

SECTION 1. BIMOLECULAR REACTIONS

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1.1 Introduction

In Table 1 (Rate Constants for Second-Order Reactions) the reactions are grouped into the classes O_x , $O(^1D)$, Singlet O_2 , HO_x , NO_x , Organic Compounds, FO_x , ClO_x , BrO_x , IO_x , SO_x and Metals. Some of the reactions in Table 1 are actually more complex than simple two-body reactions. To explain the pressure and temperature dependences occasionally seen in reactions of this type, it is necessary to consider the bimolecular class of reactions in terms of two subcategories, direct (concerted) and indirect (nonconcerted) reactions.

A direct or concerted bimolecular reaction is one in which the reactants A and B proceed to products C and D without the intermediate formation of an AB adduct that has appreciable bonding, i.e., there is no bound intermediate; only the transition state $(AB)^\ddagger$ lies between reactants and products.



The reaction of OH with CH_4 forming $H_2O + CH_3$ is an example of a reaction of this class.

Very useful correlations between the expected structure of the transition state $[AB]^\ddagger$ and the A-Factor of the reaction rate constant can be made, especially in reactions that are constrained to follow a well-defined approach of the two reactants in order to minimize energy requirements in the making and breaking of bonds. The rate constants for these reactions are well represented by the Arrhenius expression $k = A \exp(-E/RT)$ in the 200–300 K temperature range. These rate constants are not pressure dependent.

The indirect or nonconcerted class of bimolecular reactions is characterized by a more complex reaction path involving a potential well between reactants and products, leading to a bound adduct (or reaction complex) formed between the reactants A and B:



The intermediate $[AB]^*$ is different from the transition state $[AB]^\ddagger$, in that it is a bound molecule which can, in principle, be isolated. (Of course, transition states are involved in all of the above reactions, both forward and backward, but are not explicitly shown.) An example of this reaction type is $ClO + NO$, which normally produces $Cl + NO_2$. Reactions of the nonconcerted type can have a more complex temperature dependence and can exhibit a pressure dependence if the lifetime of $[AB]^*$ is comparable to the rate of collisional deactivation of $[AB]^*$. This arises because the relative rate at which $[AB]^*$ goes to products C + D vs. reactants A + B is a sensitive function of its excitation energy. Thus, in reactions of this type, the distinction between the bimolecular and termolecular classification becomes less meaningful, and it is especially necessary to study such reactions under the temperature and pressure conditions in which they are to be used in model calculation, or, alternatively, to develop a reliable theoretical basis for extrapolation of data.

The rate constant tabulation for second-order reactions (Table 1) is given in Arrhenius form:

$$k(T) = A \cdot \exp\left(-\frac{E/R}{T}\right)$$

and contains the following information:

1. Reaction stoichiometry and products (if known). The pressure dependences are included, where appropriate.
2. Arrhenius A-factor: **A**
3. Temperature dependence (“activation temperature”): **E/R**
4. Rate constant at 298 K: **k(298 K)**
5. Rate constant uncertainty factor at 298 K: **f(298 K)** (see below)
6. A parameter used to calculate the rate constant uncertainty at temperatures other than 298 K: **g** (see below)
7. Index number for a detailed note containing references to the literature, the basis of recommendation and in several cases, alternative methods to calculate the rate constant.

For a few reactions, the A-factor, E/R and k(298 K) are italicized. These represent estimates by the Panel in cases where there are no literature data or where the existing data are judged to be of insufficient quality to base a recommendation.

1.2 Uncertainty Estimates

For bimolecular rate constants in Table 1, an estimate of the uncertainty at any given temperature, f(T), may be obtained from the following expression:

$$f(T) = f(298 \text{ K}) \exp\left|g\left(\frac{1}{T} - \frac{1}{298}\right)\right|$$

Note that the exponent is an absolute value. An upper or lower bound (corresponding approximately to one standard deviation) of the rate constant at any temperature T can be obtained by multiplying or dividing the recommended value of the rate constant at that temperature by the factor f(T). The quantity f(298 K) is the uncertainty in the rate constant at T = 298 K. The quantity g has been defined in this evaluation for use with f(298 K) in the above expression to obtain the rate constant uncertainty at different temperatures. It should not be interpreted as the uncertainty in the Arrhenius activation temperature (E/R). Both uncertainty factors, f(298 K) and g, do not necessarily result from a rigorous statistical analysis of the available data. Rather, they are chosen by the evaluators to construct the appropriate uncertainty factor, f(T), shown above.

This approach is based on the fact that rate constants are almost always known with minimum uncertainty at room temperature. The overall uncertainty normally increases at other temperatures, because there are usually fewer data at other temperatures. In addition, data obtained at temperatures far distant from 298 K may be less accurate than at room temperature due to various experimental difficulties.

The uncertainty represented by f(T) is normally symmetric; i.e., the rate constant may be greater than or less than the recommended value, k(T), by the factor f(T). In a few cases in Table 1 asymmetric uncertainties are given in the temperature coefficient. For these cases, the factors by which a rate constant is to be multiplied or divided to obtain, respectively, the upper and lower limits are not equal, except at 298 K where the factor is simply f(298 K). Explicit equations are given below for the case where g is given as (+a, -b):

For T > 298 K, multiply by the factor

$$f(298) e^{a\left(\frac{1}{298} - \frac{1}{T}\right)}$$

and divide by the factor

$$f(298) e^{b\left(\frac{1}{298} - \frac{1}{T}\right)}$$

For T < 298 K, multiply by the factor

$$f(298) e^{b\left(\frac{1}{T} - \frac{1}{298}\right)}$$

and divide by the factor

$$f(298)e^{\left[\frac{1}{T} - \frac{1}{298}\right]}$$

Examples of symmetric and asymmetric error limits are shown in Figure 1.

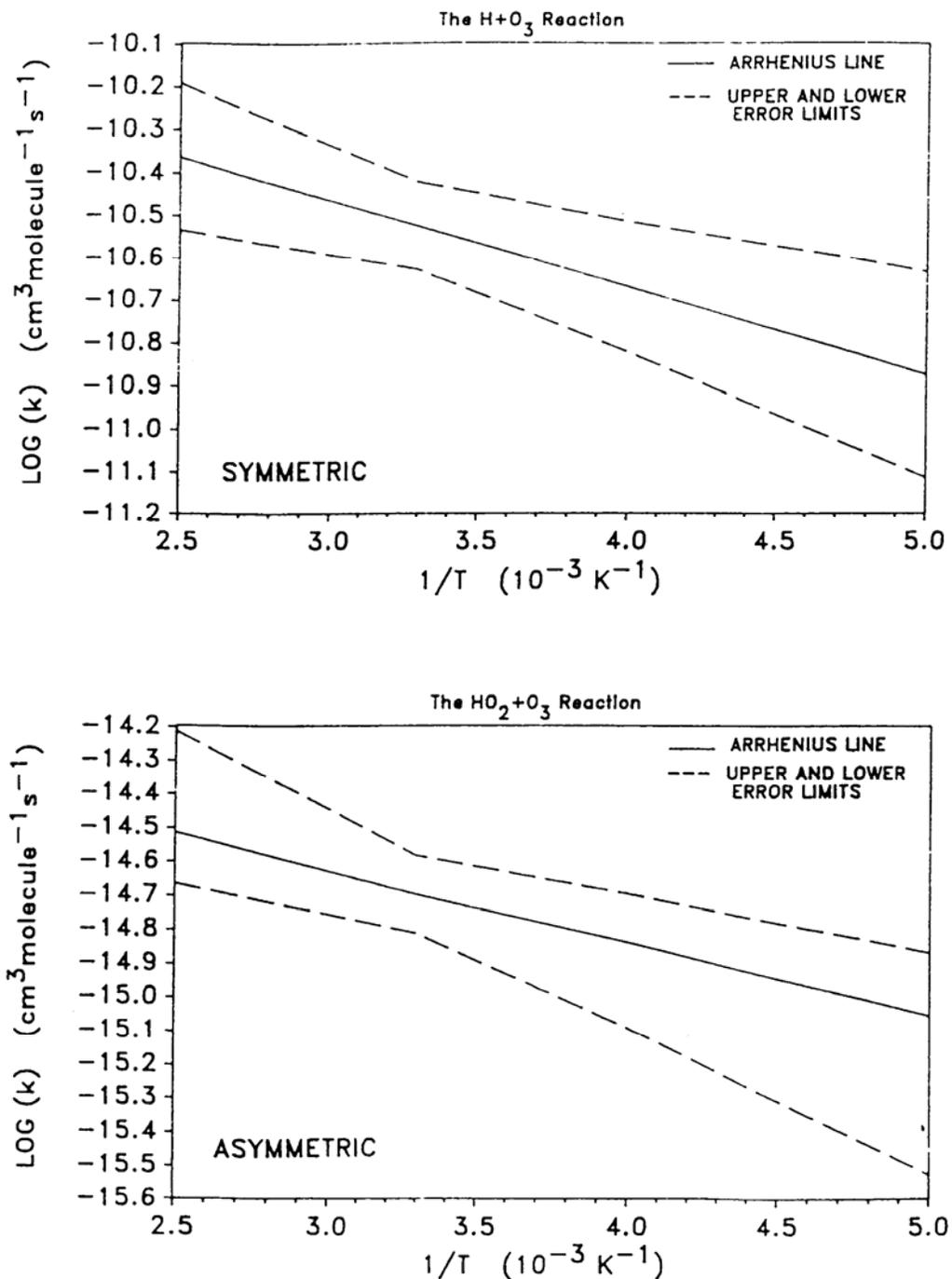


Figure 1. Symmetric and Asymmetric Error Limits

The assigned uncertainties represent the subjective judgment of the Panel. They are not determined by a rigorous, statistical analysis of the database, which generally is too limited to permit such an analysis. Rather, the

uncertainties are based on knowledge of the techniques, the difficulties of the experiments, and the potential for systematic errors.

There is obviously no way to quantify these “unknown” errors. The spread in results among different techniques for a given reaction may provide some basis for an uncertainty, but the possibility of the same, or compensating, systematic errors in all the studies must be recognized.

Furthermore, the probability distribution may not follow the normal Gaussian form. For measurements subject to large systematic errors, the true rate constant may be much further from the recommended value than would be expected based on a Gaussian distribution with the stated uncertainty. As an example, in the past the recommended rate constants for the reactions $\text{HO}_2 + \text{NO}$ and $\text{Cl} + \text{ClONO}_2$ changed by factors of 30–50. These changes could not have been allowed for with any reasonable values of σ in a Gaussian distribution.

