

# Erratum: Evaluated Kinetic Data for Combustion Modeling. Supplement I [J. Phys. Chem. Ref. Data 23, 847 (1994)]

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D. L. Baulch, C. J. Cobos, R. A. Cox, P. Frank, G. Hayman, Th. Just, J. A. Kerr, T. Murrells, M. J. Pilling, J. Troe, R. W. Walker, and J. Warnatz



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## Errata

### Erratum: Evaluated Kinetic Data for Combustion Modelling Supplement I

[J. Phys. Chem. Ref. Data, 23, 847, (1994)]

D.L. Baulch

School of Chemistry, University of Leeds, Leeds LS2 9JT, U.K.

C.J. Cobos

Institut für Physikalische Chemie, Universität Göttingen, D-3400 Göttingen, Germany

R.A. Cox

NERC, Polaris House, Swindon, SN2 1EU, U.K.

P. Frank

DLR, Institut für Physikalische Chemie der Verbrennung, D-7000 Stuttgart 80, Germany

G. Hayman

AEA Technology Consultancy Services, Harwell, Didcot OX11 0RA, U.K.

Th. Just

DLR, Institut für Physikalische Chemie der Verbrennung, D-7000 Stuttgart 80, Germany

J.A. Kerr

EAWAG, CH-8600 Dübendorf, Switzerland

T. Murrells

AEA Technology Consultancy Services, Harwell, Didcot OX11 0RA, U.K.

M.J. Pilling

School of Chemistry, University of Leeds, Leeds LS2 9JT, U.K.

J. Troe

Institut für Physikalische Chemie, Universität Göttingen, D-3400 Göttingen, Germany

R.W. Walker

School of Chemistry, University of Hull, Hull HU6 7RX, U.K.

and

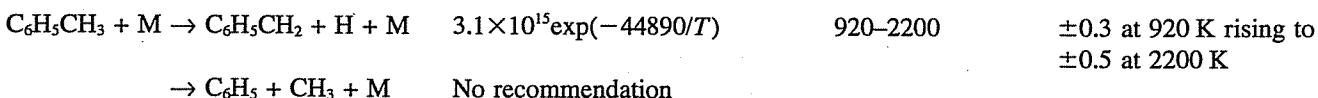
J. Warnatz

Institut für Technische Verbrennung, Universität Stuttgart, D-7000 Stuttgart 80, Germany

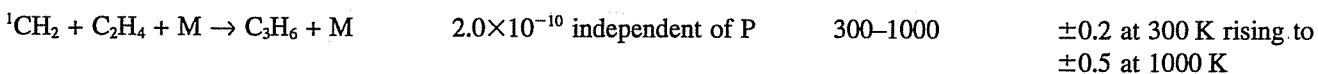
Since going to press the following errors have been noted:

**Summary Table:**

**p.869** — The entry for  $C_6H_5CH_3 + M$  should read:



**p.871** — The entry for  $^1CH_2 + C_2H_4 + M$  should read:



**p.928** —  $H + C_6H_5CH_3$  The expression for  $k_1$  should read:

$$k_1 = 3.6 \times 10^{-19} T^{2.63} \exp(-2210/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} \text{ over the range } 600\text{--}2500 \text{ K}$$

**p.940 and p.857** —  $OH + C_2H_2$ . Channel (2) for this reaction should be written as  $OH + C_2H_2 \rightarrow HOCH_2 + H$ . The thermodynamic data given on **p.940** for channel (2) refer to the formation of  $CH_2CO + H$  and should be ignored.

**p.1016** — The entry in the table of Rate Coefficient Data under the heading Reviews and Evaluations should read  $6.0 \times 10^{-12}$  not  $6.5 \times 10^{-12}$ .

**p.1025** — The recommended value for  $k_1$  should read  $3.1 \times 10^{15} \exp(-44890/T)$  not  $3.1 - 10^{15} \exp(-44890/T)$ .

Table 1 on **p.1026** should be Table 4.

Table 2 on **p.1030** should be Table 5.

In Sec. 4.2, Summary of Preferred Rate Data in Tables 1–3, page numbers of the data sheets for the corresponding reaction were omitted. Tables 1–3 are repeated here with the page numbers added. The following pages replace pp.853–872 of J. Phys. Chem. Ref. Data, 23, 847 (1994).

## 4.2. Summary of Preferred Rate Data

TABLE I. Bimolecular Reactions

[p853 of original article]

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i>O Atom Reactions</i>				
$\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$	$8.5 \times 10^{-20} T^{2.67} \exp(-3160/T)$	300–2500	$\pm 0.5$ at 300 K falling to $\pm 0.2$ for $T > 500$ K	CEC <sup>1</sup>
$\text{O} + \text{OH} \rightarrow \text{O}_2 + \text{H}$	$2.0 \times 10^{-11} \exp(112/T)$ $2.4 \times 10^{-11} \exp(-353/T)$	220–500 1000–2000	$\pm 0.2$ $\pm 0.1$	CEC <sup>1</sup>
$\text{O} + \text{HO}_2 \rightarrow \text{OH} + \text{O}_2$	$5.3 \times 10^{-11}$	300–1000	$\pm 0.3$ at 300 K rising to $\pm 0.5$ at 1000 K	CEC <sup>1</sup>
$\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{HO}_2$	$1.1 \times 10^{-12} \exp(-2000/T)$	300–500	$\pm 0.3$	CEC <sup>1</sup>
$\text{O} + \text{NO} \rightarrow \text{O}_2 + \text{N}$	$1.14 \times 10^{-15} T^{1.13} \exp(-19200/T)$	1000–5000	$\pm 0.3$	873
$\text{O} + \text{N}_2 \rightarrow \text{N} + \text{NO}$	$3.0 \times 10^{-10} \exp(-38300/T)$	1400–4000	$\pm 0.2$	875
$\text{O} + \text{NH} \rightarrow \text{NO} + \text{H}$ $\rightarrow \text{N} + \text{OH}$	$1.5 \times 10^{-10}$	1000–3380	$\pm 0.5$	878
$\text{O} + \text{NH}_3 \rightarrow \text{OH} + \text{NH}_2$	$1.6 \times 10^{-11} \exp(-3670/T)$	500–2500	$\pm 0.5$	CEC <sup>1</sup>
$\text{O} + \text{CH} \rightarrow \text{CO} + \text{H}$ $\rightarrow \text{CHO}^+ + e^-$	$6.6 \times 10^{-11}$ $4.2 \times 10^{-13} \exp(-850/T)$	300–2000 300–2500	$\pm 0.5$ $\pm 0.5$	CEC <sup>1</sup>
$\text{O} + {}^3\text{CH}_2 \rightarrow \text{CO} + 2\text{H}$ $\rightarrow \text{CO} + \text{H}_2$	$2 \times 10^{-10}$ $k_1/k = 0.6 \pm 0.3$ over whole range	300–2500	$\pm 0.2$ at 300 K rising to $\pm 0.7$ at 2500 K.	CEC <sup>1</sup>
$\text{O} + \text{CH}_3 \rightarrow \text{HCHO} + \text{H}$	$1.4 \times 10^{-10}$	300–2500	$\pm 0.2$	CEC <sup>1</sup>
$\text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3$	$1.2 \times 10^{-15} T^{1.56} \exp(-4270/T)$	300–2500	$\pm 0.3$ at 300 K falling to $\pm 0.15$ at 2500 K	CEC <sup>1</sup>
$\text{O} + \text{CHO} \rightarrow \text{OH} + \text{CO}$ $\rightarrow \text{CO}_2 + \text{H}$	$5.0 \times 10^{-11}$ $5.0 \times 10^{-11}$	300–2500 300–2500	$\pm 0.3$ $\pm 0.3$	CEC <sup>1</sup>
$\text{O} + \text{HCHO} \rightarrow \text{OH} + \text{CHO}$	$6.9 \times 10^{-13} T^{0.57} \exp(-1390/T)$	250–2200	$\pm 0.1$ at 250 K rising to $\pm 0.3$ at 2200 K	CEC <sup>1</sup>
$\text{O} + \text{CH}_3\text{O} \rightarrow \text{O}_2 + \text{CH}_3$ $\rightarrow \text{OH} + \text{HCHO}$	$2.5 \times 10^{-11}$ $k_2/k = (0.12 \pm 0.1)$ at 300 K	300–1000	$\pm 0.3$ at 300 K rising to $\pm 0.7$ at 1000 K	CEC <sup>1</sup>
$\text{O} + \text{CH}_3\text{OOH} \rightarrow \text{OH} + \text{CH}_3\text{O}_2$ $\rightarrow \text{OH} + \text{CH}_2\text{OOH}$	$3.3 \times 10^{-11} \exp(-2390/T)$	300–1000	$\pm 0.3$ at 300 K rising to $\pm 0.5$ at 100	878
$\text{O} + \text{CN} \rightarrow \text{CO} + \text{N}({}^4\text{S})$ $\rightarrow \text{CO} + \text{N}({}^2\text{D})$	$1.7 \times 10^{-11}$	300–5000	$\pm 0.2$ at 300 K rising to $\pm 0.6$ at 5000 K	CEC <sup>1</sup>
$\text{O} + \text{NCO} \rightarrow \text{NO} + \text{CO}$ $\rightarrow \text{O}_2 + \text{CN}$	$7.0 \times 10^{-11}$	1450–2600	$\pm 0.8$	CEC <sup>1</sup>
$\text{O} + \text{HCN} \rightarrow \text{NCO} + \text{H}$ $\rightarrow \text{CO} + \text{NH}$ $\rightarrow \text{OH} + \text{CN}$	$2.3 \times 10^{-18} T^{2.1} \exp(-3075/T)$	450–2500	$\pm 0.2$ at 450 K rising to $\pm 0.3$ at 2500 K	CEC <sup>1</sup>
$\text{O} + \text{C}_2\text{H} \rightarrow \text{CO} + \text{CH}$	$1.7 \times 10^{-11}$	300–2500	$\pm 1.0$	CEC <sup>1</sup>
$\text{O} + \text{C}_2\text{H}_2 \rightarrow \text{CO} + {}^3\text{CH}_2$ $\rightarrow \text{CHCO} + \text{H}$	$1.2 \times 10^{-17} T^{2.1} \exp(-790/T)$ $k_2/k = 0.7 \pm 0.2$ over whole range.	295–2500	$\pm 0.2$	879
$\text{O} + \text{C}_2\text{H}_3 \rightarrow \text{OH} + \text{C}_2\text{H}_2$ $\rightarrow \text{CO} + \text{CH}_3$ $\rightarrow \text{HCO} + \text{CH}_2$	$5 \times 10^{-11}$	300–2000	$\pm 0.5$	CEC <sup>1</sup>

[p854 of original article]

