + H_2O \rightarrow C_2H_5OH + OH$	$1.22 \times 10^{-14} \times T_g^{0.91} \times \exp(-17210.0/(0.2389 \times R \times T_g))$	28
$C_2H_5O + H_2O_2 \rightarrow C_2H_5OH + HO_2$	$1.11 \times 10^{-10}/T_g^{0.483} \times \exp(-7782.0/(0.2389 \times R \times T_g))$	28
$C_2H_5O + CH_4 \rightarrow C_2H_5OH + CH_3$	$1.42 \times 10^{-22} \times T_g^{3.336} \times \exp(-9044.0/(0.2389 \times R \times T_g))$	28
$C_2H_5O + CH_3OOH \rightarrow C_2H_5OH + CH_3O_2$	$2.15 \times 10^{-9} / T_g^{0.927} \times \exp(-6187.0 / (0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + H_{2} \rightarrow C_{2}H_{5}OH + H$	$7.35 \times 10^{-22} \times T_{\rm g}^{2.97} \times \exp(-12840.0/(0.2389 \times {\rm R} \times T_{\rm g}))$	28
$CH_{3}CHOH + OH \rightarrow C_{2}H_{5}OH + O$	$3.09 \times 10^{-22} \times T_g^{2.868} \times \exp(-8884.0/(0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + H_{2}O \rightarrow C_{2}H_{5}OH + OH$	$2.42 \times 10^{-15} \times T_g^{0.83} \times \exp(-23930.0/(0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + HO_{2} \rightarrow C_{2}H_{5}OH + O_{2}$	$3.23 \times 10^{-13} \times T_g^{0.089} \times \exp(-4879.0/(0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + H_{2}O_{2} \rightarrow C_{2}H_{5}OH + HO_{2}$	$1.43 \times 10^{-11}/T_g^{0.258} \times \exp(-9419.0/(0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + CH_{3}OOH \rightarrow C_{2}H_{5}OH + CH_{3}O_{2}$	$3.79 \times 10^{-19} \times T_g^{1.847} \times \exp(-2574.0/(0.2389 \times R \times T_g))$	28
$CH_{3}CHOH + CH_{4} \rightarrow C_{2}H_{5}OH + CH_{3}$	$7.47 \times 10^{-23} \times T_g^{3.361} \times \exp(-18590.0/(0.2389 \times R \times T_g))$	28
$CH_3CHOH + C_2H_6 \rightarrow C_2H_5OH + C_2H_5$	1.16×10 <sup>-13</sup> ×exp(-2.4/(0.2389×R× <i>T</i> <sub>g</sub> ))	28
$C_2H_5O_2 + OH \rightarrow C_2H_5O + HO_2$	0.75×1.30×10 <sup>-10</sup>	23
$C_2H_4 + OH \rightarrow CH_2CH_2OH$	9.00×10 <sup>-12</sup>	23

$CH_2CH_2OH + O \rightarrow CH_2O + CH_2OH$	$4.59 \times 10^{-10} \times (T_g/298)^{0.17} \times \exp(-4.24/(R \times T_g))$	23
$CH_2CH_2OH \rightarrow C_2H_4 + OH$	$9.94 \times 10^{16} \times (T_g/298)^{-6.54} \times \exp(-113000.0/(R \times T_g))$	23
$CH_2CH_2OH + H \rightarrow CH_3 + CH_2OH$	1.49×10 <sup>-10</sup>	29
$CH_2CH_2OH + H_2 \rightarrow C_2H_5OH + H$	$6.53 \times 10^{-25} \times T_{\rm g}^{3.826} \times \exp(-9484.0/(0.2389 \times {\rm R} \times T_{\rm g}))$	28
$CH_2CH_2OH + OH \rightarrow C_2H_5OH + O$	$1.75 \times 10^{-25} \times T_g^{3.837} \times \exp(-5580.0/(0.2389 \times \mathbb{R} \times T_g))$	28
$CH_2CH_2OH + HO_2 \rightarrow C_2H_5OH + O2$	$3.64 \times 10^{-14} \times T_g^{0.278} \times \exp(-443.0/(0.2389 \times R \times T_g))$	28
$CH_2CH_2OH + H_2O \rightarrow C_2H_5OH + OH$	$6.66 \times 10^{-16} \times T_g^{0.92} \times \exp(-17940.0/(0.2389 \times R \times T_g))$	28
$CH_2CH_2OH + H_2O_2 \rightarrow C_2H_5OH + HO_2$	$4.78 \times 10^{-21} \times T_{\rm g}^{2.481} \times \exp(-2827.0/(0.2389 \times {\rm R} \times T_{\rm g}))$	28
$CH_2CH_2OH + CH_4 \rightarrow C_2H_5OH + CH_3$	$1.05 \times 10^{-22} \times T_g^{3.48} \times \exp(-16160.0/(0.2389 \times R \times T_g))$	28
$CH_2CH_2OH + C_2H_6 \rightarrow C_2H_5OH + C_2H_5$	1.16×10 <sup>-13</sup> ×exp(-26990.0/(0.2389×R× <i>T</i> <sub>g</sub> ))	28
$CH_2CH_2OH + CH_3OOH \rightarrow C_2H_5OH + CH_3O_2$	$4.81 \times 10^{-20} \times T_{\rm g}^{2.036} \times \exp(-488.0/(0.2389 \times {\rm R} \times T_{\rm g}))$	28
$C_2H_5OH + H \rightarrow CH_2CH_2OH + H_2$	$3.12 \times 10^{-21} \times T_g^{3.20} \times \exp(-7150.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + O \rightarrow CH_2CH_2OH + OH$	$1.61 \times 10^{-21} \times T_g^{3.23} \times \exp(-4658.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + OH \rightarrow CH_2CH_2OH + H_2O$	$3.01 \times 10^{-13} \times T_g^{0.40} \times \exp(-717.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + O_2 \rightarrow CH_2CH_2OH + HO_2$	$3.32 \times 10^{-11} \times \exp(-52800.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + HO_2 \rightarrow CH_2CH_2OH + H_2O_2$	$3.95 \times 10^{-20} \times T_g^{2.55} \times \exp(-16490.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + CH_3 \rightarrow CH_2CH_2OH + CH_4$	$5.48 \times 10^{-22} \times T_g^{3.30} \times \exp(-12290.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + C_2H_5 \rightarrow CH_2CH_2OH + C_2H_6$	$8.30 \times 10^{-14} \times \exp(-13400.0/(0.2389 \times R \times T_g))$	28
$C_2H_5OH + CH_3O_2 \rightarrow CH_2CH_2OH + CH_3OOH$	$2.04 \times 10^{-20} \times T_g^{2.55} \times \exp(-15750.0/(0.2389 \times R \times T_g))$	28
$C_3H_7 + CH_3O_2 \rightarrow CH_3CHO + CH_3O + CH_3$	4.00×10 <sup>-11</sup>	23
$\rm CH_3O_2 + \rm CH_3CHO \rightarrow \rm CH_3OOH + \rm CH_3CO$	$5.00 \times 10^{-12} \times \exp(-6000.0/T_g)$	30
$C_{3}H_{7} + O \rightarrow CH_{3}CHO + CH_{3}$	8.00×10 <sup>-11</sup>	30
$C_3H_5 + O_2 \rightarrow CH_3CHO + CHO$	1.66×10 <sup>-13</sup>	30
$C_2H_4 + OH \rightarrow CH_3CHO + H$	$3.95 \times 10^{-26} \times T_g^{3.91} \times \exp(-867.0/T_g)$	30
$C_3H_5 + O_2 \rightarrow CH_3CO + CH_2O$	$1.71 \times 10^{-9} \times (T_g/298)^{-3.21} \times \exp(-17980.0/(R \times T_g))$	23
$C_3H_6 + O \rightarrow CH_3CO + CH_3$	$0.19 \times 1.25 \times 10^{-12} \times (T_g/298)^{2.15} \times \exp(3330.0/(R \times T_g))$	23
$C_2H_2 + O \rightarrow CH_2CO$	2.16×10 <sup>-13</sup>	23
$CH_3CO + H \rightarrow CH_2CO + H_2$	0.35×3.32×10 <sup>-11</sup>	23
$C_3H_5 + O \rightarrow CH_3 + CH_2CO$	9.96×10 <sup>-11</sup>	30
$C_3H_5 + OH \rightarrow CH_3 + CH_2CO + H$	8.30×10 <sup>-12</sup>	30
$C_3H_5 + HO_2 \rightarrow CH_3 + CH_2CO + OH$	3.32×10 <sup>-11</sup>	30
$C_3H_6 + O \rightarrow CH_2CO + CH_3 + H$	$4.15 \times 10^{-17} \times T_g^{1.76} \times \exp(-38.2/T_g)$	30
$CH_3CHO + CH \rightarrow CH_2CO + CH_3$	1.00×10 <sup>-10</sup>	18
$CH_2CO + OH \rightarrow CH_3 + CO_2$	1.12×10 <sup>-12</sup> ×exp(1013.0/(0.2389×R×T <sub>g</sub> ))	18

$CH_2CHO \rightarrow CH_3CO$	$1.58 \times 10^{16} / (T_g/298)^{5.49} \times \exp(-193000.0 / (R \times T_g))$	23
$CH_3CO \rightarrow CH_2CHO$	$3.00 \times 10^{15} \times \exp(-118000.0/(R \times T_g))$	23
$CH_2O + CH \rightarrow CH_2CHO$	$1.31 \times 10^{-12} \times (T_g/298)^{0.38} \times \exp(3610.0/(R \times T_g))$	23
$C_2H_3 + O \rightarrow CH_2CHO$	$5.50 \times 10^{-11} \times (T_g/298)^{0.20} \times \exp(1790.0/(R \times T_g))$	23
$C_2H_3 + O_2 \rightarrow CH_2CHO + O$	$2.13 \times 10^{-11}/(T_g/298)^{0.03} \times \exp(-18950.0/(R \times T_g))$	23
$C_2H_3 + OH \rightarrow CH_2CHO + H$	$5.58 \times 10^{-12} \times (T_g/298)^{0.26} \times \exp(1820.0/(R \times T_g))$	23
$C_2H_4 + O \rightarrow CH_2CHO + H$	$3.36 \times 10^{-12} \times (T_g/298)^{0.95} \times \exp(-7220.0/(R \times T_g))$	23
$C_3H_5 + O_2 \rightarrow CH_2CHO + CH_2O$	$4.21 \times 10^{-14} \times (T_g/298)^{0.37} \times \exp(-70750.0/(R \times T_g))$	23
$CH_{3}CHO + H \rightarrow CH_{2}CHO + H_{2}$	$2.13 \times 10^{-13} \times (T_g/298)^{3.10} \times \exp(-21780.0/(R \times T_g))$	23
$CH_3CHO + O \rightarrow CH_2CHO + OH$	$2.49 \times 10^{-11} \times \exp(-20920.0/(R \times T_g))$	23
$CH_3CHO + O_2 \rightarrow CH_2CHO + HO_2$	$3.32 \times 10^{-10} \times \exp(-203000.0/(R \times T_g))$	23
$CH_3CHO + OH \rightarrow CH_2CHO + H_2O$	$2.66 \times 10^{-11} \times \exp(-8370.0/(R \times T_g))$	23
$CH_{3}CHO + HO_{2} \rightarrow CH_{2}CHO + H_{2}O_{2}$	$1.66 \times 10^{-12} \times \exp(-58580.0/(R \times T_g))$	23
$CH_3CHO + CH_3 \rightarrow CH_2CHO + CH_4$	$9.96 \times 10^{-12} \times \exp(-46020.0/(R \times T_g))$	23
$C_2H_3 + HO_2 \rightarrow CH_2CHO + OH$	1.66×10 <sup>-11</sup>	18
$CH_{3}CHO + CH_{2} \rightarrow CH_{2}CHO + CH_{3}$	$2.76 \times 10^{-12} \times \exp(-3517.0/(0.2389 \times R \times T_g))$	18
$CH_2CHO \rightarrow CH_3 + CO$	$6.51 \times 10^{34} / T_g^{6.87} \times \exp(-47197.0 / (0.2389 \times R \times T_g))$	18
$CH_2CHO \rightarrow CH_2CO + H$	$1.32 \times 10^{34} / T_g^{6.57} \times \exp(-49460.0 / (0.2389 \times R \times T_g))$	18
$CH_2CHO + H \rightarrow CH_3CHO$	1.66×10 <sup>-10</sup>	18
$CH_2CHO + H \rightarrow CH_2CO + H_2$	3.32×10 <sup>-11</sup>	18
$CH_2CHO + OH \rightarrow H_2O + CH_2CO$	1.99×10 <sup>-11</sup>	18
$CH_2CHO + H \rightarrow CH_3 + CHO$	8.29×10 <sup>-11</sup>	18
$CH_2CHO + O \rightarrow CH_2O + CHO$	8.30×10 <sup>-11</sup>	18
$CH_2CHO + OH \rightarrow CHO + CH_2OH$	5.00×10 <sup>-10</sup>	18
$CH_2CHO + O_2 \rightarrow CO + CH_2O + OH$	$4.45 \times 10^{-7}/T_{g}^{1.84} \times \exp(-6530.0/(0.2389 \times R \times T_{g}))$	18
$CH_{3}O + C_{2}H_{4} \rightarrow CH_{3}OH + C_{2}H_{3}$	1.99×10 <sup>-13</sup> ×exp(-3400.0/ <i>T</i> <sub>g</sub> )	30
$CH_2OH + OH \rightarrow CH_3OH + O$	$3.89 \times 10^{-21} \times T_g^{2.59} \times \exp(-7956.0/(0.2389 \times R \times T_g))$	31
$CH_2OH + HO_2 \rightarrow CH_3OH + O_2$	$2.06 \times 10^{-12} / T_g^{0.24} \times \exp(3501.0 / (0.2389 \times R \times T_g))$	31
$CH_2OH + CH_3OOH \to CH_3OH + CH_3O_2$	$3.90 \times 10^{-10} / T_g^{1.03} \times \exp(-2404.0 / (0.2389 \times R \times T_g))$	31
$CH_2OH + C_2H_5OOH \rightarrow CH_3OH + C_2H_5O_2$	$3.90 \times 10^{-10} / T_g^{1.03} \times \exp(-2408.0 / (0.2389 \times \mathbb{R} \times T_g))$	31
$CH_3O_2 + OH \rightarrow CH_3O + HO_2$	0.90×2.80×10 <sup>-10</sup>	23
$CH_2(S) + H_2O_2 \rightarrow CH_3O + OH$	5.00×10 <sup>-11</sup>	29
$C_2H_5 + OH \rightarrow CH_2OH + CH_3$	4.98×10 <sup>-11</sup>	29
$CH_3O + CH_3OOH \rightarrow CH_3OH + OH + CH_2O$	$2.49 \times 10^{-13} \times \exp(-6500.0/(0.2389 \times R \times T_g))$	32
$CH_{3}O + C_{2}H_{5}OOH \rightarrow CH_{3}CHO + OH + CH_{3}OH$	$1.05 \times 10^{-12} \times \exp(-5500.0/(0.2389 \times R \times T_g))$	32
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$CH_2OH + C_2H_5OOH \rightarrow CH_3CHO + OH + CH_3OH$	$6.97 \times 10^{-13} \times \exp(-13600.0/(0.2389 \times R \times T_g))$	32
$CH_3O + CH_2CO \rightarrow CH_3OH + C_2HO$	$5.69 \times 10^{-19} \times T_g^{2.00} \times \exp(-6416.99/(0.2389 \times R \times T_g))$	33
$\rm CH_{3}O + \rm CH_{3}CHO \rightarrow \rm CH_{3}OH + \rm CH_{2}CHO$	$2.13 \times 10^{-19} \times T_{\rm g}^{2.00} \times \exp(-3702.80/(0.2389 \times {\rm R} \times T_{\rm g}))$	33
$CH_2OH + CH_2CO \rightarrow CH_3OH + C_2HO$	$3.76 \times 10^{-19} \times T_g^{2.00} \times \exp(-17077.95/(0.2389 \times R \times T_g))$	33
$CH_2OH + CH_3CHO \rightarrow CH_3OH + CH_2CHO$	$1.41 \times 10^{-19} \times T_{\rm g}^{2.00} \times \exp(-13176.14/(0.2389 \times {\rm R} \times T_{\rm g}))$	33
$CH_2CHO + H \rightarrow CH_3CO + H$	8.30×10 <sup>-12</sup>	34
$CH_3CHO + CH_2CHO \rightarrow CH_3CHO + CH_3CO$	4.15×10 <sup>-17</sup>	40
$\rm CH_3CHO + CHO \rightarrow CH_3CO + CH_2O$	$1.30 \times 10^{-10} \times \exp(-8440.0/(0.2389 \times R \times T_g))$	35
$C_2H_3 + O_2 \rightarrow CH_2CO + OH$	$1.94 \times 10^{-21} \times T_g^{2.43} \times \exp(-7074.00/(0.2389 \times R \times T_g))$	33
$C_2HO + H_2O_2 \rightarrow CH_2CO + HO_2$	$5.69 \times 10^{-20} \times T_g^{2.00} \times \exp(-1926.22/(0.2389 \times R \times T_g))$	33
$C_2HO + CH_2O \rightarrow CH_2CO + CHO$	$5.69 \times 10^{-19} \times T_g^{2.00} \times \exp(-4161.68/(0.2389 \times R \times T_g))$	33
$C_2HO + CH_3CHO \rightarrow CH_3CO + CH_2CO$	$4.26 \times 10^{-19} \times T_g^{2.00} \times \exp(-4416.11/(0.2389 \times R \times T_g))$	33
$CH_2CHO + O \rightarrow CH_2CO + OH$	$3.32 \times 10^{-11} \times \exp(-4000.0/(0.2389 \times R \times T_g))$	34
$CH_2CHO + O_2 \rightarrow CH_2CO + HO_2$	2.33×10 <sup>-13</sup>	34
$C_2HO + H_2 \rightarrow CH_2CO + H$	$1.08 \times 10^{-12} \times \exp(-840.11/(0.2389 \times R \times T_g))$	36
$C_2HO + H_2O \rightarrow CH_2CO + OH$	2.34×10 <sup>-13</sup> ×exp(-9994.98/(0.2389×R× <i>T</i> <sub>g</sub> ))	36
$CH_3 + CO \rightarrow CH_2CO + H$	$3.99 \times 10^{-12} \times \exp(-40200.05/(0.2389 \times R \times T_g))$	36
$CH_2 + CO_2 \rightarrow CH_2CO + O$	$6.21 \times 10^{-12} \times \exp(-53690.01/(0.2389 \times R \times T_g))$	36
$C_3H_7 + HO_2 \rightarrow CH_3CHO + CH_3 + OH$	3.99×10 <sup>-11</sup>	35
$C_3H_6 + OH \rightarrow CH_3CHO + CH_3$	$2.32 \times 10^{-12} \times \exp(1040.0/(0.2389 \times R \times T_g))$	37
$C_2H_3 + CH_3O_2 \rightarrow CH_2CHO + CH_3O$	3.99×10 <sup>-11</sup>	41
$CH_2 + O_2 \rightarrow COOH + H$	$0.15 \times 4.10 \times 10^{-11} \times \exp(-6240.0/(R \times T_g))$	23
$CO + OH \rightarrow COOH$	$9.34 \times 10^{-13} \times (T_g/298)^{-3.50} \times \exp(-5478.0/(R \times T_g))$	23
$CH_2O + OH \rightarrow COOH + H_2$	$1.40 \times 10^{-12} \times (T_g/298)^{1.63} \times \exp(-4410.0/(R \times T_g))$	23
$CH_3$ + COOH $\rightarrow$ CH <sub>3</sub> COOH	$5.81 \times 10^{-11} \times (T_g/298)^{0.10}$	23
$CH_{3}O_{2} + H \rightarrow CH_{4} + O_{2}$	$1.17 \times 10^{-11} \times (T_g/298)^{1.02} \times \exp(-69450.0/(R \times T_g))$	23
$CH_3O_2 + OH \rightarrow CH_3OH + O_2(e1)$	$3.53 \times 10^{-12} / (T_g/298)^{1.17} \times \exp(570.0 / (R \times T_g))$	23
$CH_{3}O_{2} + HO_{2} \rightarrow CH_{3}OH + O_{3}$	4.10×10 <sup>-13</sup> ×exp(6570.0/(R× <i>T</i> <sub>g</sub> ))	23
$CH_2OH + H \rightarrow CH_3OH$	$1.29 \times 10^{-9} / T_g^{0.247} \times \exp(-1668.0 / (0.2389 \times R \times T_g))$	26
$O_2 + CH_2OH \rightarrow CH_2O + HO_2$	1.40×10 <sup>-12</sup>	23
$CH_3 + O_2 \rightarrow CH_3O_2$	6.11×10 <sup>-14</sup>	23
$\text{HCOOH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCOO}$	$7.86 \times 10^{-16} \times (T_g/298)^{5.59} \times \exp(9910.0/(R \times T_g))$	23
$H + COOH \rightarrow HCOOH$	9.50×10 <sup>-10</sup>	38

