Summary Table of Evaluated Kinetic Data for Combustion Modeling: Supplement 1

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INTRODUCTION

This publication has been prepared by the CEC Group on Evaluation of Kinetic Data for Combustion Modeling, which was established as one of the projects within the European Energy Research and Development Programme. The CEC Group has previously published a compilation of critically evaluation kinetic data for combustion modeling in the *Journal of Physical and Chemical Reference Data* **21**:411–736 (1992). That compilation has now

been updated and together with material on a number of new reactions the update will be published in the *Journal of Physical and Chemical Reference Data* as Supplement 1 to the original article. Here we present the Summary Table giving the recommended rate constants and assigned error limits for all of the reactions considered in the original article and Supplement 1.

The formal cutoff point for the literature searching on which these evaluations are based was January 1992, but the Group continued to monitor the literature during the preparation of the data sheets and every attempt was made to incorporate the results of more recent studies of importance, in particular, the material presented at the Twenty-Fourth Symposium (International) on Combustion, held in 1992.

The reader is referred to the full article to obtain the data sheets for each reaction which contain a summary of the experimental results on which the recommendations are based.

GUIDE TO THE USE OF THE TABLES

There are three tables. Table 1 summarizes data on bimolecular reactions, Table 2 provides data for decomposition ("unimolecular") reactions and Table 3 for combination ("termolecular") processes.

Reaction Ordering

The reactions are grouped in order using a system widely adopted in publications of the National Institute of Standards and Technology. The grouping is made on the basis of the attacking atom or radical in the order set out in the following list.

O Atom Reactions

O_2 Reactions

H Atom Reactions

H_2 Reactions

OH Radical Reactions

H_2O Reactions

HO_2 Radical Reactions

H_2O_2 Reactions

N Atom Reactions

NH Radical Reactions

NH_2 Radical Reactions

NH_3 Reactions

C Atom Reactions

C_2 Radical Reactions

CH Radical Reactions

$^3CH_2$ Radical Reactions

$^1CH_2$ Radical Reactions

CH_3 Radical Reactions

CH_4 Reactions

CHO Radical Reactions

HCHO Reactions

CH_2OH Radical Reactions

CH_3O Radical Reactions

CH_3O_2 Radical Reactions

CH_3OH Reactions

CH_3OOH Reactions

CN Radical Reactions

NCO Radical Reactions

C_2H Radical Reactions

C_2H_3 Radical Reactions

C_2H_4 Reactions

C_2H_5 Radical Reactions

C_2H_6 Reactions

CHCO Radical Reactions

CH_2CHO Radical Reactions

CH_3CO Radical Reactions

CH_3CHO Reactions

C_2H_5O Radical Reactions

C_2H_5OOH Reactions

C_3H_5 Radical Reactions

$i - C_3H_7$ Radical Reactions

C_3H_8 Reactions

$t - C_4H_9$ Radical Reactions

C_6H_5 Radical Reactions

C_6H_6 Reactions

C_6H_5O Radical Reactions

$C_6H_5CH_2$ Radical Reactions

$C_6H_5CH_3$ Reactions

$p - C_6H_4(CH_3)_2$ Reactions

$C_6H_5C_2H_5$ Radical Reactions

Thus, the reaction

$$CN + CH_4 \rightarrow HCN + CH_3$$
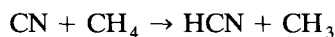
will be found under CN radical reactions. For reactions not classified by this rule, e.g., radical-radical reactions, the rule that species higher on the list take precedence over those lower applies. Thus, the reaction

$$OH + CH_3 + M \rightarrow CH_3OH + M$$
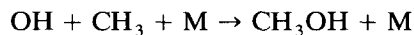
will be found under OH radical reactions. The same rule applies to reactions between species of a non-radical nature. For the purposes of the classification O_2 and NO are treated as radicals only in their reactions with non-radical species.

Tabulation of the Rate Constants

It is assumed that all reactions in the complication are elementary reactions.

The relationship between rate and rate constant for a reaction described by a stoichiometric equation such as
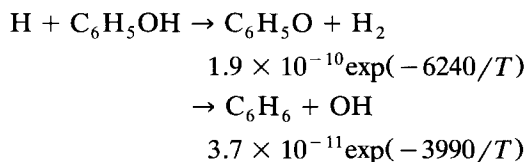
$$A + A \rightarrow B + C$$
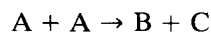
is given by

$$Rate = -(1/2)d[A]/dt$$
$$= d[B]/dt = d[C]/dt = k[A]^2.$$

For bimolecular reactions, the temperature dependence of the rate constant is expressed either as $k = A \exp(-B/T)$ or $AT^n\exp(-C/T)$, whichever is the more appropriate, where

A, n, B, and C are constants. In some cases, the form with $C = 0$, leading to $k = AT^n$, gives the best representation. The expressions used for pressure dependent combination and dissociation reactions are discussed in detail later.

Many of the reactions in the tables may lead to more than one set of products. For these multichannel reactions the most likely channels are listed and, wherever possible, an expression is given for the rate constant of each channel. The set of products first listed is assigned a rate constant, k_1, the second set a rate constant, k_2, and so on. Thus, the entry

$$H + C_6H_5OH \rightarrow C_6H_5O + H_2$$
$$1.9 \times 10^{-10}\exp(-6240/T)$$
$$\rightarrow C_6H_6 + OH$$
$$3.7 \times 10^{-11}\exp(-3990/T)$$

indicates that the rate constant for the reaction $H + C_6H_5OH \rightarrow C_6H_5O + H_2$, i.e., k_1, is given by the expression $1.9 \times 10^{-10}\exp(-6240/T)$cm^3 molecular^{-1} s^{-1} and the rate constant, k_2, for the second channel giving $C_6H_6 + OH$ is given by $3.7 \times 10^{-11}\exp(-3990/T)$cm^3 molecule^{-1} s^{-1}.
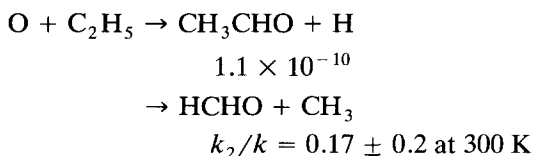
In most cases, rate data for individual channels are not available and often only the overall rate constant for removal of reactants (k) has been measured. In such cases the expression refers to k, which is equal to the sum of the rate constants for the individual product channels. Thus the entry,

$$O + HCN \rightarrow NCO + H$$
$$\rightarrow CO + NH$$
$$\rightarrow OH + CN$$
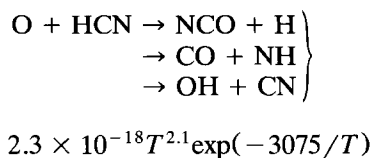
$2.3 \times 10^{-18}T^{2.1}\exp(-3075/T)$

indicates that $k = k_1 + k_2 + k_3 = 2.3 \times 10^{-18}T^{2.1}\exp(-3075/T)$cm^3 molecule^{-1} s^{-1}.

In many cases the contribution of a particular channel to the overall rate constant is indicated by quoting a branching ratio. This is particularly so when the contribution has only been measured at one temperature, or over a

very limited range. Thus, the entry

$$O + C_2H_5 \rightarrow CH_3CHO + H$$
$$1.1 \times 10^{-10}$$
$$\rightarrow HCHO + CH_3$$
$$k_2/k = 0.17 \pm 0.2 \text{ at } 300 \text{ K}$$

gives a value for the overall rate constant (in this case over the range 300–2500 K) for removal of reactants, $k = k_1 + k_2$, and indicates the contribution of channel 2 by giving a value for the branching ratio k_2/k at the only temperature at which it has been measured.

Temperature Range and Error Limits

Wherever possible, an attempt has been made to make recommendations for high temperatures even if this requires a considerable extrapolation from the low temperature data and consequent assignment of large error limits. However, in many cases, particularly for reactions likely to have a large activation energy, or where alternative reaction channels may become important, it has not been considered safe to extrapolate much beyond the range of existing measurements.

The preferred values are based almost exclusively on experimental data but in a few cases estimates have been made based on analogous reactions. No attempt has been made to include calculated values of rate parameters but theoretical and empirical estimates have not been ignored. They have often provided valuable background and guidance on whether experimental values are 'reasonable'.

The reliability of a preferred expression for k is expressed in terms of an estimated $\Delta \log k$ at the extremes of the temperature range covered by the recommended expression. Thus a quoted $\Delta \log k = \pm X$ is equivalent to the statement that the range of values of k encompassed by these error limits may be found by multiplication and division of k by a factor F, where $X = \log F$.

No attempt has been made to assign explicit error limits to the temperature coefficient of k. The assignment of error limits in $\Delta \log k$ at the extremes of the temperature range indicates how the quality of the data varies with temperature without attempting to define the form which this variation takes. In the opinion of the evaluators the available data rarely merit a more elaborate assignment of errors over a wide temperature range.

The assignment of error limits in k is a subjective assessment by the evaluators. Modern techniques are capable in favorable circumstances of measuring rate coefficients with the precision represented by a standard deviation as small as 10%. However, data obtained in different laboratories on the same reaction and often by the same technique are rarely concordant to the extent that might be expected from the precision of the measurements; mean values may differ by many standard deviations. This is indicative of systematic errors which are difficult to detect and which cannot be simply incorporated into quoted error limits.