TABLE 1. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{O} + \text{C}_2\text{H}_4 \rightarrow \text{CH}_2\text{CHO} + \text{H}$ [ $\rightarrow \text{HCO} + \text{CH}_3$ $\rightarrow \text{HCHO} + \text{CH}_2$ $\rightarrow \text{CH}_2\text{CO} + \text{H}_2$ ]	$2.25 \times 10^{-17} T^{1.88} \exp(-90/T)$ $k_1/k = 0.35 \pm 0.05$ at $p > 3$ Torr; $k_2/k = 0.6 \pm 0.10$ ; $k_3/k = 0.05 \pm 0.10$	300–2000	$\pm 0.1$ for $T < 1000$ K rising to $\pm 0.3$ at 2000 K	882
$\text{O} + \text{C}_2\text{H}_5 \rightarrow \text{CH}_3\text{CHO} + \text{H}$ [ $\rightarrow \text{HCHO} + \text{CH}_3$ ]	$1.1 \times 10^{-10}$ $k_2/k = 0.17 \pm 0.2$ at 300 K	300–2500	$\pm 0.3$ from 300 to 1000 K $\pm 0.5$ from 1000 to 2500 K	CEC <sup>1</sup>
$\text{O} + \text{C}_2\text{H}_6 \rightarrow \text{OH} + \text{C}_2\text{H}_5$	$1.66 \times 10^{-15} T^{1.5} \exp(-2920/T)$	300–1200	$\pm 0.3$ at 300 K falling to $\pm 0.15$ at 1200 K	CEC <sup>1</sup>
$\text{O} + \text{CHCO} \rightarrow 2\text{CO} + \text{H}$	$1.6 \times 10^{-10}$	300–2500	$\pm 0.3$	CEC <sup>1</sup>
$\text{O} + \text{CH}_2\text{CO} \rightarrow \text{CH}_2\text{O} + \text{CO}$ [ $\rightarrow \text{HCO} + \text{H} + \text{CO}$ $\rightarrow \text{HCO} + \text{HCO}$ ]	$3.8 \times 10^{-12} \exp(-680/T)$	230–500	$\pm 0.3$	CEC <sup>1</sup>
$\text{O} + \text{CH}_3\text{CO} \rightarrow \text{OH} + \text{CH}_2\text{CO}$ [ $\rightarrow \text{CO}_2 + \text{CH}_3$ ]	$3.2 \times 10^{-10}$ $k_1/k = 0.2 \pm 0.1$ at 298 K $k_2/k = 0.8 \pm 0.2$ at 298 K	298–1500	$\pm 0.3$ at 298 K rising to $\pm 1.0$ at 1500 K	884
$\text{O} + \text{CH}_3\text{CHO} \rightarrow \text{OH} + \text{CH}_3\text{CO}$ [ $\rightarrow \text{OH} + \text{CH}_2\text{CHO}$ ]	$9.7 \times 10^{-12} \exp(-910/T)$	298–1500	$\pm 0.05$ at 298 K rising to $\pm 0.5$ at 1500 K	885
$\text{O} + \text{C}_2\text{H}_5\text{OOH} \rightarrow \text{OH} + \text{C}_2\text{H}_4\text{OOH}$ [ $\rightarrow \text{OH} + \text{C}_2\text{H}_5\text{OO}$ ]	$3.3 \times 10^{-11} \exp(-2390/T)$ [estimate]	300–1000	$\pm 0.3$ at 300 K rising to $\pm 0.5$ at 1000 K	885
$\text{O} + \text{C}_3\text{H}_5 \rightarrow \text{CH}_2\text{CHCHO} + \text{H}$ [ $\rightarrow \text{HCHO} + \text{C}_2\text{H}_3$ ]	$3.0 \times 10^{-10}$ $< 3 \times 10^{-11}$	300–1000 2000	$\pm 0.2$ over the range 300–600 K; $\pm 0.4$ over the range 600–1000 K	1030
$\text{O} + \text{C}_6\text{H}_6 \rightarrow \text{OH} + \text{C}_6\text{H}_5$ [ $\rightarrow \text{C}_6\text{H}_5\text{O}$ ]	$(k_1 + k_2) = 5.9 \times 10^{-23} T^{3.8} \exp(-473/T)$ $k_2 = 3.7 \times 10^{-11} \exp(-2280/T)$	298–2000 298–1400	$\pm 0.3$ $\pm 0.3$ at 298 K falling to $\pm 0.2$ at 1400 K.	886
$\text{O} + \text{C}_6\text{H}_5\text{OH} \rightarrow \text{products}$	$2.1 \times 10^{-11} \exp(-1460/T)$	290–600	$\pm 0.3$	887
$\text{O} + \text{C}_6\text{H}_5\text{CH}_2 \rightarrow \text{HCO} + \text{C}_6\text{H}_6$ [ $\rightarrow \text{C}_6\text{H}_5\text{CHO} + \text{H}$ $\rightarrow \text{CH}_2\text{O} + \text{C}_6\text{H}_5$ ]	$5.5 \times 10^{-10}$ No recommendation	300	$\pm 0.3$	CEC <sup>1</sup>
$\text{O} + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{products}$	$5.3 \times 10^{-15} T^{1.21} \exp(-1260/T)$	298–2800	$\pm 0.1$ at 298 K rising to $\pm 0.4$ at 2800 K	891
$\text{O} + \text{C}_6\text{H}_5\text{CHO} \rightarrow \text{OH} + \text{C}_6\text{H}_5\text{CO}$ [ $\rightarrow \text{OH} + \text{C}_6\text{H}_4\text{CHO}$ $\rightarrow \text{C}_6\text{H}_5(\text{O})\text{CHO}$ ]	$1.0 \times 10^{-11} \exp(-910/T)$ No recommendation	298–1500	$\pm 0.3$ at 298 K rising to $\pm 0.7$ at 1500 K	888
$\text{O} + p\text{-C}_6\text{H}_4(\text{CH}_3)_2 \rightarrow \text{products}$	$5.1 \times 10^{-11} \exp(-1630/T)$	298–600	$\pm 0.3$	889
$\text{O} + \text{C}_6\text{H}_5\text{C}_2\text{H}_5 \rightarrow \text{products}$	$2.8 \times 10^{-11} \exp(-1840/T)$	298–600	$\pm 0.3$	892
<i>O<sub>2</sub> Reactions</i>				
$\text{O}_2 + \text{CH}_4 \rightarrow \text{HO}_2 + \text{CH}_3$	$6.6 \times 10^{-11} \exp(-28630/T)$	500–2000	$\pm 0.5$ at 500 K rising to $\pm 1.0$ at 2000 K	CEC <sup>1</sup>
$\text{O}_2 + \text{C}_2\text{H}_6 \rightarrow \text{HO}_2 + \text{C}_2\text{H}_5$	$1.0 \times 10^{-10} \exp(-26100/T)$	500–2000	$\pm 0.5$ at 500 K rising to $\pm 1.0$ at 2000 K	CEC <sup>1</sup>

TABLE I. Bimolecular Reactions — Continued

[p855 of original article]

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{O}_2 + \text{HCHO} \rightarrow \text{HO}_2 + \text{HCO}$	$1.0 \times 10^{-10} \exp(-20460/T)$	700–1000	$\pm 0.5$	CEC <sup>1</sup>
$\text{O}_2 + \text{CH}_3\text{CHO} \rightarrow \text{HO}_2 + \text{CH}_3\text{CO}$	$5.0 \times 10^{-11} \exp(-19700/T)$	600–1100	$\pm 0.5$ at 600 K rising to $\pm 1.0$ at 1100 K.	CEC <sup>1</sup>
$\text{O}_2 + \text{C}_3\text{H}_6 \rightarrow \text{HO}_2 + \text{CH}_2\text{CHCH}_2$	$3.2 \times 10^{-12} \exp(-19700/T)$	600–1000	$\pm 0.3$ at 800 K rising to $\pm 0.5$ at 600 K and 1000 K	892
$\text{O}_2 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{HO}_2 + \text{C}_6\text{H}_5\text{CH}_2$	$3 \times 10^{-12} \exp(-20000/T)$	700–1200	$\pm 0.7$	893
<i>H Atom Reactions</i>				
$\text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$	$1.62 \times 10^{-10} \exp(-7470/T)$	300–5000	$\pm 0.1$ at 300 K rising to $\pm 0.5$ at 5000 K	894
$\text{H} + \text{O}_2 + \text{Ar} \rightarrow \text{HO}_2 + \text{Ar}$	See Table 3			896
$\text{H} + \text{O}_2 + \text{H}_2 \rightarrow \text{HO}_2 + \text{H}_2$	See Table 3			896
$\text{H} + \text{O}_2 + \text{N}_2 \rightarrow \text{HO}_2 + \text{N}_2$	See Table 3			896
$\text{H} + \text{H} + \text{Ar} \rightarrow \text{H}_2 + \text{Ar}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{H} + \text{H}_2 \rightarrow \text{H}_2 + \text{H}_2$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{OH} + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O} + \text{H}_2\text{O}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{OH} + \text{Ar} \rightarrow \text{H}_2\text{O} + \text{Ar}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{OH} + \text{N}_2 \rightarrow \text{H}_2\text{O} + \text{N}_2$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	$7.1 \times 10^{-11} \exp(-710/T)$	300–1000	$\pm 0.3$	CEC <sup>1</sup>
$\rightarrow 2\text{OH}$	$2.8 \times 10^{-10} \exp(-440/T)$	300–1000	$\pm 0.3$	
$\rightarrow \text{H}_2\text{O} + \text{O}$	$5.0 \times 10^{-11} \exp(-866/T)$	300–1000	$\pm 0.3$	
$\text{H} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{H}_2$	$7.5 \times 10^{-16} T^{1.6} \exp(-9270/T)$	300–2500	$\pm 0.2$	CEC <sup>1</sup>
$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	$2.8 \times 10^{-12} \exp(-1890/T)$	300–1000	$\pm 0.3$	CEC <sup>1</sup>
$\rightarrow \text{OH} + \text{H}_2\text{O}$	$1.7 \times 10^{-11} \exp(-1800/T)$	300–1000	$\pm 0.3$	
$\text{H} + \text{NO} \rightarrow \text{OH} + \text{N}$	$3.6 \times 10^{-10} \exp(-24910/T)$	1500–4500	$\pm 0.5$	897
$\text{H} + \text{NH} \rightarrow \text{H}_2 + \text{N}$	$1.7 \times 10^{-11}$	1500–2500	$\pm 1.0$	CEC <sup>1</sup>
$\text{H} + \text{NH}_2 \rightarrow \text{H}_2 + \text{NH}$	$1.0 \times 10^{-11}$	2000–3000	$\pm 1.0$	CEC <sup>1</sup>
$\text{H} + \text{CO} + \text{M} \rightarrow \text{HCO} + \text{M}$	See Table 3			899
$\text{H} + {}^3\text{CH}_2 \rightarrow \text{H}_2 + \text{CH}$	$1.0 \times 10^{-11} \exp(900/T)$	300–3000	$\pm 0.7$	CEC <sup>1</sup>
$\text{H} + \text{CH}_3 \rightarrow \text{H}_2 + {}^1\text{CH}_2$	$1.0 \times 10^{-10} \exp(-7600/T)$	300–2500	$\pm 1.0$	CEC <sup>1</sup>
$\rightarrow \text{CH}_4$	See Table 3			
$\text{H} + \text{CH}_4 \rightarrow \text{H}_2 + \text{CH}_3$	$2.2 \times 10^{-20} T^{3.0} \exp(-4045/T)$	300–2500	$\pm 0.2$ at 300 K and 2500 K reducing to $\pm 0.05$ over range 500–1000 K	CEC <sup>1</sup>
$\text{H} + \text{CHO} \rightarrow \text{H}_2 + \text{CO}$	$1.5 \times 10^{-10}$	300–2500	$\pm 0.3$	CEC <sup>1</sup>
$\text{H} + \text{HCHO} \rightarrow \text{H}_2 + \text{HCO}$	$2.1 \times 10^{-16} T^{1.62} \exp(-1090/T)$	300–1700	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 1700 K	914
$\text{H} + \text{CH}_3\text{O} \rightarrow \text{H}_2 + \text{HCHO}$	$3.0 \times 10^{-11}$	300–1000	$\pm 0.5$	CEC <sup>1</sup>

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TABLE 1. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{H} + \text{HNCO} \rightarrow \text{NH}_2 + \text{CO}$ $\rightarrow \text{H}_2 + \text{NCO}$	No recommendation $3.4 \times 10^{-10} T^{-0.27} \exp(-10190/T)$	500–1000	$\pm 1.0$	CEC <sup>1</sup>
$\text{H} + \text{NCO} \rightarrow \text{NH} + \text{CO}$ $\rightarrow \text{HCN} + \text{O}$	$8.7 \times 10^{-11}$	1400–1500	$\pm 0.5$	CEC <sup>1</sup>
$\text{H} + \text{C}_2\text{H}_2 \rightarrow \text{H}_2 + \text{C}_2\text{H}$ $\rightarrow \text{C}_2\text{H}_3$	$1.1 \times 10^{-10} \exp(-14000/T)$ See Table 3	1000–3000	$\pm 1.0$	CEC <sup>1</sup>
$\text{H} + \text{C}_2\text{H}_3 \rightarrow \text{H}_2 + \text{C}_2\text{H}_2$ $\rightarrow \text{C}_2\text{H}_4$	$2.0 \times 10^{-11}$ See Table 3	300–2500	$\pm 0.5$	CEC <sup>1</sup>
$\text{H} + \text{C}_2\text{H}_4 \rightarrow \text{H}_2 + \text{C}_2\text{H}_3$ $\rightarrow \text{C}_2\text{H}_5$	$9.0 \times 10^{-10} \exp(-7500/T)$ See Table 3	700–2000	$\pm 0.5$	CEC <sup>1</sup>
$\text{H} + \text{C}_2\text{H}_5 \rightarrow 2\text{CH}_3$ $\rightarrow \text{C}_2\text{H}_6$	$6.0 \times 10^{-11}$ See Table 3	300–2000	$\pm 0.3$ at 300 K rising to $\pm 0.7$ at 2000 K	CEC <sup>1</sup>
$\text{H} + \text{C}_2\text{H}_6 \rightarrow \text{H}_2 + \text{C}_2\text{H}_5$	$2.4 \times 10^{-15} T^{1.5} \exp(-3730/T)$	300–2000	$\pm 0.15$ at 300 K rising to $\pm 0.3$ at 2000 K	CEC <sup>1</sup>
$\text{H} + \text{CHCO} \rightarrow \text{CH}_2 + \text{CO}$ $\rightarrow \text{H}_2 + \text{C}_2\text{O}$ $\rightarrow \text{HCCOH}$	$2.5 \times 10^{-10}$	300–2500	$\pm 0.4$	CEC <sup>1</sup>
$\text{H} + \text{CH}_2\text{CO} \rightarrow \text{CH}_3 + \text{CO}$ $\rightarrow \text{CH}_2\text{CHO}$	$3.0 \times 10^{-11} \exp(-1700/T)$ $k_2/k$ very small	200–2000	$\pm 0.5$ at 200 K rising to $\pm 1.0$ at 2000 K	CEC <sup>1</sup>
$\text{H} + \text{CH}_3\text{CHO} \rightarrow \text{H}_2 + \text{CH}_3\text{CO}$ $\rightarrow \text{H}_2 + \text{CH}_2\text{CHO}$	$6.8 \times 10^{-15} T^{1.16} \exp(-1210/T)$	300–2000	$\pm 0.1$ at 300 K rising to $\pm 0.4$ at 2000 K	CEC <sup>1</sup>
$\text{H} + \text{C}_3\text{H}_5 \rightarrow \text{C}_3\text{H}_6$ $\rightarrow \text{C}_2\text{H}_3 + \text{CH}_3$ $\rightarrow \text{H}_2 + \text{C}_3\text{H}_4$	$(k_1 + k_2) = 2.8 \times 10^{-10}$ $3 \times 10^{-11}$	300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 1000 K $\pm 0.5$	1030
$\text{H} + \text{C}_6\text{H}_5 + \text{M} \rightarrow \text{C}_6\text{H}_6 + \text{M}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_6 \rightarrow \text{H}_2 + \text{C}_6\text{H}_5$ $\rightarrow \text{C}_6\text{H}_7$	No recommendation See Table 3			CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_5\text{O} + \text{M} \rightarrow \text{C}_6\text{H}_5\text{OH} + \text{M}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_5\text{OH} \rightarrow \text{C}_6\text{H}_5\text{O} + \text{H}_2$ $\rightarrow \text{C}_6\text{H}_6 + \text{OH}$	$1.9 \times 10^{-10} \exp(-6240/T)$ $3.7 \times 10^{-11} \exp(-3990/T)$	1000–1150	$\pm 0.3$	CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_5\text{CH}_2 + \text{M} \rightarrow \text{C}_6\text{H}_5\text{CH}_3 + \text{M}$	See Table 3			CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{H}_2 + \text{C}_6\text{H}_5\text{CH}_2$ $\rightarrow \text{H}_2 + \text{C}_6\text{H}_4\text{CH}_3$ $\rightarrow \text{C}_6\text{H}_6 + \text{CH}_3$ $\rightarrow \text{C}_6\text{H}_6\text{CH}_3$	$3.6 \times 10^{-19} T^{2.63} \exp(-2210/T)$ No recommendation $9.6 \times 10^{-11} \exp(-4070/T)$ See Table 3	600–2500 770–1100	$\pm 0.3$ $\pm 0.3$	927
$\text{H} + p\text{-C}_6\text{H}_4(\text{CH}_3)_2 \rightarrow \text{products}$	$5.8 \times 10^{-13}$	298	$\pm 0.1$	CEC <sup>1</sup>
$\text{H} + \text{C}_6\text{H}_5\text{C}_2\text{H}_5 \rightarrow \text{H}_2 + \text{C}_6\text{H}_5\text{C}_2\text{H}_4$ $\rightarrow \text{C}_6\text{H}_6\text{C}_2\text{H}_5$	No recommendation See Table 3			CEC <sup>1</sup>