Table 1-1. Rate Constants for Second-Order Reactions

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
O_x Reactions						
$O + O_2 \xrightarrow{M} O_3$	(See Table 2)					
$O + O_3 \rightarrow O_2 + O_2$	8.0×10^{-12}	2060	8.0×10^{-15}	1.15	250	A1
O(¹D) Reactions						
$O(^1D) + O_2 \rightarrow O + O_2$	3.3×10^{-11}	-55	3.95×10^{-11}	1.1	20	A2, A3
$O(^1D) + O_3 \rightarrow O_2 + O_2$	1.2×10^{-10}	0	1.2×10^{-10}	1.2	50	A2, A4
$\quad \rightarrow O_2 + O + O$	1.2×10^{-10}	0	1.2×10^{-10}	1.2	50	A2, A4
$O(^1D) + H_2 \rightarrow OH + H$	1.1×10^{-10}	0	1.1×10^{-10}	1.1	100	A2, A5
$O(^1D) + H_2O \rightarrow OH + OH$	1.63×10^{-10}	-60	2.0×10^{-10}	1.15	45	A2, A6
$O(^1D) + N_2 \rightarrow O + N_2$	2.15×10^{-11}	-110	3.1×10^{-11}	1.10	30	A2, A7
$O(^1D) + N_2 \xrightarrow{M} N_2O$	(See Table 2-1)					
$O(^1D) + N_2O \rightarrow N_2 + O_2$ (a)	4.7×10^{-11}	-20	5.0×10^{-11}	1.15	50	A2, A8
$\quad \rightarrow NO + NO$ (b)	6.7×10^{-11}	-20	6.7×10^{-11}	1.15	50	A2, A8
$O(^1D) + NH_3 \rightarrow OH + NH_2$	2.5×10^{-10}	0	2.5×10^{-10}	1.3	100	A2, A9
$O(^1D) + CO_2 \rightarrow O + CO_2$	7.5×10^{-11}	-115	1.1×10^{-10}	1.15	40	A2, A10
$O(^1D) + CH_4 \rightarrow$ products	1.5×10^{-10}	0	1.5×10^{-10}	1.2	100	A2, A11
$O(^1D) + HCl \rightarrow$ products	1.5×10^{-10}	0	1.5×10^{-10}	1.15	50	A2, A12
$O(^1D) + HF \rightarrow$ products	5.0×10^{-11}	0	5.0×10^{-11}	2.0	100	A2, A13
$O(^1D) + NF_3 \rightarrow$ products	2.0×10^{-11}	-25	2.2×10^{-11}	2	25	A2, A14
$O(^1D) + HBr \rightarrow$ products	1.5×10^{-10}	0	1.5×10^{-10}	2.0	100	A2, A15
$O(^1D) + Cl_2 \rightarrow$ products	2.7×10^{-10}	0	2.7×10^{-10}	1.15	50	A2, A16
$O(^1D) + CCl_2O \rightarrow$ products	2.2×10^{-10}	-30	2.4×10^{-10}	1.15	50	A2, A17
$O(^1D) + CClFO \rightarrow$ products	1.9×10^{-10}	0	1.9×10^{-10}	2.0	100	A2, A18
$O(^1D) + CF_2O \rightarrow$ products	7.4×10^{-11}	0	7.4×10^{-11}	2.0	100	A2, A18

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
O(¹ D) + CCl ₄ → products (CFC-10)	3.3×10 ⁻¹⁰	0	3.3×10 ⁻¹⁰	1.2	100	A19
O(¹ D) + CH ₃ Br → products	1.8×10 ⁻¹⁰	0	1.8×10 ⁻¹⁰	1.3	100	A19, A20
O(¹ D) + CH ₂ Br ₂ → products	2.7×10 ⁻¹⁰	0	2.7×10 ⁻¹⁰	1.3	100	A19, A21
O(¹ D) + CHBr ₃ → products	6.6×10 ⁻¹⁰	0	6.6×10 ⁻¹⁰	1.5	100	A19, A22
O(¹ D) + CH ₃ F → products (HFC-41)	1.5×10 ⁻¹⁰	0	1.5×10 ⁻¹⁰	1.2	100	A19, A23
O(¹ D) + CH ₂ F ₂ → products (HFC-32)	5.1×10 ⁻¹¹	0	5.1×10 ⁻¹¹	1.3	100	A19, A24
O(¹ D) + CHF ₃ → products (HFC-23)	9.1×10 ⁻¹²	0	9.1×10 ⁻¹²	1.2	100	A19, A25
O(¹ D) + CHCl ₂ F → products (HCFC-21)	1.9×10 ⁻¹⁰	0	1.9×10 ⁻¹⁰	1.3	100	A19, A26
O(¹ D) + CHClF ₂ → products (HCFC-22)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	1.2	100	A19, A27
O(¹ D) + CHF ₂ Br → products	1.75×10 ⁻¹⁰	-70	2.2×10 ⁻¹⁰	1.2	40	A19, A28
O(¹ D) + CCl ₃ F → products (CFC-11)	2.3×10 ⁻¹⁰	0	2.3×10 ⁻¹⁰	1.2	100	A19
O(¹ D) + CCl ₂ F ₂ → products (CFC-12)	1.4×10 ⁻¹⁰	0	1.4×10 ⁻¹⁰	1.3	100	A19
O(¹ D) + CClF ₃ → products (CFC-13)	8.7×10 ⁻¹¹	0	8.7×10 ⁻¹¹	1.3	100	A19, A29
O(¹ D) + CClBrF ₂ → products (Halon-1211)	1.5×10 ⁻¹⁰	0	1.5×10 ⁻¹⁰	1.3	100	A19, A30
O(¹ D) + CBr ₂ F ₂ → products (Halon-1202)	2.2×10 ⁻¹⁰	0	2.2×10 ⁻¹⁰	1.3	100	A19, A31
O(¹ D) + CBrF ₃ → products (Halon-1301)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	1.3	100	A19, A32
O(¹ D) + CF ₄ → CF ₄ + O (CFC-14)			2.0×10 ⁻¹⁴	1.5		A19, A33
O(¹ D) + CH ₃ CH ₂ F → products (HFC-161)	2.6×10 ⁻¹⁰	0	2.6×10 ⁻¹⁰	1.3	100	A19, A34
O(¹ D) + CH ₃ CHF ₂ → products (HFC-152a)	2.0×10 ⁻¹⁰	0	2.0×10 ⁻¹⁰	1.3	100	A19, A35
O(¹ D) + CH ₃ CCl ₂ F → products (HCFC-141b)	2.6×10 ⁻¹⁰	0	2.6×10 ⁻¹⁰	1.3	100	A19, A36
O(¹ D) + CH ₃ CClF ₂ → products (HCFC-142b)	2.2×10 ⁻¹⁰	0	2.2×10 ⁻¹⁰	1.3	100	A19, A37
O(¹ D) + CH ₃ CF ₃ → products (HFC-143a)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	3.0	100	A19, A38
O(¹ D) + CH ₂ ClCClF ₂ → products (HCFC-132b)	1.6×10 ⁻¹⁰	0	1.6×10 ⁻¹⁰	2.0	100	A19, A39
O(¹ D) + CH ₂ ClCF ₃ → products (HCFC-133a)	1.2×10 ⁻¹⁰	0	1.2×10 ⁻¹⁰	1.3	100	A19, A40
O(¹ D) + CH ₂ FCF ₃ → products (HFC-134a)	4.9×10 ⁻¹¹	0	4.9×10 ⁻¹¹	1.3	100	A19, A41

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
O(¹ D) + CHCl ₂ CF ₃ → products (HCFC-123)	2.0×10 ⁻¹⁰	0	2.0×10 ⁻¹⁰	1.3	100	A19, A42
O(¹ D) + CHClFCF ₃ → products (HCFC-124)	8.6×10 ⁻¹¹	0	8.6×10 ⁻¹¹	1.3	100	A19, A43
O(¹ D) + CHF ₂ CF ₃ → products (HFC-125)	1.2×10 ⁻¹⁰	0	1.2×10 ⁻¹⁰	2.0	100	A19, A44
O(¹ D) + CCl ₃ CF ₃ → products (CFC-113a)	2×10 ⁻¹⁰	0	2×10 ⁻¹⁰	2.0	100	A19, A45
O(¹ D) + CCl ₂ FCClF ₂ → products (CFC-113)	2×10 ⁻¹⁰	0	2×10 ⁻¹⁰	2.0	100	A19, A46
O(¹ D) + CCl ₂ FCF ₃ → products (CFC-114a)	1×10 ⁻¹⁰	0	1×10 ⁻¹⁰	2.0	100	A19, A47
O(¹ D) + CClF ₂ CClF ₂ → products (CFC-114)	1.3×10 ⁻¹⁰	0	1.3×10 ⁻¹⁰	1.3	100	A19, A48
O(¹ D) + CClF ₂ CF ₃ → products (CFC-115)	5×10 ⁻¹¹	0	5×10 ⁻¹¹	1.3	100	A19, A49
O(¹ D) + CBrF ₂ CBrF ₂ → products (Halon-2402)	1.6×10 ⁻¹⁰	0	1.6×10 ⁻¹⁰	1.3	100	A19, A50
O(¹ D) + CF ₃ CF ₃ → products (CFC-116)			1.5×10 ⁻¹³	1.5		A19, A51
O(¹ D) + CHF ₂ CF ₂ CF ₂ CHF ₂ → products (HFC-338pcc)	1.8×10 ⁻¹¹	0	1.8×10 ⁻¹¹	1.5	100	A19, A52
O(¹ D) + c-C ₄ F ₈ → products			8×10 ⁻¹³	1.3		A19, A53
O(¹ D) + CF ₃ CHFCHFCF ₂ CF ₃ → products (HFC-43-10mee)	2.1×10 ⁻¹⁰	0	2.1×10 ⁻¹⁰	4	100	A19, A54
O(¹ D) + C ₅ F ₁₂ → products (CFC-41-12)			3.9×10 ⁻¹³	2		A19, A55
O(¹ D) + C ₆ F ₁₄ → products (CFC-51-14)			1×10 ⁻¹²	2		A19, A56
O(¹ D) + 1,2-(CF ₃) ₂ C-C ₄ F ₆ → products			2.8×10 ⁻¹³	2		A19, A57
O(¹ D) + SF ₆ → products			1.8×10 ⁻¹⁴	1.5		A58
Singlet O₂ Reactions						
O ₂ (¹ Δ) + O → products			<2×10 ⁻¹⁶			A59
O ₂ (¹ Δ) + O ₂ → products	3.6×10 ⁻¹⁸	220	1.7×10 ⁻¹⁸	1.2	100	A60
O ₂ (¹ Δ) + O ₃ → O + 2O ₂	5.2×10 ⁻¹¹	2840	3.8×10 ⁻¹⁵	1.2	500	A61
O ₂ (¹ Δ) + H ₂ O → products			4.8×10 ⁻¹⁸	1.5		A62
O ₂ (¹ Δ) + N → NO + O			<9×10 ⁻¹⁷			A63
O ₂ (¹ Δ) + N ₂ → products			<10 ⁻²⁰			A64
O ₂ (¹ Δ) + CO ₂ → products			<2×10 ⁻²⁰			A65

