KINETIC DATA FOR COMBUSTION MODELLING

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The following tables present evaluated rate constants and other chemical kinetic data required for modelling the combustion of hydrocarbons. The compilation was prepared as part of the project "Kinetics and Mechanisms of Chemical Processes in Combustion", which is one of the projects in the third European Community Energy Research and Development Program. The tables are reprinted from the *Journal of Physical and Chemical Reference Data* by permission of the authors and the American Institute of Physics.

Table 1 lists all the reactions studied and gives the recommended rate constant k for every bimolecular reaction, as well as the applicable temperature range and the associated error limits. Where more than one set of products is possible, rate constants or branching ratios are given for all channels considered feasible. The data for decomposition reactions and combination reactions are given in Tables 2 and 3, respectively. The reference includes a detailed data sheet for each reaction listed here, covering the thermodynamic data, kinetic measurements, and reliability assessments.

REFERENCE

Baulch, D. L., et al., *J. Phys. Chem. Ref. Data*, 21, 411-734, 1992.

Table 1
BIMOLECULAR REACTIONS

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
O Atom Reactions			
$O + H_2 \rightarrow OH + H$	$8.5 \times 10^{-20} T^{2.67} \exp(-3160/T)$	300–2500	± 0.5 at 300 K falling to ± 0.2 for $T > 500$ K
$O + OH \rightarrow O_2 + H$	$2.0 \times 10^{-11} \exp(112/T)$ $2.4 \times 10^{-11} \exp(-353/T)$	220–500 1000–2000	± 0.2 ± 0.1
$O + HO_2 \rightarrow OH + O_2$	5.3×10^{-11}	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K.
$O + H_2O_2 \rightarrow OH + HO_2$	$1.1 \times 10^{-12} \exp(-2000/T)$	300–500	± 0.3
$O + NH_3 \rightarrow OH + NH_2$	$1.6 \times 10^{-11} \exp(-3670/T)$	500–2500	± 0.5
$O + CH \rightarrow CO + H$ $\rightarrow CHO^+ + e$	6.6×10^{-11} $4.2 \times 10^{-13} \exp(-850/T)$	300–2000 300–2500	± 0.5 ± 0.5
$O + {}^3CH_2 \rightarrow CO + 2H$ $\rightarrow CO + H_2$	2×10^{-10} $k_1/k = 0.6 \pm 0.3$ over whole range	300–2500	± 0.2 at 300 K rising to ± 0.7 at 2500 K.
$O + CH_3 \rightarrow HCHO + H$	1.4×10^{-10}	300–2500	± 0.2
$O + CH_4 \rightarrow OH + CH_3$	$1.5 \times 10^{-15} T^{1.56} \exp(-4270/T)$	300–2500	± 0.3 at 300 K falling to ± 0.15 at 2500 K.
$O + CHO \rightarrow OH + CO$ $\rightarrow CO_2 + H$	5.0×10^{-11} 5.0×10^{-11}	300–2500 300–2500	± 0.3 ± 0.3
$O + HCHO \rightarrow OH + CHO$	$6.9 \times 10^{-13} T^{0.57} \exp(-1390/T)$	250–2200	± 0.1 at 250 K rising to ± 0.3 at 2200 K.
$O + CH_3O \rightarrow O_2 + CH_3$ $\rightarrow OH + HCHO$	2.5×10^{-11} $k_2/k = (0.12 \pm 0.1)$ at 300 K	300–1000	± 0.3 at 300 K rising to ± 0.7 at 1000 K.
$O + CN \rightarrow CO + N(^4S)$ $\rightarrow CO + N(^2D)$	1.7×10^{-11}	300–5000	± 0.2 at 300 K rising to ± 0.6 × 5000 K.
$O + NCO \rightarrow NO + CO$ $\rightarrow O_2 + CN$	7.0×10^{-11}	1450–2600	± 0.8

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$O + HCN \rightarrow NCO + H$ $\rightarrow CO + NH$ $\rightarrow OH + CN$	$2.3 \times 10^{-18} T^{2.1} \exp(-3075/T)$	450–2500	± 0.2 at 450 K rising to ±0.3 at 2500 K.
$O + CH_3OOH \rightarrow OH + CH_2COOH$ $\rightarrow OH + CH_3O_2$	$6.9 \times 10^{-13} T^{0.57} \exp(-1390/T)$ [estimate]	250–2200	± 0.1 at 250 K rising to ± 0.3 at 2200 K.
$O + C_2H \rightarrow CO + CH$	1.7×10^{-11}	300–2500	± 1.0
$O + C_2H_2 \rightarrow CO + {}^3CH_2$ $\rightarrow CHCO + H$	$3.6 \times 10^{-20} T^{2.8} \exp(-250/T)$ $k_1/k = 0.5 \pm 0.3$ over whole range.	300–2500	± 0.2
$O + C_2H_3 \rightarrow OH + C_2H_2$ $\rightarrow CO + CH_3$ $\rightarrow HCO + CH_2$	5×10^{-11}	300–2000	± 0.5
$O + C_2H_4 \rightarrow CH_2CHO + H$ $\rightarrow HCO + CH_3$ $\rightarrow HCHO + CH_2$ $\rightarrow CH_2CO + H_2$	$5.75 \times 10^{-18} T^{2.08}$ $k_1/k = 0.35 \pm 0.05$ at p> 3 Torr $k_2/k = 0.6 \pm 0.10$	300–2000 over whole temperature range	± 0.1 for $T < 1000$ K rising to ± 0.3 at 2000 K.
$O + C_2H_5 \rightarrow CH_3CHO + H$ $\rightarrow HCHO + CH_3$	1.1×10^{-10} $k_2/k = 0.17 \pm 0.2$ at 300 K	300–2500	± 0.3 from 300 to 1000 K ± 0.5 from 1000 to 2500 K
$O + C_2H_6 \rightarrow OH + C_2H_5$	$1.66 \times 10^{-15} T^{1.5} \exp(-2920/T)$	300–1200	± 0.3 at 300 K falling to ± 0.15 at 1200 K.
$O + CHCO \rightarrow 2CO + H$	1.6×10^{-10}	300–2500	± 0.3
$O + CH_2CO \rightarrow CH_2O + CO$ $\rightarrow HCO + H + CO$ $\rightarrow HCO + HCO$	$3.8 \times 10^{-12} \exp(-680/T)$	230–500	± 0.3
$O + CH_3CHO \rightarrow OH + CH_3CO$ $\rightarrow OH + CH_2CHO$	$9.7 \times 10^{-12} \exp(-910/T)$	300–1500	± 0.05 at 300 K rising to ± 0.5 at 1500 K.
$O + C_2H_5OOH \rightarrow OH + C_2H_4OOH$ $\rightarrow OH + C_2H_5OO$	$6.9 \times 10^{-13} T^{0.57} \exp(-1390/T)$ [estimate]	250–2200	± 0.1 at 150 K rising to ± 0.3 at 2200 K.
$O + C_6H_6 \rightarrow OH + C_6H_5$ $\rightarrow C_6H_5OH$	$1.2 \times 10^{-22} T^{3.7} \exp(-570/T)$	300–1000	± 0.5
$O + C_6H_5CH_2 \rightarrow HCO + C_6H_6$ $\rightarrow C_6H_5CH + H$	5.5×10^{-10}	300	±0.3
$\rightarrow CH_2O + C_6H_5$	No recommendation		
$O + C_6H_5CH_3 \rightarrow$ products	$5.3 \times 10^{-15} T^{1.21} \exp(-1260/T)$	300–2800	± 0.1 at 300 K rising to ± 0.4 at 2800 K
$O + p\text{-}C_6H_4(CH_3)_2 \rightarrow$ products	$2.6 \times 10^{-11} \exp(-1409/T)$	300–600	± 0.3
$O + C_6H_5C_2H_5 \rightarrow$ products	1.0×10^{-13}	298	± 0.3
O_2 Reactions			
$O_2 + CH_4 \rightarrow HO_2 + CH_3$	$6.6 \times 10^{-11} \exp(-28630/T)$	500–2000	± 0.5 at 500 K rising to ± 1.0 at 2000 K.