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{molecule}^{-1}\text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i>H<sub>2</sub> Reactions</i>				
$\text{H}_2 + \text{Ar} \rightarrow 2\text{H} + \text{Ar}$	See Table 2			CEC <sup>1</sup>
$\text{H}_2 + \text{H}_2 \rightarrow 2\text{H} + \text{H}_2$	See Table 2			CEC <sup>1</sup>
<i>OH Radical Reactions</i>				
$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$1.7 \times 10^{-16} T^{1.6} \exp(-1660/T)$	300–2500	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 2500 K	CEC <sup>1</sup>
$\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	$2.5 \times 10^{-15} T^{1.14} \exp(-50/T)$	250–2500	$\pm 0.2$	CEC <sup>1</sup>
$\text{OH} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O}_2 + \text{M}$	See Table 3			CEC <sup>1</sup>
$\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	$4.8 \times 10^{-11} \exp(250/T)$	300–2000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 2000 K	929
$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$	$1.3 \times 10^{-11} \exp(-670/T)$	300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 1000 K	931
$\text{OH} + \text{NH} \rightarrow \text{NO} + \text{H}_2$ [ $\rightarrow \text{H}_2\text{O} + \text{N}$ ]	$8.0 \times 10^{-11}$	300–1000	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{NH}_2 \rightarrow \text{O} + \text{NH}_3$ [ $\rightarrow \text{H}_2\text{O} + \text{NH}$ ]	$3.3 \times 10^{-14} T^{0.405} \exp(-250/T)$ No recommendation	500–2500	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$	$1.05 \times 10^{-17} T^{1.5} \exp(250/T)$	300–2000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 2000 K	CEC <sup>1</sup>
$\text{OH} + \text{CH}_3 \rightarrow \text{H} + \text{CH}_2\text{OH}$ [ $\rightarrow \text{H} + \text{CH}_3\text{O}$ $\rightarrow \text{H}_2\text{O} + \text{CH}_2$ $\rightarrow \text{CH}_3\text{OH}$ ]	No recommendation $1.2 \times 10^{-11} \exp(-1400/T)$ See Table 3	300–1000	$\pm 0.5$	932
$\text{OH} + \text{CH}_4 \rightarrow \text{H}_2\text{O} + \text{CH}_3$	$2.6 \times 10^{-17} T^{1.83} \exp(-1400/T)$	250–2500	$\pm 0.07$ at 250 K rising to $\pm 0.15$ at 1200 K	CEC <sup>1</sup>
$\text{OH} + \text{CHO} \rightarrow \text{H}_2\text{O} + \text{CO}$	$1.7 \times 10^{-10}$	300–2500	$\pm 0.3$	CEC <sup>1</sup>
$\text{OH} + \text{HCHO} \rightarrow \text{H}_2\text{O} + \text{CHO}$	$5.7 \times 10^{-15} T^{1.18} \exp(225/T)$	300–3000	$\pm 0.1$ at 300 K rising to $\pm 0.7$ at 3000 K	CEC <sup>1</sup>
$\text{OH} + \text{CN} \rightarrow \text{O} + \text{HCN}$ [ $\rightarrow \text{NCO} + \text{H}$ ]	$1.0 \times 10^{-10}$	1500–3000	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{HCN} \rightarrow \text{H}_2\text{O} + \text{CN}$ [ $\rightarrow \text{HO} + \text{CN} + \text{H}$ $\rightarrow \text{HNCO} + \text{H}$ ]	$1.5 \times 10^{-11} \exp(-5400/T)$ No recommendation	1500–2500	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{CH}_3\text{OOH} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{OO}$ [ $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{OOH}$ ]	$1.2 \times 10^{-12} \exp(130/T)$ $1.8 \times 10^{-12} \exp(220/T)$	300–1000 300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.4$ at 1000 K $\pm 0.1$ at 300 K rising to $\pm 0.3$ at 1000 K	CEC <sup>1</sup>
$\text{OH} + \text{C}_2\text{H}_2 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}$ [ $\rightarrow \text{H} + \text{CH}_3\text{CO}$ $\rightarrow \text{C}_2\text{H}_2\text{OH}$ ]	$1.0 \times 10^{-10} \exp(-6500/T)$ See Table 3	1000–2000	$\pm 1.0$	940
$\text{OH} + \text{C}_2\text{H}_4 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_3$	$3.4 \times 10^{-11} \exp(-2990/T)$	650–1500	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{C}_2\text{H}_6 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_5$	$1.2 \times 10^{-17} T^{2.0} \exp(-435/T)$	250–2000	$\pm 0.07$ at 250 K rising to $\pm 0.15$ at 2000 K	CEC <sup>1</sup>

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TABLE 1. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{molecule}^{-1}\text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{OH} + \text{CH}_2\text{CO} \rightarrow \text{CH}_2\text{OH} + \text{CO}$ [ $\rightarrow \text{H}_2\text{CO} + \text{HCO}$ ]	$1.7 \times 10^{-11}$	300–2000	$\pm 1.0$	CEC <sup>1</sup>
$\text{OH} + \text{CH}_3\text{CHO} \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CO}$ [ $\rightarrow \text{H}_2\text{O} + \text{CH}_2\text{CHO}$ ]	$3.9 \times 10^{-14} T^{0.73} \exp(560/T)$	250–1200	$\pm 0.1$ at 250 K rising to $\pm 0.3$ at 1200 K	CEC <sup>1</sup>
$\text{OH} + \text{C}_2\text{H}_5\text{OOH} \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_5\text{OO}$ [ $\rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_4\text{OOH}$ ]	$3.0 \times 10^{-12} \exp(190/T)$ [estimate]	250–1000	$\pm 0.3$ at 250 K rising to $\pm 0.7$ at 1000 K	CEC <sup>1</sup>
$\text{OH} + \text{C}_3\text{H}_5 \rightarrow \text{H}_2\text{O} + \text{C}_3\text{H}_4$ [ $\rightarrow \text{CH}_2\text{CHCH}_2\text{OH}$ $\rightarrow \text{CH}_2\text{CHCHO} + 2\text{H}$ ]	$1.0 \times 10^{-11}$ $(k_2^\infty + k_3) = 2.5 \times 10^{-11}$	300–1000	$\pm 0.5$	1030
$\text{OH} + \text{C}_6\text{H}_6 \rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5$ [ $\rightarrow \text{H} + \text{C}_6\text{H}_5\text{OH}$ $\rightarrow \text{C}_6\text{H}_6\text{OH}$ ]	$2.7 \times 10^{-16} T^{1.42} \exp(-730/T)$ $2.2 \times 10^{-11} \exp(-5330/T)$ See Table 3	400–1500 1000–1150	$\pm 0.3$ $\pm 0.3$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{OH} \rightarrow \text{C}_6\text{H}_5(\text{OH})_2$ [ $\rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5\text{O}$ $\rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_4\text{OH}$ ]	See Table 3 $1.0 \times 10^{-11}$	1000–1150	$\pm 0.5$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5\text{CH}_2$ [ $\rightarrow \text{C}_6\text{H}_5\text{CH}_3\text{OH}$ ]	$8.6 \times 10^{-15} T \exp(-440/T)$ See Table 3	400–1200	$\pm 0.5$ at 400 K reducing to $\pm 0.3$ at 1200 K	941
$\text{OH} + \text{C}_6\text{H}_5\text{CHO} \rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5\text{CO}$ [ $\rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_4\text{CHO}$ ]	$1.3 \times 10^{-11}$	298–1500	$\pm 0.1$ at 298 K rising to $\pm 0.5$ at 1500 K	942
$\text{OH} + p\text{-C}_6\text{H}_4(\text{CH}_3)_2 \rightarrow \text{C}_6\text{H}_4\text{CH}_2\text{CH}_3 + \text{H}_2\text{O}$ [ $\rightarrow p\text{-C}_6\text{H}_4(\text{CH}_3)_2\text{OH}$ ]	$6.4 \times 10^{-11} \exp(-1440/T)$ See Table 3	500–960	$\pm 0.1$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{C}_2\text{H}_5 \rightarrow \text{HOC}_6\text{H}_5\text{C}_2\text{H}_5$ [ $\rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_5\text{C}_2\text{H}_4$ $\rightarrow \text{H}_2\text{O} + \text{C}_6\text{H}_4\text{C}_2\text{H}_5$ ]	See Table 3 No recommendation			CEC <sup>1</sup>
<i>H<sub>2</sub>O Reactions</i>				
$\text{H}_2\text{O} + \text{M} \rightarrow \text{H} + \text{OH} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>HO<sub>2</sub> Radical Reactions</i>				
$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$7.0 \times 10^{-10} \exp(-6030/T) +$ $2.2 \times 10^{-13} \exp(820/T)$ $7.0 \times 10^{-10} \exp(-6030/T)$	550–1250 850–1250	$\pm 0.15$ between 550–800 K rising to $\pm 0.4$ at 1250 K	943
$\text{HO}_2 + \text{NH}_2 \rightarrow \text{NH}_3 + \text{O}_2$ [ $\rightarrow \text{HNO} + \text{H}_2\text{O}$ ]	$2.6 \times 10^{-11}$	300–400	$\pm 0.4$	CEC <sup>1</sup>
$\text{HO}_2 + \text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{O}$ [ $\rightarrow \text{O}_2 + \text{CH}_4$ ]	$3 \times 10^{-11}$ No recommendation	300–2500	$\pm 0.7$	CEC <sup>1</sup>
$\text{HO}_2 + \text{CH}_4 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3$	$1.5 \times 10^{-11} \exp(-12440/T)$	600–1000	$\pm 0.2$ at 600 K rising to $\pm 0.3$ at 1000 K	CEC <sup>1</sup>
$\text{HO}_2 + \text{HCHO} \rightarrow \text{H}_2\text{O}_2 + \text{CHO}$	$5.0 \times 10^{-12} \exp(-6580/T)$	600–1000	$\pm 0.5$	CEC <sup>1</sup>

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{HO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$ [ $\rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$ ]	$4.1 \times 10^{-13} \exp(790/T)$ $k_1/k = 1.0 \pm 0.1$ over whole range	298–700	$\pm 0.1$ at 298 K rising to $\pm 0.3$ at 700 K	945
$\text{HO}_2 + \text{C}_2\text{H}_4 \rightarrow \text{OH} + \text{C}_2\text{H}_4\text{O}$	$3.7 \times 10^{-12} \exp(-8650/T)$	600–900	$\pm 0.15$ at 600 K rising to $\pm 0.25$ at 900 K	CEC <sup>1</sup>
$\text{HO}_2 + \text{C}_2\text{H}_6 \rightarrow \text{H}_2\text{O}_2 + \text{C}_2\text{H}_5$	$2.2 \times 10^{-11} \exp(-10300/T)$	500–1000	$\pm 0.2$ at 500 K rising to $\pm 0.3$ at 1000 K	CEC <sup>1</sup>
$\text{HO}_2 + \text{CH}_3\text{CHO} \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CO}$	$5.0 \times 10^{-12} \exp(-6000/T)$	900–1200	$\pm 0.7$	CEC <sup>1</sup>
$\text{HO}_2 + \text{C}_3\text{H}_5 \rightarrow \text{C}_3\text{H}_6 + \text{O}_2$ [ $\rightarrow \text{CO} + \text{products}$ ]	$4.4 \times 10^{-12}$ $1.1 \times 10^{-11}$	300–1000 500–900	$\pm 0.3$ over the range 600 K to 800 K rising to 0.5 at other temperatures $\pm 0.3$	1030
$\text{HO}_2 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{C}_6\text{H}_5\text{CH}_2$ [ $\rightarrow \text{H}_2\text{O}_2 + \text{C}_6\text{H}_5\text{CH}_3$ ]	$6.6 \times 10^{-13} \exp(-7080/T)$ $9.1 \times 10^{-12} \exp(-14500/T)$	600–1000 600–1000	$\pm 0.3$ at 750 K rising to $\pm 0.5$ at 600 K and 1000 K $\pm 1.0$	948
$\text{HO}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{C}_6\text{H}_5\text{CHCH}_3$ [ $\rightarrow \text{H}_2\text{O}_2 + \text{C}_6\text{H}_5\text{CH}_2\text{CH}_2$ $\rightarrow \text{H}_2\text{O}_2 + \text{C}_6\text{H}_4\text{CH}_2\text{CH}_3$ ]	$4.4 \times 10^{-13} \exp(-5680/T)$ $5.3 \times 10^{-12} \exp(-9760/T)$ $9 \times 10^{-12} \exp(-14500/T)$	600–1000 600–1000 600–1000	$\pm 0.3$ at 750 K rising to $\pm 0.5$ at 600 K and 1000 K $\pm 0.5$ $\pm 1.0$	948
<i>H<sub>2</sub>O<sub>2</sub> Reactions</i>				
$\text{H}_2\text{O}_2 + \text{M} \rightarrow 2\text{OH} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>N Atom Reactions</i>				
$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	$1.5 \times 10^{-14} T \exp(-3270/T)$	298–5000	$\pm 0.12$ over range 300–1000 K rising to $\pm 0.3$ over range 1000–5000 K	949
$\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$	$4.7 \times 10^{-11}$	300–2500	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 2500 K	952
$\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$	$7.1 \times 10^{-11} \exp(-790/T)$	1400–4000	$\pm 0.2$	954
$\text{N} + \text{CN} \rightarrow \text{N}_2 + \text{C}$	$3 \times 10^{-10}$	300–2500	$\pm 1.0$	CEC <sup>1</sup>
$\text{N} + \text{NCO} \rightarrow \text{NO} + \text{CN}$ $\rightarrow \text{N}_2 + \text{CO}$	No recommendation $3.3 \times 10^{-11}$	1700	$\pm 0.5$	CEC <sup>1</sup>
<i>NH Radical Reactions</i>				
$\text{NH} + \text{O}_2 \rightarrow \text{NO} + \text{OH}$ [ $\rightarrow \text{NO}_2 + \text{H}$ $\rightarrow \text{HNO} + \text{O}$ ]	$(k_1 + k_2) = 1.3 \times 10^{-13} \exp(-770/T)$ $6.5 \times 10^{-11} \exp(-9000/T)$	270–550 2200–3500	$\pm 0.25$ $\pm 0.5$	957
$\text{NH} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{H}$ [ $\rightarrow \text{HN}_2 + \text{O}$ $\rightarrow \text{N}_2 + \text{OH}$ ]	$5.0 \times 10^{-11}$ $2.8 \times 10^{-10} \exp(-6400/T)$	270–380 2220–3350	$\pm 0.2$ $\pm 0.5$	958
<i>NH<sub>2</sub> Radical Reactions</i>				
$\text{NH}_2 + \text{O}_2 \rightarrow \text{products}$	$<3 \times 10^{-18}$	298		CEC <sup>1</sup>
$\text{NH}_2 + \text{NO} \rightarrow \text{N}_2 + \text{H}_2\text{O}$ [ $\rightarrow \text{N}_2 + \text{H} + \text{OH}$ $\rightarrow \text{N}_2\text{H} + \text{OH}$ $\rightarrow \text{N}_2\text{O} + \text{H}_2$ ]	$1.8 \times 10^{-12} \exp(650/T)$ $(k_2 + k_3)/k \approx 0.12$ at 298 K	220–2000	$\pm 0.5$	CEC <sup>1</sup>