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$O_2(^1\Sigma) + O \rightarrow \text{products}$			8×10^{-14}	5.0		A66
$O_2(^1\Sigma) + O_2 \rightarrow \text{products}$			3.9×10^{-17}	1.5		A67
$O_2(^1\Sigma) + O_3 \rightarrow \text{products}$	3.5×10^{-11}	135	2.2×10^{-11}	1.15	50	A68
$O_2(^1\Sigma) + H_2 \rightarrow \text{products}$ $O_2(^1\Sigma) + H_2 \rightarrow 2 OH$	6.4×10^{-12}	600	8.5×10^{-13} $< 4 \times 10^{-17}$ (see note)	1.15	100	A69
$O_2(^1\Sigma) + H_2O \rightarrow O_2 + H_2O$	3.9×10^{-12}	-125	5.9×10^{-12}	1.3	100	A70
$O_2(^1\Sigma) + N \rightarrow \text{products}$			$< 10^{-13}$			A71
$O_2(^1\Sigma) + N_2 \rightarrow \text{products}$	1.8×10^{-15}	-45	2.1×10^{-15}	1.1	100	A72
$O_2(^1\Sigma) + N_2O \rightarrow \text{products}$ $O_2(^1\Sigma) + N_2O \rightarrow NO + NO_2$	7.0×10^{-14}	-75	9.0×10^{-14} $< 2 \times 10^{-17}$ (see Note)	1.3	50	A73
$O_2(^1\Sigma) + CO_2 \rightarrow \text{products}$	4.2×10^{-13}	0	4.2×10^{-13}	1.2	200	A74
HO_x Reactions						
$O + OH \rightarrow O_2 + H$	2.2×10^{-11}	-120	3.3×10^{-11}	1.15	50	B1
$O + HO_2 \rightarrow OH + O_2$	3.0×10^{-11}	-200	5.9×10^{-11}	1.05	50	B2
$O + H_2O_2 \rightarrow OH + HO_2$	1.4×10^{-12}	2000	1.7×10^{-15}	1.3	200	B3
$H + O_2 \xrightarrow{M} HO_2$	(See Table 2-1)					
$H + O_3 \rightarrow OH + O_2$	1.4×10^{-10}	470	2.9×10^{-11}	1.1	70	B4
$H + HO_2 \rightarrow 2 OH$	7.2×10^{-11}	0	7.2×10^{-11}	1.3	100	B5
$\quad \rightarrow O + H_2O$	1.6×10^{-12}	0	1.6×10^{-12}	1.5	100	B5
$\quad \rightarrow H_2 + O_2$	6.9×10^{-12}	0	6.9×10^{-12}	1.4	100	B5
$OH + O_3 \rightarrow HO_2 + O_2$	1.7×10^{-12}	940	7.3×10^{-14}	1.2	80	B6
$OH + H_2 \rightarrow H_2O + H$	2.8×10^{-12}	1800	6.7×10^{-15}	1.05	100	B7
$OH + HD \rightarrow \text{products}$	5.0×10^{-12}	2130	4.0×10^{-15}	1.2	100	B8
$OH + OH \rightarrow H_2O + O$	1.8×10^{-12}	0	1.8×10^{-12}	1.3	100	B9
$\quad \xrightarrow{M} H_2O_2$	(See Table 2-1)					
$OH + HO_2 \rightarrow H_2O + O_2$	4.8×10^{-11}	-250	1.1×10^{-10}	1.25	80	B10

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$	See Note					B11
$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2\text{O}_2$	1.0×10^{-14}	490	1.9×10^{-15}	1.15	+160 -80	B12
$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	3.5×10^{-13}	-430	1.5×10^{-12}	1.2	200	B13
$+ \text{M} \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	$1.7 \times 10^{-33} [\text{M}]$	-1000	$4.9 \times 10^{-32} [\text{M}]$	1.2	200	B13
NO_x Reactions						
$\text{O} + \text{NO} \xrightarrow{\text{M}} \text{NO}_2$	(See Table 2-1)					
$\text{O} + \text{NO}_2 \rightarrow \text{NO} + \text{O}_2$	5.1×10^{-12}	-210	1.04×10^{-11}	1.1	20	C 1
$\text{O} + \text{NO}_2 \xrightarrow{\text{M}} \text{NO}_3$	(See Table 2-1)					
$\text{O} + \text{NO}_3 \rightarrow \text{O}_2 + \text{NO}_2$	1.0×10^{-11}	0	1.0×10^{-11}	1.5	150	C 2
$\text{O} + \text{N}_2\text{O}_5 \rightarrow \text{products}$			$< 3.0 \times 10^{-16}$			C 3
$\text{O} + \text{HNO}_3 \rightarrow \text{OH} + \text{NO}_3$			$< 3.0 \times 10^{-17}$			C 4
$\text{O} + \text{HO}_2\text{NO}_2 \rightarrow \text{products}$	7.8×10^{-11}	3400	8.6×10^{-16}	3.0	750	C 5
$\text{H} + \text{NO}_2 \rightarrow \text{OH} + \text{NO}$	4.0×10^{-10}	340	1.3×10^{-10}	1.3	300	C 6
$\text{OH} + \text{NO} \xrightarrow{\text{M}} \text{HONO}$	(See Table 2-1)					
$\text{OH} + \text{NO}_2 \xrightarrow{\text{M}} \text{HNO}_3$	(See Table 2-1)					
$\text{OH} + \text{NO}_3 \rightarrow \text{products}$			2.2×10^{-11}	1.5		C 7
$\text{OH} + \text{HONO} \rightarrow \text{H}_2\text{O} + \text{NO}_2$	1.8×10^{-11}	390	4.5×10^{-12}	1.5	+200 -500	C 8
$\text{OH} + \text{HNO}_3 \rightarrow \text{H}_2\text{O} + \text{NO}_3$	(See Note)			1.2		C 9
$\text{OH} + \text{HO}_2\text{NO}_2 \rightarrow \text{products}$	1.3×10^{-12}	-380	4.6×10^{-12}	1.3	+270 -500	C10
$\text{OH} + \text{NH}_3 \rightarrow \text{H}_2\text{O} + \text{NH}_2$	1.7×10^{-12}	710	1.6×10^{-13}	1.2	200	C11
$\text{HO}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{OH}$	3.5×10^{-12}	-250	8.1×10^{-12}	1.15	50	C12
$\text{HO}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{HO}_2\text{NO}_2$	(See Table 2-1)					
$\text{HO}_2 + \text{NO}_2 \rightarrow \text{HONO} + \text{O}_2$	(See Note)					C13
$\text{HO}_2 + \text{NO}_3 \rightarrow \text{products}$			3.5×10^{-12}	1.5		C14
$\text{HO}_2 + \text{NH}_2 \rightarrow \text{products}$			3.4×10^{-11}	2.0		C15

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	1.5×10^{-11}	3600	8.5×10^{-17}	1.25	400	C16
$\text{N} + \text{O}_3 \rightarrow \text{NO} + \text{O}_2$			$< 2.0 \times 10^{-16}$			C17
$\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$	2.1×10^{-11}	-100	3.0×10^{-11}	1.3	100	C18
$\text{N} + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{O}$	5.8×10^{-12}	-220	1.2×10^{-11}	1.5	100	C19
$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$	3.0×10^{-12}	1500	1.9×10^{-14}	1.1	200	C20
$\text{NO} + \text{NO}_3 \rightarrow 2\text{NO}_2$	1.5×10^{-11}	-170	2.6×10^{-11}	1.3	100	C21
$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$	1.2×10^{-13}	2450	3.2×10^{-17}	1.15	150	C22
$\text{NO}_2 + \text{NO}_3 \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2$	(See Note)					C23
$\text{NO}_2 + \text{NO}_3 \xrightarrow{\text{M}} \text{N}_2\text{O}_5$	(See Table 2-1)					
$\text{NO}_3 + \text{NO}_3 \rightarrow 2\text{NO}_2 + \text{O}_2$	8.5×10^{-13}	2450	2.3×10^{-16}	1.5	500	C24
$\text{NH}_2 + \text{O}_2 \rightarrow \text{products}$			$< 6.0 \times 10^{-21}$			C25
$\text{NH}_2 + \text{O}_3 \rightarrow \text{products}$	4.3×10^{-12}	930	1.9×10^{-13}	3.0	500	C26
$\text{NH}_2 + \text{NO} \rightarrow \text{products}$	4.0×10^{-12}	-450	1.8×10^{-11}	1.3	150	C27
$\text{NH}_2 + \text{NO}_2 \rightarrow \text{products}$	2.1×10^{-12}	-650	1.9×10^{-11}	3.0	250	C28
$\text{NH} + \text{NO} \rightarrow \text{products}$	4.9×10^{-11}	0	4.9×10^{-11}	1.5	300	C29
$\text{NH} + \text{NO}_2 \rightarrow \text{products}$	3.5×10^{-13}	-1140	1.6×10^{-11}	2.0	500	C30
$\text{O}_3 + \text{HNO}_2 \rightarrow \text{O}_2 + \text{HNO}_3$			$< 5.0 \times 10^{-19}$			C31
$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow 2\text{HNO}_3$			$< 2.0 \times 10^{-21}$			C32
$\text{N}_2(\text{A}, \nu) + \text{O}_2 \rightarrow \text{products}$			$2.5 \times 10^{-12}, \nu=0$	1.5		C33
$\text{N}_2(\text{A}, \nu) + \text{O}_3 \rightarrow \text{products}$			$4.1 \times 10^{-11}, \nu=0$	2.0		C34
Reactions of Organic Compounds						
$\text{O} + \text{CH}_3 \rightarrow \text{products}$	1.1×10^{-10}	0	1.1×10^{-10}	1.3	250	D1
$\text{O} + \text{HCN} \rightarrow \text{products}$	1.0×10^{-11}	4000	1.5×10^{-17}	10	1000	D2
$\text{O} + \text{C}_2\text{H}_2 \rightarrow \text{products}$	3.0×10^{-11}	1600	1.4×10^{-13}	1.3	250	D3
$\text{O} + \text{H}_2\text{CO} \rightarrow \text{products}$	3.4×10^{-11}	1600	1.6×10^{-13}	1.25	250	D4