Treatment of Combination and Dissociation Reactions

The rates of combination and the reverse dissociation reactions

$$A + B + M \rightleftharpoons AB + M,$$
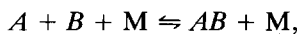
depend on the temperature, T, the nature, and the concentration of the third body [M]. The rate coefficients of these reactions have to be expressed in a form which is more complicated than those for simple bimolecular reactions. The combination reactions are described by a pseudo-second-order rate law:

$$\frac{d[AB]}{dt} = k[A][B],$$

in which the second-order rate constant depends on [M]. The low pressure third-order limit is characterized by k_0,

$$k_0([M]) = \lim_{[M] \to 0} k([M]).$$

The high pressure second-order limit is characterized by k_∞,

$$k_\infty = \lim_{[M] \to \infty} k([M]),$$

which is independent of [M]. For a combination reaction in the low-pressure range, the summary table gives a second-order rate constant expressed as the product of a third-order rate constant and the third-body concentration. The transition between the third-order and the second-order range is represented by a reduced fall off expression of k/k_∞ as a function of

$$k_0[M]/k_\infty = [M]/[M]_c,$$

where the "center of the fall-off curve" $[M]_c$ indicates the third-body concentration for which the extrapolated $k_0[M]$ would be equal to k_∞. The dependence of k on [M] in general is complicated and has to be analyzed by unimolecular rate theory. For moderately complex molecules at not too high temperatures, however, a simple approximate relationship holds:

$$k = \frac{k_0 k_\infty[M]}{k_0[M] + k_\infty} F = k_0[M]\left(\frac{1}{1 + [M]/[M]_c}\right) F$$

$$= k_\infty\left(\frac{[M]/[M]_c}{1 + [M]/[M]_c}\right) F,$$

where the first factors on the right-hand side represent the Lindemann–Hinshelwood expression, and the additional broadening factor F, at not too high temperature, is approximately given by

$$\log_{10} F \cong \frac{\log_{10} F_c}{1 + \left[\dfrac{\log_{10}([M]/[M]_c)}{N}\right]^2},$$

where $N = 0.75 - 1.27 \log_{10} F_c$. The temperature dependence of F_c, which is sometimes significant, can be estimated by the procedure of Troe and colleagues [1–3]. The results can usually be represented [3], approximately by an equation

$$F_c = (1 - a)\exp(-T/T^{***}) +$$

$$a \exp(-T/T^*) + \exp(-T^{**}/T),$$

where a, T^*, T^{**}, and T^{***} are constants. The first two terms are of importance for atmospheric conditions, but the last term in most cases becomes relevant only at high temperatures. In this way, the three quantities, k_0, k_∞, and F_c, with

$$[M]_c = \frac{k_\infty}{k_0},$$

characterize the falloff curve for the present application. Alternatively, the three quantities k_∞, $[M]_c$, and F_c (or k_0, $[M]_c$, and F_c) can be used.

The dependence of k_0 and k_∞ on the temperature is represented in the T exponent n,

$$k \propto T^{-n}$$

(except for the cases with an established energy barrier in the potential). We have used this form of temperature dependence because it often gives a better fit to the data over a wider range of temperature than does the Arrhenius expression.

In many cases values of all three parameters, k_0, k_∞, and F_c cannot be derived from the experimental data. This may not be important for modeling purposes since, if large species are concerned, the reaction may be close enough to its high pressure limit for k_∞ to be used and, correspondingly, for small reactants the low-pressure limiting rate constant, k_0, may be adequate. However, effects of pressure should always be considered and incorporated wherever possible.

In a few instances, the rate constant for the reaction has been measured under conditions where it is almost certainly pressure dependent but where the measurements cannot be analyzed to give values of k_0, k_∞ and F_c. In such cases an expression for k only is quoted.

To avoid ambiguity, the subscripts denoting infinite and zero pressure limiting rate constants have, in places, been written as superscripts, e.g., k_1^∞ or k_1^0 rather than $k_{1\infty}$ and k_{10}.

REFERENCES

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2. Troe, J., *Ber. Bunsenges. Phys. Chem.* **87**:161 (1983).
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SUMMARY OF PREFERRED RATE DATA

TABLE 1

Bimolecular Reactions

Reaction	$k(cm^3 \text{ molecule}^{-1}s^{-1})$	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
$O + OH \rightarrow O_2 + H$	$2.0 \times 10^{-11}\exp(112/T)$	220–500	± 0.2
	$2.4 \times 10^{-11}\exp(-353/T)$	1000–2000	± 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
$O + N_2 \rightarrow N + NO$	$3.0 \times 10^{-10}\exp(-38300/T)$	1400–4000	± 0.2
$O + NH \rightarrow NO + H$ $\rightarrow N + OH$	1.5×10^{-10}	1000–3380	± 0.5
$O + NH_3 \rightarrow OH + NH_2$	$1.6 \times 10^{-11}\exp(-3670/T)$	500–2500	± 0.5
$O + CH \rightarrow CO + H$	6.6×10^{-11}	300–2000	± 0.5
$\rightarrow CHO^+ + e$	$4.2 \times 10^{-13}\exp(-850/T)$	300–2500	± 0.5
$O + {}^3CH_2 \rightarrow CO + 2H$ $\rightarrow CO + H_2$	2.0×10^{-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
$O + CH_4 \rightarrow OH + CH_3$	$1.2 \times 10^{-15}T^{1.56}\exp(-4270/T)$	300–2500	± 0.3 at 300 K falling to ± 0.15 at 2500 K
$O + CHO \rightarrow OH + CO$	5.0×10^{-11}	300–2500	± 0.3
$\rightarrow CO_2 + H$	5.0×10^{-11}	300–2500	± 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
$O + CH_3OOH$ $\rightarrow OH + CH_3O_2$ $\rightarrow OH + CH_2OOH$	$3.3 \times 10^{-11}\exp(-2390/T)$	300–1000	± 0.3 at 300 K rising to ± 0.5 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 at 5000 K
$O + NCO \rightarrow NO + CO$ $\rightarrow O_2 + CN$	7.0×10^{-11}	1450–2600	± 0.8
$O + HCN \rightarrow NCO + H$ $\rightarrow CO + NH$ $\rightarrow OH + CN$	$2.3 \times 10^{-18}T^{2.1}\exp(-3075/T)$	450–2500	± 0.2 at 450 K rising to ± 0.3 at 2500 K
$O + C_2H \rightarrow CO + H$	1.7×10^{-11}	300–2500	± 1.0
$O + C_2H_2 \rightarrow CO + {}^3CH_2$ $\rightarrow CHCO + H$	$1.2 \times 10^{-17}T^{2.1}\exp(-790/T)$ $k_2/k = 0.7 \pm 0.2$ over whole range	295–2500	± 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
$O + C_2H_4 \rightarrow CH_2CHO + H$ $\rightarrow HCO + CH_3$ $\rightarrow HCHO + CH_2$ $\rightarrow CH_2CO + H_2$	$2.25 \times 10^{-17}T^{1.88}\exp(-90/T)$ $k_1/k = 0.35 \pm 0.05$ at p > 3 torr; $k_2/k = 0.6 \pm 0.10$; $k_4/k = 0.05 \pm 0.10$	300–2000	± 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

TABLE 1—(*Continued*)

Reaction	$k(cm^3\ molecule^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
$O + CHCO \rightarrow 2CO + H$	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
$O + CH_3CO \rightarrow OH + CH_2CO$ $\rightarrow CO_2 + CH_3$	3.2×10^{-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	± 0.3 at 298 K rising to ± 1.0 at 1500 K
$O + CH_3CHO \rightarrow OH + CH_3CO$ $\rightarrow OH + CH_2CHO$	$9.7 \times 10^{-12}exp(-910/T)$	298–1500	± 0.05 at 298 K rising to ± 0.5 at 1500 K
$O + C_2H_5OOH \rightarrow OH + C_2H_4OOH$ $\rightarrow OH + C_2H_5OO$	$3.3 \times 10^{-11}exp(-2390/T)$ [estimate]	300–1000	± 0.3 at 300 K rising to ± 0.5 at 1000 K
$O + C_3H_5 \rightarrow CH_2CHCHO + H$	3.0×10^{-10}	300–1000	± 0.2 over the range 300–600 K;
$\rightarrow HCHO + C_2H_3$	$< 3 \times 10^{-11}$	2000	± 0.4 over the range 600–1000 K
$O + C_6H_6 \rightarrow OH + C_6H_5$	$(k_1 + k_2) = 5.9 \times 10^{-23}T^{3.8}$ $\times exp(-473/T)$	298–2000	± 0.3
$\rightarrow C_6H_6O$	$k_2 = 3.7 \times 10^{-11}exp(-2280/T)$	298–1400	± 0.3 at 298 K falling to 0.2 at 1400K
$O + C_6H_5OH \rightarrow products$	$2.1 \times 10^{-11}exp(-1460/T)$	290–600	± 0.3
$O + C_6H_5CH_2 \rightarrow HCO + C_6H_6$ $\rightarrow C_6H_5CHO + H$	5.5×10^{-10}	300	± 0.3
$\rightarrow CH_2O + C_6H_5$	No recommendation		
$O + C_6H_5CH_3 \rightarrow products$	$5.3 \times 10^{-15}T^{1.21}exp(-1260/T)$	298–2800	± 0.1 at 298 K rising to ± 0.4 at 2800 K
$O + C_6H_5CHO \rightarrow OH + C_6H_5CO$ $\rightarrow OH + C_6H_4CHO$	$1.0 \times 10^{-11}exp(-910/T)$	298–1500	± 0.3 at 298 K rising to ± 0.7 at 1500 K
$\rightarrow C_6H_5(O)CHO$	No recommendation		
$O + p - C_6H_4(CH_3)_2 \rightarrow products$	$2.6 \times 10^{-11}exp(-1630/T)$	298–600	± 0.3
$O + C_6H_5C_2H_5 \rightarrow products$	$2.8 \times 10^{-11}exp(-1840/T)$	298–600	± 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
$O_2 + C_2H_6 \rightarrow HO_2 + C_2H_5$	$1.0 \times 10^{-10}exp(-26100/T)$	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
$O_2 + C_3H_6 \rightarrow HO_2 + CH_2CHCH_2$	$3.2 \times 10^{-12}exp(-19700/T)$	600–1000	± 0.3 at 800 K rising to ± 0.5 at 600 K and 1000 K
$O_2 + C_6H_5CH_3 \rightarrow HO_2 + C_6H_5CH_2$	$3 \times 10^{-12}exp(-20000/T)$	700–1200	± 0.7
H Atoms Reactions			
$H + O_2 \rightarrow OH + O$	$1.62 \times 10^{-10}exp(-7470/T)$	300–5000	± 0.1 at 300 K rising to ± 0.5 at 5000 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		
$H + H + Ar \rightarrow H_2 + Ar$	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		
$H + OH + N_2 \rightarrow H_2O + N_2$	See Table 3		
$H + HO_2 \rightarrow H_2 + O_2$	$7.1 \times 10^{-11}exp(-710/T)$	300–1000	± 0.3
$\rightarrow 2OH$	$2.8 \times 10^{-10}exp(-440/T)$	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