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$O_2 + C_2H_6 \rightarrow HO_2 + C_2H_5$	$1.0 \times 10^{-10} \exp(-26100/T)$	500–2000	± 0.5 at 500 K rising to ± 1.0 at 2000 K
$O_2 + HCHO \rightarrow HO_2 + HCO$	$1.0 \times 10^{-10} \exp(-20460/T)$	700–1000	± 0.5
$O_2 + CH_3CHO \rightarrow HO_2 + CH_3CO$	$5.0 \times 10^{-11} \exp(-19700/T)$	600–1100	± 0.5 at 600 K rising to ± 1.0 at 1100 K.
H Atom Reactions			
$H + O_2 \rightarrow OH + O$	$3.3 \times 10^{-10} \exp(-8460/T)$	300–2500	± 0.1 at 300 K rising to ± 0.2 at 2500 K.
$H + O_2 + Ar \rightarrow HO_2 + Ar$	See Table 3		
$H + O_2 + H_2 \rightarrow HO_2 + H_2$	See Table 3		
$H + O_2 + N_2 \rightarrow HO_2 + N_2$	See Table 3		
$H + O_2 + H_2O \rightarrow HO_2 + H_2O$	See Table 3		
$H + H + Ar \rightarrow H_2 + Ar$	See Table 3		
$H + H + H_2 \rightarrow H_2 + H_2$	See Table 3		
$H + OH + H_2O \rightarrow H_2O + H_2O$	See Table 3		
$H + OH + Ar \rightarrow H_2O + Ar$	See Table 3		
$H + HO + N_2 \rightarrow H_2O + N_2$	See Table 3		
$H + HO_2 \rightarrow H_2 + O_2$	$7.1 \times 10^{-11} \exp(-710/T)$	300–1000	± 0.3
$\rightarrow 2\,OH$	$2.8 \times 10^{-10} \exp(-440/T)$	300–1000	± 0.3
$\rightarrow H_2O + O$	$5.0 \times 10^{-11} \exp(-866/T)$	300–1000	± 0.3
$H + H_2O \rightarrow OH + H_2$	$7.5 \times 10^{-16} T^{1.6} \exp(-9270/T)$	300–2500	±0.2
$H + H_2O_2 \rightarrow H_2 + HO_2$	$2.8 \times 10^{-12} \exp(-1890/T)$	300–1000	± 0.3
$\rightarrow OH + H_2O$	$1.7 \times 10^{-11} \exp(-1800/T)$	300–1000	± 0.3
$H + NH \rightarrow H_2 + N$	1.7×10^{-11}	1500–2500	± 1.0
$H + NH_2 \rightarrow H_2 + NH$	1.0×10^{-11}	2000–3000	± 1.0
$H + {}^3CH_2 \rightarrow H_2 + CH$	$1.0 \times 10^{-11} \exp(900/T)$	300–3000	± 0.7
$H + CH_3 \rightarrow H_2 + {}^1CH_2$	$1.0 \times 10^{-10} \exp(-7600/T)$	300–2500	± 1.0
$\rightarrow CH_4$	See Table 3		
$H + CH_4 \rightarrow H_2 + CH_3$	$2.2 \times 10^{-20} T^{3.0} \exp(-4045/T)$	300–2500	± 0.2
$H + CHO \rightarrow H_2 + CO$	1.5×10^{-10}	300–2500	± 0.3
$H + HCHO \rightarrow H_2 + HCO$	$3.8 \times 10^{-14} T^{1.05} \exp(-1650/T)$	300–2200	± 0.1 at 300 K rising to ± 0.5 at 2200 K
$H + CH_3O \rightarrow H_2 + HCHO$	3.0×10^{-11}	300–1000	± 0.5
$H + HNCO \rightarrow NH_2 + CO$	No recommendation		
$\rightarrow H_2 + NCO$	$3.4 \times 10^{-10} T^{-0.27} \exp(-10190/T)$	500–1000	± 1.0
$H + NCO \rightarrow NH + CO$]	8.7×10^{-11}	1400–1500	± 0.5
$\rightarrow HCN + O$]			