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$O_2 + HOCO \rightarrow HO_2 + CO_2$			2×10^{-12} (See Note)	2		D5
$O + CH_3CHO \rightarrow CH_3CO + OH$	1.8×10^{-11}	1100	4.5×10^{-13}	1.25	200	D6
$O_3 + C_2H_2 \rightarrow$ products	1.0×10^{-14}	4100	1.0×10^{-20}	3	500	D7
$O_3 + C_2H_4 \rightarrow$ products	1.2×10^{-14}	2630	1.7×10^{-18}	1.25	100	D8
$O_3 + C_3H_6 \rightarrow$ products	6.5×10^{-15}	1900	1.1×10^{-17}	1.15	200	D9
$OH + CO \rightarrow$ Products	(See Table 2-1)					D10
$OH + CH_4 \rightarrow CH_3 + H_2O$	2.45×10^{-12}	1775	6.3×10^{-15}	1.1	100	D11
$OH + {}^{13}CH_4 \rightarrow {}^{13}CH_3 + H_2O$	(See Note)					D12
$OH + CH_3D \rightarrow$ products	3.5×10^{-12}	1950	5.0×10^{-15}	1.15	200	D13
$OH + H_2CO \rightarrow H_2O + HCO$	5.5×10^{-12}	-125	8.5×10^{-12}	1.15	50	D14
$OH + CH_3OH \rightarrow$ products	2.9×10^{-12}	345	9.1×10^{-13}	1.10	60	D15
$OH + CH_3OOH \rightarrow$ products	3.8×10^{-12}	-200	7.4×10^{-12}	1.4	150	D16
$OH + HC(O)OH \rightarrow$ products	4.0×10^{-13}	0	4.0×10^{-13}	1.2	100	D17
$OH + HC(O)C(O)H \rightarrow$ products	1.15×10^{-11}	0	1.15×10^{-11}	1.5	200	D18
$OH + HOCH_2CHO \rightarrow$ products	1.1×10^{-11}	0	1.1×10^{-11}	1.2	200	D19
$OH + HCN \rightarrow$ products	1.2×10^{-13}	400	3.1×10^{-14}	3	150	D20
$OH + C_2H_2 \xrightarrow{M} \text{products}$	(See Table 2)					
$OH + C_2H_4 \xrightarrow{M} \text{products}$	(See Table 2)					
$OH + C_2H_6 \rightarrow H_2O + C_2H_5$	8.7×10^{-12}	1070	2.4×10^{-13}	1.1	100	D21
$OH + C_3H_8 \rightarrow$ products	8.7×10^{-12}	615	1.1×10^{-12}	1.05	50	D22
$OH + C_2H_5CHO \rightarrow C_2H_5CO + H_2O$	4.9×10^{-12}	-405	1.9×10^{-11}	1.05	80	D23
$OH + 1-C_3H_7OH \rightarrow$ products	4.4×10^{-12}	-70	5.6×10^{-12}	1.05	80	D24
$OH + 2-C_3H_7OH \rightarrow$ products	3.0×10^{-12}	-180	5.5×10^{-12}	1.05	80	D25
$OH + C_2H_5C(O)OH \rightarrow$ products	1.2×10^{-12}	0	1.2×10^{-12}	1.1	200	D26

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{OH} + \text{CH}_3\text{C}(\text{O})\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{C}(\text{O})\text{CH}_2$ $\rightarrow \text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{OH}$	See Note		< 2% of k			D27
$\text{OH} + \text{CH}_3\text{CN} \rightarrow \text{products}$	7.8×10^{-13}	1050	2.3×10^{-14}	1.5	200	D28
$\text{OH} + \text{CH}_3\text{ONO}_2 \rightarrow \text{products}$	8.0×10^{-13}	1000	2.8×10^{-14}	1.7	200	D29
$\text{OH} + \text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2$ (PAN) $\rightarrow \text{products}$			$< 4 \times 10^{-14}$			D30
$\text{OH} + \text{C}_2\text{H}_5\text{ONO}_2 \rightarrow \text{products}$	1.0×10^{-12}	490	2.0×10^{-13}	1.4	150	D31
$\text{OH} + 1\text{-C}_3\text{H}_7\text{ONO}_2 \rightarrow \text{products}$	7.1×10^{-13}	0	7.1×10^{-13}	1.5	200	D32
$\text{OH} + 2\text{-C}_3\text{H}_7\text{ONO}_2 \rightarrow \text{products}$	1.2×10^{-12}	320	4.1×10^{-13}	1.5	200	D33
$\text{HO}_2 + \text{CH}_2\text{O} \rightarrow \text{adduct}$	6.7×10^{-15}	-600	5.0×10^{-14}	5	600	D34
$\text{HO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{OOH} + \text{O}_2$	4.1×10^{-13}	-750	5.2×10^{-12}	1.3	150	D35
$\text{HO}_2 + \text{C}_2\text{H}_5\text{O}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH} + \text{O}_2$	7.5×10^{-13}	-700	8.0×10^{-12}	1.5	250	D36
$\text{HO}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2 \rightarrow \text{products}$	4.3×10^{-13}	-1040	1.4×10^{-11}	2	500	D37
$\text{HO}_2 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2 \rightarrow \text{products}$	8.6×10^{-13}	-700	9.0×10^{-12}	2	300	D38
$\text{NO}_3 + \text{CO} \rightarrow \text{products}$			$< 4.0 \times 10^{-19}$			D39
$\text{NO}_3 + \text{CH}_2\text{O} \rightarrow \text{products}$			5.8×10^{-16}	1.3		D40
$\text{NO}_3 + \text{CH}_3\text{CHO} \rightarrow \text{products}$	1.4×10^{-12}	1900	2.4×10^{-15}	1.3	300	D41
$\text{CH}_3 + \text{O}_2 \rightarrow \text{products}$			$< 3.0 \times 10^{-16}$			D42
$\text{CH}_3 + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_3\text{O}_2$	(See Table 2-1)					
$\text{CH}_3 + \text{O}_3 \rightarrow \text{products}$	5.4×10^{-12}	220	2.6×10^{-12}	2	150	D43
$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	5.2×10^{-12}	0	5.2×10^{-12}	1.4	100	D44
$\text{CH}_2\text{OH} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	9.1×10^{-12}	0	9.1×10^{-12}	1.3	200	D45
$\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{HO}_2$	3.9×10^{-14}	900	1.9×10^{-15}	1.5	300	D46
$\text{CH}_3\text{O} + \text{NO} \rightarrow \text{CH}_2\text{O} + \text{HNO}$	(See Note)					D47
$\text{CH}_3\text{O} + \text{NO} \xrightarrow{\text{M}} \text{CH}_3\text{ONO}$	(See Table 2-1)					
$\text{CH}_3\text{O} + \text{NO}_2 \rightarrow \text{CH}_2\text{O} + \text{HONO}$	1.1×10^{-11}	1200	2.0×10^{-13}	5	600	D48

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{CH}_3\text{O} + \text{NO}_2 \xrightarrow{\text{M}} \text{CH}_3\text{ONO}_2$	(See Table 2-1)					
$\text{CH}_3\text{O}_2 + \text{O}_3 \rightarrow \text{products}$	2.9×10^{-16}	1000	1.0×10^{-17}	3	500	D49
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{products}$	9.5×10^{-14}	-390	3.5×10^{-13}	1.2	100	D50
$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	2.8×10^{-12}	-300	7.7×10^{-12}	1.15	100	D51
$\text{CH}_3\text{O}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{CH}_3\text{O}_2\text{NO}_2$	(See Table 2-1)					
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2 \rightarrow \text{products}$	2.0×10^{-12}	-500	1.1×10^{-11}	1.5	250	D52
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2 \rightarrow \text{products}$	7.5×10^{-13}	-500	4.0×10^{-12}	2	300	D53
$\text{C}_2\text{H}_5 + \text{O}_2 \rightarrow \text{C}_2\text{H}_4 + \text{HO}_2$			$< 2.0 \times 10^{-14}$			D54
$\text{C}_2\text{H}_5 + \text{O}_2 \xrightarrow{\text{M}} \text{C}_2\text{H}_5\text{O}_2$	(See Table 2-1)					
$\text{C}_2\text{H}_5\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2$	6.3×10^{-14}	550	1.0×10^{-14}	1.5	200	D55
$\text{C}_2\text{H}_5\text{O} + \text{NO} \xrightarrow{\text{M}} \text{products}$	(See Table 2-1)					
$\text{C}_2\text{H}_5\text{O} + \text{NO}_2 \xrightarrow{\text{M}} \text{products}$	(See Table 2-1)					
$\text{C}_2\text{H}_5\text{O}_2 + \text{C}_2\text{H}_5\text{O}_2 \rightarrow \text{products}$	6.8×10^{-14}	0	6.8×10^{-14}	2	300	D56
$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{products}$	2.6×10^{-12}	-365	8.7×10^{-12}	1.2	150	D57
$\text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2 \rightarrow \text{products}$	2.9×10^{-12}	-500	1.5×10^{-11}	1.5	150	D58
$\text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO} \rightarrow \text{products}$	8.1×10^{-12}	-270	2.0×10^{-11}	1.5	100	D59
$\text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{products}$	(See Table 2-1)					
$\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2 + \text{NO} \rightarrow \text{products}$	2.9×10^{-12}	-300	8.0×10^{-12}	1.5	300	D60
FO_x Reactions						
$\text{O} + \text{FO} \rightarrow \text{F} + \text{O}_2$	2.7×10^{-11}	0	2.7×10^{-11}	3.0	250	E 1
$\text{O} + \text{FO}_2 \rightarrow \text{FO} + \text{O}_2$	5.0×10^{-11}	0	5.0×10^{-11}	5.0	250	E 2
$\text{OH} + \text{CH}_3\text{F} \rightarrow \text{CH}_2\text{F} + \text{H}_2\text{O}$ (HFC-41)	2.5×10^{-12}	1430	2.1×10^{-14}	1.15	150	E 3
$\text{OH} + \text{CH}_2\text{F}_2 \rightarrow \text{CHF}_2 + \text{H}_2\text{O}$ (HFC-32)	1.7×10^{-12}	1500	1.1×10^{-14}	1.15	150	E 4
$\text{OH} + \text{CHF}_3 \rightarrow \text{CF}_3 + \text{H}_2\text{O}$ (HFC-23)	6.3×10^{-13}	2300	2.8×10^{-16}	1.2	200	E 5
$\text{OH} + \text{CH}_3\text{CH}_2\text{F} \rightarrow \text{products}$ (HFC-161)	2.5×10^{-12}	730	2.2×10^{-13}	1.15	150	E 6