TABLE 1—(*Continued*)

Reaction	$k(cm^3\ molecule^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
$H + H_2O_2 \rightarrow H_2 + HO_2$	$2.8 \times 10^{-12}exp(-1890/T)$	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
$H + CO + M \rightarrow HCO + M$	See Table 3		
$H + {}^3CH_2 \rightarrow H_2 + CH$	$1.0 \times 10^{-11}exp(900/T)$	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 at 300 K and 2500 K reducing to ± 0.05 over range 500–1000 K
$H + CHO \rightarrow H_2 + CO$	1.5×10^{-10}	300–2500	± 0.3
$H + HCHO \rightarrow H_2 + HCO$	$2.1 \times 10^{-16}T^{1.62}exp(-1090/T)$	300–1700	± 0.1 at 300 K rising to ± 0.3 at 1700 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
$H + NCO \rightarrow NH + CO\rbrack$	8.7×10^{-11}	1400–1500	± 0.5
$\rightarrow HCN + O\rbrack$			
$H + C_2H_2 \rightarrow H_2 + C_2H$	$1.1 \times 10^{-10}exp(-14000/T)$	1000–3000	± 1.0
$\rightarrow C_2H_3$	See Table 3		
$H + C_2H_3 \rightarrow H_2 + C_2H_2$	2.0×10^{-11}	300–2500	± 0.5
$\rightarrow C_2H_4$	See Table 3		
$H + C_2H_4 \rightarrow H_2 + C_2H_3$	$9.0 \times 10^{-10}exp(-7500/T)$	700–2000	± 0.5
$\rightarrow C_2H_5$	See Table 3		
$H + C_2H_5 \rightarrow 2CH_3$	6.0×10^{-11}	300–2000	± 0.3 at 300 K rising to$^{/}$
$\rightarrow C_2H_6$	See Table 3		± 0.7 at 2000 K
$H + C_2H_6 \rightarrow H_2 + C_2H_5$	$2.4 \times 10^{-15}T^{1.5}exp(-3730/T)$	300–2000	± 0.15 at 300 K rising to ± 0.3 at 2000 K
$H + CHCO \rightarrow CH_2 + CO\rbrack$			
$\rightarrow H_2 + C_2O\rbrack$	2.5×10^{-10}	300–2500	± 0.4
$\rightarrow HCCOH\rbrack$			
$H + CH_2CO \rightarrow CH_3 + CO$	$3.0 \times 10^{-11}exp(-1700/T)$	200–2000	± 0.5 at 200 K rising to
$\rightarrow CH_2CHO$	k_2/k very small		± 1.0 at 2000 K
$H + CH_3CHO \rightarrow H_2 + CH_3CO\rbrack$	$6.8 \times 10^{-15}T^{1.16}exp(-1210/T)$	300–2000	± 0.1 at 300 K rising to
$\rightarrow H_2 + CH_2CHO\rbrack$			± 0.4 at 2000 K
$H + C_3H_5 \rightarrow C_3H_6\rbrack$	$(k_1^{\infty} + k_2) = 2.8 \times 10^{-10}$	300–1000	± 0.2 at 300 K rising to
$\rightarrow C_2H_3 + CH_3\rbrack$			± 0.5 at 1000 K
$\rightarrow H_2 + C_3H_4$	3×10^{-11}	300–1000	± 0.5
$H + C_6H_5 + M \rightarrow C_6H_6 + M$	See Table 3		
$H + C_6H_6 \rightarrow H_2 + C_6H_5$	No recommendation		
$\rightarrow C_6H_7$	See Table 3		
$H + C_6H_5O + M \rightarrow C_6H_5OH + M$	See Table 3		
$H + C_6H_5OH \rightarrow C_6H_5O + H_2$	$1.9 \times 10^{-10}exp(-6240/T)$	1000–1150	± 0.3
$\rightarrow C_6H_6 + OH$	$3.7 \times 10^{-11}exp(-3990/T)$	1000–1150	± 0.3
$H + C_6H_5CH_2 + M$	See Table 3		
$\rightarrow C_6H_5CH_3 + M$			
$H + C_6H_5CH_3 \rightarrow H_2 + C_6H_5CH_2$	$6.6 \times 10^{-22}T^{3.44}exp(-1570/T)$	600–2500	± 0.3 at 600 K rising to ± 0.5 at 2500 K
$\rightarrow H_2 + C_6H_4CH_3$	No recommendation		
$\rightarrow C_6H_6 + CH_3$	No recommendation		
$\rightarrow C_6H_6CH_3$	See Table 3		
$H + p - C_6H_4(CH_3)_2 \rightarrow products$	5.8×10^{-13}	298	± 0.1
$H + C_6H_5C_2H_5 \rightarrow H_2 + C_6H_5C_2H_4$	No recommendation		
$\rightarrow C_6H_6C_2H_5$	See Table 3		

TABLE 1—(*Continued*)

Reaction	$k(cm^3 \text{ molecule}^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
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		
$OH + HO_2 \rightarrow H_2O + O_2$	$4.8 \times 10^{-11}\exp(250/T)$	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 at 300 K rising to ± 0.5 at 1000 K
$OH + NH \rightarrow NO + H_2$ $\rightarrow H_2O + N$	8.0×10^{-11}	300–1000	± 0.5
$OH + NH_2 \rightarrow O + NH_3$	$3.3 \times 10^{-14}T^{0.405}\exp(-250/T)$	500–2500	± 0.5
$\rightarrow H_2O + NH$	No recommendation		
$OH + CO \rightarrow H + CO_2$	$1.05 \times 10^{-17}T^{1.5}\exp(250/T)$	300–2000	± 0.2 at 300 K rising to ± 0.5 at 2000 K
$OH + CH_3 \rightarrow H + CH_2OH$ $\rightarrow H + CH_3O$	No recommendation		
$\rightarrow H_2O + {}^1CH_2$	$1.2 \times 10^{-11}\exp(-1400/T)$	300–1000	± 0.5
$\rightarrow CH_3OH$	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
$OH + C_3H_5 \rightarrow H_2O + C_3H_4$	1.0×10^{-11}	300–1000	± 0.5
$\rightarrow CH_2CHCH_2OH$ $\rightarrow CH_2CHCHO + 2H$	$(k_2^\infty + k_3) = 2.5 \times 10^{-11}$	300–1000	± 0.3
$OH + C_6H_6 \rightarrow H_2O + C_6H_5$	$2.7 \times 10^{-16}T^{1.42}\exp(-730/T)$	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		

TABLE 1—(*Continued*)

Reaction	$k(cm^3$ molecule^{-1}s$^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
OH + $C_6H_5OH \rightarrow C_6H_5(OH)_2$	See Table 3		
$\rightarrow H_2O + C_6H_5O$	1.0×10^{-11}	1000–1150	± 0.5
$\rightarrow H_2O + C_6H_4OH$			
OH + $C_6H_5CH_3 \rightarrow H_2O + C_6H_5CH_2$	$8.6 \times 10^{-15}T$ exp($-440/T$)	400–1200	± 0.5 at 400 K reducing to
$\rightarrow C_6H_5CH_3OH$	See Table 3		± 0.3 at 1200 K
OH + C_6H_5CHO			
$\rightarrow H_2O + C_6H_5CO$	1.3×10^{-11}	298–1500	± 0.1 at 298 K rising to
$\rightarrow H_2O + C_6H_4CHO$			± 0.5 at 1500 K
OH + $p - C_6H_4(CH_3)_2$			
$\rightarrow C_6H_4CH_2CH_3 + H_2O$	6.4×10^{-11}exp($-1440/T$)	500–960	± 0.1
$\rightarrow p - C_6H_4(CH_3)_2OH$	See Table 3		
OH + $C_6H_5C_2H_5$			
$\rightarrow HOC_6H_5C_2H_5$	See Table 3		
$\rightarrow H_2O + C_6H_5C_2H_4$			
$\rightarrow H_2O + C_6H_4C_2H_5$	No recommendation		
H_2O Reactions			
$H_2O + M \rightarrow H + OH + M$	See Table 2		
HO_2 Radical Reactions			
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	7.0×10^{-10}exp($-6030/T$) +	550–1250	± 0.15 between 550 and
	2.2×10^{-13}exp($820/T$)		800 K rising to
			± 0.4 at 1250 K
	7.0×10^{-10}exp($-6030/T$)	850–1250	
$HO_2 + NH_2 \rightarrow NH_3 + O_2$			
$\rightarrow HNO + H_2O$	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		
$HO_2 + CH_4 \rightarrow H_2O_2 + CH_3$	1.5×10^{-11}exp($-12440/T$)	600–1000	± 0.2 at 600 K rising to
			± 0.3 at 1000 K
$HO_2 + HCHO$			
$\rightarrow H_2O_2 + CHO$	5.0×10^{-12}exp($-6580/T$)	600–1000	± 0.5
$HO_2 + CH_3O_2$			
$\rightarrow CH_3OOH + O_2$	4.1×10^{-13}exp($790/T$)	298–700	± 0.1 at 298 K rising to
$\rightarrow HCHO + H_2O + O_2$	$k_1/k = 1.0 \pm 0.1$ over whole range		to ± 0.3 at 700 K
$HO_2 + C_2H_4 \rightarrow OH + C_2H_4O$	3.7×10^{-12}exp($-8650/T$)	600–900	± 0.15 at 600 K rising to
			± 0.25 at 900 K
$HO_2 + C_2H_6 \rightarrow H_2O_2 + C_2H_5$	2.2×10^{-11}exp($-10300/T$)	500–1000	± 0.2 at 500 K rising to
			± 0.3 at 1000 K
$HO_2 + CH_3CHO$			
$\rightarrow H_2O_2 + CH_3CO$	5.0×10^{-12}exp($-6000/T$)	900–1200	± 0.7
$HO_2 + C_3H_5 \rightarrow C_3H_6 + O_2$	4.4×10^{-12}	300–1000	± 0.3 over the range
			600–800 K
			rising to 0.5 at other
			temperatures
$\rightarrow CO$ + products	1.1×10^{-11}	500–900	± 0.3
$HO_2 + C_6H_5CH_3$			
$\rightarrow H_2O_2 + C_6H_5CH_2$	6.6×10^{-13}exp($-7080/T$)	600–1000	± 0.3 at 750 K rising to
			± 0.5 at 600 K and 1000 K
$\rightarrow H_2O_2 + C_6H_4CH_3$	9.1×10^{-12}exp($-14500/T$)	600–1000	± 1.0
$HO_2 + C_6H_5CH_2CH_3$			
$\rightarrow H_2O_2 + C_6H_5CHCH_3$	4.4×10^{-13}exp($-5680/T$)	600–1000	± 0.3 at 750 K rising to
			± 0.5 at 600 and 1000 K
$\rightarrow H_2O_2 + C_6H_5CH_2CH_2$	5.3×10^{-12}exp($-9760/T$)	600–1000	± 0.5
$\rightarrow H_2O_2 + C_6H_4CH_2CH_3$	9×10^{-12}exp($-14500/T$)	600–1000	± 1.0