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TABLE I. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i>NH<sub>3</sub> Reactions</i>				
$\text{NH}_3 + \text{M} \rightarrow \text{NH}_2 + \text{H}$ → $\text{NH} + \text{H}_2$	See Table 2 No recommendation			961
<i>C Atom Reactions</i>				
$\text{C} + \text{N}_2 \rightarrow \text{CN} + \text{N}$	$8.7 \times 10^{-11} \exp(-22600/T)$	2000–5000	± 0.2	965
$\text{C} + \text{NO} \rightarrow \text{CN} + \text{O}$ → $\text{CO} + \text{N}$	$2.5 \times 10^{-11}$ $8.0 \times 10^{-11}$ $k_1/k_2 = 0.6 \pm 0.25; k_1/k = 0.4 \pm 0.25$ over range 1500–4050 K	300 1500–4050	± 0.3 ± 0.3	966
<i><sup>1</sup>C<sub>2</sub> and <sup>3</sup>C<sub>2</sub> Radical Reactions</i>				
<i>CH Radical Reactions</i>				
$\text{CH} + \text{O}_2 \rightarrow \text{CHO} + \text{O}$ → $\text{CO} + \text{OH}$	$5.5 \times 10^{-11}$	300–2000	± 0.3 at 300 K rising to ± 0.5 at 2000 K	CEC <sup>1</sup>
$\text{CH} + \text{H}_2 \rightarrow \text{CH}_2 + \text{H}$ → $\text{CH}_3$	$2.4 \times 10^{-10} \exp(-1760/T)$	300–1000	± 0.3	CEC <sup>1</sup>
$\text{CH} + \text{H}_2\text{O} \rightarrow \text{products}$	$9.5 \times 10^{-12} \exp(380/T)$	300–1000	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N}$ → $\text{CHN}_2$	$2.6 \times 10^{-12} \exp(-9030/T)$ at p < 1 atm.	2000–4000	± 0.3	967
$\text{CH} + \text{NO} \rightarrow \text{CO} + \text{NH}$ → $\text{CN} + \text{OH}$ → $\text{HCN} + \text{O}$	$2.0 \times 10^{-10}$	300–4000	± 0.25	970
$\text{CH} + \text{CO} \rightarrow \text{products}$	$4.6 \times 10^{-13} \exp(860/T)$	300–1000	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{CO}_2 \rightarrow \text{products}$	$5.7 \times 10^{-12} \exp(-345/T)$	300–1000	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{CH}_4 \rightarrow \text{products}$	$5.0 \times 10^{-11} \exp(200/T)$	200–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{C}_2\text{H}_2 \rightarrow \text{products}$	$3.5 \times 10^{-10} \exp(61/T)$	200–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{C}_2\text{H}_4 \rightarrow \text{products}$	$2.2 \times 10^{-10} \exp(173/T)$	200–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{C}_2\text{H}_6 \rightarrow \text{products}$	$1.8 \times 10^{-10} \exp(132/T)$	200–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{C}_3\text{H}_8 \rightarrow \text{products}$	$1.9 \times 10^{-10} \exp(240/T)$	300–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + n\text{-C}_4\text{H}_{10} \rightarrow \text{products}$	$4.4 \times 10^{-10} \exp(28/T)$	250–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + i\text{-C}_4\text{H}_{10} \rightarrow \text{products}$	$2.0 \times 10^{-10} \exp(240/T)$	300–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{neo-C}_5\text{H}_{12} \rightarrow \text{products}$	$1.6 \times 10^{-10} \exp(340/T)$	300–700	± 1.0	CEC <sup>1</sup>
$\text{CH} + \text{CH}_3\text{C}_2\text{H} \rightarrow \text{products}$	No recommendation			CEC <sup>1</sup>
$\text{CH} + \text{CH}_2\text{O} \rightarrow \text{products}$	$1.6 \times 10^{-10} \exp(260/T)$	300–700	± 1.0	CEC <sup>1</sup>

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i><sup>3</sup>CH<sub>2</sub> Radical Reactions</i>				
${}^3\text{CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{H} + \text{OH}$ → CO <sub>2</sub> + H + H → CO + H <sub>2</sub> O → CO <sub>2</sub> + H <sub>2</sub> → HCHO + O	$4.1 \times 10^{-11} \exp(-750/T)$	300–1000	± 0.1 at 300 K rising to ± 0.5 at 1000 K	972
${}^3\text{CH}_2 + {}^3\text{CH}_2 \rightarrow \text{C}_2\text{H}_2 + \text{H}_2$ → C <sub>2</sub> H <sub>2</sub> + 2H	$2.0 \times 10^{-10} \exp(-400/T)$ $k_2/k = 0.9 \pm 0.1$ over range 300–3000 K.	300–3000	± 0.5	CEC <sup>1</sup>
${}^3\text{CH}_2 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_4 + \text{H}$	$7.0 \times 10^{-11}$	300–3000	± 0.3 at 300 K rising to ± 0.5 at 3000 K	CEC <sup>1</sup>
${}^3\text{CH}_2 + \text{C}_2\text{H}_2 \rightarrow \text{C}_3\text{H}_4$	See Table 3			CEC <sup>1</sup>
${}^3\text{CH}_2 + \text{C}_2\text{H}_4 \rightarrow \text{C}_3\text{H}_6$ → c-C <sub>3</sub> H <sub>6</sub> → CH <sub>2</sub> CHCH <sub>2</sub> + H	See Table 3			CEC <sup>1</sup>
<i><sup>1</sup>CH<sub>2</sub> Radical Reactions</i>				
${}^1\text{CH}_2 + \text{Ar} \rightarrow {}^3\text{CH}_2 + \text{Ar}$	$6.0 \times 10^{-12}$	300–2000	± 0.3	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{NO} \rightarrow \text{products}$	$1.6 \times 10^{-10}$	290–650	± 0.2	971
${}^1\text{CH}_2 + \text{N}_2 \rightarrow {}^3\text{CH}_2 + \text{N}_2$	$1.0 \times 10^{-11}$	300–2000	± 0.3	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{CH}_4 \rightarrow {}^3\text{CH}_2 + \text{CH}_4$	$1.2 \times 10^{-11}$	300–2000	± 0.4	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{C}_2\text{H}_2 \rightarrow {}^3\text{CH}_2 + \text{C}_2\text{H}_2$	$8.0 \times 10^{-11}$	300–2000	± 0.4	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{C}_2\text{H}_4 \rightarrow {}^3\text{CH}_2 + \text{C}_2\text{H}_4$	$4.0 \times 10^{-11}$	300–2000	± 0.4	971
${}^1\text{CH}_2 + \text{C}_2\text{H}_6 \rightarrow {}^3\text{CH}_2 + \text{C}_2\text{H}_6$	$3.6 \times 10^{-11}$	300–2000	± 0.4	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{O}_2 \rightarrow \text{CO} + \text{H} + \text{OH}$ → CO <sub>2</sub> + H <sub>2</sub> → CO + H <sub>2</sub> O → ${}^3\text{CH}_2 + \text{O}_2$	$5.2 \times 10^{-11}$	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 + \text{H}$	$1.2 \times 10^{-10}$	300–1000	± 0.1 at 300 K rising to ± 0.3 at 1000 K	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{C}_2\text{H}_2 \rightarrow \text{CH}_2\text{CCH}_2$ → CH <sub>3</sub> CCH → CH <sub>2</sub> CCH + H → ${}^3\text{CH}_2 + \text{C}_2\text{H}_2$	See Table 3			CEC <sup>1</sup>
	See earlier entry			
${}^1\text{CH}_2 + \text{C}_2\text{H}_4 \rightarrow \text{C}_3\text{H}_6$ → ${}^3\text{CH}_2 + \text{C}_2\text{H}_4$	See Table 3 See earlier entry			971
<i>CH<sub>3</sub> Radical Reactions</i>				
$\text{CH}_3 + \text{M} \rightarrow \text{CH}_2 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{O}$ → HCHO + OH → CH <sub>3</sub> O <sub>2</sub>	$2.2 \times 10^{-10} \exp(-15800/T)$ $5.5 \times 10^{-13} \exp(-4500/T)$ See Table 3	300–2500 1000–2500	± 0.5 ± 0.5	CEC <sup>1</sup>
$\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_4 + \text{H}$	$1.14 \times 10^{-20} T^{2.74} \exp(-4740/T)$	300–2500	± 0.15 in the range 300–700 K ± 0.3 in the range 700–2500 K	CEC <sup>1</sup>

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TABLE 1. BIMOLECULAR REACTIONS — CONTINUED

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{CH}_3 + \text{CO} + \text{M} \rightarrow \text{CH}_3\text{CO} + \text{M}$	See Table 3			973
$\text{CH}_3 + \text{CH}_3 \rightarrow \text{C}_2\text{H}_5 + \text{H}$ $\rightarrow \text{C}_2\text{H}_4 + \text{H}_2$ $\rightarrow \text{C}_2\text{H}_6$	$5 \times 10^{-11} \exp(-6800/T)$ No recommendation (see data sheets) See Table 3	1300–2500	$\pm 0.6$	CEC <sup>1</sup>
$\text{CH}_3 + \text{HCHO} \rightarrow \text{CH}_4 + \text{HCO}$	$1.3 \times 10^{-31} T^{6.1} \exp(-990/T)$	300–2000	$\pm 0.2$	989
$\text{CH}_3 + \text{C}_2\text{H}_2 + \text{M} \rightarrow \text{C}_3\text{H}_5 + \text{M}$ $\rightarrow \text{CH}_4 + \text{C}_2\text{H}$	See Table 3 No recommendation			CEC <sup>1</sup>
$\text{CH}_3 + \text{C}_2\text{H}_4 \rightarrow \text{CH}_4 + \text{C}_2\text{H}_3$ $\rightarrow n\text{-C}_3\text{H}_7$	$6.9 \times 10^{-12} \exp(-5600/T)$ See Table 3	400–3000	$\pm 0.5$	CEC <sup>1</sup>
$\text{CH}_3 + \text{C}_2\text{H}_5 \rightarrow \text{CH}_4 + \text{C}_2\text{H}_4$ $\rightarrow \text{C}_3\text{H}_8$	$1.9 \times 10^{-12}$ See Table 3	300–2000	$\pm 0.4$	991
$\text{CH}_3 + \text{C}_2\text{H}_6 \rightarrow \text{CH}_4 + \text{C}_2\text{H}_5$	$2.5 \times 10^{-31} T^{6.0} \exp(-3043/T)$	300–1500	$\pm 0.1$ at 300 K rising to $\pm 0.2$ at 1500 K	CEC <sup>1</sup>
$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$ $\rightarrow \text{CH}_4 + \text{CH}_2\text{CHO}$	$3.3 \times 10^{-30} T^{5.6} \exp(-1240/T)$ No recommendation (see data sheets)	300–1250	$\pm 0.3$	CEC <sup>1</sup>
$\text{CH}_3 + \text{C}_3\text{H}_5 \rightarrow \text{C}_2\text{H}_5\text{CHCH}_2$ $\rightarrow \text{CH}_4 + \text{CH}_2\text{CCH}_2$	See Table 3 $3.5 \times 10^{-13}$	500–1200	$\pm 0.5$	1030
<i>CH<sub>4</sub> Reactions</i>				
$\text{CH}_4 + \text{M} \rightarrow \text{CH}_3 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>CHO Radical Reactions</i>				
$\text{CHO} + \text{Ar} \rightarrow \text{H} + \text{CO} + \text{Ar}$	See Table 2			901
$\text{CHO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$ $\rightarrow \text{OH} + \text{CO}_2$ $\rightarrow \text{HCO}_3$	$5.0 \times 10^{-12}$	300–2500	$\pm 0.3$	CEC <sup>1</sup>
$\text{CHO} + \text{CHO} \rightarrow \text{HCHO} + \text{CO}$	$5.0 \times 10^{-11}$	300	$\pm 0.3$	CEC <sup>1</sup>
<i>HCHO Reactions</i>				
$\text{HCHO} + \text{M} \rightarrow \text{H} + \text{CHO} + \text{M}$ $\rightarrow \text{H}_2 + \text{CO} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>CH<sub>2</sub>OH Reactions</i>				
$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	$2.6 \times 10^{-7} T^{-1.0} +$ $1.2 \times 10^{-10} \exp(-1800/T)$	300–1200	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 1200 K	998
<i>CH<sub>3</sub>O Radical Reactions</i>				
$\text{CH}_3\text{O} + \text{M} \rightarrow \text{HCHO} + \text{H} + \text{M}$	See Table 2			997
$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	$3.6 \times 10^{-14} \exp(-880/T)$	300–1000	$\pm 0.1$ at 500 K rising to $\pm 0.3$ at 300 K and 1000 K	997