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CH ₃ CHF ₂ → products (HFC-152a)	9.4×10 ⁻¹³	990	3.4×10 ⁻¹⁴	1.1	100	E7
OH + CH ₂ FCH ₂ F → CHFCH ₂ F + H ₂ O (HFC-152)	1.1×10 ⁻¹²	730	9.7×10 ⁻¹⁴	1.1	150	E8
OH + CH ₃ CF ₃ → CH ₂ CF ₃ + H ₂ O (HFC-143a)	1.1×10 ⁻¹²	2010	1.3×10 ⁻¹⁵	1.1	100	E9
OH + CH ₂ FCHF ₂ → products (HFC-143)	3.9×10 ⁻¹²	1620	1.7×10 ⁻¹⁴	1.2	200	E10
OH + CH ₂ FCF ₃ → CHFCH ₂ F + H ₂ O (HFC-134a)	1.05×10 ⁻¹²	1630	4.4×10 ⁻¹⁵	1.1	200	E11
OH + CHF ₂ CHF ₂ → CF ₂ CHF ₂ + H ₂ O (HFC-134)	1.6×10 ⁻¹²	1660	6.1×10 ⁻¹⁵	1.2	200	E12
OH + CHF ₂ CF ₃ → CF ₂ CF ₃ + H ₂ O (HFC-125)	6.0×10 ⁻¹³	1700	2.0×10 ⁻¹⁵	1.2	150	E13
OH + CH ₃ CHFCH ₃ → products (HFC-281ea)	3.0×10 ⁻¹²	490	5.8×10 ⁻¹³	1.2	100	E14
OH + CF ₃ CH ₂ CH ₃ → products (HFC-263fb)	–	–	4.2×10 ⁻¹⁴	1.5	–	E15
OH + CH ₂ FCF ₂ CHF ₂ → products (HFC-245ca)	2.1×10 ⁻¹²	1620	9.2×10 ⁻¹⁵	1.2	150	E16
OH + CHF ₂ CHFCHF ₂ → products (HFC-245ea)	–	–	1.6×10 ⁻¹⁴	2.0	–	E17
OH + CF ₃ CHFCH ₂ F → products (HFC-245eb)	–	–	1.5×10 ⁻¹⁴	2.0	–	E18
OH + CHF ₂ CH ₂ CF ₃ → products (HFC-245fa)	6.1×10 ⁻¹³	1330	7.0×10 ⁻¹⁵	1.2	150	E19
OH + CF ₃ CF ₂ CH ₂ F → CF ₃ CF ₂ CHF + H ₂ O (HFC-236cb)	1.3×10 ⁻¹²	1700	4.4×10 ⁻¹⁵	2.0	200	E20
OH + CF ₃ CHFCHF ₂ → products (HFC-236ea)	9.4×10 ⁻¹³	1550	5.2×10 ⁻¹⁵	1.2	200	E21
OH + CF ₃ CH ₂ CF ₃ → CF ₃ CHCF ₃ + H ₂ O (HFC-236fa)	1.45×10 ⁻¹²	2500	3.3×10 ⁻¹⁶	1.15	150	E22
OH + CF ₃ CHFCF ₃ → CF ₃ CFCF ₃ +H ₂ O (HFC-227ea)	4.3×10 ⁻¹³	1650	1.7×10 ⁻¹⁵	1.1	150	E23
OH + CF ₃ CH ₂ CF ₂ CH ₃ → products (HFC-365mfc)	1.8×10 ⁻¹²	1660	6.9×10 ⁻¹⁵	1.3	150	E24
OH + CF ₃ CH ₂ CH ₂ CF ₃ → products (HFC-356mff)	3.4×10 ⁻¹²	1820	7.6×10 ⁻¹⁵	1.2	300	E25
OH + CF ₃ CF ₂ CH ₂ CH ₂ F → products (HFC-356mcf)	1.7×10 ⁻¹²	1100	4.2×10 ⁻¹⁴	1.3	150	E26
OH + CHF ₂ CF ₂ CF ₂ CF ₂ H → products (HFC-338pcc)	7.7×10 ⁻¹³	1540	4.4×10 ⁻¹⁵	1.2	150	E27
OH + CF ₃ CH ₂ CF ₂ CH ₂ CF ₃ → products (HFC-458mfcf)	1.1×10 ⁻¹²	1800	2.6×10 ⁻¹⁵	1.5	200	E28
OH + CF ₃ CHFCHF ₂ CF ₃ → products (HFC-43-10mee)	5.2×10 ⁻¹³	1500	3.4×10 ⁻¹⁵	1.2	150	E29
OH + CF ₃ CF ₂ CH ₂ CH ₂ CF ₂ CF ₃ → products (HFC-55-10-mcff)	3.5×10 ⁻¹²	1800	8.3×10 ⁻¹⁵	1.5	300	E30
OH + CH ₂ =CHF → products	1.5×10 ⁻¹²	–390	5.5×10 ⁻¹²	1.3	150	E31

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CH ₂ =CF ₂ → products	6.2×10^{-13}	-350	2.0×10^{-12}	1.5	150	E32
OH + CF ₂ =CF ₂ → products	3.4×10^{-12}	-320	1.0×10^{-11}	1.15	100	E33
OH + CF ₃ OH → CF ₃ O + H ₂ O			$<2 \times 10^{-17}$			E34
OH + CH ₂ (OH)CF ₃ → products	1.6×10^{-12}	830	9.8×10^{-14}	1.15	200	E35
OH + CH ₂ (OH)CF ₂ CF ₃ → products	1.15×10^{-12}	730	1.0×10^{-13}	1.2	200	E36
OH + CF ₃ CH(OH)CF ₃ → products	5.1×10^{-13}	900	2.5×10^{-14}	1.3	200	E37
OH + CH ₃ OCHF ₂ → products (HFOC-152a)	6.0×10^{-12}	1530	3.5×10^{-14}	1.3	200	E38
OH + CF ₃ OCH ₃ → CF ₃ OCH ₂ + H ₂ O (HFOC-143a)	1.5×10^{-12}	1450	1.2×10^{-14}	1.1	150	E39
OH + CF ₂ HOCHF ₂ H → CF ₂ OCF ₂ H + H ₂ O (HFOC-134)	1.1×10^{-12}	1830	2.4×10^{-15}	1.15	150	E40
OH + CF ₃ OCHF ₂ → CF ₃ OCF ₂ + H ₂ O (HFOC-125)	4.6×10^{-13}	2040	4.9×10^{-16}	1.2	200	E41
OH + CHF ₂ OCH ₂ CF ₃ → products (HFOC-245fa)	3.1×10^{-12}	1660	1.2×10^{-14}	1.2	200	E42
OH + CH ₃ OCF ₂ CHF ₂ → products	1.7×10^{-12}	1300	2.2×10^{-14}	1.3	200	E43
OH + CH ₃ OCF ₂ CF ₃ → products	1.1×10^{-12}	1370	1.1×10^{-14}	1.2	150	E44
OH + CH ₃ OCF ₂ CF ₂ CF ₃ → products	1.4×10^{-12}	1440	1.1×10^{-14}	1.15	150	E45
OH + CH ₃ OCF(CF ₃) ₂ → products	1.3×10^{-12}	1330	1.5×10^{-14}	1.3	200	E46
OH + CHF ₂ OCH ₂ CF ₂ CHF ₂ → products	1.8×10^{-12}	1410	1.6×10^{-14}	1.3	200	E47
OH + CHF ₂ OCH ₂ CF ₂ CF ₃ → products	1.6×10^{-12}	1510	1.0×10^{-14}	1.3	200	E48
F + O ₂ \xrightarrow{M} FO ₂	(See Table 2-1)					
F + O ₃ → FO + O ₂	2.2×10^{-11}	230	1.0×10^{-11}	1.5	200	E49
F + H ₂ → HF + H	1.4×10^{-10}	500	2.6×10^{-11}	1.2	200	E50
F + H ₂ O → HF + OH	1.4×10^{-11}	0	1.4×10^{-11}	1.3	200	E51
F + NO \xrightarrow{M} FNO	(See Table 2-1)					
F + NO ₂ \xrightarrow{M} FNO ₂	(See Table 2-1)					
F + HNO ₃ → HF + NO ₃	6.0×10^{-12}	-400	2.3×10^{-11}	1.3	200	E52
F + CH ₄ → HF + CH ₃	1.6×10^{-10}	260	6.7×10^{-11}	1.4	200	E53

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
FO + O ₃ → products			<1 × 10 ⁻¹⁴			E54
FO + NO → NO ₂ + F	8.2×10 ⁻¹²	-300	2.2×10 ⁻¹¹	1.5	200	E55
FO + NO ₂ \xrightarrow{M} FONO ₂	(See Table 2-1)					
FO + FO → 2F + O ₂	1.0×10 ⁻¹¹	0	1.0×10 ⁻¹¹	1.5	250	E56
FO ₂ + O ₃ → products			<3.4×10 ⁻¹⁶			E57
FO ₂ + NO → FNO + O ₂	7.5×10 ⁻¹²	690	7.5×10 ⁻¹³	2.0	400	E58
FO ₂ + NO ₂ → products	3.8×10 ⁻¹¹	2040	4.0×10 ⁻¹⁴	2.0	500	E59
FO ₂ + CO → products			<5.1×10 ⁻¹⁶			E60
FO ₂ + CH ₄ → products			<2×10 ⁻¹⁶			E61
CF ₃ + O ₂ \xrightarrow{M} CF ₃ O ₂	(See Table 2-1)					
CF ₃ O + M → F + CF ₂ O + M	(See Table 2-1)					
CF ₃ O + O ₂ → FO ₂ + CF ₂ O	<3 × 10 ⁻¹¹	5000	<1.5 × 10 ⁻¹⁸	1.3	-	E62
CF ₃ O + O ₃ → CF ₃ O ₂ + O ₂	2 × 10 ⁻¹²	1400	1.8 × 10 ⁻¹⁴		600	E63
CF ₃ O + H ₂ O → OH + CF ₃ OH	3 × 10 ⁻¹²	>3600	<2 × 10 ⁻¹⁷	1.2	-	E64
CF ₃ O + NO → CF ₂ O + FNO	3.7 × 10 ⁻¹¹	-110	5.4 × 10 ⁻¹¹		70	E65
CF ₃ O + NO ₂ → products	(See Note)					E66
\xrightarrow{M} CF ₃ ONO ₂	(See Table 2-1)					
CF ₃ O + CO → products			<2 × 10 ⁻¹⁵			E67
\xrightarrow{M} CF ₃ OCO	(See Table 2-1)					
CF ₃ O + CH ₄ → CH ₃ + CF ₃ OH	2.6 × 10 ⁻¹²	1420	2.2 × 10 ⁻¹⁴	1.1	200	E68
CF ₃ O + C ₂ H ₆ → C ₂ H ₅ + CF ₃ OH	4.9 × 10 ⁻¹²	400	1.3 × 10 ⁻¹²	1.2	100	E69
CF ₃ O ₂ + O ₃ → CF ₃ O + 2O ₂			<3 × 10 ⁻¹⁵			E70
CF ₃ O ₂ + CO → CF ₃ O + CO ₂			<5 × 10 ⁻¹⁶			E71
CF ₃ O ₂ + NO → CF ₃ O + NO ₂	5.4 × 10 ⁻¹²	-320	1.6 × 10 ⁻¹¹	1.1	150	E72
CF ₃ O ₂ + NO ₂ \xrightarrow{M} CF ₃ O ₂ NO ₂	(See Table 2-1)					