Table 1
BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits (Δ log k)
$H + C_2H_2 \rightarrow H_2 + C_2H$ $\rightarrow C_2H_3$	$1.0 \times 10^{-10} \exp(-14000/T)$ See Table 3	1000–3000	± 1.0
$H + C_2H_3 \rightarrow H_2 + C_2H_2$ $\rightarrow C_2H_4$	2.0×10^{-11} See Table 3	300–2500	± 0.5
$H + C_2H_4 \rightarrow C_2H_3 + H_2$ $\rightarrow C_2H_5$	$9.0 \times 10^{-10} \exp(-7500/T)$ See Table 3	700–2000	± 0.5
$H + C_2H_5 \rightarrow 2CH_3$ $\rightarrow C_2H_6$	6.0×10^{-11} See Table 3	300–2000	± 0.3
$H + C_2H_6 \rightarrow H_2 + C_2H_5$	$2.4 \times 10^{-15} T^{1.5} \exp(-3730/T)$	300–2000	± 0.15 at 300 K rising to ± 0.3 at 2000 K
$H + CHCO \rightarrow CH_2 + CO$ $\rightarrow H_2 + C_2O$ $\rightarrow HCCOH$	2.5×10^{-10}	300–2500	± 0.4
$H + CH_2CO \rightarrow CH_3 + CO$ $\rightarrow CH_2CHO$	$3.0 \times 10^{-11} \exp(-1700/T)$ k_2/k very small	200–2000	± 0.5 at 200 K rising to ± 1.0 at 2000 K.
$H + CH_3CHO \rightarrow H_2 + CH_3CO$ $\rightarrow H_2 + CH_2CHO$	$6.8 \times 10^{-15} T^{1.16} \exp(-1210/T)$	300–2000	± 0.1 at 300 rising to ± 0.4 at 2000 K.
$H + C_6H_5 + M \rightarrow C_6H_6 + M$	See Table 3		
$H + C_6H_6 \rightarrow H_2 + C_6H_5$ $\rightarrow C_6H_7$	No recommendation See Table 3		
$H + C_6H_5O + M \rightarrow C_6H_5OH + M$	See Table 3		
$H + C_6H_5OH \rightarrow C_6H_5O + H_2$ $\rightarrow C_6H_6 + OH$	$1.9 \times 10^{-10} \exp(-6240/T)$ $3.7 \times 10^{-11} \exp(-3990/T)$	1000–1150 1000–1150	± 0.3 ± 0.3
$H + C_6H_5CH_2 + M \rightarrow C_6H_5CH_3 + M$	See Table 3		
$H + C_6H_5CH_3 \rightarrow H_2 + C_6H_5CH_2$ $\rightarrow H_2 + C_6H_4CH_3$ $\rightarrow C_6H_6 + CH_3$ $\rightarrow C_6H_6CH_3$	$6.6 \times 10^{-22} T^{3.44} \exp(-1570/T)$ No recommendation No recommendation See Table 3	600–2800	± 0.3 at 600 K rising to ± 0.5 at 2800 K.
$H + p\text{-}C_6H_4(CH_3)_2 \rightarrow$ products	5.8×10^{-13}	298	± 0.1
$H + C_6H_5C_2H_5 \rightarrow H_2 + C_6H_5C_2H_4$ $\rightarrow C_6H_6C_2H_5$	2.4×10^{-12} See Table 3	773	± 0.1
H_2 Reactions			
$H_2 + Ar \rightarrow 2H + Ar$	See Table 2		
$H_2 + H_2 \rightarrow 2H + H_2$	See Table 2		
OH Radical Reactions			
$OH + H_2 \rightarrow H_2O + H$	$1.7 \times 10^{-16} T^{1.6} \exp(-1660/T)$	300–2500	± 0.1 at 300 K rising to ± 0.3 at 2500 K
$OH + OH \rightarrow H_2O + O$	$2.5 \times 10^{-15} T^{1.14} \exp(-50/T)$	250–2500	± 0.2
$OH + OH + M \rightarrow H_2O_2 + M$	See Table 3		

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$OH + HO_2 \rightarrow H_2O + O_2$	$4.8 \times 10^{-11} \exp(250/T)$	300–2000	± 0.2 at 300 K rising to ± 0.5 at 2000 K.
$OH + H_2O_2 \rightarrow H_2O + HO_2$	$1.3 \times 10^{-11} \exp(-670/T)$	300–1000	± 0.2
$OH + NH \rightarrow NO + H_2$ $\rightarrow H_2O + N$	8.0×10^{-11}	300–1000	± 0.5
$OH + NH_2 \rightarrow O + NH_3$ $\rightarrow H_2O + NH$	$3.3 \times 10^{-14} T^{0.405} \exp(-250/T)$ No recommendation	500–2500	± 0.5
$OH + CO \rightarrow H + CO_2$	$1.05 \times 10^{-17} T^{1.5} \exp(250/T)$	300–2000	± 0.2 at 300 K rising to ± 0.5 at 2000 K.
$OH + CH_3 \rightarrow H + CH_2OH$ $\rightarrow H + CH_3O$ $\rightarrow H_2O + {}^1CH_2$	6.0×10^{-11}	300–2000	± 0.7
$\rightarrow CH_3OH$	See Table 3		
$OH + CH_4 \rightarrow H_2O + CH_3$	$2.6 \times 10^{-17} T^{1.83} \exp(-1400/T)$	250–2500	± 0.07 at 250 K rising to ± 0.15 at 1200 K.
$OH + CHO \rightarrow H_2O + CO$	1.7×10^{-10}	300–2500	± 0.3
$OH + HCHO \rightarrow H_2O + CHO$	$5.7 \times 10^{-15} T^{1.18} \exp(225/T)$	300–3000	± 0.1 at 300 K rising to ± 0.7 at 3000 K.
$OH + CN \rightarrow O + HCN$ $\rightarrow NCO + H$	1.0×10^{-10}	1500–3000	± 0.5
$OH + HCN \rightarrow H_2O + CN$	$1.5 \times 10^{-11} \exp(-5400/T)$	1500–2500	± 0.5
$\rightarrow HOCN + H$ $\rightarrow HNCO + H$	No recommendation		
$OH + CH_3OOH \rightarrow H_2O + CH_3OO$	$1.2 \times 10^{-12} \exp(130/T)$	300–1000	± 0.2 at 300 K rising to ± 0.4 at 1000 K
$\rightarrow H_2O + CH_2OOH$	$1.8 \times 10^{-12} \exp(220/T)$	300–1000	± 0.1 at 300 K rising to ±0.3 at 1000 K.
$OH + C_2H_2 \rightarrow H_2O + C_2H$ $\rightarrow H + CH_2CO$	$1.0 \times 10^{-10} \exp(-6500/T)$	1000–2000	± 1.0
$\rightarrow C_2H_2OH$	See Table 3		
$OH + C_2H_4 \rightarrow H_2O + C_2H_3$	$3.4 \times 10^{-11} \exp(-2990/T)$	650–1500	± 0.5
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	$1.2 \times 10^{-17} T^{2.0} \exp(-435/T)$	250–2000	± 0.07 at 250 K rising to ± 0.15 at 2000 K.
$OH + CH_2CO \rightarrow CH_2OH + CO$ $\rightarrow H_2CO + HCO$	1.7×10^{-11}	300–2000	± 1.0
$OH + CH_3CHO \rightarrow H_2O + CH_3CO$ $\rightarrow H_2O + CH_2CHO$	$3.9 \times 10^{-14} T^{0.73} \exp(560/T)$	250–1200	± 0.1 at 250 K rising to ± 0.3 at 1200 K.
$OH + C_2H_5OOH \rightarrow H_2O + C_2H_5OO$ $\rightarrow H_2O + C_2H_4OOH$	$3.0 \times 10^{-12} \exp(190/T)$ [estimate]	250–1000	± 0.3 at 250 K rising to ± 0.7 at 1000 K