$CH_3 + O \rightarrow CH_2O + H$ $1.00 \times 10^{-10}$ $CH_3 + OH \rightarrow CH_3OH$ $7.70 \times 10^{-13} \times (T_g/298)^{2.08} \times exp(7360.0)/(R \times 120 \times 10^{-32})$ $H + O_2 + M \rightarrow HO_2 + M$ $1.20 \times 10^{-32}$	23 (T <sub>g</sub> )) 23 23
$CH_3 + OH \rightarrow CH_3OH$ $7.70 \times 10^{-13} \times (T_g/298)^{2.08} \times exp(7360.0)/(R \times 1.20 \times 10^{-32})^{1.08}$ $H + O_2 + M \rightarrow HO_2 + M$ $1.20 \times 10^{-32}$	(T <sub>g</sub> )) 23 23
$H + O_2 + M \rightarrow HO_2 + M$ 1.20×10 <sup>-32</sup>	23
$CH_3 + COOH \rightarrow CH_4 + CO_2 \qquad \qquad 0.40 \times 5.80 \times 10^{-11} \times exp(-60.0)(0.2389 \times R \times 10^{-11} \times 10^{$	<i>T</i> <sub>g</sub> )) 39
$CH_3 + COOH \rightarrow CH_2CO + H_2O \qquad \qquad 0.60 \times 5.80 \times 10^{-11} \times exp(-60.0)(0.2389 \times R \times 10^{-11} \times 10^{-11}$	<i>T</i> <sub>g</sub> )) 39
$COOH + CO \rightarrow CO_2 + CHO \qquad 1.00 \times 10^{-15}$	23
CH <sub>3</sub> O + H $\rightarrow$ CH <sub>3</sub> OH 4.04×10 <sup>-12</sup> × $T_g^{0.52}$ ×exp(-50.0/(0.2389×R)	× <i>T</i> <sub>g</sub> )) 27
$CH_3 + O \rightarrow CHO + H_2$ $0.40 \times 1.70 \times 10^{-10}$	23
$CH_2(S) + O \rightarrow H + CO + H$ 7.48×10 <sup>-11</sup>	29
$CH_2(S) + O \rightarrow CO + H_2$ 7.48×10 <sup>-11</sup>	29
$CH_2(S) + O_2 \rightarrow CO + OH + H$ 4.65×10 <sup>-11</sup>	29
$CH_2(S) + O_2 \rightarrow CO + H_2O$ 1.99×10 <sup>-11</sup>	29
$C_2H_4 + H \rightarrow C_2H_5 \qquad 1.25 \times 10^{-11} \times (T_g/298)^{1.07} \times \exp(-6067.0) (R)^{-10}$	× <i>T</i> <sub>g</sub> )) 42
C <sub>2</sub> H <sub>4</sub> + O $\rightarrow$ CHO + CH <sub>3</sub> 1.50×10 <sup>-12</sup> ×( $T_g$ /298) <sup>1.55</sup> ×exp(-1788.0/(R)	× <i>T</i> <sub>g</sub> )) 41
$CH_3 + CH_3CO \rightarrow C_2H_6 + CO$ $0.38 \times 1.43 \times 10^{-10}$	43
$C_2H_5 + C_2H_3 \rightarrow C_2H_6 + C_2H_2$ 0.37×6.50×10 <sup>-11</sup>	44,45
$CH_3 + M \rightarrow CH + H_2 + M$ $6.97 \times 10^{-9} \times exp(-345.0 \times 10^{3}/(R \times T_g))$	6,7
$CH_2 + M \rightarrow C + H_2 + M$ $2.16 \times 10^{-10} \times exp(-247.0 \times 10^3/(R \times T_g))$	6,7
$CH_2 + M \rightarrow CH + H + M$ $6.64 \times 10^{-9} \times exp(-348.0 \times 10^{3}/(R \times T_g))$	6,7
$C + H_2 + M \rightarrow CH_2 + M$ 6.89×10 <sup>-32</sup>	6,7
CH + M $\rightarrow$ C + H + M 3.16×10 <sup>-10</sup> ×exp(-280.0×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
$C_2 + M \rightarrow C + C + M$ 2.49×10 <sup>-8</sup> ×exp(-595.0×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
$C + CO + M \rightarrow C_2O + M$ 6.31×10 <sup>-32</sup>	6,7
$H_2 + M \rightarrow H + H + M$ $1.88 \times 10^{-8} \times (T_g/298)^{-1.1} \times \exp(-437.0 \times 10^{3}/(10^{-10} \times 10^{-10})^{-1.1})$	(R× <i>T</i> <sub>g</sub> )) 6,7
$H + H + M \rightarrow H_2 + M$ $6.04 \times 10^{-33} \times (T_g/298)^{-1.00}$	6,7
$O + CO + M \rightarrow CO_2 + M$ $8.20 \times 10^{-34} \times exp(-1510.0/T_g) \times 2.000$	6,7
$O_3 + M \rightarrow O_2 + O + M$ $4.12 \times 10^{-10} \times exp(-11430.0/T_g)$	6,7
$O + O_2 + M \rightarrow O_3 + M$ $5.51 \times 10^{-34} \times (T_g/298)^{-2.6}$	6,7
$O_2 + M \rightarrow O + O + M$ $3.00 \times 10^{-6} \times T_g^{-1} \times exp(-5.938 \times 10^4/T_g)$	6,7
$O + O + M \rightarrow O_2 + M$ $5.21 \times 10^{-35} \times \exp(900.0/T_g)$	6,7
$CO_2 + M \rightarrow CO + O + M$ $6.06 \times 10^{-10} \times exp(-5.2525 \times 10^4/T_g)$	6,7
O + C + M $\rightarrow$ CO + M 2.14×10 <sup>-29</sup> ×( $T_g$ /300) <sup>-3.08</sup> ×exp(-2114.0/ $T_g$ )	) 6,7
H + O + M $\rightarrow$ OH + M 4.36×10 <sup>-32</sup> ×( $T_g$ /300) <sup>-1.00</sup>	6,7