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
ClO_x Reactions						
O + ClO → Cl + O ₂	2.8×10 ⁻¹¹	-85	3.7×10 ⁻¹¹	1.10	50	F 1
O + OCIO → ClO + O ₂	2.4×10 ⁻¹²	960	1.0×10 ⁻¹³	2.0	300	F 2
O + OCIO \xrightarrow{M} ClO ₃	(See Table 2-1)					
O + Cl ₂ O → ClO + ClO	2.7×10 ⁻¹¹	530	4.5×10 ⁻¹²	1.3	150	F 3
O + HCl → OH + Cl	1.0×10 ⁻¹¹	3300	1.5×10 ⁻¹⁶	2.0	350	F 4
O + HOCl → OH + ClO	1.7×10 ⁻¹³	0	1.7×10 ⁻¹³	3.0	300	F 5
O + ClONO ₂ → products	2.9×10 ⁻¹²	800	2.0×10 ⁻¹³	1.5	200	F 6
O ₃ + OCIO → products	2.1×10 ⁻¹²	4700	3.0×10 ⁻¹⁹	2.5	1000	F 7
O ₃ + Cl ₂ O ₂ → products			<1.0×10 ⁻¹⁹			F 8
OH + Cl ₂ → HOCl + Cl	1.4×10 ⁻¹²	900	6.7×10 ⁻¹⁴	1.2	400	F 9
OH + ClO → Cl + HO ₂ → HCl + O ₂	7.4×10 ⁻¹² 6.0×10 ⁻¹³	-270 -230	1.8×10 ⁻¹¹ 1.3×10 ⁻¹²	1.4 3.0	100 150	F10
OH + OCIO → HOCl + O ₂	4.5×10 ⁻¹³	-800	6.8×10 ⁻¹²	2.0	200	F11
OH + HCl → H ₂ O + Cl	2.6×10 ⁻¹²	350	8.0×10 ⁻¹³	1.1	100	F12
OH + HOCl → H ₂ O + ClO	3.0×10 ⁻¹²	500	5.0×10 ⁻¹³	3.0	500	F13
OH + ClNO ₂ → HOCl + NO ₂	2.4×10 ⁻¹²	1250	3.6×10 ⁻¹⁴	2.0	300	F14
OH + ClONO ₂ → products	1.2×10 ⁻¹²	330	3.9×10 ⁻¹³	1.5	200	F15
OH + CH ₃ Cl → CH ₂ Cl + H ₂ O	2.4×10 ⁻¹²	1250	3.6×10 ⁻¹⁴	1.15	100	F16
OH + CH ₂ Cl ₂ → CHCl ₂ + H ₂ O	1.9×10 ⁻¹²	870	1.0×10 ⁻¹³	1.15	100	F17
OH + CHCl ₃ → CCl ₃ + H ₂ O	2.2×10 ⁻¹²	920	1.0×10 ⁻¹³	1.15	150	F18
OH + CCl ₄ → products	~1.0×10 ⁻¹²	>2300	<5.0×10 ⁻¹⁶	-	-	F19
OH + CH ₂ FCl → CHClF + H ₂ O (HCFC-31)	2.4×10 ⁻¹²	1210	4.1×10 ⁻¹⁴	1.15	200	F20
OH + CHFCl ₂ → CFCl ₂ + H ₂ O (HCFC-21)	1.2×10 ⁻¹²	1100	3.0×10 ⁻¹⁴	1.2	150	F21
OH + CHF ₂ Cl → CF ₂ Cl + H ₂ O (HCFC-22)	1.05×10 ⁻¹²	1600	4.8×10 ⁻¹⁵	1.1	150	F22
OH + CFCl ₃ → products (CFC-11)	~1.0×10 ⁻¹²	>3700	<5.0×10 ⁻¹⁸			F23

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CF ₂ Cl ₂ → products (CFC-12)	$\sim 1.0 \times 10^{-12}$	>3600	$< 6.0 \times 10^{-18}$			F24
OH + CH ₂ ClCH ₃ → products	5.4×10^{-12}	800	3.7×10^{-13}	1.2	100	F25
OH + CH ₃ CCl ₃ → CH ₂ CCl ₃ + H ₂ O	1.64×10^{-12}	1520	1.0×10^{-14}	1.15	100	F26
OH + CH ₃ CFCl ₂ → CH ₂ CFCl ₂ + H ₂ O (HCFC-141b)	1.25×10^{-12}	1600	5.8×10^{-15}	1.15	150	F27
OH + CH ₃ CF ₂ Cl → CH ₂ CF ₂ Cl + H ₂ O (HCFC-142b)	1.3×10^{-12}	1770	3.4×10^{-15}	1.2	150	F28
OH + CH ₂ ClCF ₂ Cl → CHClCF ₂ Cl + H ₂ O (HCFC-132b)	3.6×10^{-12}	1600	1.7×10^{-14}	1.5	200	F29
OH + CH ₂ ClCF ₃ → CHClCF ₃ + H ₂ O (HCFC-133a)	5.6×10^{-13}	1100	1.4×10^{-14}	1.3	200	F30
OH + CHCl ₂ CF ₂ Cl → CCl ₂ CF ₂ Cl (HCFC-122) + H ₂ O	7.7×10^{-13}	810	5.1×10^{-14}	1.2	150	F31
OH + CHFClCFCl ₂ → CFCICFCl ₂ (HCFC-122a) + H ₂ O	7.1×10^{-13}	1140	1.6×10^{-14}	1.3	150	F32
OH + CHCl ₂ CF ₃ → CCl ₂ CF ₃ + H ₂ O (HCFC-123)	6.3×10^{-13}	850	3.6×10^{-14}	1.2	100	F33
OH + CHFClCF ₂ Cl → CFCICF ₂ Cl + H ₂ O (HCFC-123a)	8.6×10^{-13}	1250	1.3×10^{-14}	1.3	200	F34
OH + CHFClCF ₃ → CFCICF ₃ + H ₂ O (HCFC-124)	7.1×10^{-13}	1300	9.0×10^{-15}	1.15	100	F35
OH + CH ₃ CF ₂ CFCl ₂ → products (HCFC-243cc)	7.7×10^{-13}	1720	2.4×10^{-15}	1.3	200	F36
OH + CHCl ₂ CF ₂ CF ₃ → products (HCFC-225ca)	6.3×10^{-13}	960	2.5×10^{-14}	1.2	200	F37
OH + CHFClCF ₂ CF ₂ Cl → products (HCFC-225cb)	5.5×10^{-13}	1230	8.9×10^{-15}	1.2	150	F38
OH + CH ₂ =CHCl → products	1.3×10^{-12}	-500	6.9×10^{-12}	1.2	100	F39
OH + CH ₂ =CCl ₂ → products	1.9×10^{-12}	-530	1.1×10^{-11}	1.15	150	F40
OH + CHCl=CCl ₂ → products	8.0×10^{-13}	-300	2.2×10^{-12}	1.2	100	F41
OH + CCl ₂ =CCl ₂ → products	4.7×10^{-12}	990	1.7×10^{-13}	1.2	200	F42
OH + CH ₃ OCl → products	2.5×10^{-12}	370	7.1×10^{-13}	2.0	150	F43
OH + CCl ₃ CHO → H ₂ O + CCl ₃ CO	9.1×10^{-12}	580	1.3×10^{-12}	1.3	200	F44
HO ₂ + Cl → HCl + O ₂	1.8×10^{-11}	-170	3.2×10^{-11}	1.5	200	F45
→ OH + ClO	4.1×10^{-11}	450	9.1×10^{-12}	2.0	200	F45
HO ₂ + ClO → HOCl + O ₂	2.7×10^{-12}	-220	5.6×10^{-12}	1.3	200	F46
H ₂ O + ClONO ₂ → products			$< 2.0 \times 10^{-21}$			F47

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{NO} + \text{OCIO} \rightarrow \text{NO}_2 + \text{ClO}$	2.5×10^{-12}	600	3.4×10^{-13}	2.0	300	F48
$\text{NO} + \text{Cl}_2\text{O}_2 \rightarrow \text{products}$			$< 2.0 \times 10^{-14}$			F49
$\text{NO}_3 + \text{OCIO} \xrightarrow{\text{M}} \text{O}_2\text{ClONO}_2$	(See Table 2-1)					
$\text{NO}_3 + \text{HCl} \rightarrow \text{HNO}_3 + \text{Cl}$			$< 5.0 \times 10^{-17}$			F50
$\text{HO}_2\text{NO}_2 + \text{HCl} \rightarrow \text{products}$			$< 1.0 \times 10^{-21}$			F51
$\text{Cl} + \text{O}_2 \xrightarrow{\text{M}} \text{ClOO}$	(See Table 2-1)					
$\text{Cl} + \text{O}_3 \rightarrow \text{ClO} + \text{O}_2$	2.3×10^{-11}	200	1.2×10^{-11}	1.15	50	F52
$\text{Cl} + \text{H}_2 \rightarrow \text{HCl} + \text{H}$	3.05×10^{-11}	2270	1.5×10^{-14}	1.1	100	F53
$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	1.1×10^{-11}	980	4.1×10^{-13}	1.3	300	F54
$\text{Cl} + \text{NO} \xrightarrow{\text{M}} \text{NOCl}$	(See Table 2-1)					
$\text{Cl} + \text{NO}_2 \xrightarrow{\text{M}} \text{ClONO} (\text{ClONO}_2)$	(See Table 2-1)					
$\text{Cl} + \text{NO}_3 \rightarrow \text{ClO} + \text{NO}_2$	2.4×10^{-11}	0	2.4×10^{-11}	1.5	400	F55
$\text{Cl} + \text{N}_2\text{O} \rightarrow \text{ClO} + \text{N}_2$	(See Note)					F56
$\text{Cl} + \text{HNO}_3 \rightarrow \text{products}$			$< 2.0 \times 10^{-16}$			F57
$\text{Cl} + \text{HO}_2\text{NO}_2 \rightarrow \text{products}$			$< 1 \times 10^{-13}$			F58
$\text{Cl} + \text{CO} \xrightarrow{\text{M}} \text{ClCO}$	(See Table 2-1)					
$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3$	7.3×10^{-12}	1280	1.0×10^{-13}	1.05	50	F59
$\text{Cl} + \text{CH}_3\text{D} \rightarrow \text{products}$	7.0×10^{-12}	1380	6.8×10^{-14}	1.07	50	F60
$\text{Cl} + \text{H}_2\text{CO} \rightarrow \text{HCl} + \text{HCO}$	8.1×10^{-11}	30	7.3×10^{-11}	1.15	100	F61
$\text{Cl} + \text{HC(O)OH} \rightarrow \text{products}$			2.0×10^{-13}	1.5		F62
$\text{Cl} + \text{CH}_3\text{O}_2 \rightarrow \text{products}$			1.6×10^{-10}	1.5		F63
$\text{Cl} + \text{CH}_3\text{OH} \rightarrow \text{CH}_2\text{OH} + \text{HCl}$	5.5×10^{-11}	0	5.5×10^{-11}	1.2	100	F64
$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{products}$			5.7×10^{-11}	2.0		F65
$\text{Cl} + \text{CH}_3\text{ONO}_2 \rightarrow \text{products}$	1.3×10^{-11}	1200	2.3×10^{-13}	1.5	300	F66
$\text{Cl} + \text{C}_2\text{H}_2 \xrightarrow{\text{M}} \text{ClC}_2\text{H}_2$	(See Table 2-1)					