TABLE 1—(*Continued*)

Reaction	$k(cm^3$ molecule$^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
H_2O_2 *Reactions*			
$H_2O_2 + M \rightarrow 2OH + M$	See Table 2		
N Atom Reactions			
$N + O_2 \rightarrow NO + O$	$1.5 \times 10^{-14}T$ exp($-3270/T$)	298–5000	± 0.12 over range 300–1000 K rising to ± 0.3 over range 1000–5000 K
$N + OH \rightarrow NO + H$	4.7×10^{-11}	300–2500	± 0.1 at 300 K rising to ± 0.3 at 2500 K
$N + NO \rightarrow N_2 + O$	7.1×10^{-11}exp($-790/T$)	1400–4000	± 0.2
$N + CN \rightarrow N_2 + C$	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
NH Radical Reactions			
$NH + O_2 \rightarrow NO + OH$ ⎤	$(k_1 + k_2) = 1.3$		
$\rightarrow HNO + O$ ⎦	$\times 10^{-13}$exp($-770/T$)	270–550	± 0.25
$\rightarrow HNO + O$	6.5×10^{-11}exp($-9000/T$)	2200–3500	± 0.5
$NH + NO \rightarrow N_2O + H$ ⎤			
$\rightarrow HN_2 + O$ ⎥	5.0×10^{-11}	270–380	± 0.2
$\rightarrow N_2 + OH$ ⎦	2.8×10^{-10}exp($-6400/T$)	2220–3350	± 0.5
NH$_2$ Radical Reactions			
$NH_2 + O_2 \rightarrow$ products	$< 3 \times 10^{-18}$	298	
$NH_2 + NO \rightarrow N_2 + H_2O$ ⎤			
$\rightarrow N_2 + H + OH$ ⎥	1.8×10^{-12}exp($650/T$)	220–2000	± 0.5
$\rightarrow N_2H + OH$ ⎥	$(k_2 + k_3)/k \approx 0.12$ at 298 K		
$\rightarrow N_2O + H_2$ ⎦			
NH$_3$ Reactions			
$NH_3 + M \rightarrow NH_2 + H$	See Table 2		
$\rightarrow NH + H_2$	No recommendation		
C Atom Reactions			
$C + N_2 \rightarrow CN + N$	8.7×10^{-11}exp($-22600/T$)	2000–5000	± 0.2
$C + NO \rightarrow CN + O$ ⎤	2.5×10^{-11}	300	± 0.3
$\rightarrow CO + N$ ⎦	8.0×10^{-11}	1500–4050	± 0.3
	$k_1/k_2 = 0.6 \pm 0.25$;		
	$k_1/k = 0.4 \pm 0.25$		
	over range 1500–4050 K		
$^1C_2$ *and* $^3C_2$ *Radical Reactions*	See data sheets		
CH Radical Reactions			
$CH + O_2 \rightarrow CHO + O$ ⎤	5.5×10^{-11}	300–2000	± 0.3 at 300 K rising to ± 0.5 at 2000 K
$\rightarrow CO + OH$ ⎦			
$CH + H_2 \rightarrow CH_2 + H$ ⎤	2.4×10^{-10}exp($-1760/T$)	300–1000	± 0.3
$\rightarrow CH_3$ ⎦			
$CH + H_2O \rightarrow$ products	9.5×10^{-12}exp($380/T$)	300–1000	± 1.0
$CH + N_2 \rightarrow HCN + N$ ⎤	2.6×10^{-12}exp($-9030/T$)	2000–4000	± 0.3
$\rightarrow CHN_2$ ⎦	at $p < 1$ atm		
$CH + NO \rightarrow CO + NH$ ⎤			
$\rightarrow CN + OH$ ⎥	2.0×10^{-10}	300–4000	± 0.25
$\rightarrow HCN + O$ ⎦			
$CH + CO \rightarrow$ products	4.6×10^{-13}exp($860/T$)	300–1000	± 1.0
$CH + CO_2 \rightarrow$ products	5.7×10^{-12}exp($-345/T$)	300–1000	± 1.0
$CH + CH_4 \rightarrow$ products	5.0×10^{-11}exp($200/T$)	200–700	± 1.0
$CH + C_2H_2 \rightarrow$ products	3.5×10^{-10}exp($61/T$)	200–700	± 1.0
$CH + C_2H_4 \rightarrow$ products	2.2×10^{-10}exp($173/T$)	200–700	± 1.0
$CH + C_2H_6 \rightarrow$ products	1.8×10^{-10}exp($132/T$)	200–700	± 1.0

TABLE 1—(*Continued*)

Reaction	$k(cm^3 \text{ molecule}^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
$CH + C_3H_8 \rightarrow$ products	$1.9 \times 10^{-10}\exp(240/T)$	300–700	± 1.0
$CH + n - C_4H_{10} \rightarrow$ products	$4.4 \times 10^{-10}\exp(28/T)$	250–700	± 1.0
$CH + i - C_4H_{10} \rightarrow$ 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
$^3CH_2$ *Radical Reactions*			
$\begin{array}{l} ^3CH_2 + O_2 \rightarrow CO + H + OH \\ \rightarrow CO_2 + H + H \\ \rightarrow CO + H_2O \\ \rightarrow CO_2 + H_2 \\ \rightarrow HCHO + O \end{array}$	$4.1 \times 10^{-11}\exp(-750/T)$	300–1000	± 0.1 at 300 K rising to ± 0.5 at 1000 K
$\begin{array}{l} ^3CH_2 + {}^3CH_2 \rightarrow C_2H_2 + H_2 \\ \rightarrow C_2H_2 + 2H \end{array}$	$2.0 \times 10^{-10}\exp(-400/T)$ $k_2/k = 0.9 \pm 0.1$ 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		
$\begin{array}{l} ^3CH_2 + C_2H_4 \\ \rightarrow C_3H_6 \\ \rightarrow c\text{-}C_3H_6 \\ \rightarrow CH_2CHCH_2 + H \end{array}$	See Table 3		
$^1CH_2$ *Radical Reactions*			
$^1CH_2 + Ar \rightarrow {}^3CH_2 + Ar$	6.0×10^{-12}	300–2000	± 0.3
$^1CH_2 + NO \rightarrow$ products	1.6×10^{-10}	290–650	± 0.2
$^1CH_2 + N_2 \rightarrow {}^3CH_2 + N_2$	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
$^1CH_2 + C_2H_4 \rightarrow {}^3CH_2 + C_2H_4$	4.0×10^{-11}	300–2000	± 0.4
$^1CH_2 + C_2H_6 \rightarrow {}^3CH_2 + C_2H_6$	3.6×10^{-11}	300–2000	± 0.4
$\begin{array}{l} ^1CH_2 + O_2 \rightarrow CO + H + OH \\ \rightarrow CO_2 + H_2 \\ \rightarrow CO + H_2O \\ \rightarrow {}^3CH_2 + O_2 \end{array}$	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
$\begin{array}{l} ^1CH_2 + C_2H_2 \rightarrow CH_2CCH_2 \\ \rightarrow CH_3CCH \\ \rightarrow CH_2CCH + H \end{array}$	See Table 3		
$\rightarrow {}^3CH_2 + C_2H_2$	See earlier entry		
$\begin{array}{l} ^1CH_2 + C_2H_4 \rightarrow C_3H_6 \\ \rightarrow {}^3CH_2 + C_2H_4 \end{array}$	See Table 3 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		
$CH_3 + H_2 \rightarrow CH_4 + H$	$1.14 \times 10^{-20}T^{2.74}\exp(-4740/T)$	300–2500	± 0.15 in the range 300–700 K ± 0.3 in the range 700–2500 K
$CH_3 + CO + M \rightarrow CH_3CO + M$	See Table 3		
$CH_3 + CH_3 \rightarrow C_2H_5 + H$	$5 \times 10^{-11}\exp(-6800/T)$	1300–2500	± 0.6
$\rightarrow C_2H_4 + H_2$	No recommendation (see data sheets)		
$\rightarrow C_2H_6$	See Table 3		

TABLE 1—(*Continued*)