$CH + CO + M \rightarrow C_2HO + M$	4.15×10 <sup>-30</sup> ×( <i>T</i> <sub>g</sub> /298) <sup>-1.90</sup>	6,7
$H + CO + M \rightarrow CHO + M$	4.80×10 <sup>-35</sup>	6,7
$H + OH + M \rightarrow H_2O + M$	4.38×10 <sup>-30</sup> ×( <i>T</i> <sub>g</sub> /298) <sup>-2.0</sup>	6,7
$OH + OH + M \rightarrow H_2O_2 + M$	$6.04 \times 10^{-31} \times (T_g/298)^{-3.0}$	6,7
$OH + M \rightarrow O + H + M$	$4.00 \times 10^{-9} \times \exp(-416 \times 10^{3}/(R \times T_g))$	6,7
$H_2O + M \rightarrow OH + H + M$	5.80×10 <sup>-9</sup> ×exp(-440.0×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CH_3OH + M \rightarrow CH_3 + OH + M$	3.32×10 <sup>-7</sup> ×exp(-286.0×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
$H_2O_2 + M \rightarrow OH + OH + M$	$2.03 \times 10^{-3} \times (T_g/298)^{-4.86} \times \exp(-223 \times 10^{3}/(R \times T_g))$	6,7
$HO_2 + M \rightarrow H + O_2 + M$	$2.41 \times 10^{-8} \times (T_g/298)^{-1.18} \times \exp(-203.0 \times 10^3/(R \times T_g))$	6,7
$CHO + M \to H + CO + M$	$2.61 \times 10^{-10} \times \exp(-65.93 \times 10^{3}/(\text{R} \times T_g))$	6,7
$CH_3OH + M \rightarrow CH_2OH + H + M$	2.16×10 <sup>-8</sup> ×exp(-279.0×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$CH_{3}O_{2} + M \rightarrow CH_{3} + O_{2} + M$	$2.03 \times (T_g/298)^{-10.0} \times \exp(-139.0 \times 10^3/(R \times T_g))$	6,7
$C_2HO + M \rightarrow CO + CH + M$	1.08×10 <sup>-8</sup> ×exp(-246.0×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$C_2H_2 + H \rightarrow C_2H_3$	9.13×10 <sup>-12</sup> ×exp(-1.01×10 <sup>4</sup> /(R× $T_g$ ))	46
$C_3H_8 \rightarrow C_3H_7 + H$	1.58×10 <sup>16</sup> ×exp(-408.0×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$C_3H_7 \rightarrow C_3H_6$ + H	$1.09 \times 10^{13} \times (T_g/298)^{0.17} \times \exp(-1.49 \times 10^{5}/(R \times T_g))$	6,7
$C_3H_6 \rightarrow C_3H_5$ + H	2.50×10 <sup>15</sup> ×exp(-363.0×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$C_3H_6 \rightarrow CH_3 + C_2H_3$	$1.18 \times 10^{18} \times (T_g/298)^{-1.20} \times \exp(-409.0 \times 10^3/(R \times T_g))$	6,7
$C_2H_2 + CH_3 \rightarrow C_3H_5$	$1.00 \times 10^{-12} \times \exp(-32.26 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_3 + H \rightarrow C_2H_4$	2.01×10 <sup>-10</sup>	47
$C_2H + H \rightarrow C_2H_2$	3.01×10 <sup>-10</sup>	6,7
$C_2H_4 \rightarrow C_2H_3 + H$	2.00×10 <sup>16</sup> ×exp(-4.61×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	48
$CH_4 \rightarrow CH_3 + H$	3.72×10 <sup>15</sup> ×exp(-4.34×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	41
$C_2H_5 \rightarrow C_2H_4$ + H	$6.86 \times 10^{12} \times (T_g/298)^{0.95} \times \exp(-1.55 \times 10^{5}/(R \times T_g))$	42
$C_2H_3 \rightarrow C_2H_2$ + H	2.00×10 <sup>14</sup> ×exp(-1.66×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	49
$C_2H_2 \rightarrow C_2H + H$	2.63×10 <sup>15</sup> ×exp(-5.19×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	41
$C_3H_8 \rightarrow C_2H_5 + CH_3$	$2.78 \times 10^{18} \times (T_g/298)^{-1.80} \times \exp(-3.71 \times 10^{5}/(R \times T_g))$	50
$C_2H_4 \rightarrow C_2H_2 + H_2$	$9.75 \times 10^{13} \times (T_g/298)^{0.44} \times \exp(-3.72 \times 10^{5}/(R \times T_g))$	41
$CH_3CO \rightarrow CO + CH_3$	$3.87 \times 10^{13} \times (T_g/298)^{0.63} \times \exp(-70.70 \times 10^3/(R \times T_g))$	6,7
$CHO + H \to CH_2O$	7.77×10 <sup>-14</sup> ×exp(1.90×10 <sup>4</sup> /(R× <i>T</i> <sub>g</sub> ))	51
$CH_2OH \rightarrow CH_2O + H$	$1.16 \times 10^{17} \times (T_g/298)^{-7.11} \times \exp(-1.84 \times 10^{5/(R \times T_g)})$	52
$CH_3O \rightarrow CH_2O + H$	$1.69 \times 10^{14} \times (T_g/298)^{0.39} \times \exp(-1.10 \times 10^5/(R \times T_g))$	42
$HCOOH \rightarrow CO + H2O$	9.12×10 <sup>12</sup> ×exp(-2.52×10 <sup>5</sup> /(R×T <sub>g</sub> ))	6,7
$C_2H_5O + H \rightarrow C_2H_5OH$	$8.32 \times 10^{-11} \times (T_g/298)^{0.44} \times \exp(-54.04/(R \times T_g))$	53
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$C_2H_5OH \rightarrow C_2H_5 + OH$	$1.34 \times 10^{17} \times (T_g/298)^{-2.16} \times \exp(-4.04 \times 10^{5}/(R \times T_g))$	54
$C_2H_5OH \rightarrow C_2H_5O + H$	$1.53 \times 10^{16} \times (T_g/298)^{0.31} \times \exp(-4.24 \times 10^{5}/(R \times T_g))$	53
$C_2H_5OOH \rightarrow C_2H_5O + OH$	$4.00 \times 10^{15} \times \exp(-1.80 \times 10^{5}/(R \times T_g))$	55
$CH_{3}CHOH + H \rightarrow C_{2}H_{5}OH$	$8.43 \times 10^{-11} \times (T_g/298)^{0.06} \times \exp(-1829.0/(R \times T_g))$	53
$CH_3CHOH \rightarrow CH_3CHO + H$	$1.20 \times 10^{15} \times (T_g/298)^{-5.19} \times \exp(-1.49 \times 10^{5/(R \times T_g)})$	56
$CH_{3}CHOH \rightarrow CH_{2}O + CH_{3}$	$1.49 \times 10^{13} \times (T_g/298)^{-3.59} \times \exp(-1.45 \times 10^{5/(R \times T_g)})$	56
$C_2H_5OH \rightarrow CH_3CHOH + H$	$1.57 \times 10^{16} \times (T_g/298)^{-0.28} \times \exp(-3.93 \times 10^{5/(R \times T_g)})$	53
$CH_3 \rightarrow CH_2 + H$	$1.90 \times 10^{16} \times (T_g/298)^{0.09} \times \exp(-4.59 \times 10^5/(R \times T_g))$	57
$CH_3 + C_2H_3 \to C_3H_6$	1.20×10 <sup>-10</sup>	44
$C_2H_5 + H \rightarrow C_2H_6$	$2.55 \times 10^{-10} \times (T_g/298)^{0.16}$	58
$C_{3}H_{7} + H \rightarrow C_{3}H_{8}$	6.00×10 <sup>-11</sup>	59
$C_{3}H_{6} + H \rightarrow C_{3}H_{7}$	$6.64 \times 10^{-12} \times \exp(-1.10 \times 10^4 / (R \times T_g))$	46
$C_{3}H_{5} + H \rightarrow C_{3}H_{6}$	$2.64 \times 10^{-10} \times (T_g/298)^{0.18} \times \exp(524/(R \times T_g))$	60
$C_2H_6 \rightarrow CH_3 + CH_3$	$1.54 \times 10^{18} \times (T_g/298)^{-2.14} \times \exp(-3.80 \times 10^{5/(R \times T_g)})$	55
$CH_2CO \rightarrow CO + CH_2$	$3.00 \times 10^{14} \times \exp(-2.97 \times 10^{5}/(R \times T_g))$	46
$C_2H_5 + OH \rightarrow C_2H_5OH$	1.28×10 <sup>-10</sup>	61
$C_2H_5OH \rightarrow C_2H_4 + H_2O$	$6.91 \times 10^{16} \times (T_g/298)^{-3.68} \times \exp(-2.96 \times 10^{5/(R \times T_g)})$	62
$C_2H_5OH \rightarrow CH_3 + CH_2OH$	$7.91 \times 10^{24} \times (T_g/298)^{-10.59} \times \exp(-4.22 \times 10^{5/(R \times T_g)})$	62
$C_2H_5 + O_2 \rightarrow C_2H_5O_2$	$1.09 \times 10^{-7} \times (T_g/298)^{-10.30} \times \exp(-2.54 \times 10^4/(R \times T_g))$	63
$C_2H_5O_2 \rightarrow C_2H_5 + O_2$	$5.30 \times 10^{15} \times (T_g/298)^{-0.83} \times \exp(-1.43 \times 10^{5/(R \times T_g)})$	64
$CH_3 + CO \rightarrow CH_3CO$	8.40×10 <sup>-13</sup> ×exp(-2.88×10 <sup>4</sup> /(R× <i>T</i> <sub>g</sub> ))	55
$C_2H_4 + O \rightarrow CH_2O + CH_2$	$8.08 \times 10^{-13} \times (T_g/298)^{1.99} \times \exp(-1.20 \times 10^4/(R \times T_g))$	65
$CH_2O + O_2 \rightarrow CHO + HO_2$	3.40×10 <sup>-11</sup> ×exp(-1.63×10 <sup>5</sup> /(R×T <sub>g</sub> ))	41
$C_2H_4 + OH \rightarrow C_2H_3 + H_2O$	$2.29 \times 10^{-13} \times (T_g/298)^{2.74} \times \exp(-9271.0/(R \times T_g))$	66
$C_2H_3 + H \rightarrow C_2H_2 + H_2$	3.32×10 <sup>-11</sup>	46
$CH_3 + C_2H_5 \rightarrow C_2H_4 + CH_4$	1.88×10 <sup>-12</sup> ×( <i>T</i> <sub>g</sub> /298) <sup>-0.50</sup>	41
$H + CH_3CHO \rightarrow H_2 + CH_3CO$	$6.64 \times 10^{-11} \times \exp(-1.76 \times 10^4 / (\text{R} \times T_g))$	46
$CH + C_2H_5 \rightarrow C_3H_5 + H$	$3.80 \times 10^{-8} \times T_g^{-0.859} \times \exp(-33.5/T_g)$	67
$CH_3CO + H \rightarrow CH_3CHO$	$1.50 \times 10^{-10} \times (T_g/298)^{0.16}$	68
$C_2H_5O_2 \rightarrow CH_3CHO$ + OH	$7.27 \times 10^{10} \times (T_g/298)^{2.63} \times \exp(-1.55 \times 10^{5}/(R \times T_g))$	69
$C_2H_3$ + OH $\rightarrow$ CH <sub>3</sub> CHO	5.00×10 <sup>-11</sup>	41
$C_2H_5 + O_2 \rightarrow CH_3CHO + OH$	$1.00 \times 10^{-13} \times \exp(-2.87 \times 10^4 / (R \times T_g))$	41
$CH_{3}CHO + H \rightarrow CO + H_{2} + CH_{3}$	$4.88 \times 10^{-13} \times (T_g/298)^{2.75} \times \exp(-4041.0/(R \times T_g))$	70
$CH_3CHO + O_2 \rightarrow CH_3CO + HO_2$	5.00×10 <sup>-11</sup> ×exp(-1.64×10 <sup>5</sup> /(R×T <sub>g</sub> ))	49
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$CH_{3}CHO + C_{2}H_{3} \rightarrow C_{2}H_{4} + CH_{3}CO$	$1.35 \times 10^{-13} \times \exp(-1.54 \times 10^4 / (R \times T_g))$	71
$CH + H_2O \rightarrow CH_2OH$	9.48×10 <sup>-12</sup> ×exp(3159.0/(R× <i>T</i> <sub>g</sub> ))	72
$C_2H_3 + OH \rightarrow CH_3CO + H$	$2.92 \times 10^{-11} \times (T_g/298)^{-1.01} \times \exp(-1621.0/(R \times T_g))$	68
$CH_3CO + O_2 \rightarrow CO_2 + CH_3O$	$7.37 \times 10^{-14} \times \exp(4506.0/(R \times T_g))$	73
$CH_3O + HO_2 \rightarrow CH_3OH + O_2$	4.70×10 <sup>-11</sup>	74
$C_2H_3 + OH \rightarrow CH_3 + CHO$	$2.88 \times 10^{-10} \times (T_g/298)^{-1.85} \times \exp(-4166.0/(R \times T_g))$	68
$\rm CO + CH_3O \rightarrow CH_2O + CHO$	3.26×10 <sup>-33</sup>	75
$CH_3CHO + H \rightarrow CH_4 + CHO$	8.80×10 <sup>-14</sup>	76
$CHO + H \to O + CH_2$	$6.61 \times 10^{-11} \times \exp(-4.29 \times 10^{5}/(\text{R} \times T_{g}))$	77
$CHO \rightarrow CO + H$	$2.00 \times 10^5 \times \exp(-1.10 \times 10^5/(R \times T_g))$	78
$CH_3 + CHO \rightarrow CH_3CHO$	3.01×10 <sup>-11</sup>	41
$CH_3 + O_2 \rightarrow CH_2O + OH$	$2.81 \times 10^{-13} \times \exp(-4.14 \times 10^4 / (R \times T_g))$	23,79
$CH_3 + OH \rightarrow CH_2O + H_2$	$2.59 \times 10^{-13} \times (T_g/298)^{-0.53} \times \exp(-4.52 \times 10^4/(R \times T_g))$	80
$CH_3O + CH_3CO \rightarrow CH_2O + CH_3CHO$	1.00×10 <sup>-11</sup>	41
$CH_3O_2 + HO_2 \rightarrow CH_2O + H_2O + O_2$	$1.60 \times 10^{-15} \times \exp(-1.44 \times 10^4 / (R \times T_g))$	81
$CH_3O_2 + CH_2OH \rightarrow CH_2O + CH_3OOH$	$4.75 \times 10^{-18} \times (T_g/298)^{2.69} \times \exp(1.43 \times 10^4/(R \times T_g))$	82
$CH_3O_2 \rightarrow CH_2O + OH$	$5.86 \times 10^{10} \times (T_g/298)^{2.98} \times \exp(-1.63 \times 10^{5}/(R \times T_g))$	83
$C_3H_5 + O_2 \rightarrow CH_2O + C_2H_2 + OH$	$3.37 \times 10^{-10} \times (T_g/298)^{-2.70} \times \exp(-1.05 \times 10^{5}/(R \times T_g))$	84
$CH_{3}OH + OH \rightarrow CH_{2}O + H_{2}O + H$	$1.10 \times 10^{-12} \times (T_g/298)^{1.44} \times \exp(-474.0/(R \times T_g))$	85
$CH_2O + H \rightarrow CH_2OH$	$2.41 \times 10^{-13} \times (T_g/298)^{-1.40} \times \exp(-2.17 \times 10^4/(R \times T_g))$	52
$CH_2O + H \rightarrow CH_3O$	$3.99 \times 10^{-11} \times \exp(-1.72 \times 10^4 / (R \times T_g))$	42
$CH_3 + C_2H_3 \rightarrow C_3H_5 + H$	$2.59 \times 10^{-9} \times (T_g/298)^{-1.25} \times \exp(-3.21 \times 10^4/(R \times T_g))$	86
$CH+CH\toC_2H_2$	1.99×10 <sup>-10</sup>	87
$CH + H_2 \rightarrow CH_3$	2.01×10 <sup>-10</sup> ×( <i>T</i> <sub>g</sub> /298) <sup>0.15</sup>	88
$C_2H_4 + O \rightarrow CH_3CO + H$	$9.11 \times 10^{-13} \times (T_g/298)^{-0.48} \times \exp(-8192.0/(R \times T_g))$	65
$C_2H_4 + O_2 \rightarrow C_2H_3 + HO_2$	$7.01 \times 10^{-11} \times \exp(-2.41 \times 10^{5}/(R \times T_g))$	41
$CH_2CO + CH_2 \rightarrow C_2H_4 + CO$	2.09×10 <sup>-10</sup>	89
$CH_2CO + H \rightarrow CH_3CO$	$2.66 \times 10^{-11} \times \exp(-6279.0/(R \times T_g))$	90
$CH_2CO + OH \rightarrow CH_2O + CHO$	4.65×10 <sup>-11</sup>	91
$CH_2CO + CH_3 \rightarrow CO + C_2H_5$	$9.54 \times 10^{-14} \times (T_g/298)^{2.29} \times \exp(-4.45 \times 10^4/(R \times T_g))$	92
$CH_2CO + CH_2 \rightarrow CH_3 + C_2HO$	1.00×10 <sup>-17</sup>	93
$CH_2CO + CH_3 \rightarrow CH_4 + C_2HO$	$5.94 \times 10^{-14} \times (T_g/298)^{3.38} \times \exp(-4.40 \times 10^4/(R \times T_g))$	92
$CH_{3}CO + CH_{3}CO \rightarrow CH_{3}CHO + CH_{2}CO$	1.49×10 <sup>-11</sup>	94
$CH_3 + CH_3CO \rightarrow CH_4 + CH_2CO$	1.01×10 <sup>-11</sup>	94