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$OH + C_6H_6 \rightarrow H_2O + C_6H_5$	$2.7 \times 10^{-16}\, T^{1.42} \exp(-730/T)$	400–1500	± 0.3
$\rightarrow H + C_6H_5OH$	$2.2 \times 10^{-11} \exp(-5330/T)$	1000–1150	± 0.3
$\rightarrow C_6H_6OH$	See Table 3		
$OH + C_6H_5OH \rightarrow C_6H_5(OH)_2$	See Table 3		
$\rightarrow H_2O + C_6H_5O$]			
$\rightarrow H_2O + C_6H_4OH$]	1.0×10^{-11}	1000–1150	± 0.5
$OH + C_6H_5CH_3 \rightarrow H_2O + C_6H_5CH_2$	$8.6 \cdot 10^{-15}\, T \exp(-1440/T)$	400–1200	± 0.5 at 400 K reducing to ±0.3 at 1200 K.
	See Table 3		
$OH + p\text{-}C_6H_4(CH_3)_2 \rightarrow C_6H_4CH_2CH_3 + H_2O$	$6.4 \times 10^{-11} \exp(-1440/T)$	500–960	±0.1
$\rightarrow p\text{-}C_6H_4(CH_3)_2OH$	See Table 3		
$OH + C_6H_5C_2H_5 \rightarrow HOC_6H_5C_2H_5$	See Table 3		
$\rightarrow H_2O + C_6H_5C_2H_4$]	8.7×10^{-12}	773	± 0.1
$\rightarrow H_2O + C_6H_4C_2H_5$]			
H_2O Reactions			
$H_2O + M \rightarrow H + OH + M$	See Table 2		
HO_2 Radical Reactions			
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$3.1 \times 10^{-12} \exp(-775/T)$	550–1250	± 0.15 at 550 K rising to ± 0.3 at 1250 K.
$HO_2 + NH_2 \rightarrow NH_3 + O_2$]			
$\rightarrow HNO + H_2O$]	2.6×10^{-11}	300–400	± 0.4
$HO_2 + CH_3 \rightarrow OH + CH_3O$	3×10^{-11}	300–2500	± 0.7
$\rightarrow O_2 + CH_4$	No recommendation		
$HO_2 + CH_4 \rightarrow H_2O_2 + CH_3$	$1.5 \times 10^{-11} \exp(-12400/T)$	600–1000	± 0.2 at 600 K rising to ± 0.3 at 1000 K.
$HO_2 + HCHO \rightarrow H_2O_2 + CHO$	$5.0 \times 10^{-12} \exp(-6580/T)$	600–1000	± 0.5
$HO_2 + C_2H_4 \rightarrow OH + C_2H_4O$	$3.7 \times 10^{-12} \exp(-8650/T)$	600–900	± 0.15 at 600 K rising to ± 0.25 at 900 K.
$HO_2 + C_2H_6 \rightarrow H_2O_2 + C_2H_5$	$2.2 \times 10^{-11} \exp(-10300/T)$	500–1000	± 0.2 at 500 K rising to ± 0.3 at 1000 K.
$HO_2 + CH_3CHO \rightarrow H_2O_2 + CH_3CO$	$5.0 \times 10^{-12} \exp(-6000/T)$	900–1200	± 0.7
H_2O_2 Reactions			
$H_2O_2 + M \rightarrow 2OH + M$	See Table 2		
N Atom Reactions			
$N + CN \rightarrow N_2 + C$	3×10^{-10}	300–2500	± 1.0
$N + NCO \rightarrow NO + CN$	No recommendation		
$\rightarrow N_2 + CO$	3.3×10^{-11}	1700	± 0.5

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
NH Radical Reactions			
$NH + O_2 \rightarrow NO + OH$ $\rightarrow NO_2 + H$ $\rightarrow HNO + O$	$1.26 \times 10^{-13} \exp(-770/T)$	270–550	± 0.2 at 270 K rising to ± 0.5 at 550 K.
$NH + NO \rightarrow N_2O + H$ $\rightarrow HN_2 + O$ $\rightarrow N_2 + OH$	5.0×10^{-11}	270–380	± 0.2
NH_2 Radical Reactions			
$NH_2 + O_2 \rightarrow$ products	$< 3 \times 10^{-18}$	298	
$NH_2 + NO \rightarrow N_2 + H_2O$ $\rightarrow N_2 + H + OH$ $\rightarrow N_2H + OH$ $\rightarrow N_2O + H_2$	$1.8 \times 10^{-12} \exp(650/T)$ $(k_2 + k_3)/k \approx 0.12$ at 298 K.	220–2000	± 0.5
$^1C_2$ and $^3C_2$ Radical Reactions	See data sheets.		
CH Radical Reactions			
$CH + O_2 \rightarrow CHO + O$ $\rightarrow CO + OH$	5.5×10^{-11}	300–2000	± 0.3 at 300 K rising to ± 0.5 at 2000 K.
$CH + H_2 \rightarrow CH_2 + H$ $\rightarrow CH_3$	$2.4 \times 10^{-10} \exp(-1760/T)$	300–1000	± 0.3
$CH + H_2O \rightarrow$ products	$9.5 \times 10^{-12} \exp(380/T)$	300–1000	± 1.0
$CH + CO \rightarrow$ products	$4.6 \times 10^{-13} \exp(860/T)$	300–1000	± 1.0
$CH + CO_2 \rightarrow$ products	$5.7 \times 10^{-12} \exp(-345/T)$	300–1000	± 1.0
$CH + CH_4 \rightarrow$ products	$5.0 \times 10^{-11} \exp(200/T)$	200–700	± 1.0
$CH + C_2H_2 \rightarrow$ products	$3.5 \times 10^{-10} \exp(61/T)$	200–700	± 1.0
$CH + C_2H_4 \rightarrow$ products	$2.2 \times 10^{-10} \exp(173/T)$	200–700	± 1.0
$CH + C_2H_6 \rightarrow$ products	$1.8 \times 10^{-10} \exp(132/T)$	200–700	± 1.0
$CH + C_3H_8 \rightarrow$ products	$1.9 \times 10^{-10} \exp(240/T)$	300–700	± 1.0
$CH + n\text{-}C_4H_{10} \rightarrow$ products	$4.4 \times 10^{-10} \exp(28/T)$	250–700	± 1.0
$CH + i\text{-}C_4H_{10} \rightarrow$ products	$2.0 \times 10^{-10} \exp(240/T)$	300–700	± 1.0
$CH +$ neo-$C_5H_{12} \rightarrow$ products	$1.6 \times 10^{-10} \exp(340/T)$	300–700	± 1.0
$CH + CH_3C_2H \rightarrow$ products	No recommendation		
$CH + CH_2O \rightarrow$ products	$1.6 \times 10^{-10} \exp(260/T)$	300–700	± 1.0