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{Cl} + \text{C}_2\text{H}_4 \xrightarrow{\text{M}} \text{ClC}_2\text{H}_4$	(See Table 2-1)					
$\text{Cl} + \text{C}_2\text{H}_6 \rightarrow \text{HCl} + \text{C}_2\text{H}_5$	7.2×10^{-11}	70	5.7×10^{-11}	1.07	20	F67
$\text{Cl} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow \text{ClO} + \text{C}_2\text{H}_5\text{O}$			7.4×10^{-11}	2.0		F68
$\rightarrow \text{HCl} + \text{C}_2\text{H}_4\text{O}_2$			7.7×10^{-11}	2.0		F68
$\text{Cl} + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{products}$	9.6×10^{-11}	0	9.6×10^{-11}	1.2	100	F69
$\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{OH} \rightarrow \text{products}$			2.8×10^{-14}	2.0		F70
$\text{Cl} + \text{CH}_3\text{CN} \rightarrow \text{products}$	1.6×10^{-11}	2140	1.2×10^{-14}	2.0	300	F71
$\text{Cl} + \text{C}_2\text{H}_5\text{ONO}_2 \rightarrow \text{products}$	1.5×10^{-11}	400	3.9×10^{-12}	1.5	200	F72
$\text{Cl} + \text{CH}_3\text{CO}_3\text{NO}_2 \rightarrow \text{products}$			$< 1 \times 10^{-14}$			F73
$\text{Cl} + \text{C}_3\text{H}_8 \rightarrow \text{HCl} + \text{CH}_3\text{CHCH}_3$	6.54×10^{-11}		8.0×10^{-11}	1.1	20	F74
$\rightarrow \text{HCl} + \text{CH}_2\text{CH}_2\text{CH}_3$	7.85×10^{-11}	80	6.0×10^{-11}	1.05	20	F74
$\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{CH}_2 + \text{HCl}$	7.7×10^{-11}	1000	2.7×10^{-12}	1.3	500	F75
$\text{Cl} + \text{C}_2\text{H}_5\text{CO}_3\text{NO}_2 \rightarrow \text{products}$			1.1×10^{-12}	2.0		F76
$\text{Cl} + 1\text{-C}_3\text{H}_7\text{ONO}_2 \rightarrow \text{products}$	4.5×10^{-11}	200	2.3×10^{-11}	1.5	200	F77
$\text{Cl} + 2\text{-C}_3\text{H}_7\text{ONO}_2 \rightarrow \text{products}$	2.3×10^{-11}	400	6.0×10^{-12}	2.0	200	F78
$\text{Cl} + \text{OCIO} \rightarrow \text{ClO} + \text{ClO}$	3.4×10^{-11}	-160	5.8×10^{-11}	1.25	200	F79
$\text{Cl} + \text{ClOO} \rightarrow \text{Cl}_2 + \text{O}_2$	2.3×10^{-10}	0	2.3×10^{-10}	3.0	250	F80
$\rightarrow \text{ClO} + \text{ClO}$	1.2×10^{-11}	0	1.2×10^{-11}	3.0	250	F80
$\text{Cl} + \text{Cl}_2\text{O} \rightarrow \text{Cl}_2 + \text{ClO}$	6.2×10^{-11}	-130	9.6×10^{-11}	1.2	130	F81
$\text{Cl} + \text{Cl}_2\text{O}_2 \rightarrow \text{products}$			1.0×10^{-10}	2.0		F82
$\text{Cl} + \text{HOCl} \rightarrow \text{products}$	2.5×10^{-12}	130	1.6×10^{-12}	1.5	250	F83
$\text{Cl} + \text{ClNO} \rightarrow \text{NO} + \text{Cl}_2$	5.8×10^{-11}	-100	8.1×10^{-11}	1.5	200	F84
$\text{Cl} + \text{ClONO}_2 \rightarrow \text{products}$	6.5×10^{-12}	-135	1.0×10^{-11}	1.2	50	F85
$\text{Cl} + \text{CH}_3\text{Cl} \rightarrow \text{CH}_2\text{Cl} + \text{HCl}$	2.17×10^{-11}	1130	4.9×10^{-13}	1.07	50	F86
$\text{Cl} + \text{CH}_2\text{Cl}_2 \rightarrow \text{HCl} + \text{CHCl}_2$	7.4×10^{-12}	910	3.5×10^{-13}	1.07	100	F87

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Cl + CHCl ₃ → HCl + CCl ₃	3.310 ⁻¹²	990	1.2x10 ⁻¹³	1.15	100	F88
Cl + CH ₃ F → HCl + CH ₂ F (HFC-41)	1.96x10 ⁻¹¹	1200	3.5x10 ⁻¹³	1.15	150	F89
Cl + CH ₂ F ₂ → HCl + CHF ₂ (HFC-32)	4.9x10 ⁻¹²	1500	3.2x10 ⁻¹⁴	1.5	200	F90
Cl + CHF ₃ → HCl + CF ₃ (HFC-23)			<5.0x10 ⁻¹⁶			F91
Cl + CH ₂ FCI → HCl + CHFCl (HCFC-31)	5.9x10 ⁻¹²	1200	1.05x10 ⁻¹³	1.1	200	F92
Cl + CHFCl ₂ → HCl + CFCl ₂ (HCFC-21)	6.0x10 ⁻¹²	1700	2.0x10 ⁻¹⁴	1.2	200	F93
Cl + CHF ₂ Cl → HCl + CF ₂ Cl (HCFC-22)	5.6x10 ⁻¹²	2430	1.6x10 ⁻¹⁵	1.15	200	F94
Cl + CH ₃ CCl ₃ → CH ₂ CCl ₃ + HCl	3.23x10 ⁻¹²	1770	8.5x10 ⁻¹⁵	1.2	200	F95
Cl + CH ₃ CH ₂ F → HCl + CH ₃ CHF (HFC-161)	1.82x10 ⁻¹¹	330	6.0x10 ⁻¹²	1.1	100	F96
→ HCl + CH ₂ CH ₂ F	1.4x10 ⁻¹¹	940	6.0x10 ⁻¹³	1.15	100	F96
Cl + CH ₃ CHF ₂ → HCl + CH ₃ CF ₂ (HFC-152a)	5.8x10 ⁻¹²	950	2.4x10 ⁻¹³	1.1	100	F97
→ HCl + CH ₂ CHF ₂	6.25x10 ⁻¹²	2320	2.6x10 ⁻¹⁵	1.15	200	F97
Cl + CH ₂ FCH ₂ F → HCl + CHFCH ₂ F (HFC-152)	2.27x10 ⁻¹¹	1050	6.7x10 ⁻¹³	1.15	200	F98
Cl + CH ₃ CFCl ₂ → HCl + CH ₂ CFCl ₂ (HCFC-141b)	3.4x10 ⁻¹²	2200	2.1x10 ⁻¹⁵	1.15	200	F99
Cl + CH ₃ CF ₂ Cl → HCl + CH ₂ CF ₂ Cl (HCFC-142b)	1.35x10 ⁻¹²	2400	4.3x10 ⁻¹⁶	1.15	200	F100
Cl + CH ₃ CF ₃ → HCl + CH ₂ CF ₃ (HFC-143a)	1.44x10 ⁻¹¹	3940	2.6x10 ⁻¹⁷	3.0	300	F101
Cl + CH ₂ FCHF ₂ → HCl + CH ₂ FCF ₂ (HFC-143)	6.8x10 ⁻¹²	1670	2.5x10 ⁻¹⁴	1.3	200	F102
→ HCl + CHFCHF ₂	9.1x10 ⁻¹²	1770	2.4x10 ⁻¹⁴	1.3	200	F102
Cl + CH ₂ ClCF ₃ → HCl + CHClCF ₃ (HCFC-133a)	1.83x10 ⁻¹²	1680	6.5x10 ⁻¹⁵	1.2	200	F103
Cl + CH ₂ FCF ₃ → HCl + CHF ₂ CF ₃ (HFC-134a)	2.4x10 ⁻¹²	2200	1.5x10 ⁻¹⁵	1.1	200	F104
Cl + CHF ₂ CHF ₂ → HCl + CF ₂ CHF ₂ (HFC-134)	7.0x10 ⁻¹²	2430	2.0x10 ⁻¹⁵	1.2	200	F105
Cl + CHCl ₂ CF ₃ → HCl + CCl ₂ CF ₃ (HCFC-123)	5.0x10 ⁻¹²	1800	1.2x10 ⁻¹⁴	1.15	200	F106
Cl + CHFClCF ₃ → HCl + CFCICF ₃ (HCFC-124)	1.13x10 ⁻¹²	1800	2.7x10 ⁻¹⁵	1.2	200	F107
Cl + CHF ₂ CF ₃ → HCl + CF ₂ CF ₃ (HFC-125)	1.8x10 ⁻¹²	2600	3.0x10 ⁻¹⁶	1.5	300	F108
Cl + C ₂ Cl ₄ \xrightarrow{M} C ₂ Cl ₅	(See Table 2-1)					