$C_2H_4 + O \rightarrow CH_2CO + H_2$	3.82×10 <sup>-14</sup>	95
$CH_3CHO \to CH_2CO + H_2$	3.00×10 <sup>14</sup> ×exp(-3.51×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	96
$CH_3CO \rightarrow CH_2CO + H$	$6.54 \times 10^{-4} \times (T_g/298)^{-4.34} \times \exp(-1.94 \times 10^{5}/(R \times T_g))$	97
$C_2H_3 + OH \rightarrow CH_2CO + H_2$	$2.22 \times 10^{-12} \times (T_g/298)^{-1.52} \times \exp(-3018.0/(R \times T_g))$	68
$OH + C_2HO \rightarrow CH_2CO + O$	$1.76 \times 10^{-13} \times (T_g/298)^{1.99} \times \exp(-4.72 \times 10^4/(R \times T_g))$	98
$CH_3 + CH_2OH \rightarrow C_2H_5OH$	2.01×10 <sup>-11</sup>	99
$C_2H_5OH + H \rightarrow C_2H_5 + H_2O$	$9.80 \times 10^{-13} \times \exp(-1.45 \times 10^4 / (R \times T_g))$	100
$C_2H_5OH + OH \rightarrow C_2H_5O + H_2O$	$1.67 \times 10^{-14} \times (T_g/298)^{3.15} \times \exp(2380.0/(R \times T_g))$	101
$C_2H_5O \rightarrow CH_3CHO + H$	$1.07 \times 10^{14} \times (T_g/298)^{-0.69} \times \exp(-9.30 \times 10^4/(R \times T_g))$	42
$C_2H_5O + C_2H_5O_2 \rightarrow CH_3CHO + C_2H_5OOH$	1.54×10 <sup>-11</sup>	102
$C_2H_5O + H \rightarrow CH_3 + CH_2OH$	$1.23 \times 10^{-10} \times (T_g/298)^{0.70} \times \exp(-1447.0/(R \times T_g))$	53
$C_2H_5O + H \rightarrow C_2H_5 + OH$	$1.25 \times 10^{-12} \times (T_g/298)^{1.27} \times \exp(-1305.0/(R \times T_g))$	53
$C_2H_5O + H \rightarrow CH_3CHO + H_2$	$8.69 \times 10^{-12} \times (T_g/298)^{1.15} \times \exp(-2819.0/(R \times T_g))$	53
$C_2H_5O + H \rightarrow C_2H_4 + H_2O$	$9.69 \times 10^{-12} \times (T_g/298)^{-0.81} \times \exp(-2985.0/(R \times T_g))$	53
$C_2H_5O + H \rightarrow CH_2O + CH_4$	$3.88 \times 10^{-16} \times (T_g/298)^{2.21} \times \exp(752.0/(R \times T_g))$	53
$CH_{3}CHO + H \rightarrow C_{2}H_{5}O$	$1.33 \times 10^{-11} \times \exp(-2.68 \times 10^4 / (R \times T_g))$	42
$CH_2O + CH_3 \rightarrow C_2H_5O$	$4.98 \times 10^{-13} \times \exp(-2.65 \times 10^4 / (R \times T_g))$	42
$C_2H_5 + O_2 \rightarrow C_2H_5O + O$	$6.14 \times 10^{-12} \times (T_g/298)^{-0.20} \times \exp(-1.17 \times 10^{5}/(R \times T_g))$	63
$C_2H_5 + HO_2 \rightarrow C_2H_5O + OH$	4.98×10 <sup>-11</sup>	63
$C_2H_5O_2 + O_3 \rightarrow C_2H_5O + O_2 + O_2$	9.27×10 <sup>-18</sup>	103
$C_2H_5O_2 + C_2H_5O_2 \rightarrow CH_3CHO + C_2H_5O + HO_2$	$1.21 \times 10^{-15} \times \exp(-0.07/(R \times T_g))$	104
$C_2H_5O_2 \rightarrow C_2H_5O + O$	$1.78 \times 10^{15} \times (T_g/298)^{-0.09} \times \exp(-2.58 \times 10^{5}/(R \times T_g))$	105
$C_2H_5 + O \rightarrow C_2H_5O$	$6.31 \times 10^{-11} \times (T_g/298)^{0.03} \times \exp(1648.0/(R \times T_g))$	106
$C_2H_5 + O_3 \rightarrow C_2H_5O + O_2$	3.32×10 <sup>-14</sup>	107
$CH_{3}CHOH + O_{2} \rightarrow CH_{3}CHO + HO_{2}$	1.90×10 <sup>-11</sup>	108
$CH_{3}CHOH + O \rightarrow CH_{3}CHO + OH$	3.16×10 <sup>-10</sup>	108
$CH_{3}CHOH + H \rightarrow CH_{3}CHO + H_{2}$	3.32×10 <sup>-11</sup>	108
$CH_3CHOH + H \rightarrow CH_3 + CH_2OH$	$8.99 \times 10^{-10} \times (T_g/298)^{-0.89} \times \exp(-1.21 \times 10^4/(R \times T_g))$	53
$CH_{3}CHOH + H \rightarrow C_{2}H_{5}O + H$	$9.31 \times 10^{-16} \times (T_g/298)^{2.94} \times \exp(-3.55 \times 10^4/(R \times T_g))$	53
$CH_{3}CHOH + H \rightarrow C_{2}H_{5} + OH$	$3.55 \times 10^{-11} \times (T_g/298)^{-0.83} \times \exp(-2.01 \times 10^4/(R \times T_g))$	53
$CH_{3}CHOH + H \rightarrow C_{2}H_{4} + H_{2}O$	$2.63 \times 10^{-10} \times (T_g/298)^{-3.02} \times \exp(-1.19 \times 10^4/(R \times T_g))$	53
$CH_{3}CHOH + H \rightarrow CH_{2}O + CH_{4}$	$8.73 \times 10^{-17} \times (T_g/298)^{2.10} \times \exp(-890.0/(R \times T_g))$	53
$C_2H_5OH + H \rightarrow H_2 + CH_3CHOH$	$1.64 \times 10^{-11} \times (T_g/298)^{-0.33} \times \exp(-2.25 \times 10^4/(R \times T_g))$	101
$C_2H_5OH + OH \rightarrow CH_3CHOH + H_2O$	$5.28 \times 10^{-11} \times (T_g/298)^{0.54} \times \exp(420.0/(\text{R} \times T_g))$	6

$C_2H_5OH + HO_2 \rightarrow CH_3CHOH + H_2O_2$	$3.09 \times 10^{-10} \times (T_g/298)^{-1.81} \times \exp(-6.89 \times 10^4/(R \times T_g))$	101
$C_2H_5OH + CH_3 \rightarrow CH_4 + CH_3CHOH$	$8.87 \times 10^{-15} \times (T_g/298)^{3.37} \times \exp(-3.29 \times 10^4/(R \times T_g))$	101
$C_2H_5OH + O \rightarrow CH_3CHOH + OH$	1.03×10 <sup>-13</sup>	110
$C_2H_5O \rightarrow CH_3CHOH$	$1.87 \times (T_g/298)^{12.40} \times \exp(-1.77 \times 10^4/(R \times T_g))$	111
CH <sub>3</sub> CHO + H → CH <sub>3</sub> CHOH	$8.02 \times 10^{-13} \times (T_g/298)^{2.20} \times \exp(-3.14 \times 10^4/(R \times T_g))$	70
$CH_3CHO + HO_2 \rightarrow CH_3CHOH + O_2$	$4.19 \times 10^{-10} \times (T_g/298)^{-1.80} \times \exp(-1.09 \times 10^{5}/(\mathbb{R} \times T_g))$	95
$C_2H_6 + C_2H_5O_2 \rightarrow C_2H_5 + C_2H_5OOH$	$2.87 \times 10^{-14} \times (T_g/298)^{3.76} \times \exp(-71960/(R \times T_g))$	6,7
$C_2H_5 + CH_3O_2 \rightarrow CH_3O + C_2H_5O$	4.00×10 <sup>-11</sup>	6,7
$C_2H_4 + O_3 \rightarrow CH_2O + CO_2 + H_2$	7.06×10 <sup>-19</sup>	6,7
$C_2H_4 + O_3 \rightarrow CH_2O + CO + H_2O$	7.06×10 <sup>-19</sup>	6,7
$C_2H_4 + O_3 \rightarrow CH_2O + CH_2O + O$	2.69×10 <sup>-19</sup>	6,7
$H_2 + C_2 \rightarrow C_2 H_2$	1.77×10 <sup>-10</sup> ×exp(-1470.0/ <i>T</i> <sub>g</sub> )	6,7
$CH_4 + C_2 \rightarrow C_2H + CH_3$	5.50×10 <sup>-11</sup> ×exp(-297.0/ <i>T</i> <sub>g</sub> )	6,7
$CH_3 + C_2H_5OH \rightarrow CH_4 + C_2H_5O$	3.11×10 <sup>-19</sup>	6,7
$CH_3 + O_3 \rightarrow CH_3O + O_2$	9.79×10 <sup>-31</sup>	6,7
$H + C_2H_5OH \rightarrow H_2 + C_2H_5O$	$1.33 \times 10^{-20} \times (T_g/298)^{10.58} \times \exp(18650/(R \times T_g))$	6,7
$H + O_3 \rightarrow OH + O_2$	2.83×10 <sup>-11</sup>	6,7
$CO_2 + C \rightarrow CO + CO$	1.00×10 <sup>-15</sup>	6,7
$O_3 + CO \rightarrow CO_2 + O_2$	4.00×10 <sup>-25</sup>	6,7
$O_2 + C_2 O \rightarrow CO_2 + CO$	3.30×10 <sup>-13</sup>	6,7
$O + C_2 O \rightarrow CO + CO$	9.51×10 <sup>-11</sup>	6,7
$O + O_3 \rightarrow O_2 + O_2$	8.00×10 <sup>-12</sup> ×exp(-2056.0/ <i>T</i> <sub>g</sub> )	6,7
$O_3 + O_2 \rightarrow O + O_2 + O_2$	2.29×10 <sup>-26</sup>	6,7
$O_3 + O_3 \rightarrow O + O_2 + O_3$	5.18×10 <sup>-26</sup>	6,7
$O_3 + O \rightarrow O + O_2 + O$	3.14×10 <sup>-27</sup>	6,7
$O_3 + OH \rightarrow O_2 + HO_2$	$3.76 \times 10^{-13} \times (T_g/298)^{1.99} \times \exp(-5.02 \times 10^3/(R \times T_g))$	6,7
$O_3 + HO_2 \rightarrow O_2 + O_2 + OH$	$1.97 \times 10^{-16} \times (T_g/298)^{4.57} \times \exp(5.76 \times 10^3/(R \times T_g))$	6,7
$O_3 + CH_3O_2 \rightarrow CH_3O + O_2 + O_2$	1.00×10 <sup>-17</sup>	6,7
$O + C_2H_5OOH \rightarrow C_2H_5O_2 + OH$	$3.30 \times 10^{-11} \times \exp(-19.87 \times 10^{3}/(R \times T_g))$	6,7
$O_2 + C_2 H_5 O \rightarrow CH_3 CHO + HO_2$	8.12×10 <sup>-15</sup>	6,7
$HO_2 + C_2H_5O_2 \rightarrow C_2H_5OOH + O_2$	7.63×10 <sup>-12</sup>	6,7
$C_2H_5O_2 + C_2H_5O_2 \rightarrow C_2H_5OH + CH_3CHO + O_2$	2.43×10 <sup>-14</sup>	6,7
$C_2H_5O_2 + C_2H_5O_2 \rightarrow C_2H_5O + C_2H_5O + O_2$	3.97×10 <sup>-14</sup>	6,7
$CH_3CHO + HO_2 \rightarrow C_2H_5O + O_2$	$6.96 \times 10^{-14} \times (T_g/298)^{1.62} \times \exp(-64.6 \times 10^3/(R \times T_g))$	6,7

$OH + C_2H_5OOH \rightarrow H_2O + C_2H_5O_2$	$1.61 \times 10^{-13} \times (T_g/298)^{2.32} \times \exp(6.66 \times 10^3/(R \times T_g))$	6,7
$CH_3 + C_3H_7 \rightarrow C_2H_5 + C_2H_5$	$3.20 \times 10^{-11} \times T_{g}^{-0.32}$	6,7
$C_3H_7 + H \rightarrow CH_3 + C_2H_5$	$6.74 \times 10^{-18} \times T_g^{2.19} \times \exp(-890.0/(1.987 \times T_g))$	6,7
$C_2H_4 + CH_2 \rightarrow C_3H_6$	$5.30 \times 10^{-12} \times \exp(-2660/T_g)$	6,7
$CH + C_2H_6 \rightarrow C_3H_6 + H$	3.00×10 <sup>-11</sup>	6,7
$C_2H_6 + CH \rightarrow C_2H_4 + CH_3$	$1.79 \times 10^{-10} \times \exp(263.0/(1.987 \times T_g))$	6,7
$C_2H_6 + CH_2 \rightarrow C_2H_5 + CH_3$	9.00×10 <sup>-33</sup> ×7g <sup>6.4162</sup>	6,7
$C_2H_4 + H_2 \rightarrow C_2H_6$	$4.75 \times 10^{-16} \times \exp(-180000.0/(R \times T_g))$	6,7
$CH_3 + C_2H_5 \rightarrow C_2H_6 + CH_2$	3.00×10 <sup>-44</sup> ×7 <sup>9.0956</sup>	6,7
$C_2H_5 + C_2H_3 \rightarrow C_2H_4 + C_2H_4$	0.68×6.50×10 <sup>-11</sup>	6,7
$CH + CH_3 \rightarrow C_2H_3 + H$	4.98×10 <sup>-11</sup>	6,7
$C_2H + C_2H \rightarrow C_2H_2 + C_2$	3.01×10 <sup>-12</sup>	6,7
$C + CH_2 \rightarrow CH + CH$	$2.69 \times 10^{-12} \times \exp(-196.0 \times 10^3 / (R \times T_g))$	6,7
$C + CH_2 \rightarrow H + C_2 H$	8.30×10 <sup>-11</sup>	6,7
$C_2H + H \rightarrow H_2 + C_2$	$5.99 \times 10^{-11} \times \exp(-118000/(R \times T_g))$	6,7
$H_2 + C_2 \rightarrow C_2 H + H$	$1.10 \times 10^{-10} \times \exp(-33.26 \times 10^{3}/(R \times T_g))$	6,7
$CH_4 + CH_2 \rightarrow CH_3 + CH_3$	3.01×10 <sup>-19</sup>	6,7
$CH_4 + CH \rightarrow C_2H_4 + H$	9.97×10 <sup>-11</sup>	6,7
$CH_4 + C_2H_5 \rightarrow C_2H_6 + CH_3$	$2.51 \times 10^{-15} \times (T_g/298)^{4.14} \times \exp(-52550/(R \times T_g))$	6,7
$CH_4 + C_2H_3 \rightarrow C_2H_4 + CH_3$	$2.13 \times 10^{-14} \times (T_g/298)^{4.02} \times \exp(-22860/(R \times T_g))$	6,7
$CH_4 + C_2H \rightarrow C_2H_2 + CH_3$	$3.01 \times 10^{-12} \times \exp(-2080/(R \times T_g))$	6,7
$CH_4 + C_3H_7 \rightarrow C_3H_8 + CH_3$	$3.54 \times 10^{-16} \times (T_g/298)^{4.02} \times \exp(-45480/(R \times T_g))$	6,7
$CH_4 + C_3H_5 \rightarrow C_3H_6 + CH_3$	$1.71 \times 10^{-14} \times (T_g/298)^{3.40} \times \exp(-97280/(R \times T_g))$	6,7
$CH_4 + H \rightarrow CH_3 + H_2$	$9.86 \times 10^{-13} \times (T_g/298)^{3.0} \times \exp(-36670.0/(\mathbb{R} \times T_g))$	6,7
$CH_3 + CH_3 \rightarrow C_2H_5 + H$	$1.46 \times 10^{-11} \times (T_g/298)^{0.1} \times \exp(-44400/(R \times T_g))$	6,7
$CH_3 + CH_2 \rightarrow C_2H_4 + H$	7.01×10 <sup>-11</sup>	6,7
$CH_3 + C_2H_6 \rightarrow C_2H_5 + CH_4$	$1.74 \times 10^{-16} \times (T_g/298)^{6.0} \times \exp(-25280/(R \times T_g))$	6,7
$CH_3 + C_2H_4 \rightarrow C_2H_3 + CH_4$	$6.91 \times 10^{-12} \times \exp(-46.56 \times 10^3 / (R \times T_g))$	6,7
$CH_3 + C_2H_3 \rightarrow C_2H_2 + CH_4$	3.00×10 <sup>-11</sup>	6,7
$CH_3 + C_2H_2 \rightarrow CH_4 + C_2H$	$3.01 \times 10^{-13} \times \exp(-72340/(R \times T_g))$	6,7
$CH_3 + C_3H_8 \rightarrow C_3H_7 + CH_4$	$1.61 \times 10^{-15} \times (T_g/298)^{3.65} \times \exp(-29930/(R \times T_g))$	6,7
$CH_3 + C_3H_7 \rightarrow C_3H_6 + CH_4$	$3.07 \times 10^{-12} \times (T_g/298)^{-0.32}$	6,7
$CH_3 + C_3H_6 \rightarrow C_3H_5 + CH_4$	$1.68 \times 10^{-15} \times (T_g/298)^{3.50} \times \exp(-23780/(R \times T_g))$	6,7
$CH_3 + H_2 \rightarrow CH_4 + H$	$2.52 \times 10^{-14} \times (T_g/298)^{3.12} \times \exp(-36420.0/(R \times T_g))$	6,7