Table 1
BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$^3CH_2$ Radical Reactions			
$^3CH_2 + O_2 \rightarrow CO + H + OH$ $\rightarrow CO_2 + H + H$ $\rightarrow CO + H_2O$ $\rightarrow CO_2 + H_2$ $\rightarrow HCHO + O$	$4.1 \times 10^{-11} \exp(-750/T)$	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K.
$^3CH_2 + {}^3CH_2 \rightarrow C_2H_2 + H_2$ $\rightarrow C_2H_2 + 2H$	$2.0 \times 10^{-10} \exp(-400/T)$ $k_2/k = 0.9 \pm 0.1$ over range 300–3000 K.	300–3000	± 0.5
$^3CH_2 + CH_3 \rightarrow C_2H_4 + H$	7.0×10^{-11}	300–3000	± 0.3 at 300 K rising to ± 0.5 at 3000 K.
$^3CH_2 + C_2H_2 \rightarrow C_3H_4$	See Table 3		
$^3CH_2 + C_2H_4 \rightarrow C_3H_6$ $\rightarrow c\text{-}C_3H_6$ $\rightarrow CH_2CHCH_2 + H$	See Table 3		
$^1CH_2$ Radical Reactions			
$^1CH_2 + Ar \rightarrow {}^3CH_2 + Ar$	6.0×10^{-12}	300–2000	± 0.3
$^1CH_2 + N_2 \rightarrow {}^3CH_2 + N_2$	1.0×10^{-11}	300–2000	± 0.3
$^1CH_2 + CH_4 \rightarrow {}^3CH_2 + CH_4$	1.2×10^{-11}	300–2000	± 0.4
$^1CH_2 + C_2H_2 \rightarrow {}^3CH_2 + C_2H_2$	8.0×10^{-11}	300–2000	± 0.4
$^1CH_2 + C_2H_4 \rightarrow {}^3CH_2 + C_2H_4$	2.3×10^{-11}	300–2000	± 0.4
$^1CH_2 + C_2H_6 \rightarrow {}^3CH_2 + C_2H_6$	3.6×10^{-11}	300–2000	± 0.4
$^1CH_2 + O_2 \rightarrow CO + H + OH$ $\rightarrow CO_2 + H_2$ $\rightarrow CO + H_2O$ $\rightarrow {}^3CH_2 + O_2$	5.2×10^{-11}	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K
$^1CH_2 + H_2 \rightarrow CH_3 + H$	1.2×10^{-10}	300–1000	± 0.1 at 300 K rising to ± 0.3 at 1000 K
$^1CH_2 + C_2H_2 \rightarrow CH_2CCH_2$ $\rightarrow CH_3CCH$ $\rightarrow CH_2CCH + H$	See Table 3		
$\rightarrow {}^3CH_2 + C_2H_2$	See earlier entry		
$^1CH_2 + C_2H_4 \rightarrow C_3H_6$	See Table 3		
$\rightarrow {}^3CH_2 + C_2H_4$	See earlier entry		
CH_3 Radical Reactions			
$CH_3 + M \rightarrow CH_2 + H + M$	See Table 2		
$CH_3 + O_2 \rightarrow CH_3O + O$	$2.2 \times 10^{-10} \exp(-15800/T)$	300–2500	± 0.5
$\rightarrow HCHO + OH$	$5.5 \times 10^{-13} \exp(-4500/T)$	1000–2500	± 0.5
$\rightarrow CH_3O_2$	See Table 3		

Table 1
BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$CH_3 + H_2 \rightarrow CH_4 + H$	$1.14 \times 10^{-20} T^{2.74} \exp(-4740/T)$	300–2500	± 0.15 in the range 300–700 K. ± 0.3 in the range 700–2500 K.
$CH_3 + CH_3 \rightarrow C_2H_5 + H$	$5 \times 10^{-11} \exp(-6800/T)$	1300–2500	± 0.6
$\rightarrow C_2H_4 + H_2$	No recommendation (see data sheets)		
$\rightarrow C_2H_6$	See Table 3		
$CH_3 + HCHO \rightarrow CH_4 + HCO$	$6.8 \times 10^{-12} \exp(-4450/T)$	300–1000	± 0.3
$CH_3 + C_2H_2 + M \rightarrow C_3H_5 + M$	See Table 3		
$\rightarrow CH_4 + C_2H$	No recommendation		
$CH_3 + C_2H_4 \rightarrow CH_4 + C_2H_3$	$6.9 \times 10^{-12} \exp(-5600/T)$	400–3000	± 0.5
$\rightarrow n\text{-}C_3H_7$	See Table 3		
$CH_3 + C_2H_5 \rightarrow CH_4 + C_2H_4$	1.9×10^{-12}	300–800	± 0.4
$\rightarrow C_3H_8$	See Table 3		
$CH_3 + C_2H_6 \rightarrow CH_4 + C_2H_5$	$2.5 \times 10^{-31} T^{6.0} \exp(-3043/T)$	300–1500	± 0.1 at 300 K rising to ± 0.2 at 1500 K.
$CH_3 + CH_3CHO \rightarrow CH_4 + CH_3CO$	$3.3 \times 10^{-30} T^{5.64} \exp(-1240/T)$	300–1250	± 0.3
$\rightarrow CH_4 + CH_2CHO$	No recommendation (see data sheets)		
CH_4 Reactions			
$CH_4 + M \rightarrow CH_3 + H + M$	See Table 2		
CHO Radical Reactions			
$CHO + O_2 \rightarrow CO + HO_2$ $\rightarrow OH + CO_2$ $\rightarrow HCO_3$	5.0×10^{-12}	300–2500	± 0.3
$CHO + CHO \rightarrow HCHO + CO$	5.0×10^{-11}	300	± 0.3
HCHO Reactions			
$HCHO + M \rightarrow H + CHO + M$ $\rightarrow H_2 + CO + M$	See Table 2		
CH_2OH Reactions			
$CH_2OH + O_2 \rightarrow CH_2O + HO_2$	$2.6 \times 10^{-9} T^{-1.0} +$ $1.2 \times 10^{-10} \exp(-1800/T)$	300–1200	± 0.1 at 300 K rising to ± 0.3 at 1200 K.
CH_3O Radical Reactions			
$CH_3O + M \rightarrow HCHO + H + M$	See Table 2		
$CH_3O + O_2 \rightarrow HCHO + HO_2$	$6.7 \times 10^{-14} \exp(-1070/T)$	300–1000	± 0.2 at 500 K rising to ± 0.3 at 300 K and 1000 K.

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
CH_3OOH Reactions			
$CH_3OOH + M \rightarrow CH_3O + OH + M$	See Table 2		
CN Radical Reactions			
$CN + O_2 \rightarrow NCO + O$	$1.1 \times 10^{-11} \exp(205/T)$	300–2500	± 0.25 at 300 K rising to ± 0.5 at 2500 K.
$CN + H_2O \rightarrow HCN + OH$ $\rightarrow HOCN + H$	$1.3 \times 10^{-11} \exp(-3750/T)$	500–3000	± 0.3 at 500 K rising to ± 0.5 at 3000 K.
$CN + CH_4 \rightarrow HCN + CH_3$	$1.5 \times 10^{-11} \exp(-940/T)$	260–400	± 0.3
NCO Radical Reactions			
$NCO + M \rightarrow N + CO + M$	See Table 2		
$NCO + NO \rightarrow N_2O + CO$ $\rightarrow N_2 + CO_2$ $\rightarrow N_2 + CO + O$	$1.7 \times 10^{-11} \exp(200/T)$	300–600	± 0.5
C_2H Radical Reactions			
$C_2H + O_2 \rightarrow CO_2 + CH$ $\rightarrow 2CO + H$ $\rightarrow C_2HO + O$ $\rightarrow CO + HCO$	3.0×10^{-11}	300	± 0.5
$C_2H + H_2 \rightarrow C_2H_2 + H$	$2.5 \times 10^{-11} \exp(-1560/T)$	300–2500	± 0.3 at 300 K rising to ± 0.7 at 2500 K
$C_2H + C_2H_2 \rightarrow C_4H_2 + H$	5.0×10^{-11}	300–2700	± 0.3
$C_2H + CH_4 \rightarrow$ products	2.0×10^{-12}	298	± 1
$C_2H + C_2H_6 \rightarrow$ products	No recommendation		
C_2H_3 Radical Reactions			
$C_2H_3 + M \rightarrow C_2H_2 + H + M$	See Table 2		
$C_2H_3 + O_2 \rightarrow HCHO + CHO$	9.0×10^{-12}	300–2000	± 0.3 at 300 K rising to ± 0.5 at 2000 K
C_2H_5 Radical Reactions			
$C_2H_5 + O_2 \rightarrow C_2H_4 + HO_2$	$1.7 \times 10^{-14} \exp(1100/T)$	600–1200	± 0.3
$C_2H_5 + C_2H_5 \rightarrow C_2H_6 + C_2H_4$ $\rightarrow n\text{-}C_4H_{10}$	2.4×10^{-12} See Table 3	300–1200	± 0.4
C_2H_6 Reactions			
$C_2H_6 + M \rightarrow CH_3 + CH_3 + M$	See Table 2		