Reaction	$k(cm^3 \text{ molecule}^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
$CH_3 + HCHO \rightarrow CH_4 + HCO$	$1.3 \times 10^{-31}T^{6.1}\exp(-990/T)$	300–2000	± 0.2
$CH_3 + C_2H_2 + M \rightarrow C_3H_5 + M$	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
$\rightarrow n - C_3H_7$	See Table 3		
$CH_3 + C_2H_5 \rightarrow CH_4 + C_2H_4$	1.9×10^{-12}	300–2000	± 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
$CH_3 + CH_3CHO$			
$\rightarrow CH_4 + CH_3CO$	$3.3 \times 10^{-30}T^{5.6}\exp(-1240/T)$	300–1250	± 0.3
$\rightarrow CH_4 + CH_2CHO$	No recommendation (see data sheets)		
$CH_3 + C_3H_5 \rightarrow C_2H_5CHCH_2$	See Table 3		
$\rightarrow CH_4 + CH_2CCH_2$	3.5×10^{-13}	500–1200	± 0.5
CH_4 Reactions			
$CH_4 + M \rightarrow CH_3 + H + M$	See Table 2		
CHO Radical Reactions			
$CHO + Ar \rightarrow H + CO + Ar$	See Table 2		
$CHO + O_2 \rightarrow CO + HO_2$			
$\rightarrow OH + CO_2$	5.0×10^{-12}	300–2500	± 0.3
$\rightarrow HCO_3$			
$CHO + CHO \rightarrow HCHO + CO$	5.0×10^{-11}	300	± 0.3
HCHO Reactions			
$HCHO + M$			
$\rightarrow H + CHO + M$	See Table 2		
$\rightarrow H_2 + CO + M$			
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		
$CH_3O + O_2 \rightarrow HCHO + HO_2$	$3.6 \times 10^{-14}\exp(-880/T)$	300–1000	± 0.1 at 500 K rising to ± 0.3 at 300 K and 1000 K
CH_3O_2 Radical Reactions			
$CH_3O_2 + CH_3O_2$			
$\rightarrow CH_3O + CH_3O + O_2$	$9.1 \times 10^{-14}\exp(420/T)$	298–700	± 0.1 at 298 K increasing to ± 0.3 at 700 K
$\rightarrow CH_3OH + HCHO + O_2$	$k_1/k_2 = 25 \exp(-1170/T)$;		
$\rightarrow CH_3OOCH_3 + O_2$	$k_3 = 0$ over whole range		
$CH_3O_2 + C_3H_5$			
$\rightarrow CH_3O + CH_2CHCH_2O$	2.0×10^{-11}	500–1200	± 0.5
CH_3OH Reactions			
$CH_3OH + Ar \rightarrow CH_3 + OH + Ar$	See Table 2		
$\rightarrow CH_2OH + H + Ar$			
$\rightarrow {}^1CH_2 + H_2O + Ar$			
CH_3OOH Reactions			
$CH_3OOH + M$			
$\rightarrow CH_3O + OH + M$	See Table 2		
CN Radical Reactions			
$CN + O_2 \rightarrow NCO + O$	$1.2 \times 10^{-11}\exp(210/T)$	290–4500	± 0.15 over the range 290–4500 K
$CN + H_2 \rightarrow HCN + H$	$3.2 \times 10^{-20}T^{2.87}\exp(-820/T)$	200–3500	± 0.2 at 200 K rising to ± 0.5 at 3500 K
$CN + H_2O \rightarrow HCN + OH$			± 0.3 at 500 K rising to
$\rightarrow HOCN + H$	$1.3 \times 10^{-11}\exp(-3750/T)$	500–3000	± 0.5 at 3000 K
$CN + CH_4 \rightarrow HCN + CH_3$	$1.5 \times 10^{-19}T^{2.64}\exp(150/T)$	290–1500	± 0.3
NCO Radical Reactions			
$NCO + M \rightarrow N + CO + M$	See Table 2		

TABLE 1—(*Continued*)

Reaction	$k(cm^3\ molecule^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
NCO + NO → N$_2$O + CO → N$_2$ + CO$_2$ → N$_2$ + CO + O	$2.3 \times 10^{-6}T^{-1.73}exp(-380/T)$	290–3000	±0.25
C$_2$H Radical Reactions			
C$_2$H + O$_2$ → CO$_2$ + CH → 2CO + H → C$_2$HO + O → CO + HCO	3.0×10^{-11}	300	±0.5
C$_2$H + H$_2$ → C$_2$H$_2$ + H	$1.8 \times 10^{-11}exp(-1090/T)$	300–2500	±0.3 at 300 K rising to ±0.5 at 2500 K
C$_2$H + C$_2$H$_2$ → C$_4$H$_2$ + H	1.5×10^{-10}	300–2700	±0.5
C$_2$H + CH$_4$ → products	3.0×10^{-12}	298	±1
C$_2$H + C$_2$H$_6$ → products	No recommendation		
C$_2$H$_3$ Radical Reactions			
C$_2$H$_3$ + M → C$_2$H$_2$ + H + M	See Table 2		
C$_2$H$_3$ + O$_2$ → HO$_2$ + C$_2$H$_2$ → H$_2$CO + CHO → C$_2$H$_3$O + O → C$_2$H$_3$O$_2$	9.0×10^{-12}	300–2000	±0.3 over range 300–600 K; ±0.5 over range 600–2000 K
C$_2$H$_4$ Reactions			
C$_2$H$_4$ + M → C$_2$H$_2$ + H$_2$ + M → C$_2$H$_3$ + H + M	See Table 2		
C$_2$H$_5$ Radical Reactions			
C$_2$H$_5$ + M → C$_2$H$_4$ + H + M	See Table 2		
C$_2$H$_5$ + O$_2$ → C$_2$H$_4$ + HO$_2$	$1.7 \times 10^{-14}exp(1100/T)$	600–1200	±0.3
C$_2$H$_5$ + H$_2$ → C$_2$H$_6$ + H	$5.1 \times 10^{-24}T^{3.6}exp(-4250/T)$	700–1200	±0.2 at 700 K rising to ±0.6 at 1200 K
C$_2$H$_5$ + C$_2$H$_2$ → C$_2$H$_5$CHCH	$5.6 \times 10^{-14}exp(-3520/T)$	300–600	±0.5
C$_2$H$_5$ + C$_2$H$_4$ → $n - C_4H_9$	$1.8 \times 10^{-13}exp(-3670/T)$	300–600	±0.5
C$_2$H$_5$ + C$_2$H$_5$ → $n - C_4H_{10}$ → C$_2$H$_6$ + C$_2$H$_4$	See Table 3 2.4×10^{-12}	300–1200	±0.4
C$_2$H$_5$ + C$_2$H$_5$CHO → C$_2$H$_6$ + C$_2$H$_5$CO	$2.9 \times 10^{-13}exp(-3660/T)$	300–700	±0.3
C$_2$H$_5$ + C$_3$H$_5$ → CH$_3$CH$_2$CH$_2$CHCH$_2$ → C$_2$H$_6$ + CH$_2$CCH$_2$ → C$_2$H$_4$ + C$_3$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	 ±0.3 ±0.4
C$_2$H$_6$ Reactions			
C$_2$H$_6$ + M → CH$_3$ + CH$_3$ + M	See Table 2		
CHCO Reactions			
CHCO + O$_2$ → CO$_2$ + HCO → 2CO + OH → C$_2$O + HO$_2$ → CHO$_2$CO	$2.7 \times 10^{-12}exp(-430/T)$ M = He, 2 torr	300–550	±0.7
CH$_2$CHO Radical Reactions			
CH$_2$CHO + O$_2$ → HO$_2$ + CH$_2$CO → HCHO + CO + OH → O$_2$CH$_2$CHO	$k_\infty = 2.6 \times 10^{-13}$ $k_2 = 3.0 \times 10^{-14}$	250–500 300	±0.2 ±0.3
CH$_3$CO Radical Reactions			
CH$_3$CO + O$_2$ + M → CH$_3$CO$_3$ + M	See Table 3		
CH$_3$CHO Reactions			
CH$_3$CHO + M → CH$_3$ + HCO + M	See Table 2		

TABLE 1—(*Continued*)