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<b><i>CH<sub>3</sub>O<sub>2</sub> Radical Reactions</i></b>				
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{O} + \text{O}_2$ $\rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{O}_2$ $\rightarrow \text{CH}_3\text{OOCH}_3 + \text{O}_2$	$9.1 \times 10^{-14} \exp(420/T)$ $k_1/k_2 = 25 \exp(-1170/T);$ $k_3 = 0$ over whole range	298–700	$\pm 0.1$ at 298 K increasing to $\pm 0.3$ at 700 K	1000
$\text{CH}_3\text{O}_2 + \text{C}_3\text{H}_5 \rightarrow \text{CH}_3\text{O} + \text{CH}_2\text{CHCH}_2\text{O}$	$2.0 \times 10^{-11}$	500–1200	$\pm 0.5$	1030
<b><i>CH<sub>3</sub>OH Reactions</i></b>				
$\text{CH}_3\text{OH} + \text{Ar} \rightarrow \text{CH}_3 + \text{OH} + \text{Ar}$ $\rightarrow \text{CH}_2\text{OH} + \text{H} + \text{Ar}$ $\rightarrow {}^1\text{CH}_2 + \text{H}_2\text{O} + \text{Ar}$	See Table 2			935
<b><i>CH<sub>3</sub>OOH Reactions</i></b>				
$\text{CH}_3\text{OOH} + \text{M} \rightarrow \text{CH}_3\text{O} + \text{OH} + \text{M}$	See Table 2			1004
<b><i>CN Radical Reactions</i></b>				
$\text{CN} + \text{O}_2 \rightarrow \text{NCO} + \text{O}$	$1.2 \times 10^{-11} \exp(210/T)$	290–4500	$\pm 0.15$ over the range 290–4500 K	1005
$\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$	$3.2 \times 10^{-20} T^{2.87} \exp(-820/T)$	200–3500	$\pm 0.2$ at 200 K rising to $\pm 0.5$ at 3500 K	1007
$\text{CN} + \text{H}_2\text{O} \rightarrow \text{HCN} + \text{OH}$ $\rightarrow \text{HOCHN} + \text{H}$	$1.3 \times 10^{-11} \exp(-3750/T)$	500–3000	$\pm 0.3$ at 500 K rising to $\pm 0.5$ at 3000 K	CEC <sup>1</sup>
$\text{CN} + \text{CH}_4 \rightarrow \text{HCN} + \text{CH}_3$	$1.5 \times 10^{-19} T^{2.64} \exp(150/T)$	290–1500	$\pm 0.3$	1009
<b><i>NCO Radical Reactions</i></b>				
$\text{NCO} + \text{M} \rightarrow \text{N} + \text{CO} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\text{NCO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{CO}$ $\rightarrow \text{N}_2 + \text{CO}_2$ $\rightarrow \text{N}_2 + \text{CO} + \text{O}$	$2.3 \times 10^{-6} T^{-1.73} \exp(-380/T)$	290–3000	$\pm 0.25$	1011
<b><i>C<sub>2</sub>H Radical Reactions</i></b>				
$\text{C}_2\text{H} + \text{O}_2 \rightarrow \text{CO}_2 + \text{CH}$ $\rightarrow 2\text{CO} + \text{H}$ $\rightarrow \text{C}_2\text{HO} + \text{O}$ $\rightarrow \text{CO} + \text{HCO}$	$3.0 \times 10^{-11}$	300	$\pm 0.5$	CEC <sup>1</sup>
$\text{C}_2\text{H} + \text{H}_2 \rightarrow \text{C}_2\text{H}_2 + \text{H}$	$1.8 \times 10^{-11} \exp(-1090/T)$	300–2500	$\pm 0.3$ at 300 K rising to $\pm 0.5$ at 2500 K	1013
$\text{C}_2\text{H} + \text{C}_2\text{H}_2 \rightarrow \text{C}_4\text{H}_2 + \text{H}$	$1.5 \times 10^{-10}$	300–2700	$\pm 0.5$	1017
$\text{C}_2\text{H} + \text{CH}_4 \rightarrow \text{products}$	$3.0 \times 10^{-12}$	298	$\pm 1$	1015
$\text{C}_2\text{H} + \text{C}_2\text{H}_6 \rightarrow \text{products}$	No recommendation			1016

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TABLE 1. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{molecule}^{-1}\text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<b><i>C<sub>2</sub>H<sub>3</sub> Radical Reactions</i></b>				
$\text{C}_2\text{H}_3 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\text{C}_2\text{H}_3 + \text{O}_2 \rightarrow \text{HO}_2 + \text{C}_2\text{H}_2$ $\quad \rightarrow \text{H}_2\text{CO} + \text{CHO}$ $\quad \rightarrow \text{C}_2\text{H}_3\text{O} + \text{O}$ $\quad \rightarrow \text{C}_2\text{H}_3\text{O}_2$	$9.0 \times 10^{-12}$	300–2000	$\pm 0.3$ over range 300–600 K; $\pm 0.5$ over range 600–2000 K	1019
<b><i>C<sub>2</sub>H<sub>4</sub> Reactions</i></b>				
$\text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}$ $\quad \rightarrow \text{C}_2\text{H}_3 + \text{H} + \text{M}$	See Table 2			1020
<b><i>C<sub>2</sub>H<sub>5</sub> Radical Reactions</i></b>				
$\text{C}_2\text{H}_5 + \text{M} \rightarrow \text{C}_2\text{H}_4 + \text{H} + \text{M}$	See Table 2			1026
$\text{C}_2\text{H}_5 + \text{O}_2 \rightarrow \text{C}_2\text{H}_4 + \text{HO}_2$	$1.7 \times 10^{-14} \exp(1100/T)$	600–1200	$\pm 0.3$	
$\text{C}_2\text{H}_5 + \text{H}_2 \rightarrow \text{C}_2\text{H}_6 + \text{H}$	$5.1 \times 10^{-24} T^{3.6} \exp(-4250/T)$	700–1200	$\pm 0.2$ at 700 K rising to $\pm 0.6$ at 1200 K	1026
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_2 \rightarrow \text{C}_2\text{H}_5\text{CHCH}_2$	$5.6 \times 10^{-14} \exp(-3520/T)$	300–600	$\pm 0.5$	1026
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_4 \rightarrow n\text{-C}_4\text{H}_9$	$1.8 \times 10^{-13} \exp(-3670/T)$	300–600	$\pm 0.5$	1026
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_5 \rightarrow n\text{-C}_4\text{H}_{10}$ $\quad \rightarrow \text{C}_2\text{H}_6 + \text{C}_2\text{H}_4$	See Table 3 $2.4 \times 10^{-12}$	300–1200	$\pm 0.4$	1026
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_5\text{CHO} \rightarrow \text{C}_2\text{H}_6 + \text{C}_2\text{H}_5\text{CO}$	$2.9 \times 10^{-13} \exp(-3660/T)$	300–700	$\pm 0.3$	1026
$\text{C}_2\text{H}_5 + \text{C}_3\text{H}_5 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2$ $\quad \rightarrow \text{C}_2\text{H}_6 + \text{CH}_2\text{CCH}_2$ $\quad \rightarrow \text{C}_2\text{H}_4 + \text{C}_3\text{H}_6$	See Table 3 $1.6 \times 10^{-12} \exp(66/T)$ $4.3 \times 10^{-12} \exp(66/T)$	500–1200 500–1200	$\pm 0.3$ $\pm 0.4$	1026
<b><i>C<sub>2</sub>H<sub>6</sub> Reactions</i></b>				
$\text{C}_2\text{H}_6 + \text{M} \rightarrow \text{CH}_3 + \text{CH}_3 + \text{M}$	See Table 2			CEC <sup>1</sup>
<b><i>CHCO Reactions</i></b>				
$\text{CHCO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{HCO}$ $\quad \rightarrow 2\text{CO} + \text{OH}$ $\quad \rightarrow \text{C}_2\text{O} + \text{HO}_2$ $\quad \rightarrow \text{CHO}_2\text{CO}$	$2.7 \times 10^{-12} \exp(-430/T)$ M = He, 2 Torr	300–550	$\pm 0.7$	CEC <sup>1</sup>
<b><i>CH<sub>2</sub>CHO Radical Reactions</i></b>				
$\text{CH}_2\text{CHO} + \text{O}_2 \rightarrow \text{HO}_2 + \text{CH}_2\text{CO}$ $\quad \rightarrow \text{HCHO} + \text{CO} + \text{OH}$ $\quad \rightarrow \text{O}_2\text{CH}_2\text{CHO}$	$k_\infty = 2.6 \times 10^{-13}$ $k_2 = 3.0 \times 10^{-14}$	250–500 300	$\pm 0.2$ $\pm 0.3$	CEC <sup>1</sup>
<b><i>CH<sub>3</sub>CO Radical Reactions</i></b>				
$\text{CH}_3\text{CO} + \text{O}_2 + \text{M} \rightarrow \text{CH}_3\text{CO}_3 + \text{M}$	See Table 3			CEC <sup>1</sup>
<b><i>CH<sub>3</sub>CHO Reactions</i></b>				
$\text{CH}_3\text{CHO} + \text{M} \rightarrow \text{CH}_3 + \text{HCO} + \text{M}$	See Table 2			CEC <sup>1</sup>

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i>C<sub>2</sub>H<sub>5</sub>O Reactions</i>				
$\text{C}_2\text{H}_5\text{O} + \text{M} \rightarrow \text{HCHO} + \text{CH}_3 + \text{M}$ → $\text{CH}_3\text{CHO} + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\text{C}_2\text{H}_5\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	$1.0 \times 10^{-13} \exp(-830/T)$	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K	CEC <sup>1</sup>
<i>C<sub>2</sub>H<sub>5</sub>OOH Reactions</i>				
$\text{C}_2\text{H}_5\text{OOH} + \text{M} \rightarrow \text{C}_2\text{H}_5\text{O} + \text{OH} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>C<sub>3</sub>H<sub>5</sub> Radical Reactions</i>				
$\text{C}_3\text{H}_5 + \text{M} \rightarrow \text{CH}_2\text{CCH}_2 + \text{H} + \text{M}$	See Table 2			1030
$\text{C}_3\text{H}_5 + \text{O}_2 \rightarrow \text{CH}_2\text{CCH}_2 + \text{HO}_2$ → CO + products	$1.7 \times 10^{-12} \exp(-11400/T)$ $7.6 \times 10^{-12} \exp(-9450/T)$	600–1200 600–1200	± 0.3 at 600 K rising to ± 0.5 at 1200 K ± 0.3	1030
$\text{C}_3\text{H}_5 + \text{H}_2 \rightarrow \text{C}_3\text{H}_6 + \text{H}$	$1.8 \times 10^{-19} T^{2.4} \exp(-9550/T)$	300–1100	± 0.7 at 300 K reducing to ± 0.3 at 1100 K	1030
$\text{C}_3\text{H}_5 + \text{CH}_4 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_3$	$6.6 \times 10^{-23} T^{3.4} \exp(-11670/T)$	300–1200	± 0.4	1030
$\text{C}_3\text{H}_5 + \text{C}_2\text{H}_4 \rightarrow \text{C}_3\text{H}_6 + \text{C}_2\text{H}_3$ → c-C <sub>3</sub> H <sub>8</sub> + H	$6.6 \times 10^{-23} T^{3.4} \exp(-13120/T)$ $1.0 \times 10^{-13} \exp(-9620/T)$	600–1200 600–1200	± 0.5 ± 0.7	1030
$\text{C}_3\text{H}_5 + \text{C}_2\text{H}_6 \rightarrow \text{C}_3\text{H}_6 + \text{C}_2\text{H}_5$	$3.9 \times 10^{-22} T^{3.3} \exp(-9990/T)$	300–1200	± 0.4	1030
$\text{C}_3\text{H}_5 + \text{C}_3\text{H}_5 \rightarrow \text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}_2$ → C <sub>3</sub> H <sub>6</sub> + CH <sub>2</sub> CCH <sub>2</sub>	See Table 3 $1.0 \times 10^{-13} \exp(132/T)$	300–1000	± 0.7	1030
$\text{C}_3\text{H}_5 + \text{C}_3\text{H}_8 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_3\text{CH}_2\text{CH}_2$ → C <sub>3</sub> H <sub>6</sub> + CH <sub>3</sub> CHCH <sub>3</sub>	$3.9 \times 10^{-22} T^{3.3} \exp(-9990/T)$ $1.3 \times 10^{-22} T^{3.3} \exp(-8660/T)$	300–1200 300–1200	± 0.4 over the range 600 to 1000 K rising to ± 0.7 at other temperatures	1030
$\text{C}_3\text{H}_5 + 2\text{-C}_4\text{H}_8 \rightarrow \text{C}_3\text{H}_6 + \text{CH}_2\text{CHCHCH}_3$ → C <sub>3</sub> H <sub>6</sub> + CH <sub>3</sub> CCHCH <sub>3</sub> → CH <sub>2</sub> CHCH <sub>2</sub> CH(CH <sub>3</sub> )CHCH <sub>3</sub>	$6.6 \times 10^{-12} \exp(-8180/T)$ $3.3 \times 10^{-23} T^{3.4} \exp(-12160/T)$ See Table 3	600–1000 600–1000	± 0.5 ± 0.5	1030
$\text{C}_3\text{H}_5 + i\text{-C}_4\text{H}_{10} \rightarrow \text{C}_3\text{H}_6 + (\text{CH}_3)_2\text{CHCH}_2$ → C <sub>3</sub> H <sub>6</sub> + (CH <sub>3</sub> ) <sub>3</sub> C	$5.9 \times 10^{-22} T^{3.3} \exp(-9990/T)$ $0.7 \times 10^{-22} T^{3.3} \exp(-7800/T)$	300–1200 300–1200	± 0.4 over the range 600 to 1000 K rising to ± 0.7 at other temperatures	1030
$\text{C}_3\text{H}_5 + \text{HCHO} \rightarrow \text{C}_3\text{H}_6 + \text{HCO}$	$1.2 \times 10^{-16} T^{1.8} \exp(-9155/T)$	300–1000	± 0.4	1030
$\text{C}_3\text{H}_5 + \text{C}_6\text{H}_5\text{CH}_3 \rightarrow \text{C}_3\text{H}_6 + \text{C}_6\text{H}_5\text{CH}_2$	$3.3 \times 10^{-12} \exp(-8660/T)$	600–1000	± 0.4	1030
<i>i-C<sub>3</sub>H<sub>7</sub> Radical Reactions</i>				
$i\text{-C}_3\text{H}_7 + \text{M} \rightarrow \text{C}_3\text{H}_6 + \text{H} + \text{M}$	See Table 2			1026
$i\text{-C}_3\text{H}_7 + \text{O}_2 \rightarrow \text{C}_3\text{H}_6 + \text{HO}_2$	$3.3 \times 10^{-14} \exp(+1290/T)$	600–800	± 0.5	1026
$i\text{-C}_3\text{H}_7 + \text{H}_2 \rightarrow \text{C}_3\text{H}_8 + \text{H}$	$1.3 \times 10^{-23} T^{3.28} \exp(-4360/T)$	300–1200	± 0.5	1026
$i\text{-C}_3\text{H}_7 + \text{C}_2\text{H}_2 \rightarrow (\text{CH}_3)_2\text{CHCHCH}$	$5.3 \times 10^{-14} \exp(-3470/T)$	300–600	± 0.5	1026
$i\text{-C}_3\text{H}_7 + \text{C}_2\text{H}_4 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$	$7.5 \times 10^{-14} \exp(-3470/T)$	300–600	± 0.5	1026