$CH_3 + H \rightarrow CH_2 + H_2$	1.00×10 <sup>-10</sup> ×exp(-63190/(R× <i>T</i> <sub>g</sub> ))	6,7
$CH_2 + CH_2 \rightarrow C_2H_2 + H + H$	$3.32 \times 10^{-10} \times \exp(-45.98 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$CH_2 + C_2H_5 \rightarrow C_2H_4 + CH_3$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + C_2H_3 \to C_2H_2 + CH_3$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + C_2H \rightarrow C_2H_2 + CH$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + C_3H_8 \rightarrow C_3H_7 + CH_3$	$1.61 \times 10^{-15} \times (T_g/298)^{3.65} \times \exp(-29930/(R \times T_g))$	6,7
$CH_2 + C_3H_7 \rightarrow C_2H_4 + C_2H_5$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + C_3H_7 \rightarrow C_3H_6 + CH_3$	3.01×10 <sup>-12</sup>	6,7
$CH_2 + C_3H_6 \rightarrow C_3H_5 + CH_3$	1.20×10 <sup>-12</sup> ×exp(-25940/(R×T <sub>g</sub> ))	6,7
$CH_2 + H_2 \rightarrow CH_3 + H$	5.00×10 <sup>-15</sup>	6,7
$CH_2 + H \rightarrow CH + H_2$	$1.00 \times 10^{-11} \times \exp(7480/(R \times T_g))$	6,7
$CH + H_2 \rightarrow CH_2 + H$	$1.48 \times 10^{-11} \times (T_g/298)^{1.79} \times \exp(-6.98 \times 10^3/(R \times T_g))$	6,7
$CH + H \rightarrow C + H_2$	1.31×10 <sup>-10</sup> ×exp(-6700/(R×T <sub>g</sub> ))	6,7
$C + H_2 \rightarrow CH + H$	6.64×10 <sup>-10</sup> ×exp(-97.28×10 <sup>3</sup> /(R×T <sub>g</sub> ))	6,7
$C_2H_6 + C_2H_3 \rightarrow C_2H_5 + C_2H_4$	$1.46 \times 10^{-13} \times (T_g/298)^{3.30} \times \exp(-43900/(R \times T_g))$	6,7
$C_2H_6 + C_2H \rightarrow C_2H_2 + C_2H_5$	5.99×10 <sup>-12</sup>	6,7
$C_2H_6 + C_3H_7 \rightarrow C_3H_8 + C_2H_5$	$1.19 \times 10^{-15} \times (T_g/298)^{3.82} \times \exp(-37830/(R \times T_g))$	6,7
$C_2H_6 + C_3H_5 \rightarrow C_3H_6 + C_2H_5$	$5.71 \times 10^{-14} \times (T_g/298)^{3.30} \times \exp(-83060/(R \times T_g))$	6,7
$C_2H_6 + H \rightarrow C_2H_5 + H_2$	$1.23 \times 10^{-11} \times (T_g/298)^{1.50} \times \exp(-31010/(R \times T_g))$	6,7
$C_2H_5 + C_2H_5 \rightarrow C_2H_6 + C_2H_4$	2.41×10 <sup>-12</sup>	6,7
$C_2H_5 + C_2H_4 \rightarrow C_2H_6 + C_2H_3$	$5.83 \times 10^{-14} \times (T_g/298)^{3.13} \times \exp(-75330/(R \times T_g))$	6,7
$C_2H_5 + C_2H_2 \rightarrow C_2H_6 + C_2H$	4.50×10 <sup>-13</sup> ×exp(-98110/(R× <i>T</i> <sub>g</sub> ))	6,7
$C_2H_5 + C_2H \rightarrow C_2H_4 + C_2H_2$	3.01×10 <sup>-12</sup>	6,7
$C_2H_5 + C_3H_8 \rightarrow C_2H_6 + C_3H_7$	$1.61 \times 10^{-15} \times (T_g/298)^{3.65} \times \exp(-38250/(R \times T_g))$	6,7
$C_2H_5 + C_3H_7 \rightarrow C_3H_8 + C_2H_4$	1.91×10 <sup>-12</sup>	6,7
$C_2H_5 + C_3H_7 \rightarrow C_3H_6 + C_2H_6$	2.41×10 <sup>-12</sup>	6,7
$C_2H_5 + C_3H_6 \rightarrow C_3H_5 + C_2H_6$	$1.69 \times 10^{-15} \times (T_g/298)^{3.50} \times \exp(-27770/(R \times T_g))$	6,7
$C_2H_5 + C_3H_5 \rightarrow C_3H_6 + C_2H_4$	$4.30 \times 10^{-12} \times \exp(550/(R \times T_g))$	6,7
$C_2H_5 + H_2 \rightarrow C_2H_6 + H$	$4.12 \times 10^{-15} \times (T_g/298)^{3.60} \times \exp(-35340/(R \times T_g))$	6,7
$C_2H_5 + H \rightarrow CH_3 + CH_3$	5.99×10 <sup>-11</sup>	6,7
$C_2H_5 + H \rightarrow C_2H_4 + H_2$	3.01×10 <sup>-12</sup>	6,7
$C_2H_4 + C_2H \rightarrow C_2H_2 + C_2H_3$	1.40×10 <sup>-10</sup>	6,7
$C_2H_4 + H \rightarrow C_2H_3 + H_2$	$4.00 \times 10^{-12} \times (T_g/298)^{2.53} \times \exp(-51220/(R \times T_g))$	6,7
$C_2H_3 + C_2H_3 \rightarrow C_2H_4 + C_2H_2$	1.60×10 <sup>-12</sup>	6,7

$C_2H_3 + C_2H \rightarrow C_2H_2 + C_2H_2$	1.60×10 <sup>-12</sup>	6,7
$C_2H_3+C_3H_8\rightarrow C_2H_4+C_3H_7$	$1.46 \times 10^{-13} \times (T_g/298)^{3.30} \times \exp(-43900/(R \times T_g))$	6,7
$C_2H_3 + C_3H_7 \rightarrow C_3H_8 + C_2H_2$	2.01×10 <sup>-12</sup>	6,7
$C_2H_3 + C_3H_7 \rightarrow C_3H_6 + C_2H_4$	2.01×10 <sup>-12</sup>	6,7
$C_2H_3 + C_3H_6 \rightarrow C_3H_5 + C_2H_4$	$1.68 \times 10^{-15} \times (T_g/298)^{3.50} \times \exp(-19620/(R \times T_g))$	6,7
$C_2H_3 + C_3H_5 \rightarrow C_3H_6 + C_2H_2$	8.00×10 <sup>-12</sup>	6,7
$C_2H_3 + H_2 \rightarrow C_2H_4 + H$	$1.61 \times 10^{-13} \times (T_g/298)^{2.63} \times \exp(-35750/(R \times T_g))$	6,7
$C_2H_2 + H \rightarrow C_2H + H_2$	1.00×10 <sup>-10</sup> ×exp(-93120/(R× <i>T</i> <sub>g</sub> ))	6,7
$C_2H + C_3H_8 \rightarrow C_2H_2 + C_3H_7$	5.99×10 <sup>-12</sup>	6,7
$C_2H + C_3H_7 \rightarrow C_3H_6 + C_2H_2$	1.00×10 <sup>-11</sup>	6,7
$C_2H + C_3H_6 \rightarrow C_3H_5 + C_2H_2$	5.99×10 <sup>-12</sup>	6,7
$C_2H + H_2 \rightarrow C_2H_2 + H$	$8.95 \times 10^{-13} \times (T_g/298)^{2.57} \times \exp(-1080/(\mathbb{R} \times T_g))$	6,7
$C_3H_8 + C_3H_5 \rightarrow C_3H_6 + C_3H_7$	$5.71 \times 10^{-14} \times (T_g/298)^{3.30} \times \exp(-83060/(R \times T_g))$	6,7
$C_3H_8 + H \rightarrow C_3H_7 + H_2$	$4.23 \times 10^{-12} \times (T_g/298)^{2.54} \times \exp(-28270/(R \times T_g))$	6,7
$C_3H_7 + C_3H_7 \rightarrow C_3H_6 + C_3H_8$	2.81×10 <sup>-12</sup>	6,7
$C_3H_7 + C_3H_6 \rightarrow C_3H_5 + C_3H_8$	$1.69 \times 10^{-15} \times (T_g/298)^{3.50} \times \exp(-27770/(R \times T_g))$	6,7
$C_3H_7 + C_3H_5 \rightarrow C_3H_6 + C_3H_6$	$2.41 \times 10^{-12} \times \exp(550/(R \times T_g))$	6,7
$C_3H_7 + H_2 \rightarrow C_3H_8 + H$	$3.19 \times 10^{-14} \times (T_g/298)^{2.84} \times \exp(-38250/(R \times T_g))$	6,7
$C_3H_7 + H \rightarrow C_3H_6 + H_2$	3.01×10 <sup>-12</sup>	6,7
$C_3H_6 + H \rightarrow C_3H_5 + H_2$	$4.40 \times 10^{-13} \times (T_g/298)^{2.50} \times \exp(-10390/(R \times T_g))$	6,7
$C_3H_5 + H_2 \rightarrow C_3H_6 + H$	$1.39 \times 10^{-13} \times (T_g/298)^{2.38} \times \exp(-79490/(R \times T_g))$	6,7
$CH_4 + O \rightarrow CH_3 + OH$	$8.32 \times 10^{-12} \times (T_g/298)^{1.56} \times \exp(-35503/(R \times T_g))$	6,7
$CH_3 + OH \rightarrow CH_4 + O$	$3.22 \times 10^{-14} \times (T_g/298)^{2.20} \times \exp(-18.62 \times 10^3/(R \times T_g))$	6,7
$CH_3 + O \rightarrow CO + H_2 + H$	0.46×1.70×10 <sup>-10</sup>	6,7
$CH_2 + O \rightarrow CO + H_2$	5.53×10 <sup>-11</sup>	6,7
$CH_2 + O \rightarrow CO + H + H$	8.29×10 <sup>-11</sup>	6,7
$CH_2 + O_2 \rightarrow CO_2 + H_2$	$2.99 \times 10^{-11} \times (T_g/298)^{-3.30} \times \exp(-11.97 \times 10^3/(R \times T_g))$	6,7
$CH_2 + O_2 \rightarrow CO + H_2O$	1.42×10 <sup>-12</sup>	6,7
$CH_2 + O_2 \rightarrow CH_2O + O$	5.39×10 <sup>-13</sup>	6,7
$CH + O \rightarrow CO + H$	6.59×10 <sup>-11</sup>	6,7
$CH + O_2 \rightarrow CO_2 + H$	1.20×10 <sup>-11</sup>	6,7
$CH + O_2 \rightarrow CO + OH$	8.00×10 <sup>-12</sup>	6,7
$CH + O_2 \rightarrow CHO + O$	8.00×10 <sup>-12</sup>	6,7
$CH + O_2 \rightarrow CO + H + O$	1.20×10 <sup>-11</sup>	6,7

$C_2H_6 + O \rightarrow C_2H_5 + OH$	$8.54 \times 10^{-12} \times (T_g/298)^{1.50} \times \exp(-24280/(R \times T_g))$	6,7
$C_2H_5 + O \rightarrow CH_3CHO + H$	8.80×10 <sup>-11</sup>	6,7
$C_2H_5 + O \rightarrow CH_2O + CH_3$	6.90×10 <sup>-11</sup>	6,7
$C_2H_5 + O \rightarrow C_2H_4 + OH$	$6.31 \times 10^{-12} \times (T_g/298)^{0.03} \times \exp(1.65 \times 10^3/(R \times T_g))$	6,7
$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	3.80×10 <sup>-15</sup>	6,7
$C_2H_3 + O \rightarrow C_2H_2 + OH$	$5.50 \times 10^{-12} \times (T_g/298)^{0.20} \times \exp(1.79 \times 10^3/(R \times T_g))$	6,7
$C_2H_3 + O \rightarrow CO + CH_3$	1.25×10 <sup>-11</sup>	6,7
$C_2H_3 + O \rightarrow CHO + CH_2$	1.25×10 <sup>-11</sup>	6,7
$C_2H_3 + O \rightarrow CH_2CO + H$	1.60×10 <sup>-10</sup>	6,7
$C_2H_3 + O_2 \rightarrow CH_2O + CHO$	9.00×10 <sup>-12</sup>	6,7
$C_2H_2 + O \rightarrow CH_2 + CO$	$3.49 \times 10^{-12} \times (T_g/298)^{1.50} \times \exp(-7.07 \times 10^3/(R \times T_g))$	6,7
$C_2H + O \rightarrow CH + CO$	1.69×10 <sup>-11</sup>	6,7
$C_2H + O_2 \rightarrow CHO + CO$	3.00×10 <sup>-11</sup>	6,7
$C_2H + O_2 \rightarrow C_2HO + O$	1.00×10 <sup>-12</sup>	6,7
$C_{3}H_{8} + O \rightarrow C_{3}H_{7} + OH$	$1.37 \times 10^{-12} \times (T_g/298)^{2.68} \times \exp(-15548/(R \times T_g))$	6,7
$H_2 + O \rightarrow OH + H$	$3.44 \times 10^{-13} \times (T_g/298)^{2.67} \times \exp(-26274/(R \times T_g))$	6,7
$H + O_2 \rightarrow OH + O$	$3.07 \times 10^{-13} \times (T_g/298)^{2.70} \times \exp(-26190.0/(R \times T_g))$	6,7
$CH_4 + OH \rightarrow CH_3 + H_2O$	$4.16 \times 10^{-13} \times (T_g/298)^{2.18} \times \exp(-10240/(R \times T_g))$	6,7
$CH_4 + HO_2 \rightarrow CH_3 + H_2O_2$	$3.01 \times 10^{-13} \times \exp(-77740/(R \times T_g))$	6,7
$CH_4 + CHO \rightarrow CH_3 + CH_2O$	$1.36 \times 10^{-13} \times (T_g/298)^{2.85} \times \exp(-93954/(R \times T_g))$	6,7
$CH_4 + CH_3O \rightarrow CH_3OH + CH_3$	$2.61 \times 10^{-13} \times \exp(-37000/(\text{R} \times T_g))$	6,7
$CH_4 + CH_3O_2 \rightarrow CH_3 + CH_3OOH$	$3.01 \times 10^{-13} \times \exp(-77320/(R \times T_g))$	6,7
$CH_3 + H_2O \rightarrow CH_4 + OH$	$1.20 \times 10^{-14} \times (T_g/298)^{2.90} \times \exp(-62190/(R \times T_g))$	6,7
$CH_3 + OH \rightarrow CH_2 + H_2O$	$1.20 \times 10^{-10} \times \exp(-11640/(R \times T_g))$	6,7
$CH_3 + OH \rightarrow CH_2OH + H$	$1.54 \times 10^{-9} \times (T_g/298)^{-1.80} \times \exp(-33.76 \times 10^3/(R \times T_g))$	6,7
$CH_3 + OH \rightarrow CH_3O + H$	$2.57 \times 10^{-12} \times (T_g/298)^{-0.23} \times \exp(-58.28 \times 10^3/(R \times T_g))$	6,7
$CH_3 + HO_2 \rightarrow CH_3O + OH$	$7.68 \times 10^{-12} \times (T_g/298)^{0.27} \times \exp(2.88 \times 10^3/(\text{R} \times T_g))$	6,7
$CH_3 + HO_2 \rightarrow CH_4 + O_2$	5.99×10 <sup>-12</sup>	6,7
$CH_3 + CH_2O \rightarrow CH_4 + CHO$	$1.60 \times 10^{-16} \times (T_g/298)^{6.10} \times \exp(-8230/(R \times T_g))$	6,7
$CH_3 + CHO \rightarrow CH_4 + CO$	2.01×10 <sup>-10</sup>	6,7
$CH_3 + CH_3O \rightarrow CH_4 + CH_2O$	4.00×10 <sup>-11</sup>	6,7
$CH_3 + CH_3CHO \rightarrow CH_4 + CH_3CO$	$2.97 \times 10^{-16} \times (T_g/298)^{5.64} \times \exp(-10310/(R \times T_g))$	6,7
$CH_3 + CH_3O_2 \rightarrow CH_3O + CH_3O$	4.00×10 <sup>-11</sup>	6,7
$CH_2 + \overline{CO_2} \rightarrow CH_2O + CO$	3.90×10 <sup>-14</sup>	6,7