Reaction	$k(cm^3 \text{ molecule}^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
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_3H_5 *Radical Reactions*			
$C_3H_5 + M \rightarrow CH_2CCH_2 + H + M$	See Table 2		
$C_3H_5 + O_2 \rightarrow CH_2CCH_2 + HO_2$	$1.7 \times 10^{-12}\exp(-11400/T)$	600–1200	± 0.3 at 600 K rising to ± 0.5 at 1200 K
$\rightarrow CO + $ products	$7.6 \times 10^{-12}\exp(-9450/T)$	600–1200	± 0.3
$C_3H_5 + H_2 \rightarrow C_3H_6 + H$	$1.8 \times 10^{-19}T^{2.4}\exp(-9550/T)$	300–1100	± 0.7 at 300 K reducing to ± 0.3 at 1100 K
$C_3H_5 + CH_4 \rightarrow C_3H_6 + CH_3$	$6.6 \times 10^{-23}T^{3.4}\exp(-11670/T)$	300–1200	± 0.4
$C_3H_5 + C_2H_4 \rightarrow C_3H_6 + C_2H_3$	$6.6 \times 10^{-23}T^{3.4}\exp(-13120/T)$	600–1200	± 0.5
$\rightarrow c - C_5H_8 + H$	$1.0 \times 10^{-13}\exp(-9620/T)$	600–1200	± 0.7
$C_3H_5 + C_2H_6 \rightarrow C_3H_6 + C_2H_5$	$3.9 \times 10^{-22}T^{3.3}\exp(-9990/T)$	300–1200	± 0.4
$C_3H_5 + C_3H_5$			
$\rightarrow CH_2CHCH_2CH_2CHCH_2$	See Table 3		
$\rightarrow C_3H_6 + CH_2CCH_2$	$1.0 \times 10^{-13}\exp(132/T)$	300–1000	± 0.7
$C_3H_5 + C_3H_8$			
$\rightarrow C_3H_6 + CH_3CH_2CH_2$	$3.9 \times 10^{-22}T^{3.3}\exp(-9990/T)$	300–1200	± 0.4 over the range 600 to
$\rightarrow C_3H_6 + CH_3CHCH_3$	$1.3 \times 10^{-22}T^{3.3}\exp(-8660/T)$	300–1200	1000 K rising to ± 0.7 at other temperatures
$C_3H_5 + 2 - C_4H_8$			
$\rightarrow C_3H_6 + CH_2CHCHCH_3$	$6.6 \times 10^{-12}\exp(-8180/T)$	600–1000	± 0.5
$\rightarrow C_3H_6 + CH_3CCHCH_3$	$3.3 \times 10^{-23}T^{3.4}\exp(-12160/T)$	600–1000	± 0.5
$\rightarrow CH_2CHCH_2CH(CH_3)CHCH_3$	See Table 3		± 0.4 over the range
$C_3H_5 + i - C_4H_{10}$			
$\rightarrow C_3H_6 + (CH_3)_2CHCH_2$	$5.9 \times 10^{-22}T^{3.3}\exp(-9990/T)$	300–1200	± 0.4 over the range
$\rightarrow C_3H_6 + (CH_3)_3C$	$0.7 \times 10^{-22}T^{3.3}\exp(-7800/T)$	300–1200	600 to 1000 K rising to ± 0.7 at other temperatures
$C_3H_5 + HCHO \rightarrow C_3H_6 + HCO$	$1.2 \times 10^{-16}T^{1.8}\exp(-9155/T)$	300–1000	± 0.4
$C_3H_5 + C_6H_5CH_3$			
$\rightarrow C_3H_6 + C_6H_5CH_2$	$3.3 \times 10^{-12}\exp(-8660/T)$	600–1000	± 0.4
$i - C_3H_7$ *Radical Reactions*			
$i - C_3H_7 + M \rightarrow C_3H_6 + H + M$	See Table 2		
$i - C_3H_7 + O_2 \rightarrow C_3H_6 + HO_2$	$3.3 \times 10^{-14}\exp(+1290/T)$	600–800	± 0.5
$i - C_3H_7 + H_2 \rightarrow C_3H_8 + H$	$1.3 \times 10^{-23}T^{3.28}\exp(-4360/T)$	300–1200	± 0.5
$i - C_3H_7 + C_2H_2$			
$\rightarrow (CH_3)_2CHCHCH$	$5.3 \times 10^{-14}\exp(-3470/T)$	300–600	± 0.5
$i - C_3H_7 + C_2H_4$			
$\rightarrow (CH_3)_2CHCH_2CH_2$	$7.5 \times 10^{-14}\exp(-3470/T)$	300–600	± 0.5
$i - C_3H_7 + i - C_3H_7$			
$\rightarrow C_6H_{14}$	See Table 3	300–1000	± 0.1 at 300 K rising to ± 0.3 at 1000 K
$\rightarrow C_3H_8 + C_3H_6$	4.2×10^{-12}	300–1000	± 0.1 at 300 K rising to ± 0.5 at 1000 K
$i - C_3H_7 + i - C_3H_7CHO$			
$\rightarrow C_3H_8 + (CH_3)_2CHCO$ $\rightarrow C_3H_8 + (CH_3)_2CCHO$	$6.6 \times 10^{-14}\exp(-3170/T)$	300–650	± 0.5
$\rightarrow C_3H_8 + CH_2CH(CH_3)CHO$	$5.3 \times 10^{-14}\exp(-4780/T)$	500–650	± 0.5

<div style="text-align:center">**TABLE 1**—(*Continued*)</div>

Reaction	$k(cm^3\ molecule^{-1}s^{-1})$	Temp (K)	Error limits ($\Delta \log k$)
C_3H_8 *Reactions*			
$C_3H_8 + M \rightarrow CH_3 + C_2H_5 + M$	See Table 2		
$t - C_4H_9$ *Radical Reactions*			
$t - C_4H_9 + M$			
$\rightarrow i - C_4H_8 + H + M$	See Table 2		
$t - C_4H_9 + O_2 \rightarrow i - C_4H_8 + HO_2$	$5 \times 10^{-14}\exp(+2115/T)$	600–800	± 0.5
$t - C_4H_9 + H_2 \rightarrow i - C_4H_{10} + H$	$3.1 \times 10^{-26}T^{4.24}\exp(-4510/T)$	300–1200	± 0.5
$t - C_4H_9 + C_2H_2$			
$\rightarrow (CH_3)_3CCHCH$	$1.2 \times 10^{-13}\exp(-4320/T)$	300–600	± 0.5
$t - C_4H_9 + C_2H_4$			
$\rightarrow (CH_3)_2CCH_2CH_2$	$3.3 \times 10^{-14}\exp(-4020/T)$	300–650	± 0.5
$t - C_4H_9 + t - C_4H_9$			
$\rightarrow C_8H_{18}$	See Table 3		
$\rightarrow i - C_4H_{10} + i - C_4H_8$	$1.2 \times 10^{-7}T^{-1.73}$	300–1000	± 0.15 at 300 K rising to ± 0.5 at 1000 K
$t - C_4H_9 + t - C_4H_9CHO$			
$\rightarrow i - C_4H_{10} + t - C_4H_9CO$	$1.0 \times 10^{-14}\exp(-3200/T)$	300–700	± 0.5
$\rightarrow i - C_4H_{10}$			
$+ CH_2C(CH_3)_2CHO$	$3.9 \times 10^{-14}\exp(-5540/T)$	500–700	± 0.5
C_6H_5 *Radical Reactions*			
$C_6H_5 + M \rightarrow C_2H_2 + C_4H_3 + M$ ⎤			
$\rightarrow C_2H_3 + C_4H_2 + M$ ⎟	See Table 2		
$\rightarrow linear - C_6H_5 + M$ ⎦			
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*			
$C_6H_5CH_2 + M$			
$\rightarrow C_3H_3 + 2C_2H_2 + M$ ⎤			
$\rightarrow C_4H_4 + C_3H_3 + M$ ⎟			
$\rightarrow C_5H_5 + C_2H_2 + M$ ⎟	See Table 2		
$\rightarrow C_7H_7 + M$ ⎦			
$C_6H_5CH_3$ *Reactions*			
$C_6H_5CH_3 + M$			
$\rightarrow C_6H_5CH_2 + H + M$ ⎤	See Table 2		
$\rightarrow C_6H_5 + CH_3 + M$ ⎦			
$p - C_6H_4(CH_3)_2$ *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*			
$C_6H_5C_2H_5 + M$			
$\rightarrow C_6H_5CH_2 + CH_3 + M$ ⎤			
$\rightarrow C_6H_6 + C_2H_4 + M$ ⎟			
$\rightarrow C_6H_5CHCH_2 + H_2 + M$ ⎟	See Table 2		
$\rightarrow C_6H_5 + C_2H_5 + M$ ⎟			
$\rightarrow C_6H_5CHCH_3 + H + M$ ⎦			

TABLE 2

Decomposition Reactions

Reaction	$k_\infty(s^{-1})$ k_0 (cm^3 molecule^{-1} s^{-1}) F_c $k\,(s^{-1}) = \dfrac{k_0 k_\infty[M]}{k_0[M] + k_\infty}F$	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
$H_2O_2 + M \rightarrow 2OH + M$	$k_0(Ar) = 3 \times 10^{-8}\exp(-21600/T)$	1000–1500	±0.2
	$k_0(N_2) = 2 \times 10^{-7}\exp(-22900/T)$	700–1500	±0.2
	$k_\infty = 3 \times 10^{14}\exp(-24400/T)$	1000–1500	±0.5
	$F_c(Ar) = 0.5$	700–1500	$\Delta F_c = \pm0.1$
$NH_3 + Ar \rightarrow NH_2 + H + Ar$	$k_0 = 7.4 \times 10^{-9}\exp(-41560/T)$	2000–3000	±0.3
	$k_\infty = 8.3 \times 10^{15}\exp(-55170/T)$	2000–3000	±0.4
	$F_c = 0.58\exp(-T/4581)$		
	$\quad + 0.42\exp(-T/102)$	2000–3000	$\Delta F_c = \pm0.1$
$CH_3 + M \rightarrow CH_2 + H + M$	$k_0 = 1.7 \times 10^{-8}\exp(-45600/T)$	1500–3000	±0.5
$CH_4 + M \rightarrow CH_3 + H + M$	$k_0(Ar) = 7.5 \times 10^{-7}\exp(-45700/T)$	1000–1700	±0.3
	$k_0(Ar) = 7.8 \times 10^{23}T^{-8.2}\exp(-59200/T)$	1700–5000	±0.3
	$k_0(CH_4) = 1.4 \times 10^{-6}\exp(-45700/T)$	1000–2000	±0.3
	$k_\infty = 2.4 \times 10^{16}\exp(-52800/T)$	1000–3000	±0.5
	$F_c(Ar) = \exp(-T/1350)$		
	$\quad + \exp(-7830/T)$	1000–5000	$\Delta F_c = \pm0.1$
	$F_c(CH_4) = 0.31\exp(-T/90)$		
	$\quad + 0.69(-T/2210)$	1000–2000	$\Delta F_c = \pm0.1$
$HCO + Ar \rightarrow H + CO + Ar$	$k_0 = 2.6 \times 10^{-10}\exp(-7930/T)$	600–2500	±0.5
$HCHO + M \rightarrow H + CHO + M$ ⎤	$k_0(Ar) = 2.7$		
$\qquad \rightarrow H_2 + CO + M$ ⎦	$\quad \times 10^{12}T^{-5.54}\exp(-48660/T)$	1700–3200	±0.3
	$k_0(2)/k_0 = 0.7 \pm 0.4$	2000–3000	
$CH_3O + M \rightarrow HCHO + H + M$	$k_0 = 9.0 \times 10^{-11}\exp(-6790/T)$	300–1700	±0.3
$CH_3OH + Ar$ ⎤	$k_0 = 1.1 \times 10^{-7}\exp(-33080/T)$	1000–2000	±0.3
$\quad \rightarrow CH_3 + OH + Ar$ ⎥	$k_\infty = 1.7 \times 10^{16}\exp(-45740/T)$	1000–2000	±0.5
$\quad \rightarrow CH_2OH + H + Ar$ ⎥	$F_c = 0.18\exp(-T/200)$	1000–2000	$\Delta F_c = \pm0.1$
$\quad \rightarrow {}^1CH_2 + H_2O + Ar$ ⎦	$\quad + 0.82\exp(-T/1438)$		
$CH_3OOH + M$			
$\quad \rightarrow CH_3O + OH + M$	$k_\infty = 6 \times 10^{14}\exp(-21300/T)$	500–800	±0.2 at 600 K rising to ±0.5 at 500 and 800 K
$NCO + Ar \rightarrow N + CO + Ar$	$k_0 = 1.7 \times 10^{-9}\exp(-23500/T)$	1450–2600	±0.4
$C_2H_3 + M \rightarrow C_2H_2 + H + M$	$k_0 = 6.9 \times 10^{17}T^{-7.5}\exp(-22900/T)$	500–2500	±0.5
	$k_\infty = 2 \times 10^{14}\exp(-20000/T)$	500–2500	±0.5
	$F_c = 0.35$	500–2500	$\Delta F_c = \pm0.1$
$C_2H_4 + M \rightarrow C_2H_2 + H_2 + M$	$k_0(Ar, Kr) = 5.8$		
	$\quad \times 10^{-8}\exp(-36000/T)$	1500–3200	±0.3
$\qquad \rightarrow C_2H_3 + H + M$	$k_0(Ar) = 4.3 \times 10^{-7}\exp(-48600/T)$	1500–3200	±0.5
$C_2H_5 + C_2H_6$			
$\quad \rightarrow C_2H_4 + H + C_2H_6$	$k_0 = 1.7 \times 10^{-6}\exp(-16800/T)$	700–900	±0.3
	$k_\infty = 8.2 \times 10^{13}\exp(-20070/T)$	700–1100	±0.3
	$F_c = 0.25\exp(-T/97)$		
	$\quad + 0.75\exp(-T/1379)$	700–1100	$\Delta F_c = \pm0.1$
$C_2H_6 + M \rightarrow 2CH_3 + M$	$k_0(Ar) = 1.1$		
	$\quad \times 10^{25}T^{-8.24}\exp(-47090/T)$	300–2000	±0.5
	$k_0(C_2H_6) = 4.5$		
	$\quad \times 10^{-2}\exp(-41930/T)$	800–1000	±0.5
	$k_\infty = 1.8$		
	$\quad \times 10^{21}T^{-1.24}\exp(-45700/T)$	300–2000	±0.3
	$F_c(Ar) = 0.38\exp(-T/73)$		
	$\quad + 0.62\exp(-T/1180)$	300–2000	$\Delta F_c = \pm0.1$