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TABLE 1. Bimolecular Reactions — Continued

Reaction	$k/\text{cm}^3 \text{ molecule}^{-1}\text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
$i\text{-C}_3\text{H}_7 + i\text{-C}_3\text{H}_7 \rightarrow \text{C}_6\text{H}_{14}$	See Table 3	300–1000	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 1000 K	1026
$\rightarrow \text{C}_3\text{H}_8 + \text{C}_3\text{H}_6$	$4.2 \times 10^{-12}$	300–1000	$\pm 0.1$ at 300 K rising to $\pm 0.5$ at 1000 K	
$i\text{-C}_3\text{H}_7 + i\text{-C}_3\text{H}_7\text{CHO} \rightarrow \text{C}_3\text{H}_8 + (\text{CH}_3)_2\text{CHCO}$	$6.6 \times 10^{-14} \exp(-3170/T)$	300–650	$\pm 0.5$	1026
$\rightarrow \text{C}_3\text{H}_8 + (\text{CH}_3)_2\text{CCHO}$				
$\rightarrow \text{C}_3\text{H}_8 + \text{CH}_2\text{CH}(\text{CH}_3)\text{CHO}$	$5.3 \times 10^{-14} \exp(-4780/T)$	500–650	$\pm 0.5$	
<i>C<sub>3</sub>H<sub>8</sub> Reactions</i>				
$\text{C}_3\text{H}_8 + \text{M} \rightarrow \text{CH}_3 + \text{C}_2\text{H}_5 + \text{M}$	See Table 2			992
<i>t-C<sub>4</sub>H<sub>9</sub> Radical Reactions</i>				
$t\text{-C}_4\text{H}_9 + \text{M} \rightarrow i\text{-C}_4\text{H}_8 + \text{H} + \text{M}$	See Table 2			1026
$t\text{-C}_4\text{H}_9 + \text{O}_2 \rightarrow i\text{-C}_4\text{H}_8 + \text{HO}_2$	$5 \times 10^{-14} \exp(+2115/T)$	600–800	$\pm 0.5$	1026
$t\text{-C}_4\text{H}_9 + \text{H}_2 \rightarrow i\text{-C}_4\text{H}_{10} + \text{H}$	$3.1 \times 10^{-26} T^{4.24} \exp(-4510/T)$	300–1200	$\pm 0.5$	1026
$t\text{-C}_4\text{H}_9 + \text{C}_2\text{H}_2 \rightarrow (\text{CH}_3)_3\text{CCHCH}$	$1.2 \times 10^{-13} \exp(-4320/T)$	300–600	$\pm 0.5$	1026
$t\text{-C}_4\text{H}_9 + \text{C}_2\text{H}_4 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2$	$3.3 \times 10^{-14} \exp(-4020/T)$	300–650	$\pm 0.5$	1026
$t\text{-C}_4\text{H}_9 + t\text{-C}_4\text{H}_9 \rightarrow \text{C}_8\text{H}_{18}$	See Table 3			1026
$\rightarrow i\text{-C}_4\text{H}_{10} + i\text{-C}_4\text{H}_8$	$1.2 \times 10^{-7} T^{-1.73}$	300–1000	$\pm 0.15$ at 300 K rising to $\pm 0.5$ at 1000 K	
$t\text{-C}_4\text{H}_9 + t\text{-C}_4\text{H}_9\text{CHO} \rightarrow i\text{-C}_4\text{H}_{10} + t\text{-C}_4\text{H}_9\text{CO}$	$1.0 \times 10^{-14} \exp(-3200/T)$	300–700	$\pm 0.5$	1026
$\rightarrow i\text{-C}_4\text{H}_{10} + \text{CH}_2\text{C}(\text{CH}_3)_2\text{CHO}$	$3.9 \times 10^{-14} \exp(-5540/T)$	500–700	$\pm 0.5$	
<i>C<sub>6</sub>H<sub>5</sub> Radical Reactions</i>				
$\text{C}_6\text{H}_5 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{C}_4\text{H}_3 + \text{M}$	See Table 2			
$\rightarrow \text{C}_2\text{H}_3 + \text{C}_4\text{H}_2 + \text{M}$				
$\rightarrow \text{linear-C}_6\text{H}_5 + \text{M}$				CEC <sup>1</sup>
<i>C<sub>6</sub>H<sub>6</sub> Reactions</i>				
$\text{C}_6\text{H}_6 + \text{M} \rightarrow \text{C}_6\text{H}_5 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\rightarrow \text{C}_4\text{H}_4 + \text{C}_2\text{H}_2 + \text{M}$				
<i>C<sub>6</sub>H<sub>5</sub>O Radical Reactions</i>				
$\text{C}_6\text{H}_5\text{O} + \text{M} \rightarrow \text{C}_5\text{H}_5 + \text{CO} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub> Radical Reactions</i>				
$\text{C}_6\text{H}_5\text{CH}_2 + \text{M} \rightarrow \text{C}_3\text{H}_3 + 2\text{C}_2\text{H}_2 + \text{M}$	See Table 2			
$\rightarrow \text{C}_4\text{H}_4 + \text{C}_3\text{H}_3 + \text{M}$				
$\rightarrow \text{C}_5\text{H}_5 + \text{C}_2\text{H}_2 + \text{M}$				
$\rightarrow \text{C}_7\text{H}_7 + \text{M}$				CEC <sup>1</sup>
<i>C<sub>6</sub>H<sub>5</sub>CH<sub>3</sub> Reactions</i>				
$\text{C}_6\text{H}_5\text{CH}_3 + \text{M} \rightarrow \text{C}_6\text{H}_5\text{CH}_2 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
$\rightarrow \text{C}_6\text{H}_5 + \text{CH}_3 + \text{M}$				

TABLE 1. Bimolecular Reactions — Continued

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Reaction	$k/\text{cm}^3 \text{ molecule}^{-1} \text{s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	Page
<i>p-C<sub>6</sub>H<sub>4</sub>(CH<sub>3</sub>)<sub>2</sub> Reactions</i>				
$p\text{-C}_6\text{H}_4(\text{CH}_3)_2 + \text{M} \rightarrow \text{C}_6\text{H}_4\text{CH}_2\text{CH}_3 + \text{H} + \text{M}$	See Table 2			CEC <sup>1</sup>
<i>C<sub>6</sub>H<sub>5</sub>C<sub>2</sub>H<sub>5</sub> Reactions</i>				
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{M} \rightarrow \text{C}_6\text{H}_5\text{CH}_2 + \text{CH}_3 + \text{M}$				
$\rightarrow \text{C}_6\text{H}_6 + \text{C}_2\text{H}_4 + \text{M}$				
$\rightarrow \text{C}_6\text{H}_5\text{CHCH}_2 + \text{H}_2 + \text{M}$				
$\rightarrow \text{C}_6\text{H}_5 + \text{C}_2\text{H}_5 + \text{M}$				
$\rightarrow \text{C}_6\text{H}_5\text{CHCH}_3 + \text{H} + \text{M}$				
	See Table 2			CEC <sup>1</sup>

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TABLE 2. Decomposition Reactions

Reaction	$k_{\infty} \text{ s}^{-1}$ $k_0 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	T/K	Error limits ( $\Delta \log k$ )	
	$F_c$			
	$k/\text{s}^{-1} = \frac{k_0 k_{\infty} [\text{M}]}{k_0[\text{M}] + k_{\infty}} F$			
$\text{H}_2 + \text{Ar} \rightarrow 2\text{H} + \text{Ar}$	$k_0 = 3.7 \times 10^{-10} \exp(-48350/T)$	2500–8000	$\pm 0.3$	CEC <sup>1</sup>
$\text{H}_2 + \text{H}_2 \rightarrow 2\text{H} + \text{H}_2$	$k_0 = 1.5 \times 10^{-9} \exp(-48350/T)$	2500–8000	$\pm 0.5$	CEC <sup>1</sup>
$\text{H}_2\text{O} + \text{N}_2 \rightarrow \text{H} + \text{OH} + \text{N}_2$	$k_0 = 5.8 \times 10^{-9} \exp(-52920/T)$	2000–6000	$\pm 0.5$	CEC <sup>1</sup>
$\text{H}_2\text{O}_2 + \text{M} \rightarrow 2\text{OH} + \text{M}$	$k_0(\text{Ar}) = 3 \times 10^{-8} \exp(-21600/T)$ $k_0(\text{N}_2) = 2 \times 10^{-7} \exp(-22900/T)$ $k_{\infty} = 3 \times 10^{14} \exp(-24400/T)$ $F_c(\text{Ar}) = 0.5$	1000–1500 700–1500 1000–1500 700–1500	$\pm 0.2$ $\pm 0.2$ $\pm 0.5$ $\Delta F_c = \pm 0.1$	CEC <sup>1</sup>
$\text{NH}_3 + \text{Ar} \rightarrow \text{NH}_2 + \text{H} + \text{Ar}$	$k_0(1) = 7.4 \times 10^{-9} \exp(-41560/T)$ $k_{\infty}(1) = 8.3 \times 10^{15} \exp(-55170/T)$ $F_c = 0.58 \exp(-T/4581) + 0.42 \exp(-T/102)$	2000–3000 2000–3000 2000–3000	$\pm 0.3$ $\pm 0.4$ $\Delta F_c = \pm 0.1$	961
$\text{CH}_3 + \text{M} \rightarrow \text{CH}_2 + \text{H} + \text{M}$	$k_0 = 1.7 \times 10^{-8} \exp(-45600/T)$	1500–3000	$\pm 0.5$	CEC <sup>1</sup>
$\text{CH}_4 + \text{M} \rightarrow \text{CH}_3 + \text{H} + \text{M}$	$k_0(\text{Ar}) = 7.5 \times 10^{-7} \exp(-45700/T)$ $k_0(\text{Ar}) = 7.8 \times 10^{23} T^{-8.2} \exp(-59200/T)$ $k_0(\text{CH}_4) = 1.4 \times 10^{-6} \exp(-45700/T)$ $k_{\infty} = 2.4 \times 10^{16} \exp(-52800/T)$ $F_c(\text{Ar}) = \exp(-T/1350) + \exp(-7830/T)$ $F_c(\text{CH}_4) = 0.31 \exp(-T/90) + 0.69(-T/2210)$	1000–1700 1700–5000 1000–2000 1000–3000 1000–5000 1000–2000	$\pm 0.3$ $\pm 0.3$ $\pm 0.3$ $\pm 0.5$ $\Delta F_c = \pm 0.1$ $\Delta F_c = \pm 0.1$	907
$\text{HCO} + \text{Ar} \rightarrow \text{H} + \text{CO} + \text{Ar}$	$k_0 = 2.6 \times 10^{-10} \exp(-7930/T)$	600–2500	$\pm 0.5$	901
$\text{HCHO} + \text{M} \rightarrow \text{H} + \text{CHO} + \text{M}$ [ $\rightarrow \text{H}_2 + \text{CO} + \text{M}$ ]	$k_0(\text{Ar}) = 2.7 \times 10^{12} T^{-5.54} \exp(-48660/T)$ $k_0(2)/k_0 = 0.7 \pm 0.4$	1700–3200 2000–3000	$\pm 0.3$	995
$\text{CH}_3\text{O} + \text{M} \rightarrow \text{HCHO} + \text{H} + \text{M}$	$k_0 = 9.0 \times 10^{-11} \exp(-6790/T)$	300–1700	$\pm 0.3$	997
$\text{CH}_3\text{OH} + \text{Ar} \rightarrow \text{CH}_3 + \text{OH} + \text{Ar}$ [ $\rightarrow \text{CH}_2\text{OH} + \text{H} + \text{Ar}$ $\rightarrow {}^1\text{CH}_2 + \text{H}_2\text{O} + \text{Ar}$ ]	$k_0 = 1.1 \times 10^{-7} \exp(-33080/T)$ $k_{\infty} = 1.7 \times 10^{16} \exp(-45740/T)$ $F_c = 0.18 \exp(-T/200) + 0.82 \exp(-T/1438)$	1000–2000 1000–2000 1000–2000	$\pm 0.3$ $\pm 0.5$ $\Delta F_c = \pm 0.1$	935
$\text{CH}_3\text{OOH} + \text{M} \rightarrow \text{CH}_3\text{O} + \text{OH} + \text{M}$	$k_{\infty} = 6 \times 10^{14} \exp(-21300/T)$	500–800	$\pm 0.2$ at 600 K rising to $\pm 0.5$ at 500 and 800 K	1004
$\text{NCO} + \text{Ar} \rightarrow \text{N} + \text{CO} + \text{Ar}$	$k_0 = 1.7 \times 10^{-9} \exp(-23500/T)$	1450–2600	$\pm 0.4$	CEC <sup>1</sup>
$\text{C}_2\text{H}_3 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{H} + \text{M}$	$k_0 = 6.9 \times 10^{17} T^{-7.5} \exp(-22900/T)$ $k_{\infty} = 2 \times 10^{14} \exp(-20000/T)$ $F_c = 0.35$	500–2500 500–2500 500–2500	$\pm 0.5$ $\pm 0.5$ $\Delta F_c = \pm 0.1$	CEC <sup>1</sup>
$\text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{H}_2 + \text{M}$ [ $\rightarrow \text{C}_2\text{H}_3 + \text{H} + \text{M}$ ]	$k_0(\text{Ar}, \text{Kr}) = 5.8 \times 10^{-8} \exp(-36000/T)$ $k_0(\text{Ar}) = 4.3 \times 10^{-7} \exp(-48600/T)$	1500–3200 1500–3200	$\pm 0.3$ $\pm 0.5$	1020
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_4 + \text{H} + \text{C}_2\text{H}_6$	$k_0 = 1.7 \times 10^{-6} \exp(-16800/T)$ $k_{\infty} = 8.2 \times 10^{13} \exp(-20070/T)$ $F_c = 0.25 \exp(-T/97) + 0.75 \exp(-T/1379)$	700–900 700–1100 700–1100	$\pm 0.3$ $\pm 0.3$ $\Delta F_c = \pm 0.1$	921
$\text{C}_2\text{H}_6 + \text{M} \rightarrow 2\text{CH}_3 + \text{M}$	$k_0(\text{Ar}) = 1.1 \times 10^{25} T^{-8.24} \exp(-47090/T)$ $k_0(\text{N}_2) = 1.1 \times 10^{25} T^{-8.24} \exp(-47090/T)$ $k_0(\text{C}_2\text{H}_6) = 4.5 \times 10^{-2} \exp(-41930/T)$ $k_{\infty} = 1.8 \times 10^{21} T^{-1.24} \exp(-45700/T)$ $F_c(\text{Ar}, \text{N}_2) = 0.38 \exp(-T/73) + 0.62 \exp(-T/1180)$ $F_c(\text{C}_2\text{H}_6) = 0.54 \exp(-T/1250)$	300–2000 300–2000 800–1000 300–2000 300–2000 800–1000	$\pm 0.5$ $\pm 0.5$ $\pm 0.5$ $\pm 0.3$ $\Delta F_c = \pm 0.1$ $\Delta F_c = \pm 0.1$	984