KINETIC DATA FOR COMBUSTION MODELLING (continued)

Table 1

BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
CHCO Reactions			
$CHCO + O_2 \rightarrow CO_2 + HCO$ $\rightarrow 2CO + OH$ $\rightarrow C_2O + HO_2$ $\rightarrow CHO_2CO$	$2.7 \times 10^{-12} \exp(430/T)$ M = He, 2 Torr	300–550	± 0.7
CH_2CHO Radical Reactions			
$CH_2CHO + O_2 \rightarrow HO_2 + CH_2CHO$ $\rightarrow HCHO + CO + OH$ $\rightarrow O_2CH_2CHO$	$k_\infty = 2.6 \times 10^{-13}$ $k_2 = 3.0 \times 10^{-14}$	250–1000 300	± 0.2 ± 0.3
CH_3CO Radical Reactions			
$CH_3CO + O_2 + M \rightarrow CH_3CO_3 + M$	See Table 3		
CH_3CHO Reactions			
$CH_3CHO + M \rightarrow CH_3 + HCO + M$	See Table 2		
C_2H_5O Reactions			
$C_2H_5O + M \rightarrow HCHO + CH_3 + M$ $\rightarrow CH_3CHO + H + M$	See Table 2		
$C_2H_5O + O_2 \rightarrow CH_3CHO + HO_2$	$1.0 \times 10^{-13} \exp(-830/T)$	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K
C_2H_5OOH Reactions			
$C_2H_5OOH + M \rightarrow C_2H_5O + OH + M$	See Table 2		
C_6H_5 Radical Reactions			
$C_6H_5 + M \rightarrow C_2H_2 + C_4H_3 + M$ $\rightarrow C_2H_3 + C_4H_2 + M$ $\rightarrow$ linear-$C_6H_5 + M$	See Table 2		
C_6H_6 Reactions			
$C_6H_6 + M \rightarrow C_6H_5 + H + M$ $\rightarrow C_4H_4 + C_2H_2 + M$	See Table 2		
C_6H_5O Radical Reactions			
$C_6H_5O + M \rightarrow C_5H_5 + CO + M$	See Table 2		
$C_6H_5CH_2$ Radical Reactions			
$C_6H_5CH_2 + M \rightarrow C_3H_3 + 2C_2H_2 + M$ $\rightarrow C_4H_4 + C_3H_3 + M$ $\rightarrow C_5H_5 + C_2H_2 + M$ $\rightarrow C_7H_7$(BCH) + M	See Table 2		

Table 1
BIMOLECULAR REACTIONS (continued)

Reaction	k/cm^3 molecule^{-1}s^{-1}	Temp/K	Error limits ($\Delta \log k$)
$C_6H_5CH_3$ Reactions			
$C_6H_5CH_3 + M \rightarrow C_6H_5CH_2 + H + M$ $\rightarrow C_6H_5 + CH_3 + M$	See Table 2		
p-$C_6H_4(CH_3)_2$ Reactions			
p-$C_6H_4(CH_3)_2 + M \rightarrow C_6H_4CH_2CH_3 + H + M$	See Table 2		
$C_6H_5C_2H_5$ Reactions			
$C_6H_5C_2H_5 + M \rightarrow C_6H_5CH_2 + CH + M$ $\rightarrow C_6H_6 + C_2H_4 + M$ $\rightarrow C_6H_5CHCH_2 + H_2 + M$ $\rightarrow C_6H_5 + C_2H_5 + M$ $\rightarrow C_6H_5CHCH_3 + H + M$	See Table 2		

Table 2
DECOMPOSITION REACTIONS

Reaction	k_∞/s^{-1} k_0/cm^3 molecule^{-1} s^{-1} F_c $k/s^{-1} = \frac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp/K	Error limits ($\Delta \log k$)
$H_2 + Ar \rightarrow 2H + Ar$	$k_0 = 3.7 \times 10^{-10} \exp(-48350/T)$	2500–8000	± 0.3
$H_2 + H_2 \rightarrow 2H + H_2$	$k_0 = 1.5 \times 10^{-9} \exp(-48350/T)$	2500–8000	± 0.5
$H_2O + N_2 \rightarrow H + OH + N_2$	$k_0 = 5.8 \times 10^{-9} \exp(-52920/T)$	2000–6000	± 0.5
$H_2O_2 + M \rightarrow 2\,OH + M$	$k_0(Ar) = 3 \times 10^{-8} \exp(-21600/T)$ $k_0(N_2) = 2 \times 10^{-7} \exp(-22900/T)$ $k_\infty = 3 \times 10^{14} \exp(-24400/T)$ $F_c(Ar) = 0.5$	1000–1500 700–1500 1000–1500 700–1500	± 0.2 ± 0.2 ± 0.5 $\Delta F_c = \pm 0.1$
$CH_3 + M \rightarrow CH_2 + H + M$	$k_0 = 1.7 \times 10^{-8} \exp(-45600/T)$	1500–3000	± 0.5
$CH_4 + M \rightarrow CH_3 + H + M$	$k_0(Ar) = 1.2 \times 10^{-6} \exp(-47000/T)$ $k_0(CH_4) = 1.4 \times 10^{-5} \exp(-48100/T)$ $k_\infty = 2.4 \times 10^{16} \exp(-52800/T)$ F_c (Ar) $= \exp(-0.45 - T/3231)$ F_c (CH_4) $= \exp(-0.37 - T/2210)$	1000–3000 1000–2000 1000–3000 1000–3000 1000–2000	± 0.3 ± 0.3 ± 0.5 $\Delta F_c = \pm 0.1$ $\Delta F_c = \pm 0.1$
$HCHO + M \rightarrow H + CHO + M$ $\rightarrow H_2 + CO + M$	$k_0(1) = 2.1 \times 10^{-8} \exp(-39200/T)$ $k_1/k_2 = 0.5$ at 2200 K	1500–2500	± 0.3
$CH_3O + M \rightarrow HCHO + H + M$	$k_0 = 3.16 \times 10^2\, T^{-2.7} \exp(-15400/T)$ [estimate]	300–1000	± 1.0
$CH_3OOH + M \rightarrow CH_3O + OH + M$	$k_\infty = 4 \times 10^{15} \exp(-21600/T)$	400–1000	± 0.5 at 600 K rising to ± 1.0 at 400 and 1000 K
$NCO + Ar \rightarrow N + CO + Ar$	$k_0 = 1.7 \times 10^{-9} \exp(-23500/T)$	1450–2600	± 0.4