TABLE 2—(*Continued*)

Reaction	$k_\infty(\text{s}^{-1})$ k_0 (cm^3 molecule^{-1} s^{-1}) F_c k (s^{-1}) $= \dfrac{k_0 k_\infty [\text{M}]}{k_0[\text{M}] + k_\infty} F$	Temp (K)	Error limits ($\Delta \log k$)
	$F_c(\text{C}_2\text{H}_6) = 0.54 \exp(-T/1250)$	800–1000	$\Delta F_c = \pm 0.1$
CH$_3$CO + M $\rightarrow$ CH$_3$ + CO + M	$k_0(\text{He}) = 1.0 \times 10^{-8}\exp(-7080/T)$	400–500	± 0.2
	$k_0(\text{Ar}) = 7.0 \times 10^{-18}$	353	± 0.4
	$k_\infty = 2.8 \times 10^{13}\exp(-8630/T)$	300–500	± 0.5
	$F_c(\text{He}) = 0.5$	400–500	$\Delta F_c = \pm 0.1$
CH$_3$CHO + M $\rightarrow$ CH$_3$ + CHO + M	$k(1 \text{ atm}) = 7$ $\times 10^{15}\exp(-41100/T)$ (pressure-dependent region)	750–1200	± 0.4
C$_2$H$_5$O + M $\rightarrow$ HCHO + CH$_3$ + M	$k_\infty = 8 \times 10^{13}\exp(-10830/T)$ [estimate]	300–600	± 1.0
C$_2$H$_5$OOH + M $\rightarrow$ C$_2$H$_5$O + OH + M	$k_\infty = 4 \times 10^{15}\exp(-21600/T)$	400–800	± 0.3
C$_3$H$_5$ + M $\rightarrow$ CH$_2$CCH$_2$ + H + M	$k_\infty = 1.5 \times 10^{11}T^{0.84}\exp(-30050/T)$	800–1500	± 0.3
i – C$_3$H$_7$ + He $\rightarrow$ C$_3$H$_6$ + H + He	$k_0 = 3.6 \times 10^{-7}\exp(-14200/T)$	750–830	± 0.3
	$k_\infty = 8.76$ $\times 10^7 T^{1.76}\exp(-17870/T)$	170–1000	± 0.3
	$F_c(\text{He}) = 0.35$	750–830	$\Delta F_c = \pm 0.1$
C$_3$H$_8$ + Ar $\rightarrow$ CH$_3$ + C$_2$H$_5$ + Ar	$k_0 = 1.3 \times 10^{-5}\exp(-32700/T)$	700–2000	± 0.5
	$k_\infty = 1.1 \times 10^{17}\exp(-42470/T)$	700–2000	± 0.3
	$F_c = 0.24 \exp(-T/1946)$ $+ 0.76 \exp(T/38)$	700–2000	$\Delta F_c = \pm 0.2$
t – C$_4$H$_9$ + M $\rightarrow i$ – C$_4$H$_8$ + H + M	$k_\infty = 8.3 \times 10^{13}\exp(-19200/T)$	300–800	± 0.5
C$_6$H$_5$ + M $\rightarrow$ C$_2$H$_2$ + C$_4$H$_3$ + M ⎤ $\rightarrow$ C$_2$H$_3$ + C$_4$H$_2$ + M ⎦	No recommendation		
$\rightarrow$ linear – C$_6$H$_5$ + M	$4.0 \times 10^{13}\exp(-36700/T)$	1450–1900	± 0.4
C$_6$H$_6$ + M $\rightarrow$ C$_6$H$_5$ + H + M ⎤ $\rightarrow$ C$_4$H$_4$ + C$_2$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$_6$H$_5$O + M $\rightarrow$ C$_5$H$_5$ + CO + M	$2.5 \times 10^{11}\exp(-22100/T)$	1000–1580	± 0.2
C$_6$H$_5$CH$_2$ + M $\rightarrow$ C$_3$H$_3$ + 2C$_2$H$_2$ + M ⎤ $\rightarrow$ C$_4$H$_4$ + C$_3$H$_3$ + M ⎪ $\rightarrow$ C$_5$H$_5$ + C$_2$H$_2$ + M ⎪ $\rightarrow$ C$_7$H$_7$(BCH) + M ⎦	$5.1 \times 10^{13}\exp(-36370/T)$	1350–1900	± 0.3 at 1350 K rising to ± 0.5 at 1900 K
C$_6$H$_5$CH$_3$ + M $\rightarrow$ C$_6$H$_5$CH$_2$ + H + M	$3.1 \times 10^{15}\exp(-44890/T)$	920–2200	± 0.3 at 920 K rising to ± 0.5 at 2200 K
$\rightarrow$ C$_6$H$_5$ + CH$_3$ + M	No recommendation		
p-C$_6$H$_4$(CH$_3$) + M $\rightarrow$ C$_6$H$_4$(CH$_3$)CH$_2$ + H + M	$4.0 \times 10^{15}\exp(-42600/T)$	1400–1800	± 0.5
C$_6$H$_5$C$_2$H$_5$ + M $\rightarrow$ C$_6$H$_5$CH$_2$ + CH$_3$ + M ⎤ $\rightarrow$ C$_6$H$_6$ + C$_2$H$_4$ + M ⎪ $\rightarrow$ C$_6$H$_5$CHCH$_2$ + H$_2$ + M ⎪	$6.1 \times 10^{15}\exp(-37800/T)$	770–1800	± 0.1 at 770 K rising to ± 0.4 at 1800 K
$\rightarrow$ C$_6$H$_5$ + C$_2$H$_5$ + M ⎪ $\rightarrow$ C$_6$H$_5$CHCH$_3$ + H + M ⎦	No recommendation		