TABLE 2. Decomposition Reactions — Continued

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Reaction	$k_{\infty}/\text{s}^{-1}$ $k_0/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $F_c$ $k/\text{s}^{-1} = \frac{k_0 k_{\infty} [\text{M}]}{k_0[\text{M}] + k_{\infty}} F$	T/K	Error limits ( $\Delta \log k$ )
$\text{CH}_3\text{CO} + \text{M} \rightarrow \text{CH}_3 + \text{CO} + \text{M}$	$k_0(\text{He}) = 1.0 \times 10^{-8} \exp(-7080/T)$ $k_0(\text{Ar}) = 7.0 \times 10^{-18}$ $k_{\infty} = 2.8 \times 10^{13} \exp(-8630/T)$ $F_c(\text{He}) = 0.5$	400–500 353 300–500 400–500	$\pm 0.2$ $\pm 0.4$ $\pm 0.5$ $\Delta F_c = \pm 0.1$
$\text{CH}_3\text{CHO} + \text{M} \rightarrow \text{CH}_3 + \text{CHO} + \text{M}$	$k(1 \text{ atm.}) = 7 \times 10^{15} \exp(-41100/T)$ (pressure dependent region)	750–1200	$\pm 0.4$
$\text{C}_2\text{H}_5\text{O} + \text{M} \rightarrow \text{HCHO} + \text{CH}_3 + \text{M}$	$k_{\infty} = 8 \times 10^{13} \exp(-10830/T)$ [estimate]	300–600	$\pm 1.0$
$\text{C}_2\text{H}_5\text{OOH} + \text{M} \rightarrow \text{C}_2\text{H}_5\text{O} + \text{OH} + \text{M}$	$k_{\infty} = 4 \times 10^{15} \exp(-21600/T)$ [estimate]	400–800	$\pm 0.3$
$\text{C}_3\text{H}_5 + \text{M} \rightarrow \text{CH}_2\text{CCH}_2 + \text{H} + \text{M}$	$k_{\infty} = 1.5 \times 10^{11} T^{0.84} \exp(-30050/T)$	800–1500	$\pm 0.3$
$\text{i-C}_3\text{H}_7 + \text{He} \rightarrow \text{C}_3\text{H}_6 + \text{H} + \text{He}$	$k_0 = 3.6 \times 10^{-7} \exp(-14200/T)$ $k_{\infty} = 8.76 \times 10^7 T^{1.76} \exp(-17870/T)$ $F_c(\text{He}) = 0.35$	750–830 170–1000 750–830	$\pm 0.3$ $\pm 0.3$ $\Delta F_c = \pm 0.1$
$\text{C}_3\text{H}_8 + \text{Ar} \rightarrow \text{CH}_3 + \text{C}_2\text{H}_5 + \text{Ar}$	$k_0 = 1.3 \times 10^{-5} \exp(-32700/T)$ $k_{\infty} = 1.1 \times 10^{17} \exp(-42470/T)$ $F_c = 0.24 \exp(-T/1946) + 0.76 \exp(-T/38)$	700–2000 700–2000 700–2000	$\pm 0.5$ $\pm 0.3$ $\Delta F_c = \pm 0.2$
$t\text{-C}_4\text{H}_9 + \text{M} \rightarrow \text{i-C}_4\text{H}_8 + \text{H} + \text{M}$	$k_{\infty} = 8.3 \times 10^{13} \exp(-19200/T)$	300–800	$\pm 0.5$
$\text{C}_6\text{H}_5 + \text{M} \rightarrow \text{C}_2\text{H}_2 + \text{C}_4\text{H}_3 + \text{M}$ $\rightarrow \text{C}_2\text{H}_3 + \text{C}_4\text{H}_2 + \text{M}$ $\rightarrow \text{linear-C}_6\text{H}_5 + \text{M}$	No recommendation  $4.0 \times 10^{13} \exp(-36700/T)$	1450–1900	$\pm 0.4$
$\text{C}_6\text{H}_6 + \text{M} \rightarrow \text{C}_6\text{H}_5 + \text{H} + \text{M}$ $\rightarrow \text{C}_4\text{H}_4 + \text{C}_2\text{H}_2 + \text{M}$	$9.0 \times 10^{15} \exp(-54060/T)$	1200–2500	$\pm 0.4$ at 1200 K reducing to $\pm 0.3$ at 2500 K
$\text{C}_6\text{H}_5\text{O} + \text{M} \rightarrow \text{C}_5\text{H}_5 + \text{CO} + \text{M}$	$2.5 \times 10^{11} \exp(-22100/T)$	1000–1580	$\pm 0.2$
$\text{C}_6\text{H}_5\text{CH}_2 + \text{M} \rightarrow \text{C}_3\text{H}_3 + 2\text{C}_2\text{H}_2 + \text{M}$ $\rightarrow \text{C}_4\text{H}_4 + \text{C}_3\text{H}_3 + \text{M}$ $\rightarrow \text{C}_5\text{H}_5 + \text{C}_2\text{H}_2 + \text{M}$ $\rightarrow \text{C}_7\text{H}_7 (\text{BCH}) + \text{M}$	$5.1 \times 10^{13} \exp(-36370/T)$	1350–1900	$\pm 0.3$ at 1350 K rising to $\pm 0.5$ at 1900 K
$\text{C}_6\text{H}_5\text{CH}_3 + \text{M} \rightarrow \text{C}_6\text{H}_5\text{CH}_2 + \text{H} + \text{M}$ $\rightarrow \text{C}_6\text{H}_5 + \text{CH}_3 + \text{M}$	$3.1 \times 10^{15} \exp(-44890/T)$ No recommendation	920–2200 1500–2000	$\pm 0.3$ at 920 K rising to $\pm 0.5$ at 2200 K $\pm 0.7$
$p\text{-C}_6\text{H}_4 (\text{CH}_3)_2 + \text{M} \rightarrow \text{C}_6\text{H}_4(\text{CH}_3)\text{CH}_2 + \text{H} + \text{M}$	$4.0 \times 10^{15} \exp(-42600/T)$	1400–1800	$\pm 0.5$
$\text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{M} \rightarrow \text{C}_6\text{H}_5\text{CH}_2 + \text{CH}_3 + \text{M}$ $\rightarrow \text{C}_6\text{H}_6 + \text{C}_2\text{H}_4 + \text{M}$ $\rightarrow \text{C}_6\text{H}_5\text{CHCH}_2 + \text{H}_2 + \text{M}$ $\rightarrow \text{C}_6\text{H}_5 + \text{C}_2\text{H}_5 + \text{M}$ $\rightarrow \text{C}_6\text{H}_5\text{CHCH}_3 + \text{H} + \text{M}$	$6.1 \times 10^{15} \exp(-37800/T)$ No recommendation	770–1800	$\pm 0.1$ at 770 K rising to $\pm 0.4$ at 1800 K

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TABLE 3. Combination Reactions