Table 2
DECOMPOSITION REACTIONS (continued)

Reaction	k_∞/s^{-1} k_0/cm^3 molecule^{-1} s^{-1} F_c $k/s^{-1} = \frac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp/K	Error limits ($\Delta \log k$)
$C_2H_3 + M \rightarrow C_2H_2 + H + M$	$k_0 = 6.9 \times 10^{17} T^{-7.5} \exp(-22900/T)$	500–2500	± 0.5
	$k_\infty = 2 \times 10^{14} \exp(-20000/T)$	500–2500	± 0.5
	$F_c = 0.35$	500–2500	ΔF_c = ± 0.1
$C_2H_6 + M \rightarrow 2CH_3 + M$	$k_0(Ar) = 1.1 \times 10^{25} T^{-8.24} \exp(-47090/T)$	300–2000	± 0.5
	$k_0(C_2H_6) = 4.5 \times 10^{-2} \exp(-41930/T)$	800–1000	± 0.5
	$k_\infty = 1.8 \times 10^{21} T^{-1.24} \exp(-45700/T)$	300–2000	± 0.3
	$F_c(Ar) = 0.38 \exp(-T/73) + 0.62 \exp(-T/1180)$	300–2000	ΔF_c = ± 0.1
	$F_c(C_2H_6) = 0.54 \exp(-T/1250)$	800–1000	ΔF_c = ± 0.1
$CH_3CHO + M \rightarrow CH_3 + CHO + M$	k(1 atm.) $= 7 \times 10^{15} \exp(-41100/T)$ (pressure dependent region)	750–1200	± 0.4
$C_2H_5O + M \rightarrow HCHO + CH_3 + M$	$k_\infty = 8 \times 10^{13} \exp(-10830/T)$ [estimate]	300–600	± 1.0
$C_2H_5OOH + M \rightarrow C_2H_5O + OH + M$	k_∞ $4 \times 10^{15} \exp(-21600/T)$	400–1000	± 1.0
$C_6H_5 + M \rightarrow C_2H_2 + C_4H_3 + M$ $\rightarrow C_2H_3 + C_4H_2 + M$	No recommendation		
$\rightarrow$ linear-$CH_5 + M$	$4.0 \times 10^{13} \exp(-36700/T)$	1450–1900	± 0.4
$C_6H_6 + M \rightarrow C_6H_5 + H + M$ $\rightarrow C_4H_4 + H_2 + M$	$9.0 \times 10^{15} \exp(-54060/T)$	1200–2500	± 0.4 at 1200 K reducing to ± 0.3 at 2500 K
$C_6H_5O + M \rightarrow C_5H_5 + CO + M$	$2.5 \times 10^{11} \exp(-22100/T)$	1000–1580	± 0.2
$C_6H_5CH_2 + M \rightarrow C_3H_3 + 2C_2H_2 + M$ $\rightarrow C_4H_4 + C_3H_3 + M$ $\rightarrow C_5H_5 + C_2H_2 + M$ $\rightarrow C_7H_7$ (BCH) + M	$5.1 \times 10^{13} \exp(-36370/T)$	1350–1900	± 0.3 at 1350 K rising to ± 0.5 1900 K
$C_6H_5CH_3 + M \rightarrow C_6H_5CH_2 + H + M$	$3.1 \times 10^{15} \exp(-44890/T)$	920–2200	± 0.3 at 900 K rising to ± 0.5 at 2200 K
$\rightarrow C_6H_5 + CH_3 + M$	No recommendation		
p-$C_6H_4(CH_3)_2 + M \rightarrow p$-$C_6H_4CH_2CH_3 + H + M$	$4.0 \times 10^{15} \exp(-42600/T)$	1400–1800	± 0.5
$C_6H_5C_2H_5 + M \rightarrow C_6H_5CH_2 + CH + M$	$6.1 \times 10^{15} \exp(-37800/T)$	770–1800	± 0.1 at 770 K rising to ± 0.4 at
$\rightarrow C_6H_6 + C_2H_4 + M$ $\rightarrow C_6H_5CHCH_2 + H_2 + M$ $\rightarrow C_6H_5 + C_2H_5 + M$ $\rightarrow C_6H_5CHCH_3 + H + M$	No recommendations		

Table 3
COMBINATION REACTIONS

Reaction	k_∞/cm^3 molecule$^{-1}s^{-1}$ k_0/cm^6 molecule^{-2} s^{-1} F_c k/cm^3 molecule$^{-1}s^{-1} = \frac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp/K	Error limits ($\Delta \log k$)
$H + O_2 + Ar \rightarrow HO_2 + Ar$	$k_0 = 1.7 \times 10^{-30} T^{-0.8}$	300–2000	± 0.5

Table 3

COMBINATION REACTIONS (continued)