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}) $= \dfrac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp (K)	Error limits ($\Delta \log k$)
H + O$_2$ + Ar → HO$_2$ + Ar	$k_0 = 1.7 \times 10^{-30} T^{-0.8}$	300–2000	±0.5
H + O$_2$ + H$_2$ → HO$_2$ + H$_2$	$k_0 = 5.8 \times 10^{-30} T^{-0.8}$	300–2000	±0.5
H + O$_2$ + N$_2$ → HO$_2$ + N$_2$	$k_0 = 3.9 \times 10^{-30} T^{-0.8}$	300–2000	±0.5
H + H + Ar → H$_2$ + Ar	$k_0 = 1.8 \times 10^{-30} T^{-1.0}$	300–2500	±0.5
H + H + H$_2$ → H$_2$ + H$_2$	$k_0 = 2.7 \times 10^{-31} T^{-0.6}$	100–5000	±0.5
H + OH + H$_2$O → H$_2$O + H$_2$O	$k_0 = 3.9 \times 10^{-25} T^{-2.0}$	300–3000	±0.5
H + OH + Ar → H$_2$O + Ar	$k_0 = 2.3 \times 10^{-26} T^{-2.0}$	300–3000	±0.3
H + OH + N$_2$ → H$_2$O + N$_2$	$k_0 = 6.1 \times 10^{-26} T^{-2.0}$	300–3000	±0.5
H + CO + Ar → HCO + Ar	$k_0 = 5.3 \times 10^{-34} \exp(-370/T)$	300–2500	±0.5
H + CH$_3$ + M → CH$_4$ + M	$k_0(\text{He}) = 1.8 \times 10^{-24} T^{-1.8}$	300–1000	±0.3
	$k_0(\text{Ar}) = 1.7 \times 10^{-24} T^{-1.8}$	300–1000	±0.5
	$k_0(\text{C}_2\text{H}_6) = 8.6 \times 10^{-24} T^{-1.8}$	300–1000	±0.5
	$k_\infty = 3.5 \times 10^{-10}$	300–1000	±0.3
	$F_c(\text{He, Ar}) = 0.63 \exp(-T/3315)$ $+ 0.37 \exp(-T/61)$	300–1000	$\Delta F_c = \pm 0.1$
	$F_c(\text{C}_2\text{H}_6) = 0.71 \exp(-T/3079)$ $+ 0.29 \exp(-T/54)$	300–1000	$\Delta F_c = \pm 0.1$
H + C$_2$H$_2$ + He → C$_2$H$_3$ + 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	$\Delta F_c = \pm 0.1$
H + C$_2$H$_3$ + M → C$_2$H$_4$ + M	No recommendation		
H + C$_2$H$_4$ + He → C$_2$H$_5$ + He	$k_0 = 1.3 \times 10^{-29} \exp(-380/T)$	300–800	±0.3
	$k_\infty = 6.6$ $\times 10^{-15} T^{1.28} \exp(-650/T)$	200–1100	±0.3
	$F_c = 0.24 \exp(-T/40)$ $+ 0.76 \exp(-T/1025)$	300–800	$\Delta F_c = \pm 0.1$
H + C$_2$H$_5$ + M → C$_2$H$_6$ + M	No recommendation		
H + C$_3$H$_5$ + M → C$_3$H$_6$ + M → C$_2$H$_3$ + CH$_3$ + M	$(k_1^\infty + k_2) = 2.8 \times 10^{-10}$	300–1000	±0.2 at 300 K rising to ±0.5 at 1000 K
H + C$_6$H$_5$ + M → C$_6$H$_6$ + M	$k_\infty = 1.3 \times 10^{-10}$	1400–1700	±0.5
H + C$_6$H$_6$ + M → C$_6$H$_7$ + M	$k_\infty = 6.7 \times 10^{-11} \exp(-2170/T)$	300–1000	±0.2
H + C$_6$H$_5$O + M → C$_6$H$_5$OH + M	$k_\infty = 4.2 \times 10^{-10}$	1000	±0.3
H + C$_6$H$_5$CH$_2$ + M → C$_6$H$_5$CH$_3$ + M	$k_\infty = 5.5 \times 10^{-10}$	300–2000	±0.2 at 300 K rising to ±0.7 at 2000 K
H + C$_6$H$_5$CH$_3$ + M → C$_6$H$_6$CH$_3$ + M	$k_\infty = 1.2 \times 10^{-13}$	298	±0.2
H + C$_6$H$_5$C$_2$H$_5$ + M → C$_6$H$_6$C$_2$H$_5$ + M	$k_\infty = 3.3 \times 10^{-13}$	298	±0.1
OH + OH + M → H$_2$O$_2$ + M	$k_0(\text{N}_2) = 6.1 \times 10^{-29} T^{-0.76}$	250–1400	±0.4
	$k_0(\text{H}_2\text{O}) = 4 \times 10^{-30}$	300–400	±0.4
	$k_\infty = 1.2 \times 10^{-10} T^{-0.37}$	200–1500	±0.5
	$F_c(\text{N}_2) = 0.5$	200–1500	$\Delta F_c = \pm 0.2$
OH + CH$_3$ + M → CH$_3$OH + M	$k_0(\text{He}) = 2.3 \times 10^{-27}$	300	±0.3
	$k_0(\text{Ar}) = 4.4 \times 10^{-4} T^{-8.2}$	1000–2000	±0.5
	$k_\infty = 1.0 \times 10^{-10}$	300–2000	±0.3
	$F_c(\text{Ar}) = 0.18 \exp(-T/200)$ $+ 0.82(-T/1438)$	1000–2000	$\Delta F_c = \pm 0.1$
OH + C$_2$H$_2$ + M → C$_2$H$_2$OH + M	See data sheet		

TABLE 3—(*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}) $= \dfrac{k_0 k_\infty [\text{M}]}{k_0[\text{M}] + k_\infty} F$	Temp (K)	Error limits ($\Delta \log k$)

OH + C$_3$H$_5$ + M
  → CH$_2$CHCH$_2$OH + M $\Big]$
  → CH$_2$CHCHO + 2H + M
	$(k_1^\infty + k_2) = 2.5 \times 10^{-11}$	300–1000	±0.3

OH + C$_6$H$_6$ + M → C$_6$H$_6$OH + M	$k_\infty = 3.8 \times 10^{-12} \exp(-340/T)$	240–340	±0.2
OH + C$_6$H$_5$CH$_3$ + M → C$_6$H$_5$(OH)$_2$ + M	$k_\infty = 2.8 \times 10^{-11}$	298	±0.1
OH + C$_6$H$_5$CH$_3$ + M → HOC$_6$H$_5$CH$_3$ + M	$k_\infty = 3.8 \times 10^{-12} \exp(180/T)$	200–300	±0.4
OH + C$_6$H$_4$(CH$_3$)$_2$ + M → C$_6$H$_4$(CH$_3$)$_2$OH + M	$k_\infty = 1.4 \times 10^{-11}$	300	±0.1
OH + C$_6$H$_5$C$_2$H$_5$ + M → HOC$_6$H$_5$C$_2$H$_5$ + M	7.5×10^{-12} at p ≤ 1 atm	298	±0.1
^{3}CH$_2$ + C$_2$H$_2$ + M → C$_3$H$_4$ + M	$2.0 \times 10^{-11} \exp(-3330/T)$ at $p = \leq 10$ torr	300–1000	±0.3

^{3}CH$_2$ + C$_2$H$_4$ + M
  → C$_3$H$_6$ + M $\Big]$
  → c − C$_3$H$_6$ + M
  → C$_3$H$_5$ + H
	$5.3 \times 10^{-12} \exp(-2660/T)$	300–1000	±0.2 at 300 K rising to
			±0.3 at 1000 K

^{1}CH$_2$ + C$_2$H$_2$ + M
  → CH$_2$CCH$_2$ + M $\Big]$
  → CH$_3$CCH + M
  → CH$_2$CCH + H + M
	2.9×10^{-10} independent of p	300–1000	±0.3 at 300 K rising to
			±0.7 at 1000 K

^{1}CH$_2$ + C$_2$H$_4$ + M → C$_3$H$_6$ + M	1.6×10^{-10} independent of p	300–1000	±0.2 at 300 K rising to ±0.5 at 1000 K
CH$_3$ + O$_2$ + M → CH$_3$O$_2$ + M	$k_0(\text{Ar}) = 1.55 \times 10^{-22} T^{-3.3}$	300–800	±0.3
	$k_0(\text{N}_2) = 1.6 \times 10^{-22} T^{-3.3}$	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	$\Delta F_c = \pm 0.1$
CH$_3$ + CO + M → CH$_3$CO + M	$k_0(\text{He}) = 3.0 \times 10^{-34} \exp(-1910/T)$	400–500	±0.2
	$k_0(\text{CO}) = 4.2 \times 10^{-36}$	300–350	±0.5
	$k_\infty = 8.4 \times 10^{-13} \exp(-3460/T)$	300–500	±0.5
	$F_c(\text{He}) = 0.5$	400–500	$\Delta F_c = \pm 0.1$
	$F_c(\text{CO}) = 0.6$	300–350	$\Delta F_c = \pm 0.1$
CH$_3$ + CH$_3$ + Ar → C$_2$H$_6$ + Ar	$k_\infty = 6.0 \times 10^{-11}$	300–2000	±0.3
	$k_0 = 3.5 \times 10^{-7} T^{-7.0} \exp(-1390/T)$	300–2000	±0.3
	$F_c = 0.38 \exp(-T/73)$ $+ 0.62 \exp(-T/1180)$	300–2000	$\Delta F_c = \pm 0.1$
CH$_3$ + C$_2$H$_2$ + M → C$_3$H$_5$ + M	$k_\infty = 1 \times 10^{-12} \exp(-3900/T)$	300–600	±0.5
CH$_3$ + C$_2$H$_4$ + M → n − C$_3$H$_7$ + M	$3.5 \times 10^{-13} \exp(-3700/T)$	300–600	±0.3
CH$_3$ + C$_2$H$_5$ + M → C$_3$H$_8$ + M	$k_\infty = 5.6 \times 10^{-11}$	300–2000	±0.3
CH$_3$ + C$_3$H$_5$ + M → C$_2$H$_5$CHCH$_2$ + M	$k_\infty = 1.7 \times 10^{-10} T^{-0.32} \exp(66/T)$	500–1200	±0.2
C$_2$H$_5$ + C$_2$H$_5$ + M → n − C$_4$H$_{10}$ + M	$k_\infty = 1.9 \times 10^{-11}$	300–1200	±0.3
C$_2$H$_5$ + C$_3$H$_5$ + M → CH$_3$CH$_2$CH$_2$CHCH$_2$ + M	$k_\infty = 3.3 \times 10^{-11} \exp(66/T)$	500–1200	±0.3
CH$_3$CO + O$_2$ + M → CH$_3$CO$_3$ + M	2×10^{-12} for $p = 1 - 4$ torr	300	±0.3

TABLE 3—(*Continued*)

Reaction	k_∞ (cm³ molecule^{-1}s^{-1}) k_0 (cm⁶ molecule^{-2}s^{-1}) F_c k (cm³ molecule^{-1}s^{-1}) $= \dfrac{k_0 k_\infty [M]}{k_0[M] + k_\infty} F$	Temp (K)	Error limits ($\Delta \log k$)
$C_3H_5 + C_3H_5 + M \rightarrow$ $CH_2CHCH_2CH_2CHCH_2 + M$	$k_\infty = 1.7 \times 10^{-11} \exp(132/T)$ $k_\infty = 2.0 \times 10^{-11}$	300–600 600–1000	± 0.2 ± 0.4
$C_3H_5 + 2 - C_4H_8 + M \rightarrow$ $CH_2CHCH_2CH(CH_3)CHCH_3 + M$	$k_\infty = 1.0 \times 10^{-13} \exp(-9620/T)$	600–1200	± 0.7
$i - C_3H_7 + i - C_3H_7 + M \rightarrow$ $(CH_3)_2CHCH_2CH_2 + M$	$k_\infty = 6.8 \times 10^{-12}$	300–1000	± 0.1 at 300 K rising to ± 0.3 at 1000 K
$t - C_4H_9 + t - C_4H_9 + M \rightarrow C_8H_{18}$	$k_\infty = 5.2 \times 10^{-8} T^{-1.73}$	300–1000	± 0.15 at 300 K rising to ± 0.3 at 1000 K