$CH_2 + H_2O \rightarrow CH_3 + OH$	1.60×10 <sup>-16</sup>	6,7
$CH_2 + OH \rightarrow CH_2O + H$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + HO_2 \rightarrow CH_2O + OH$	3.00×10 <sup>-11</sup>	6,7
$CH_2 + CH_2O \rightarrow CH_3 + CHO$	1.00×10 <sup>-14</sup>	6,7
$CH_2 + CHO \rightarrow CH_3 + CO$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + CH_3O \rightarrow CH_3 + CH_2O$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + CH_3O_2 \rightarrow CH_2O + CH_3O$	3.01×10 <sup>-11</sup>	6,7
$CH + CO_2 \rightarrow CHO + CO$	9.68×10 <sup>-13</sup>	6,7
$CH + CO_2 \rightarrow CO + CO + H$	9.68×10 <sup>-13</sup>	6,7
$C_2H_6 + OH \rightarrow C_2H_5 + H_2O$	$3.97 \times 10^{-13} \times (T_g/298)^{2.0} \times \exp(-2519/(\mathbb{R} \times T_g))$	6,7
$C_2H_6 + HO_2 \rightarrow C_2H_5 + H_2O_2$	$4.90 \times 10^{-13} \times \exp(-65520/(R \times T_g))$	6,7
$C_2H_6 + CHO \rightarrow C_2H_5 + CH_2O$	$4.18 \times 10^{-13} \times (T_g/298)^{2.72} \times \exp(-76330/(R \times T_g))$	6,7
$C_2H_6 + CH_3O \rightarrow C_2H_5 + CH_3OH$	$4.00 \times 10^{-13} \times \exp(-29680/(R \times T_g))$	6,7
$C_2H_6 + CH_3O_2 \rightarrow C_2H_5 + CH_3OOH$	$4.90 \times 10^{-13} \times \exp(-62520/(R \times T_g))$	6,7
$C_2H_5 + H_2O \rightarrow C_2H_6 + OH$	$2.06 \times 10^{-14} \times (T_g/298)^{1.44} \times \exp(-84810/(R \times T_g))$	6,7
$C_2H_5 + OH \rightarrow C_2H_4 + H_2O$	4.00×10 <sup>-11</sup>	6,7
$C_2H_5 + HO_2 \rightarrow C_2H_6 + O_2$	5.00×10 <sup>-13</sup>	6,7
$C_2H_5 + HO_2 \rightarrow C_2H_4 + H_2O_2$	5.00×10 <sup>-13</sup>	6,7
$C_2H_5$ + $CH_2O \rightarrow C_2H_6$ + $CHO$	$8.19 \times 10^{-14} \times (T_g/298)^{2.81} \times \exp(-24530/(R \times T_g))$	6,7
$C_2H_5 + CHO \rightarrow C_2H_6 + CO$	2.01×10 <sup>-10</sup>	6,7
$C_2H_5 + CH_3O \rightarrow C_2H_6 + CH_2O$	4.00×10 <sup>-11</sup>	6,7
$C_2H_4 + HO_2 \rightarrow CH_3CHO + OH$	$1.00 \times 10^{-14} \times \exp(-33260/(R \times T_g))$	6,7
$C_2H_3 + H_2O \rightarrow C_2H_4 + OH$	$1.20 \times 10^{-14} \times (T_g/298)^{2.9} \times \exp(-62190/(\mathbb{R} \times T_g))$	6,7
$C_2H_3 + OH \rightarrow C_2H_2 + H_2O$	5.00×10 <sup>-11</sup>	6,7
$C_2H_3 + CH_2O \rightarrow C_2H_4 + CHO$	$8.07 \times 10^{-14} \times (T_g/298)^{2.81} \times \exp(-24530/(R \times T_g))$	6,7
$C_2H_3$ + CHO $\rightarrow$ $C_2H_4$ + CO	1.50×10 <sup>-10</sup>	6,7
$C_2H_3 + CH_3O \rightarrow C_2H_4 + CH_2O$	4.00×10 <sup>-11</sup>	6,7
$C_2H_2 + OH \rightarrow C_2H + H_2O$	$5.00 \times 10^{-12} \times (T_g/298)^{2.0} \times \exp(-58530.0/(R \times T_g))$	6,7
$C_2H_2 + HO_2 \rightarrow CH_2CO + OH$	$1.00 \times 10^{-14} \times \exp(-33260/(R \times T_g))$	6,7
$C_2H + OH \rightarrow CH_2 + CO$	3.01×10 <sup>-11</sup>	6,7
$C_2H + OH \rightarrow C_2H_2 + O$	3.01×10 <sup>-11</sup>	6,7
$C_2H + HO_2 \rightarrow C_2H_2 + O_2$	3.01×10 <sup>-11</sup>	6,7
$C_2H + HO_2 \rightarrow C_2HO + OH$	3.01×10 <sup>-11</sup>	6,7
$C_2H + CHO \rightarrow C_2H_2 + CO$	1.00×10 <sup>-10</sup>	6,7

$C_2H + CH_3O \rightarrow C_2H_2 + CH_2O$	4.00×10 <sup>-11</sup>	6,7
$C_2H + CH_3O_2 \rightarrow CH_3O + C_2HO$	4.00×10 <sup>-11</sup>	6,7
$C_3H_8 + OH \rightarrow C_3H_7 + H_2O$	$1.44 \times 10^{-12} \times (T_g/298) \times \exp(-1.08 \times 10^3/(R \times T_g))$	6,7
$C_3H_8 + HO_2 \rightarrow C_3H_7 + H_2O_2$	$1.61 \times 10^{-13} \times (T_g/298)^{2.55} \times \exp(-69010/(R \times T_g))$	6,7
$C_3H_8 + CHO \rightarrow C_3H_7 + CH_2O$	$5.21 \times 10^{-13} \times (T_g/298)^{2.50} \times \exp(-77160/(R \times T_g))$	6,7
$C_3H_8 + CH_3O \rightarrow C_3H_7 + CH_3OH$	7.21×10 <sup>-13</sup> ×exp(-27020/(R× <i>T</i> <sub>g</sub> ))	6,7
$C_{3}H_{8} + CH_{3}O_{2} \rightarrow C_{3}H_{7} + CH_{3}OOH$	1.00×10 <sup>-11</sup> ×exp(-81070/(R× <i>T</i> <sub>g</sub> ))	6,7
$C_3H_7 + CH_2O \rightarrow C_3H_8 + CHO$	$7.49 \times 10^{-14} \times (T_g/298)^{2.9} \times \exp(-24530/(R \times T_g))$	6,7
$C_3H_7$ + CHO $\rightarrow C_3H_8$ + CO	1.00×10 <sup>-10</sup>	6,7
$C_3H_7 + CH_3O \rightarrow C_3H_8 + CH_2O$	4.00×10 <sup>-11</sup>	6,7
$C_3H_7 + CH_3O_2 \rightarrow C_2H_5 + CH_2O$	5.99×10 <sup>-11</sup>	6,7
$H_2 + OH \rightarrow H + H_2O$	$2.06 \times 10^{-12} \times (T_g/298)^{1.52} \times \exp(-14470/(R \times T_g))$	6,7
$H_2 + HO_2 \rightarrow H + H_2O_2$	$5.00 \times 10^{-11} \times \exp(-109000/(R \times T_g))$	6,7
$H_2 + CHO \rightarrow H + CH_2O$	$2.66 \times 10^{-13} \times (T_g/298)^{2.0} \times \exp(-74580/(R \times T_g))$	6,7
$H_2 + CH_3O_2 \rightarrow H + CH_3OOH$	5.00×10 <sup>-11</sup> ×exp(-109000/(R× <i>T</i> <sub>g</sub> ))	6,7
$H + CO_2 \rightarrow CO + OH$	$2.51 \times 10^{-10} \times \exp(-111000.0/(R \times T_g))$	6,7
$H + H_2O \rightarrow H_2 + OH$	$6.82 \times 10^{-12} \times (T_g/298)^{1.60} \times \exp(-80820/(R \times T_g))$	6,7
$H + OH \rightarrow H_2 + O$	$6.86 \times 10^{-14} \times (T_g/298)^{2.80} \times \exp(-16210/(R \times T_g))$	6,7
$H + HO_2 \rightarrow H_2 + O_2$	$1.10 \times 10^{-10} \times \exp(-8.90 \times 10^{3}/(R \times T_{g}))$	6,7
$H + HO_2 \rightarrow H_2O + O$	$5.00 \times 10^{-11} \times \exp(-7.20 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$H + HO_2 \rightarrow OH + OH$	$2.81 \times 10^{-10} \times \exp(-3.66 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$H + CH_2O \rightarrow H_2 + CHO$	$2.14 \times 10^{-12} \times (T_g/298)^{1.62} \times \exp(-9060/(R \times T_g))$	6,7
$H + CHO \rightarrow H_2 + CO$	5.50×10 <sup>-10</sup>	6,7
$H + CH_3O \rightarrow H_2 + CH_2O$	2.32×10 <sup>-11</sup>	6,7
$H + CH_3O \to CH_3 + OH$	9.93×10 <sup>-12</sup>	6,7
$H + CH_2CO \rightarrow CH_3 + CO$	1.04×10 <sup>-13</sup>	6,7
$H + C_2HO \rightarrow CH_2 + CO$	2.50×10 <sup>-10</sup>	6,7
$H + CH_3O_2 \rightarrow OH + CH_3O$	1.60×10 <sup>-10</sup>	6,7
$O + H_2O \rightarrow OH + OH$	$1.25 \times 10^{-11} \times (T_g/298)^{1.3} \times \exp(-71500/(R \times T_g))$	6,7
$O + OH \rightarrow H + O_2$	$2.41 \times 10^{-11} \times \exp(-2.94 \times 10^{3}/(R \times T_g))$	6,7
$O + HO_2 \rightarrow O_2 + OH$	$2.91 \times 10^{-11} \times \exp(1.66 \times 10^{3} / (R \times T_g))$	6,7
$O + CH_2O \rightarrow OH + CHO$	$1.78 \times 10^{-11} \times (T_g/298)^{0.57} \times \exp(-11560/(R \times T_g))$	6,7
$O + CHO \rightarrow CO + OH$	5.00×10 <sup>-11</sup>	6,7
$O + CHO \rightarrow H + CO_2$	5.00×10 <sup>-11</sup>	6,7

$O + CH_3O \rightarrow CH_3 + O_2$	2.20×10 <sup>-11</sup>	6,7
$O + CH_3O \rightarrow OH + CH_2O$	1.00×10 <sup>-11</sup>	6,7
$O + CH_3CHO \rightarrow OH + CH_3CO$	$8.30 \times 10^{-12} \times \exp(-7.50 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$O + CH_2CO \rightarrow CH_2 + CO_2$	2.29×10 <sup>-13</sup>	6,7
$O + CH_2CO \rightarrow CH_2O + CO$	7.88×10 <sup>-14</sup>	6,7
$O + CH_2CO \rightarrow CHO + CO + H$	4.33×10 <sup>-14</sup>	6,7
$O + CH_2CO \rightarrow CHO + CHO$	4.33×10 <sup>-14</sup>	6,7
$O + C_2 HO \rightarrow CO + CO + H$	1.60×10 <sup>-10</sup>	6,7
$O + CH_3O_2 \rightarrow CH_3O + O_2$	5.99×10 <sup>-11</sup>	6,7
$O + CH_3OOH \rightarrow CH_3O_2 + OH$	5.63×10 <sup>-15</sup>	6,7
$O_2$ + CHO $\rightarrow$ CO + HO <sub>2</sub>	7.14×10 <sup>-11</sup>	6,7
$O_2 + CH_3O \rightarrow CH_2O + HO_2$	1.97×10 <sup>-15</sup>	6,7
$O_2 + C_2HO \rightarrow CO + CO + OH$	6.46×10 <sup>-13</sup>	6,7
$CO + OH \rightarrow CO_2 + H$	$5.40 \times 10^{-14} \times (T_g/298)^{1.50} \times \exp(2080/(R \times T_g))$	6,7
$CO + HO_2 \rightarrow CO_2 + OH$	$2.51 \times 10^{-10} \times \exp(-98940/(R \times T_g))$	6,7
$\rm CO + CH_3O \rightarrow CO_2 + CH_3$	$2.61 \times 10^{-11} \times \exp(-49390/(R \times T_g))$	6,7
$H_2O + CHO \rightarrow CH_2O + OH$	$8.54 \times 10^{-13} \times (T_g/298)^{1.35} \times \exp(-109000/(R \times T_g))$	6,7
$H_2O + CH_3O \rightarrow CH_3OH + OH$	$1.46 \times 10^{-15} \times (T_g/298)^{3.80} \times \exp(-48060/(R \times T_g))$	6,7
$OH + OH \rightarrow H_2O + O$	$1.65 \times 10^{-12} \times (T_g/298)^{1.14} \times \exp(-0.42 \times 10^3/(R \times T_g))$	6,7
$OH + HO_2 \rightarrow O_2 + H_2O$	$4.80 \times 10^{-11} \times \exp(2.08 \times 10^{3}/(\text{R} \times T_g))$	6,7
$OH + CH_2O \rightarrow H_2O + CHO$	$4.73 \times 10^{-12} \times (T_g/298)^{1.18} \times \exp(1.87 \times 10^3/(R \times T_g))$	6,7
$OH + CHO \rightarrow CO + H_2O$	1.69×10 <sup>-10</sup>	6,7
$OH + CH_3O \rightarrow CH_2O + H_2O$	3.01×10 <sup>-11</sup>	6,7
$OH + CH_3CHO \rightarrow CH_3CO + H_2O$	1.49×10 <sup>-11</sup>	6,7
$OH + CH_2CO \to CO + CH_2OH$	1.14×10 <sup>-11</sup>	6,7
$OH + CH_3O_2 \rightarrow CH_3OH + O_2$	1.00×10 <sup>-10</sup>	6,7
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	1.63×10 <sup>-12</sup>	6,7
$\mathrm{HO}_{2} + \mathrm{CH}_{2}\mathrm{O} \rightarrow \mathrm{CHO} + \mathrm{H}_{2}\mathrm{O}_{2}$	$3.30 \times 10^{-12} \times \exp(-48810/(R \times T_g))$	6,7
$HO_2 + CHO \rightarrow OH + H + CO_2$	5.00×10 <sup>-11</sup>	6,7
$\mathrm{HO}_{2} + \mathrm{CH}_{3}\mathrm{O} \rightarrow \mathrm{CH}_{2}\mathrm{O} + \mathrm{H}_{2}\mathrm{O}_{2}$	5.00×10 <sup>-13</sup>	6,7
$\mathrm{HO}_{2} + \mathrm{CH}_{3}\mathrm{O}_{2} \rightarrow \mathrm{CH}_{3}\mathrm{OOH} + \mathrm{O}_{2}$	5.12×10 <sup>-12</sup>	6,7
$CH_2O + CH_3O \rightarrow CH_3OH + CHO$	1.69×10 <sup>-13</sup> ×exp(-12470/(R×T <sub>g</sub> ))	6,7
$CH_2O + CH_3O_2 \rightarrow CHO + CH_3OOH$	$3.30 \times 10^{-12} \times \exp(-48810/(R \times T_g))$	6,7
$CHO+CHO\toCH_2O+CO$	5.00×10 <sup>-11</sup>	6,7