Reaction	$k_\infty/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	$k_0/\text{cm}^6 \text{molecule}^{-2} \text{s}^{-1}$	$F_c$	T/K	Error limits ( $\Delta \log k$ )	Page
			$k_\infty/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} = \frac{k_0 k_\infty [\text{M}]}{k_0 [\text{M}] + k_\infty} F$			
H + O <sub>2</sub> + Ar → HO <sub>2</sub> + Ar	$k_0 = 1.7 \times 10^{-30} T^{-0.8}$			300–2000	$\pm 0.5$	896
H + O <sub>2</sub> + H <sub>2</sub> → HO <sub>2</sub> + H <sub>2</sub>	$k_0 = 5.8 \times 10^{-30} T^{-0.8}$			300–2000	$\pm 0.5$	896
H + O <sub>2</sub> + N <sub>2</sub> → HO <sub>2</sub> + N <sub>2</sub>	$k_0 = 3.9 \times 10^{-30} T^{-0.8}$			300–2000	$\pm 0.5$	896
H + H + Ar → H <sub>2</sub> + Ar	$k_0 = 1.8 \times 10^{-30} T^{-1.0}$			300–2500	$\pm 0.5$	CEC <sup>1</sup>
H + H + H <sub>2</sub> → H <sub>2</sub> + H <sub>2</sub>	$k_0 = 2.7 \times 10^{-31} T^{-0.6}$			100–5000	$\pm 0.5$	CEC <sup>1</sup>
H + OH + H <sub>2</sub> O → H <sub>2</sub> O + H <sub>2</sub> O	$k_0 = 3.9 \times 10^{-25} T^{-2.0}$			300–3000	$\pm 0.5$	CEC <sup>1</sup>
H + OH + Ar → H <sub>2</sub> O + Ar	$k_0 = 2.3 \times 10^{-26} T^{-2.0}$			300–3000	$\pm 0.3$	CEC <sup>1</sup>
H + OH + N <sub>2</sub> → H <sub>2</sub> O + N <sub>2</sub>	$k_0 = 6.1 \times 10^{-26} T^{-2.0}$			300–3000	$\pm 0.5$	CEC <sup>1</sup>
H + CO + Ar → HCO + Ar	$k_0 = 5.3 \times 10^{-34} \exp(-370/T)$			300–2500	$\pm 0.5$	899
H + CH <sub>3</sub> + M → CH <sub>4</sub> + M	$k_0(\text{He}) = 1.8 \times 10^{-24} T^{-1.8}$ $k_0(\text{Ar}) = 1.7 \times 10^{-24} T^{-1.8}$ $k_0(\text{C}_2\text{H}_6) = 8.6 \times 10^{-24} T^{-1.8}$ $k_\infty = 3.5 \times 10^{-10}$ $F_c(\text{He,Ar}) = 0.63 \exp(-T/3315) + 0.37 \exp(-T/61)$ $F_c(\text{C}_2\text{H}_6) = 0.71 \exp(-T/3079) + 0.29 \exp(-T/54)$			300–1000	$\pm 0.3$	905
H + C <sub>2</sub> H <sub>2</sub> + He → C <sub>2</sub> H <sub>3</sub> + He	$k_\infty = 1.4 \times 10^{-11} \exp(-1300/T)$ $k_0 = 3.3 \times 10^{-30} \exp(-740/T)$ $F_c = 0.44$			200–400	$\pm 0.3$	CEC <sup>1</sup>
H + C <sub>2</sub> H <sub>3</sub> + M → C <sub>2</sub> H <sub>4</sub> + M	No recommendation					CEC <sup>1</sup>
H + C <sub>2</sub> H <sub>4</sub> + M → C <sub>2</sub> H <sub>5</sub> + M	$k_0(\text{He}) = 1.3 \times 10^{-29} \exp(-380/T)$ $k_0(\text{N}_2) = 7.7 \times 10^{-30} \exp(-380/T)$ $k_\infty = 6.6 \times 10^{-15} T^{1.28} \exp(-650/T)$ $F_c = (\text{He,N}_2) 0.24 \exp(-T/40) + 0.76 \exp(-T/1025)$			300–800	$\pm 0.3$	916
H + C <sub>2</sub> H <sub>5</sub> + M → C <sub>2</sub> H <sub>6</sub> + M	No recommendation					CEC <sup>1</sup>
H + C <sub>3</sub> H <sub>5</sub> + M → C <sub>3</sub> H <sub>6</sub> + M → C <sub>2</sub> H <sub>3</sub> + CH <sub>3</sub> + M	$(k_1 + k_2) = 2.8 \times 10^{-10}$			300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 1000 K	1030
H + C <sub>6</sub> H <sub>5</sub> + M → C <sub>6</sub> H <sub>6</sub> + M	$k_\infty = 1.3 \times 10^{-10}$			1400–1700	$\pm 0.5$	CEC <sup>1</sup>
H + C <sub>6</sub> H <sub>6</sub> + M → C <sub>6</sub> H <sub>7</sub> + M	$k_\infty = 6.7 \times 10^{-11} \exp(-2170/T)$			300–1000	$\pm 0.2$	CEC <sup>1</sup>
H + C <sub>6</sub> H <sub>5</sub> O + M → C <sub>6</sub> H <sub>5</sub> OH + M	$k_\infty = 4.2 \times 10^{-10}$			1000	$\pm 0.3$	CEC <sup>1</sup>
H + C <sub>6</sub> H <sub>5</sub> CH <sub>2</sub> + M → C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> + M	$k_\infty = 4.8 \times 10^{-10}$			300–2000	$\pm 0.2$ at 300 K rising to $\pm 0.7$ at 2000 K	926
H + C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub> + M → C <sub>6</sub> H <sub>6</sub> CH <sub>3</sub> + M	$k_\infty = 1.2 \times 10^{-13}$			298	$\pm 0.2$	927
H + C <sub>6</sub> H <sub>5</sub> C <sub>2</sub> H <sub>5</sub> + M → C <sub>6</sub> H <sub>6</sub> C <sub>2</sub> H <sub>5</sub> + M	$k_\infty = 3.3 \times 10^{-13}$			298	$\pm 0.1$	CEC <sup>1</sup>
OH + OH + M → H <sub>2</sub> O <sub>2</sub> + M	$k_0(\text{N}_2) = 6.1 \times 10^{-29} T^{-0.76}$ $k_0(\text{H}_2\text{O}) = 4 \times 10^{-30}$ $k_\infty = 1.2 \times 10^{-10} T^{-0.37}$ $F_c(\text{N}_2) = 0.5$			250–1400 300–400 200–1500 200–1500	$\pm 0.4$ $\pm 0.4$ $\pm 0.5$ $\Delta F_c = \pm 0.2$	CEC <sup>1</sup>

TABLE 3. Combination Reactions — Continued

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Reaction	$k_{\text{c}}/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ $k_0/\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$ $F_c$ $k/\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} = \frac{k_0 k_{\infty} [\text{M}]}{k_0 [\text{M}] + k_{\infty}} F$	T/K	Error limits ( $\Delta \log k$ )	Page
$\text{OH} + \text{CH}_3 + \text{M} \rightarrow \text{CH}_3\text{OH} + \text{M}$	$k_0(\text{He}) = 2.3 \times 10^{-27}$ $k_0(\text{Ar}) = 4.4 \times 10^{-4} T^{-8.2}$ $k_{\infty} = 1.0 \times 10^{-10}$ $F_c(\text{Ar}) = 0.18 \exp(-T/200) + 0.82 (-T/1438)$	300 1000–2000 300–2000 1000–2000	$\pm 0.3$ $\pm 0.5$ $\pm 0.3$ $\Delta F_c = \pm 0.1$	032
$\text{OH} + \text{C}_2\text{H}_2 + \text{M} \rightarrow \text{C}_2\text{H}_2\text{OH} + \text{M}$	See data sheet			940
$\text{OH} + \text{C}_3\text{H}_5 + \text{M} \rightarrow \text{CH}_2\text{CHCH}_2\text{OH} + \text{M}$ $\rightarrow \text{CH}_2\text{CHCHO} + 2\text{H} + \text{M}$	$(k_1'' + k_2) = 2.5 \times 10^{-11}$	300–1000	$\pm 0.3$	1030
$\text{OH} + \text{C}_6\text{H}_6 + \text{M} \rightarrow \text{C}_6\text{H}_6\text{OH} + \text{M}$	$k_{\infty} = 3.8 \times 10^{-12} \exp(-340/T)$	240–340	$\pm 0.2$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{OH} + \text{M} \rightarrow \text{C}_6\text{H}_5(\text{OH})_2 + \text{M}$	$k_{\infty} = 2.8 \times 10^{-11}$	298	$\pm 0.1$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{CH}_3 + \text{M} \rightarrow \text{HOCH}_2\text{CH}_2\text{CH}_3 + \text{M}$	$k_{\infty} = 3.8 \times 10^{-12} \exp(180/T)$	200–300	$\pm 0.4$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_4(\text{CH}_3)_2 + \text{M} \rightarrow \text{C}_6\text{H}_4(\text{CH}_3)_2\text{OH} + \text{M}$	$k_{\infty} = 1.4 \times 10^{-11}$	300	$\pm 0.1$	CEC <sup>1</sup>
$\text{OH} + \text{C}_6\text{H}_5\text{C}_2\text{H}_5 + \text{M} \rightarrow \text{HOCH}_2\text{CH}_2\text{CH}_3 + \text{M}$	$7.5 \times 10^{-12}$ at $p \leq 1 \text{ atm.}$	298	$\pm 0.1$	CEC <sup>1</sup>
${}^3\text{CH}_2 + \text{C}_2\text{H}_2 + \text{M} \rightarrow \text{C}_3\text{H}_4 + \text{M}$	$2.0 \times 10^{-11} \exp(-3330/T)$ at $p = \leq 10 \text{ Torr.}$	300–1000	$\pm 0.3$	CEC <sup>1</sup>
${}^3\text{CH}_2 + \text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_3\text{H}_6 + \text{M}$ $\rightarrow c\text{-C}_3\text{H}_6 + \text{M}$ $\rightarrow \text{C}_3\text{H}_5 + \text{H} + \text{M}$	$5.3 \times 10^{-12} \exp(-2660/T)$	300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.3$ at 1000 K	CEC <sup>1</sup>
${}^1\text{CH}_2 + \text{C}_2\text{H}_2 + \text{M} \rightarrow \text{CH}_2\text{CCH}_2 + \text{M}$ $\rightarrow \text{CH}_3\text{CCH} + \text{M}$ $\rightarrow \text{CH}_2\text{CCH} + \text{H} + \text{M}$	$2.9 \times 10^{-10}$ independent of $p$	300–1000	$\pm 0.3$ at 300 K rising to $\pm 0.7$ at 1000 K	
${}^1\text{CH}_2 + \text{C}_2\text{H}_4 + \text{M} \rightarrow \text{C}_3\text{H}_6 + \text{M}$	$1.6 \times 10^{-10}$ independent of $p$	300–1000	$\pm 0.2$ at 300 K rising to $\pm 0.5$ at 1000 K	971
$\text{CH}_3 + \text{O}_2 + \text{M} \rightarrow \text{CH}_3\text{O}_2 + \text{M}$	$k_0(\text{Ar}) = 1.55 \times 10^{-22} T^{-3.3}$ $k_0(\text{N}_2) = 1.6 \times 10^{-22} T^{-3.3}$ $k_{\infty} = 1.3 \times 10^{-15} T^{1.2}$ $F_c = 0.466 - 1.30 \times 10^{-4} T$	300–800 300–800 300–800 300–800	$\pm 0.3$ $\pm 0.3$ $\pm 0.3$ $\Delta F_c = \pm 0.1$	CEC <sup>1</sup>
$\text{CH}_3 + \text{CO} + \text{M} \rightarrow \text{CH}_3\text{CO} + \text{M}$	$k_0(\text{He}) = 3.0 \times 10^{-34} \exp(-1910/T)$ $k_0(\text{N}_2) = 4.2 \times 10^{-36}$ $k_{\infty} = 8.4 \times 10^{-13} \exp(-3460/T)$ $F_c(\text{He}) = 0.5$ $F_c(\text{N}_2) = 0.6$	400–500 300–350 300–500 400–500 300–350	$\pm 0.2$ $\pm 0.5$ $\pm 0.5$ $\Delta F_c = \pm 0.1$ $\Delta F_c = \pm 0.1$	973
$\text{CH}_3 + \text{CH}_3 + \text{Ar} \rightarrow \text{C}_2\text{H}_6 + \text{Ar}$	$k_{\infty} = 6.0 \times 10^{-11}$ $k_0 = 3.5 \times 10^{-7} T^{-7.0} \exp(-1390/T)$ $F_c = 0.38 \exp(-T/73) + 0.62 \exp(-T/1180)$	300–2000 300–2000 300–2000	$\pm 0.3$ $\pm 0.3$ $\Delta F_c = \pm 0.1$	980
$\text{CH}_3 + \text{C}_2\text{H}_2 + \text{M} \rightarrow \text{C}_3\text{H}_5 + \text{M}$	$k_{\infty} = 1 \times 10^{-12} \exp(-3900/T)$	300–600	$\pm 0.5$	CEC <sup>1</sup>
$\text{CH}_3 + \text{C}_2\text{H}_4 + \text{M} \rightarrow n\text{-C}_3\text{H}_7 + \text{M}$	$3.5 \times 10^{-13} \exp(-3700/T)$	300–600	$\pm 0.3$	CEC <sup>1</sup>
$\text{CH}_3 + \text{C}_2\text{H}_5 + \text{M} \rightarrow \text{C}_3\text{H}_8 + \text{M}$	$k_{\infty} = 5.6 \times 10^{-11}$	300–2000	$\pm 0.3$	991
$\text{CH}_3 + \text{C}_3\text{H}_5 + \text{M} \rightarrow \text{C}_2\text{H}_5\text{CHCH}_2 + \text{M}$	$k_{\infty} = 1.7 \times 10^{-10} T^{-0.32} \exp(66/T)$	500–1200	$\pm 0.2$	1030
$\text{C}_2\text{H}_5 + \text{C}_2\text{H}_5 + \text{M} \rightarrow n\text{-C}_4\text{H}_{10} + \text{M}$	$k_{\infty} = 1.9 \times 10^{-11}$	300–1200	$\pm 0.3$	1026
$\text{C}_2\text{H}_5 + \text{C}_3\text{H}_5 + \text{M} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2 + \text{M}$	$k_{\infty} = 3.3 \times 10^{-11} \exp(66/T)$	500–1200	$\pm 0.3$	1026

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TABLE 3. Combination Reactions — Continued

Reaction	$k_\infty/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1}$	$T/\text{K}$	Error limits ( $\Delta \log k$ )	Page
	$k_0/\text{cm}^6 \text{molecule}^{-2} \text{s}^{-1}$			
	$F_c$			
	$k/\text{cm}^3 \text{molecule}^{-1} \text{s}^{-1} = \frac{k_0 k_\infty [\text{M}]}{k_0 [\text{M}] + k_\infty} F$			
$\text{CH}_3\text{CO} + \text{O}_2 + \text{M} \rightarrow \text{CH}_3\text{CO}_3 + \text{M}$	$2 \times 10^{-12}$ for $p = 1\text{--}4$ Torr.	300	$\pm 0.3$	CEC <sup>1</sup>
$\text{C}_3\text{H}_5 + \text{C}_3\text{H}_5 + \text{M} \rightarrow$ $\text{CH}_2\text{CHCH}_2\text{CH}_2\text{CHCH}_2 + \text{M}$	$k_\infty = 1.7 \times 10^{-11} \exp(132/T)$ $k_\infty = 2.0 \times 10^{-11}$	300–600 600–1000	$\pm 0.2$ $\pm 0.4$	1030
$\text{C}_3\text{H}_5 + 2\text{-C}_4\text{H}_8 + \text{M} \rightarrow$ $\text{CH}_2\text{CHCH}_2\text{CH}(\text{CH}_3)\text{CHCH}_3 + \text{M}$	$k_\infty = 1.0 \times 10^{-13} \exp(-9620/T)$	600–1200	$\pm 0.7$	1030
$i\text{-C}_3\text{H}_7 + i\text{-C}_3\text{H}_7 + \text{M} \rightarrow$ $(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 + \text{M}$	$k_\infty = 6.8 \times 10^{-12}$	300–1000	$\pm 0.1$ at 300 K rising to $\pm 0.3$ at 1000 K	1026
$t\text{-C}_4\text{H}_9 + t\text{-C}_4\text{H}_9 \rightarrow \text{C}_8\text{H}_{18}$	$k_\infty = 5.2 \times 10^{-8} T^{-1.73}$	300–1000	$\pm 0.15$ at 300 K rising to $\pm 0.3$ at 1000 K	1026

**Reference**

<sup>1</sup>CEC Group on Evaluation of Kinetic Data for Combustion Modelling, D. L. Baulch, C. J. Cobos, R. A. Cos, C. Esser, P. Franck, Th. Just, J. A. Kerr, M. J. Pilling, J. Troe, R. W. Walker, and J. Warnatz, *J. Phys. Chem. Ref. Data* **21**, 411 (1992).