Reaction	k_∞/cm^3 molecule^{-1}s^{-1} k_0/cm^6 molecule^{-2} s^{-1} F_c $k = \frac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp/K	Error limits ($\Delta \log k$)
$H + O_2 + H_2 \rightarrow HO_2 + H_2$	$k_0 = 5.8 \times 10^{-30} T^{-0.8}$	300–2000	± 0.5
$H + O_2 + N_2 \rightarrow HO_2 + N_2$	$k_0 = 3.9 \times 10^{-30} T^{-0.8}$	300–2000	± 0.5
$H + O_2 + H_2O \rightarrow HO_2 + H_2O$	$k_0 = 4.3 \times 10^{-30} T^{-0.8}$	300–2000	± 0.5
$H + H + Ar \rightarrow H_2 + Ar$	$k_0 = 1.8 \times 10^{-30} T^{-1.0}$	300–2500	± 0.5
$H + H + H_2 \rightarrow H_2 + H_2$	$k_0 = 2.7 \times 10^{-31} T^{-0.6}$	100–5000	± 0.5
$H + OH + H_2O \rightarrow H_2O + H_2O$	$k_0 = 3.9 \times 10^{-25} T^{-2.0}$	300–3000	± 0.3
$H + OH + Ar \rightarrow H_2O + Ar$	$k_0 = 2.3 \times 10^{-26} T^{-2.0}$	300–3000	± 0.3
$H + OH + N_2 \rightarrow H_2O + N_2$	$k_0 = 6.1 \times 10^{-26} T^{-2.0}$	300–3000	± 0.3
$H + CH_3 + M \rightarrow CH_4 + M$	$k_0(He) = 6.2 \times 10^{-29} (T/3000)^{-1.8}$	300–1000	± 0.3
	$k_0(Ar) = 6 \times 10^{-29} (T/300)^{-1.8}$	300–1000	± 0.5
	$k_0(C_2H_6) = 3 \times 10^{-28} (T/300)^{-1.8}$	300–1000	± 0.5
	$k_\infty = 3.5 \times 10^{-10}$	300–1000	± 0.3
	$F_c(He,Ar) = \exp(-0.45 - T/3231)$	300–1000	ΔF_c = ± 0.1
	$F_c(C_2H_6) = \exp(-0.34 - T/3053)$	300–1000	ΔF_c = ± 0.1
$H + C_2H_2 + He \rightarrow C_2H_3 + He$	$k_\infty = 1.4 \times 10^{-11} \exp(-1300/T)$	200–400	± 0.3
	$k_0 = 3.3 \times 10^{-30} \exp(-740/T)$	200–400	± 0.5
	$F_c = 0.44$	200–400	ΔF_c = ± 0.1
$H + C_2H_3 + M \rightarrow C_2H_4 + M$	No recommendation		
$H + C_2H_4 + M \rightarrow C_2H_5 + M$	No recommendation		
$H + C_2H_5 + M \rightarrow C_2H_6 + M$	No recommendation		
$H + C_6H_5 + M \rightarrow C_6H_6 + M$	$k_\infty = 1.3 \times 10^{-10}$	1400–1700	± 0.5
$H + C_6H_6 + M \rightarrow C_6H_7 + M$	$k_\infty = 6.7 \times 10^{-11} \exp(-2170/T)$	300–1000	± 0.2
$H + C_6H_5O + M \rightarrow C_6H_5OH + M$	$k_\infty = 4.2 \times 10^{-10}$	1000	± 0.3
$H + C_6H_5CH_2 + M \rightarrow C_6H_5CH_3 + M$	$k_\infty = 5.5 \times 10^{-10}$	300–2000	± 0.2 at 300 K rising to ± 0.7 at 2000 K.
$H + C_6H_5CH_3 + M \rightarrow C_6H_6CH_3 + M$	$k_\infty = 1.2 \times 10^{-13}$	298	± 0.2
$H + C_6H_5C_2H_5 + M \rightarrow C_6H_6C_2H_5 + M$	$k_\infty = 3.3 \times 10^{-13}$	298	± 0.1
$OH + OH + M \rightarrow H_2O_2 + M$	$k_0(N_2) = 8 \times 10^{-31} (T/300)^{-0.76}$	250–1400	± 0.4
	$k_0(H_2O) = 4 \times 10^{-30}$	300–400	
	$k_\infty = 1.5 \times 10^{-11} (T/300)^{-0.37}$	200–1500	± 0.5
	$F_c(N_2) = 0.5$	200–1500	ΔF_c = ± 0.2
$OH + CH_3 + M \rightarrow CH_3OH + M$	No data available for this channel (See Table 1)		

Table 3

COMBINATION REACTIONS (continued)

Reaction	k_∞/cm^3 molecule^{-1}s^{-1} k_0/cm^6 molecule^{-2} s^{-1} F_c k/cm^3 molecule^{-1}s^{-1} = $\frac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp/K	Error limits ($\Delta \log k$)
$OH + C_2H_2 + M \rightarrow C_2H_2OH + M$	See data sheet		
$OH + C_6H_6 + M \rightarrow C_6H_6OH + M$	$k_\infty = 3.8 \times 10^{-12} \exp(-340/T)$	240–340	± 0.2
$OH + C_6H_5OH + M \rightarrow C_6H_5(OH)_2 + M$	$k_\infty = 2.8 \times 10^{-11}$	298	± 0.1
$OH + C_6H_5CH_3 + M \rightarrow HOC_6H_5CH_3 + M$	$k_\infty = 3.8 \times 10^{-12} \exp(180/T)$	200–300	± 0.4
$OH + C_6H_4(CH_3)_2 + M \rightarrow C_6H_4(CH_3)_2OH + M$	$k_\infty = 1.4 \times 10^{-11}$	300–320	± 0.1
$OH + C_6H_5C_2H_5 + M \rightarrow HOC_6H_5C_2H_5 + M$	7.5×10^{-12} at p ≤ 1 atm.	298	± 0.1
$^3CH_2 + C_2H_2 + M \rightarrow C_3H_4 + M$	$2.0 \times 10^{-11} \exp(-3330/T)$ at p = ≤ 10 Torr.	300–1000	± 0.3
$^3CH_2 + C_2H_4 + M \rightarrow C_3H_6 + M$ $\rightarrow c\text{-}C_3H_6 + M$ $\rightarrow C_3H_5 + H + M$	$5.3 \times 10^{-12} \exp(-2660/T)$	300–1000	± 0.2 at 300 K rising to ± 0.3 at 1000 K
$^1CH_2 + C_2H_2 + M \rightarrow CH_2CCH_2 + M$ $\rightarrow CH_3CCH + M$ $\rightarrow CH_2CCH + H + M$	3.7×10^{-10} independent of p	300–1000	± 0.3 at 300 K rising to ± 0.7 at 1000 K.
$^1CH_2 + C_2H_4 + M \rightarrow C_3H_6$	1.1×10^{-10} independent of p	300–1000	± 0.2 at 300 K rising to ± 0.5 at 1000 K.
$CH_3 + O_2 + M \rightarrow CH_3O_2 + M$	$k_0(Ar) = 1.5 \times 10^{-22} T^{-3.3}$	300–800	± 0.3
	$k_0(N_2) = 1.6 \times 10^{-22} T^{-3.3}$	300–800	± 0.3
	$k_\infty = 1.3 \times 10^{-15} T^{-1.2}$	300–800	± 0.3
	$F_c = 0.466 - 1.30 \times 10^{-4} T$	300–800	
$CH_3 + CH_3 + Ar \rightarrow C_2H_6 + Ar$	$k_\infty = 6 \times 10^{-11}$	300–2000	± 0.05 at 300 K rising to ± 0.3 at 2000 K
	$k_0 = 3.5 \times 10^{-7} T^{-7.0} \exp(-1390/T)$	300–2000	± 0.3
	$F_c = 0.38 \exp(-T/73)$ + $0.62\exp(-T/1180)$	300–2000	ΔF_c = ± 0.1
$CH_3 + C_2H_2 + M \rightarrow C_3H_5 + M$	$k_\infty = 1 \times 10^{-12} \exp(-3900/T)$	300–600	± 0.5
$CH_3 + C_2H_4 + M \rightarrow n\text{-}C_3H_7 + M$	$3.5 \times 10^{-13} \exp(-3700/T)$	300–600	± 0.3
$CH_3 + C_2H_5 + M \rightarrow C_3H_8 + M$	$k_\infty = 4.7 \times 10^{-11}$	300–800	± 0.3
$C_2H_5 + C_2H_5 + M \rightarrow n\text{-}C_4H_{10} + M$	$k_\infty = 1.9 \times 10^{-11}$	300–1200	± 0.3
$CH_3CO + O_2 + M \rightarrow CH_3CO_3 + M$	2×10^{-12} for p = 1–4 Torr.	300	± 0.3