$CHO + CH_3O \to CH_3OH + CO$	1.50×10 <sup>-10</sup>	6,7
$CHO + CH_3O_2 \rightarrow CH_3O + H + CO_2$	5.00×10 <sup>-11</sup>	6,7
$CH_3O + CH_3O \rightarrow CH_2O + CH_3OH$	1.00×10 <sup>-10</sup>	6,7
$CH_{3}O + CH_{3}O_{2} \rightarrow CH_{2}O + CH_{3}OOH$	5.00×10 <sup>-13</sup>	6,7
$CH_3O_2 + CH_3O_2 \rightarrow CH_3OH + CH_2O + O_2$	2.19×10 <sup>-13</sup>	6,7
$CH_3O_2 + CH_3O_2 \rightarrow CH_3O + CH_3O + O_2$	1.29×10 <sup>-13</sup>	6,7
$\rm CH_4 + \rm CH_3\rm CO \rightarrow \rm CH_3\rm CHO + \rm CH_3$	$4.82 \times 10^{-14} \times (T_g/298)^{2.88} \times \exp(-89800/(R \times T_g))$	6,7
$CH_4 + CH_2OH \rightarrow CH_3OH + CH_3$	$1.68 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-67930/(R \times T_g))$	6,7
$CH_3 + H_2O_2 \rightarrow CH_4 + HO_2$	$2.01 \times 10^{-14} \times \exp(2490/(R \times T_g))$	6,7
$CH_3 + CH_3OH \rightarrow CH_4 + CH_3O$	$1.12 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-29020/(R \times T_g))$	6,7
$CH_3 + CH_3OH \rightarrow CH_4 + CH_2OH$	$4.38 \times 10^{-15} \times (T_g/298)^{3.20} \times \exp(-30020/(R \times T_g))$	6,7
$CH_3 + CH_2OH \rightarrow CH_4 + CH_2O$	4.00×10 <sup>-12</sup>	6,7
$CH_2 + H_2O_2 \rightarrow CH_3 + HO_2$	1.00×10 <sup>-14</sup>	6,7
$\mathrm{CH}_2 + \mathrm{CH}_3\mathrm{CO} \to \mathrm{CH}_2\mathrm{CO} + \mathrm{CH}_3$	3.01×10 <sup>-11</sup>	6,7
$CH_2 + CH_3OH \rightarrow CH_3O + CH_3$	$1.12 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-29020/(R \times T_g))$	6,7
$CH_2 + CH_3OH \rightarrow CH_2OH + CH_3$	$4.38 \times 10^{-15} \times (T_g/298)^{3.20} \times \exp(-30020/(R \times T_g))$	6,7
$CH_2 + CH_2OH \to CH_2O + CH_3$	2.01×10 <sup>-12</sup>	6,7
$CH_2 + CH_2OH \rightarrow C_2H_4 + OH$	4.00×10 <sup>-11</sup>	6,7
$C_2H_6 + CH_3C \rightarrow CH_3CHO + C_2H_5$	$1.91 \times 10^{-13} \times (T_g/298)^{2.75} \times \exp(-73334/(R \times T_g))$	6,7
$C_2H_6 + CH_2OH \rightarrow CH_3OH + C_2H_5$	$8.73 \times 10^{-15} \times (T_g/298)^{3.00} \times \exp(-58451/(R \times T_g))$	6,7
$C_2H_5 + H_2O_2 \rightarrow C_2H_6 + HO_2$	$1.45 \times 10^{-14} \times \exp(-4070/(R \times T_g))$	6,7
$C_2H_5 + CH_3OH \rightarrow C_2H_6 + CH_3O$	$1.12 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-37420/(R \times T_g))$	6,7
$C_2H_5 + CH_3OH \rightarrow C_2H_6 + CH_2OH$	$4.38 \times 10^{-15} \times (T_g/298)^{3.20} \times \exp(-38330/(R \times T_g))$	6,7
$C_2H_5 + CH_2OH \rightarrow C_2H_6 + CH_2O$	4.00×10 <sup>-12</sup>	6,7
$C_2H_5 + CH_2OH \rightarrow CH_3OH + C_2H_4$	4.00×10 <sup>-12</sup>	6,7
$C_2H_3 + H_2O_2 \rightarrow C_2H_4 + HO_2$	$2.01 \times 10^{-14} \times \exp(2490/(R \times T_g))$	6,7
$C_2H_3 + CH_3OH \rightarrow C_2H_4 + CH_3O$	$1.12 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-29020/(R \times T_g))$	6,7
$C_2H_3 + CH_3OH \rightarrow C_2H_4 + CH_2OH$	$4.38 \times 10^{-15} \times (T_g/298)^{3.20} \times \exp(-30020/(R \times T_g))$	6,7
$C_2H_3 + CH_2OH \rightarrow C_2H_4 + CH_2O$	5.00×10 <sup>-11</sup>	6,7
$C_2H_3 + CH_2OH \rightarrow C_3H_5 + OH$	2.01×10 <sup>-11</sup>	6,7
$C_2H_2 + CH_2OH \rightarrow C_2H_3 + CH_2O$	1.20×10 <sup>-12</sup> ×exp(-37660/(R×T <sub>g</sub> ))	6,7
$C_2H + CH_3OH \rightarrow C_2H_2 + CH_3O$	2.01×10 <sup>-12</sup>	6,7
$C_2H + CH_3OH \rightarrow C_2H_2 + CH_2OH$	1.00×10 <sup>-11</sup>	6,7
$C_2H + CH_2OH \rightarrow C_2H_2 + CH_2O$	5.99×10 <sup>-11</sup>	6,7

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$C_3H_8$ + $CH_3CO \rightarrow CH_3CHO$ + $C_3H_7$	$1.89 \times 10^{-13} \times (T_g/298)^{2.60} \times \exp(-73916/(R \times T_g))$	6,7
$C_3H_8 + CH_2OH \rightarrow CH_3OH + C_3H_7$	$6.56 \times 10^{-15} \times (T_g/298)^{2.95} \times \exp(-58451/(R \times T_g))$	6,7
$C_3H_7 + OH \rightarrow C_3H_6 + H_2O$	4.00×10 <sup>-11</sup>	6,7
$C_3H_7 + H_2O_2 \rightarrow C_3H_8 + HO_2$	$5.15 \times 10^{-15} \times (T_g/298)^{2.11} \times \exp(-10730/(R \times T_g))$	6,7
$C_3H_7 + CH_3OH \rightarrow C_3H_8 + CH_3O$	$1.12 \times 10^{-15} \times (T_g/298)^{3.10} \times \exp(-37420/(R \times T_g))$	6,7
$C_3H_7 + CH_3OH \rightarrow C_3H_8 + CH_2OH$	$3.90 \times 10^{-15} \times (T_g/298)^{3.17} \times \exp(-38330/(R \times T_g))$	6,7
$C_3H_7 + CH_2OH \rightarrow C_3H_8 + CH_2O$	1.60×10 <sup>-12</sup>	6,7
$C_3H_7 + CH_2OH \rightarrow C_3H_6 + CH_3OH$	8.00×10 <sup>-13</sup>	6,7
$C_3H_6 + O \rightarrow C_3H_5 + OH$	$1.56 \times 10^{-11} \times (T_g/298)^{0.70} \times \exp(-24610/(R \times T_g))$	6,7
$C_3H_6 + OH \rightarrow C_3H_5 + H_2O$	$4.60 \times 10^{-13} \times (T_g/298)^{2.0} \times \exp(1250/(R \times T_g))$	6,7
$C_3H_6 + HO_2 \rightarrow C_3H_5 + H_2O_2$	$4.33 \times 10^{-14} \times (T_g/298)^{2.6} \times \exp(-58200/(R \times T_g))$	6,7
$C_3H_6 + CHO \rightarrow C_3H_5 + CH_2O$	$9.05 \times 10^{-13} \times (T_g/298)^{1.9} \times \exp(-71170/(\mathbb{R} \times T_g))$	6,7
$C_3H_6 + CH_3O \rightarrow C_3H_5 + CH_3OH$	$2.97 \times 10^{-15} \times (T_g/298)^{2.95} \times \exp(-50140/(R \times T_g))$	6,7
$C_3H_6 + CH_3O_2 \rightarrow C_3H_5 + CH_3OOH$	$3.30 \times 10^{-12} \times \exp(-71340/(R \times T_g))$	6,7
$C_3H_6 + CH_3CO \rightarrow C_3H_5 + CH_3CHO$	$7.82 \times 10^{-13} \times (T_g/298)^{2.00} \times \exp(-67930/(R \times T_g))$	6,7
$C_3H_6 + CH_2OH \rightarrow C_3H_5 + CH_3OH$	$1.99 \times 10^{-15} \times (T_g/298)^{2.95} \times \exp(-50140/(R \times T_g))$	6,7
$C_3H_5 + HO_2 \rightarrow C_3H_6 + O_2$	4.40×10 <sup>-12</sup>	6,7
$C_3H_5 + H_2O_2 \rightarrow C_3H_6 + HO_2$	$7.67 \times 10^{-14} \times (T_g/298)^{2.05} \times \exp(-56790/(R \times T_g))$	6,7
$C_3H_5 + CH_2O \rightarrow C_3H_6 + CHO$	$1.05 \times 10^{-11} \times (T_g/298)^{1.9} \times \exp(-76080/(R \times T_g))$	6,7
$C_3H_5$ + CHO $\rightarrow$ $C_3H_6$ + CO	1.00×10 <sup>-10</sup>	6,7
$C_3H_5 + CH_3O \rightarrow C_3H_6 + CH_2O$	5.00×10 <sup>-11</sup>	6,7
$C_3H_5 + CH_3OH \rightarrow C_3H_6 + CH_2OH$	$4.33 \times 10^{-14} \times (T_g/298)^{2.9} \times \exp(-85640/(R \times T_g))$	6,7
$C_3H_5 + CH_2OH \rightarrow C_3H_6 + CH_2O$	3.01×10 <sup>-11</sup>	6,7
$H_2 + CH_3CO \rightarrow CH_3CHO + H$	$2.18 \times 10^{-13} \times (T_g/298)^{1.82} \times \exp(-73670/(R \times T_g))$	6,7
$H_2 + CH_2OH \rightarrow CH_3OH + H$	$9.96 \times 10^{-14} \times (T_g/298)^{2.0} \times \exp(-55870/(R \times T_g))$	6,7
$H + H_2O_2 \rightarrow H_2O + OH$	$1.69 \times 10^{-11} \times \exp(-14970/(R \times T_g))$	6,7
$H + H_2O_2 \rightarrow H_2 + HO_2$	$2.81 \times 10^{-12} \times \exp(-15710/(R \times T_g))$	6,7
$H + CH_3OH \rightarrow CH_2OH + H_2$	$2.42 \times 10^{-12} \times (T_g/298)^{2.0} \times \exp(-18870/(R \times T_g))$	6,7
$H + CH_3OH \rightarrow CH_3O + H_2$	3.18×10 <sup>-16</sup>	6,7
$H + CH_2OH \rightarrow CH_2O + H_2$	1.00×10 <sup>-11</sup>	6,7
$H + CH_2OH \rightarrow CH_3 + OH$	1.60×10 <sup>-10</sup>	6,7
$H + CH_3OOH \rightarrow H_2O + CH_3O$	5.88×10 <sup>-15</sup>	6,7
$H + CH_3OOH \rightarrow H_2 + CH_3O_2$	7.11×10 <sup>-15</sup>	6,7

$O + H_2O_2 \rightarrow O_2 + H_2O$	8.91×10 <sup>-16</sup>	6,7
$O+CH_3CO\toOH+CH_2CO$	8.75×10 <sup>-11</sup>	6,7
$O + CH_3CO \rightarrow CO_2 + CH_3$	2.63×10 <sup>-10</sup>	6,7
$O + CH_3OH \rightarrow OH + CH_2OH$	$5.71 \times 10^{-11} \times \exp(-22.86 \times 10^{3}/(\text{R} \times T_g))$	6,7
$O + CH_3OH \rightarrow OH + CH_3O$	$1.66 \times 10^{-11} \times \exp(-19.62 \times 10^{3}/(R \times T_g))$	6,7
$O + CH_2OH \rightarrow CH_2O + OH$	7.00×10 <sup>-11</sup>	6,7
$OH + H_2O_2 \rightarrow HO_2 + H_2O$	$1.30 \times 10^{-11} \times \exp(-5.57 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$OH + CH_3CO \rightarrow CH_2CO + H_2O$	2.01×10 <sup>-11</sup>	6,7
$OH + CH_3CO \rightarrow CH_3 + CO + OH$	5.00×10 <sup>-11</sup>	6,7
$OH + CH_3OH \rightarrow H_2O + CH_2OH$	1.06×10 <sup>-12</sup>	6,7
$OH + CH_3OH \rightarrow H_2O + CH_3O$	$1.66 \times 10^{-11} \times \exp(-7.10 \times 10^{3}/(R \times T_g))$	6,7
$OH + CH_2OH \rightarrow CH_2O + H_2O$	4.00×10 <sup>-11</sup>	6,7
$OH + CH_3OOH \rightarrow H_2O + CH_3O_2$	1.79×10 <sup>-12</sup> ×exp(1.83×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$HO_2 + CH_3CO \rightarrow CH_3 + CO_2 + OH$	5.00×10 <sup>-11</sup>	6,7
$HO_2 + CH_3OH \rightarrow CH_2OH + H_2O_2$	1.60×10 <sup>-13</sup> ×exp(-52630/(R×7 <sub>g</sub> ))	6,7
$HO_2 + CH_2OH \rightarrow CH_2O + H_2O_2$	2.01×10 <sup>-11</sup>	6,7
$CH_2O + CH_3CO \rightarrow CH_3CHO + CHO$	$3.01 \times 10^{-13} \times \exp(-54040/(R \times T_g))$	6,7
$CH_2O + CH_2OH \rightarrow CH_3OH + CHO$	$7.72 \times 10^{-14} \times (T_g/298)^{2.8} \times \exp(-24530/(R \times T_g))$	6,7
$CHO + H_2O_2 \rightarrow CH_2O + HO_2$	$1.69 \times 10^{-13} \times \exp(-29020/(R \times T_g))$	6,7
$CHO + CH_3CO \to CH_3CHO + CO$	1.50×10 <sup>-11</sup>	6,7
$CHO + CH_3OH \to CH_2O + CH_2OH$	$2.41 \times 10^{-13} \times (T_g/298)^{2.9} \times \exp(-54880/(R \times T_g))$	6,7
$CHO + CH_2OH \to CH_2O + CH_2O$	3.01×10 <sup>-10</sup>	6,7
$CHO + CH_2OH \to CH_3OH + CO$	2.01×10 <sup>-10</sup>	6,7
$\rm CH_3O + \rm CH_3CO \rightarrow \rm CH_3OH + \rm CH_2CO$	1.00×10 <sup>-11</sup>	6,7
$CH_3O + CH_3OH \rightarrow CH_3OH + CH_2OH$	$5.00 \times 10^{-13} \times \exp(-17040/(R \times T_g))$	6,7
$CH_3O + CH_2OH \rightarrow CH_2O + CH_3OH$	4.00×10 <sup>-11</sup>	6,7
$CH_{3}O_{2} + H_{2}O_{2} \rightarrow CH_{3}OOH + HO_{2}$	$4.00 \times 10^{-12} \times \exp(-41570/(R \times T_g))$	6,7
$CH_3O_2 + CH_3CO \rightarrow CH_3 + CO_2 + CH_3O$	4.00×10 <sup>-11</sup>	6,7
$CH_{3}O_{2} + CH_{3}OH \rightarrow CH_{2}OH + CH_{3}OOH$	$3.01 \times 10^{-12} \times \exp(-57370/(R \times T_g))$	6,7
$CH_{3}O_{2} + CH_{2}OH \rightarrow CH_{3}O + OH + CH_{2}O$	2.00×10 <sup>-11</sup>	6,7
$H_2O_2 + CH_3CO \rightarrow CH_3CHO + HO_2$	$3.01 \times 10^{-13} \times \exp(-34420/(R \times T_g))$	6,7
$H_2O_2 + CH_2OH \rightarrow CH_3OH + HO_2$	$5.00 \times 10^{-15} \times \exp(-10810/(R \times T_g))$	6,7
$CH_3CO + CH_3OH \rightarrow CH_3CHO + CH_2OH$	2.13×10 <sup>-13</sup> ×( $T_g$ /298) <sup>3.00</sup> ×exp(-51630/(R× $T_g$ ))	6,7
$CH_3OH + CH_2OH \rightarrow CH_3OH + CH_3O$	$1.30 \times 10^{-14} \times \exp(-50470/(R \times T_g))$	6,7

$CH_2OH + CH_2OH \to CH_2O + CH_3OH$	8.00×10 <sup>-12</sup>	6,7
$CH_2 + CH_2 \rightarrow C_2H_4$	1.70×10 <sup>-12</sup>	6,7
$C_2H_6 + H \rightarrow CH_4 + CH_3$	$8.97 \times 10^{-20} \times \exp(-48.64 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$O + H_2O \rightarrow HO_2 + H$	$4.48 \times 10^{-12} \times (T_g/298)^{0.97} \times \exp(-287.0 \times 10^3/(R \times T_g))$	6,7
$O + H_2 O \rightarrow H_2 + O_2$	$4.48 \times 10^{-12} \times (T_g/298)^{0.97} \times \exp(-287.0 \times 10^3/(R \times T_g))$	6,7
$O + CH_2 \rightarrow CHO + H$	5.01×10 <sup>-11</sup>	6,7
$CH_3 + O \rightarrow CH_3O$	$7.51 \times 10^{-14} \times (T_g/298)^{-2.12} \times \exp(-2.61 \times 10^{3/}(R \times T_g))$	6,7
$CH + H_2O \rightarrow CH_2O + H$	$2.82 \times 10^{-11} \times (T_g/298)^{-1.22} \times \exp(-0.10 \times 10^{3/}(R \times T_g))$	6,7
$C_2H_2 + H_2 \rightarrow C_2H_4$	$5.00 \times 10^{-13} \times \exp(-163.0 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_2 + CO \rightarrow C_2H + CHO$	$8.00 \times 10^{-10} \times \exp(-446.0 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_2 + OH \rightarrow CO + CH_3$	$9.13 \times 10^{-11} \times \exp(-57.29 \times 10^{3}/(\text{R} \times T_g))$	6,7
$CO + CH_3 \rightarrow C_2H_2 + OH$	6.31×10 <sup>-11</sup> ×exp(-253×10 <sup>3</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$C_2H_2 + H_2 \rightarrow C_2H_3 + H$	$4.00 \times 10^{-12} \times \exp(-272.0 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_4 + H_2 \rightarrow C_2H_5 + H$	$1.69 \times 10^{-11} \times \exp(-285.0 \times 10^{3}/(R \times T_g))$	6,7
$H_2 + O_2 \rightarrow HO_2 + H$	$2.41 \times 10^{-10} \times \exp(-237.0 \times 10^{3}/(R \times T_g))$	6,7
$H_2 + CH_3O \rightarrow CH_3OH + H$	$1.66 \times 10^{-15} \times (T_g/298)^{4.0} \times \exp(-20.54 \times 10^3/(R \times T_g))$	6,7
$OH + O_2 \rightarrow HO_2 + O$	$3.70 \times 10^{-11} \times \exp(-220000.0/(R \times T_g))$	6,7
$C_2H_5 + OH \rightarrow C_2H_6 + O$	$9.85 \times 10^{-19} \times (T_g/298)^{8.8} \times \exp(-2.08 \times 10^3/(R \times T_g))$	6,7
$C_2H + H_2O \rightarrow C_2H_2 + OH$	$7.74 \times 10^{-14} \times (T_g/298)^{3.05} \times \exp(-3.13 \times 10^{3}/(R \times T_g))$	6,7
$OH + OH \rightarrow HO_2 + H$	$3.32 \times 10^{-12} \times (T_g/298)^{0.51} \times \exp(-211 \times 10^3/(R \times T_g))$	6,7
$H_2O + O_2 \rightarrow HO_2 + OH$	$7.72 \times 10^{-12} \times \exp(-310000.0/(R \times T_g))$	6,7
$HO_2 + H_2O \rightarrow OH + H_2O_2$	$4.65 \times 10^{-11} \times \exp(-137.0 \times 10^{3}/(R \times T_g))$	6,7
$CH_2OH + H_2O \rightarrow CH_3OH + OH$	$4.12 \times 10^{-14} \times (T_g/298)^{3.0} \times \exp(-86.80 \times 10^3/(R \times T_g))$	6,7
$C_2H_6 \rightarrow C_2H_5 + H$	$8.11 \times 10^{17} \times (T_g/298)^{-1.23} \times \exp(-427.0 \times 10^3/(R \times T_g))$	6,7
$CH_3 + CH_3 \rightarrow CH_4 + CH_2$	$7.14 \times 10^{-12} \times \exp(-41.99 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_4+C_3H_6\rightarrow C_3H_5+C_2H_5$	$9.60 \times 10^{-11} \times \exp(-216.0 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_4 + C_2H_2 \rightarrow C_2H_3 + C_2H_3$	$4.00 \times 10^{-11} \times \exp(-286.0 \times 10^{3}/(R \times T_g))$	6,7
$C_2H_2 + C_2H_2 \rightarrow C_2H + C_2H_3$	$1.60 \times 10^{-11} \times \exp(-353.0 \times 10^{3}/(\text{R} \times T_g))$	6,7
$C_2H_4 + C_3H_6 \rightarrow C_2H_3 + C_3H_7$	$1.00 \times 10^{-10} \times \exp(-316.0 \times 10^{3}/(R \times T_g))$	6,7
$C_3H_6 + C_2H_2 \rightarrow C_2H_3 + C_3H_5$	$6.71 \times 10^{-11} \times \exp(-196.0 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$C_3H_6 + C_3H_6 \rightarrow C_3H_7 + C_3H_5$	$4.20 \times 10^{-10} \times \exp(-231.0 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$CH_4 + O_2 \rightarrow CH_3 + HO_2$	6.59×10 <sup>-11</sup> ×exp(-238000.0/(R×T <sub>g</sub> ))	6,7
$C_2H_6 + O_2 \rightarrow C_2H_5 + HO_2$	$1.00 \times 10^{-10} \times \exp(-217000.0/(R \times T_g))$	6,7
$CO + C_2H_4 \rightarrow CHO + C_2H_3$	$2.51 \times 10^{-10} \times \exp(-379000.0/(R \times T_g))$	6,7

$C_2H_2 + O_2 \rightarrow C_2H + HO_2$	$2.01 \times 10^{-11} \times \exp(-312000.0/(R \times T_g))$	6,7
$CH_3 + O_2 \rightarrow CH_3O + O$	$1.25 \times 10^{-11} \times \exp(-118000.0/(R \times T_g))$	6,7
$H_2O_2 + O_2 \rightarrow HO_2 + HO_2$	$9.00 \times 10^{-11} \times \exp(-166000.0/(R \times T_g))$	6,7
$CH_{3}CHO + C_{2}H_{5} \rightarrow C_{2}H_{6} + CH_{3}CO$	$2.09 \times 10^{-12} \times \exp(-35.59 \times 10^{3}/(R \times T_g))$	6,7
$CH_{3}CHO + C_{3}H_{5} \rightarrow C_{3}H_{6} + CH_{3}CO$	$6.31 \times 10^{-13} \times \exp(-30.18 \times 10^{3}/(\text{R} \times T_{g}))$	6,7
$C_3H_6 + O_2 \rightarrow C_3H_5 + HO_2$	$9.00 \times 10^{-11} \times \exp(-166000.0/(R \times T_g))$	6,7
$CH_2O + HO_2 \rightarrow CH_2OH + O_2$	$5.63 \times 10^{-12} \times \exp(-79.99 \times 10^{3}/(R \times T_g))$	6,7
$CH_{3}CHO + HO_{2} \rightarrow H_{2}O_{2} + CH_{3}CO$	$5.00 \times 10^{-12} \times \exp(-49.89 \times 10^{3}/(R \times T_g))$	6,7
$CH_{3}CHO + CH_{2}OH \rightarrow CH_{3}CO + CH_{3}OH$	8.30×10 <sup>-15</sup>	6,7
$C_2H_2 + HO_2 \rightarrow C_2H_3 + O_2$	$5.00 \times 10^{-14} \times (T_g/298)^{1.61} \times \exp(-59.28 \times 10^3/(R \times T_g))$	6,7
$C_2H_3 + O_2 \rightarrow C_2H_2 + HO_2$	$2.14 \times 10^{-14} \times (T_g/298)^{1.61} \times \exp(1.60 \times 10^3/(R \times T_g))$	6,7
$C_2H_4+C_2H_4\rightarrow C_2H_5+C_2H_3$	$8.00 \times 10^{-10} \times \exp(-299.0 \times 10^3 / (R \times T_g))$	6,7
$CH_4 + CH_3 \rightarrow H + C_2H_6$	$1.33 \times 10^{-10} \times \exp(-167000.0/(R \times T_g))$	6,7
$C_2H_4 + CH_3 \rightarrow C_3H_7$	$4.00 \times 10^{-14} \times (T_g/298)^{2.48} \times \exp(-25.65 \times 10^3/(\text{R} \times T_g))$	6,7
$C_3H_5 \rightarrow C_2H_2 + CH_3$	$1.26 \times 10^{13} \times \exp(-140 \times 10^{3}/(R \times T_g))$	6,7
$CH + CH_2 \to C_2H_2 + H$	6.64×10 <sup>-11</sup>	6,7
$CH_2 + CH_2 \to C_2H_2 + H_2$	$2.66 \times 10^{-9} \times \exp(-11944.0/(1.987 \times T_g))$	6,7
$C + CH_3 \rightarrow H + C_2H_2$	8.30×10 <sup>-11</sup>	6,7
$CH + C_2H_3 \rightarrow CH_2 + C_2H_2$	8.30×10 <sup>-11</sup>	6,7
$C_2H_2 + CH \rightarrow C_2H + CH_2$	$3.50 \times 10^{-10} \times \exp(172.0/(1.987 \times T_g))$	6,7
$CO_2 + O \rightarrow CO + O_2$	$7.95 \times 10^{-12} \times \exp(-1.81612 \times 10^4)/T_g)$	6,7
$O_2 + CO \rightarrow CO_2 + O$	$3.99 \times 10^{-14} \times \exp(-1.527467 \times 10^4/T_g)$	6,7
$O_2 + C \rightarrow CO + O$	$1.99 \times 10^{-10} \times \exp(-2.01 \times 10^3/T_g)$	6,7
$HCOOH \rightarrow CO_2 + H_2$	4.46×10 <sup>13</sup> ×exp(-2.86×10 <sup>5</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$\text{HCOOH + OH} \rightarrow \text{COOH + H}_2\text{O}$	$9.85 \times 10^{-13} \times \exp(-8614.0/(R \times T_g))$	6,7
$CO + H_2O_2 \rightarrow COOH + OH$	$9.60 \times 10^{-14} \times (T_g/298)^{2.09} \times \exp(-2.28 \times 10^4/(R \times T_g))$	6,7
$COOH \rightarrow CO + OH$	$29.85 \times (T_g/298)^{0.13} \times \exp(-1.53 \times 10^5/(R \times T_g))$	6,7
$COOH \rightarrow CO_2 + H$	$125.0 \times (T_g/298)^{0.41} \times \exp(-1.48 \times 10^5/(R \times T_g))$	6,7
$COOH + O \to CO_2 + OH$	1.44×10 <sup>-11</sup>	6,7
$COOH + OH \rightarrow CO_2 + H_2O$	1.03×10 <sup>-11</sup>	6,7
$HCOO \rightarrow CO + OH$	$1.21 \times 10^{14} \times (T_g/298)^{0.53} \times \exp(-1.42 \times 10^{5}/(R \times T_g))$	6,7
$HCOO \rightarrow CO_2 + H$	$1.00 \times 10^{13} \times (T_g/298)^{0.31} \times \exp(-1.38 \times 10^5/(R \times T_g))$	6,7
$C_2H_4 + O \rightarrow C_2H_3 + OH$	$1.33 \times 10^{-12} \times (T_g/298)^{1.91} \times \exp(-1.56 \times 10^4/(R \times T_g))$	6,7
$C_2H_5O + C_2H_6 \rightarrow C_2H_5OH + C_2H_5$	$4.00 \times 10^{-13} \times \exp(-29680/(R \times T_g))$	6,7

$C_2H_5O + CHO \rightarrow C_2H_5OH + CO$	1.50×10 <sup>-10</sup>	6,7
$CH_3 + C_2H_5 \rightarrow C_3H_8$	$3.47 \times 10^{-11} \times (T_g/298)^{-0.34} \times \exp(2150.0/(R \times T_g))$	6,7
$CH_3 + H \rightarrow CH_4$	3.50×10 <sup>-10</sup>	6,7
$C_2H_5O \rightarrow CH_2O + CH_3$	1.00×10 <sup>15</sup> ×exp(-9.06×10 <sup>4</sup> /(R× <i>T</i> <sub>g</sub> ))	6,7
$H + H_2 \rightarrow H + H + H$	$\exp(@B+@C \times T_g+@D \times T_g^2+(@$	6,7
	$E) \times T_g^3 + @F \times Log(T_g) + @G \times exp(T_g/11600))$	

@B = -496.794, @C = -0.0237, @D = 4.729×10<sup>-7</sup>, @E = -4.327×10<sup>-11</sup>, @F = 47.387, @G = 113.761

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