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
ClO + O ₃ → ClOO + O ₂ → OCIO + O ₂	<i>1.0×10⁻¹²</i>	>4000	<1.4×10 ⁻¹⁷ <1.0×10 ⁻¹⁸			F109 F109
ClO + H ₂ → products	~1.0×10 ⁻¹²	>4800	<1.0×10 ⁻¹⁹			F110
ClO + NO → NO ₂ + Cl	6.4×10 ⁻¹²	-290	1.7×10 ⁻¹¹	1.15	100	F111
ClO + NO ₂ \xrightarrow{M} ClONO ₂	(See Table 2-1)					
ClO + NO ₃ → ClOO + NO ₂	4.7×10 ⁻¹³	0	4.7×10 ⁻¹³	1.5	400	F112
ClO + N ₂ O → products	~1.0×10 ⁻¹²	>4300	<6.0×10 ⁻¹⁹			F113
ClO + CO → products	~1.0×10 ⁻¹²	>3700	<4.0×10 ⁻¹⁸			F114
ClO + CH ₄ → products	~1.0×10 ⁻¹²	>3700	<4.0×10 ⁻¹⁸			F115
ClO + H ₂ CO → products	~1.0×10 ⁻¹²	>2100	<1.0×10 ⁻¹⁵			F116
ClO + CH ₃ O ₂ → products	3.3×10 ⁻¹²	115	2.2×10 ⁻¹²	1.5	115	F117
ClO + ClO → Cl ₂ + O ₂ → ClOO + Cl → OCIO + Cl	1.0×10 ⁻¹² 3.0×10 ⁻¹¹ 3.5×10 ⁻¹³	1590 2450 1370	4.8×10 ⁻¹⁵ 8.0×10 ⁻¹⁵ 3.5×10 ⁻¹⁵	1.5 1.5 1.5	300 500 300	F118 F118 F118
ClO + ClO \xrightarrow{M} Cl ₂ O ₂	(See Table 2-1)					
ClO + OCIO \xrightarrow{M} Cl ₂ O ₃	(See Table 2-1)					
HCl + ClONO ₂ → products			<1.0×10 ⁻²⁰			F119
CH ₂ Cl + O ₂ \xrightarrow{M} CH ₂ ClO ₂	(See Table 2-1)					
CHCl ₂ + O ₂ \xrightarrow{M} CHCl ₂ O ₂	(See Table 2-1)					
CCl ₃ + O ₂ \xrightarrow{M} CCl ₃ O ₂	(See Table 2-1)					
CFCl ₂ + O ₂ \xrightarrow{M} CFCl ₂ O ₂	(See Table 2-1)					
CF ₂ Cl + O ₂ \xrightarrow{M} CF ₂ ClO ₂	(See Table 2-1)					
CCl ₃ O ₂ + NO ₂ \xrightarrow{M} CCl ₃ O ₂ NO ₂	(See Table 2-1)					
CFCl ₂ O ₂ + NO ₂ \xrightarrow{M} CFCl ₂ O ₂ NO ₂	(See Table 2-1)					
CF ₂ ClO ₂ + NO ₂ \xrightarrow{M} CF ₂ ClO ₂ NO ₂	(See Table 2-1)					

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{CH}_2\text{ClO} + \text{O}_2 \rightarrow \text{CHClO} + \text{HO}_2$			6×10^{-14}	5		F120
$\text{CH}_2\text{ClO}_2 + \text{HO}_2 \rightarrow \text{CH}_2\text{ClO}_2\text{H} + \text{O}_2$	3.3×10^{-13}	-820	5.2×10^{-12}	1.5	200	F121
$\text{CH}_2\text{ClO}_2 + \text{NO} \rightarrow \text{CH}_2\text{ClO} + \text{NO}_2$	7×10^{-12}	-300	1.9×10^{-11}	1.5	200	F122
$\text{CCl}_3\text{O}_2 + \text{NO} \rightarrow \text{CCl}_2\text{O} + \text{NO}_2 + \text{Cl}$	7.3×10^{-12}	-270	1.8×10^{-11}	1.3	200	F123
$\text{CCl}_2\text{FO}_2 + \text{NO} \rightarrow \text{CClFO} + \text{NO}_2 + \text{Cl}$	4.5×10^{-12}	-350	1.5×10^{-11}	1.3	200	F124
$\text{CClF}_2\text{O}_2 + \text{NO} \rightarrow \text{CF}_2\text{O} + \text{NO}_2 + \text{Cl}$	3.8×10^{-12}	-400	1.5×10^{-11}	1.2	200	F125
BrO_x Reactions						
$\text{O} + \text{BrO} \rightarrow \text{Br} + \text{O}_2$	1.9×10^{-11}	-230	4.1×10^{-11}	1.5	150	G 1
$\text{O} + \text{HBr} \rightarrow \text{OH} + \text{Br}$	5.8×10^{-12}	1500	3.8×10^{-14}	1.3	200	G 2
$\text{O} + \text{HOBr} \rightarrow \text{OH} + \text{BrO}$	1.2×10^{-10}	430	2.8×10^{-11}	3.0	300	G 3
$\text{O} + \text{BrONO}_2 \rightarrow \text{NO}_3 + \text{BrO}$	1.9×10^{-11}	-215	3.9×10^{-11}	1.25	40	G 4
$\text{OH} + \text{Br}_2 \rightarrow \text{HOBr} + \text{Br}$	2.1×10^{-11}	-240	4.6×10^{-11}	1.1	50	G 5
$\text{OH} + \text{BrO} \rightarrow \text{products}$	1.7×10^{-11}	-250	3.9×10^{-11}	1.4	100	G 6
$\text{OH} + \text{HBr} \rightarrow \text{H}_2\text{O} + \text{Br}$	5.5×10^{-12}	-200	1.1×10^{-11}	1.1	100	G 7
$\text{OH} + \text{CH}_3\text{Br} \rightarrow \text{CH}_2\text{Br} + \text{H}_2\text{O}$	2.35×10^{-12}	1300	3.0×10^{-14}	1.1	100	G 8
$\text{OH} + \text{CH}_2\text{Br}_2 \rightarrow \text{CHBr}_2 + \text{H}_2\text{O}$	2.0×10^{-12}	840	1.2×10^{-13}	1.15	150	G 9
$\text{OH} + \text{CHBr}_3 \rightarrow \text{CBr}_3 + \text{H}_2\text{O}$	1.35×10^{-12}	600	1.8×10^{-13}	1.5	100	G10
$\text{OH} + \text{CHF}_2\text{Br} \rightarrow \text{CF}_2\text{Br} + \text{H}_2\text{O}$	1.0×10^{-12}	1380	1.0×10^{-14}	1.1	100	G11
$\text{OH} + \text{CH}_2\text{ClBr} \rightarrow \text{CHClBr} + \text{H}_2\text{O}$	2.4×10^{-12}	920	1.1×10^{-13}	1.1	100	G12
$\text{OH} + \text{CF}_2\text{ClBr} \rightarrow \text{products}$ (Halon-1211)	$\sim 1 \times 10^{-12}$	>2600	$< 1.5 \times 10^{-16}$			G13
$\text{OH} + \text{CF}_2\text{Br}_2 \rightarrow \text{products}$ (Halon-1202)	$\sim 1 \times 10^{-12}$	>2200	$< 5.0 \times 10^{-16}$			G14
$\text{OH} + \text{CF}_3\text{Br} \rightarrow \text{products}$ (Halon-1301)	$\sim 1 \times 10^{-12}$	>3600	$< 6.0 \times 10^{-18}$			G15
$\text{OH} + \text{CH}_2\text{BrCH}_3 \rightarrow \text{products}$	2.9×10^{-12}	640	3.4×10^{-13}	1.2	150	G16
$\text{OH} + \text{CH}_2\text{BrCF}_3 \rightarrow \text{CHBrCF}_3 + \text{H}_2\text{O}$	1.4×10^{-12}	1340	1.6×10^{-14}	1.2	150	G17
$\text{OH} + \text{CHFBrCF}_3 \rightarrow \text{CFBrCF}_3 + \text{H}_2\text{O}$	7.3×10^{-13}	1120	1.7×10^{-14}	1.2	100	G18

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CHClBrCF ₃ → CClBrCF ₃ + H ₂ O	1.1×10 ⁻¹²	940	4.7×10 ⁻¹⁴	1.2	150	G19
OH + CHFClCF ₂ Br → CFCICF ₂ Br + H ₂ O	8.4×10 ⁻¹³	1220	1.4×10 ⁻¹⁴	1.3	200	G20
OH + CF ₂ BrCF ₂ Br → products (Halon-2402)	~1×10 ⁻¹²	>3600	<6×10 ⁻¹⁸			G21
OH + CH ₂ BrCH ₂ CH ₃ → products	3.0×10 ⁻¹²	330	1.0×10 ⁻¹²	1.1	50	G22
OH + CH ₃ CHBrCH ₃ → products	1.85×10 ⁻¹²	270	7.5×10 ⁻¹³	1.15	50	G23
HO ₂ + Br → HBr + O ₂	4.8×10 ⁻¹²	310	1.7×10 ⁻¹²	1.3	150	G24
HO ₂ + BrO → products	4.5×10 ⁻¹²	-460	2.1×10 ⁻¹¹	1.15	100	G25
NO ₃ + HBr → HNO ₃ + Br			<1.0×10 ⁻¹⁶			G26
Cl + CH ₂ ClBr → HCl + CHClBr	6.8×10 ⁻¹²	870	3.7×10 ⁻¹³	1.2	100	G27
Cl + CH ₃ Br → HCl + CH ₂ Br	1.4×10 ⁻¹¹	1030	4.4×10 ⁻¹³	1.05	50	G28
Cl + CH ₂ Br ₂ → HCl + CHBr ₂	6.3×10 ⁻¹²	800	4.3×10 ⁻¹³	1.1	50	G29
Cl + CHBr ₃ → CBr ₃ + HCl	4.85×10 ⁻¹²	850	2.8×10 ⁻¹³	1.3	200	G30
Br + O ₃ → BrO + O ₂	1.7×10 ⁻¹¹	800	1.2×10 ⁻¹²	1.2	200	G31
Br + H ₂ O ₂ → HBr + HO ₂	1.0×10 ⁻¹¹	>3000	<5.0×10 ⁻¹⁶			G32
Br + NO ₂ \xrightarrow{M} BrNO ₂	(See Table 2-1)					
Br + NO ₃ → BrO + NO ₂			1.6×10 ⁻¹¹	2.0		G33
Br + H ₂ CO → HBr + HCO	1.7×10 ⁻¹¹	800	1.1×10 ⁻¹²	1.3	200	G34
Br + OCIO → BrO + ClO	2.6×10 ⁻¹¹	1300	3.4×10 ⁻¹³	2.0	300	G35
Br + Cl ₂ O → BrCl + ClO	2.1×10 ⁻¹¹	470	4.3×10 ⁻¹²	1.3	150	G36
Br + Cl ₂ O ₂ → products			3.0×10 ⁻¹²	2.0		G37
BrO + O ₃ → products	~1.0×10 ⁻¹²	>3200	<2.0×10 ⁻¹⁷			G38
BrO + NO → NO ₂ + Br	8.8×10 ⁻¹²	-260	2.1×10 ⁻¹¹	1.15	130	G39
BrO + NO ₂ \xrightarrow{M} BrONO ₂	(See Table 2-1)					
BrO + NO ₃ → products			1.0×10 ⁻¹²	3.0		G40
BrO + ClO → Br + OCIO	9.5×10 ⁻¹³	-550	6.0×10 ⁻¹²	1.25	150	G41

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\rightarrow \text{Br} + \text{ClOO}$	2.3×10^{-12}	-260	5.5×10^{-12}	1.25	150	G41
$\rightarrow \text{BrCl} + \text{O}_2$	4.1×10^{-13}	-290	1.1×10^{-12}	1.25	150	G41
$\text{BrO} + \text{BrO} \rightarrow \text{products}$	1.5×10^{-12}	-230	3.2×10^{-12}	1.15	150	G42
$\text{CH}_2\text{BrO}_2 + \text{NO} \rightarrow \text{CH}_2\text{O} + \text{NO}_2 + \text{Br}$	4×10^{-12}	-300	1.1×10^{-11}	1.5	200	G43
IO_x Reactions						
$\text{O} + \text{I}_2 \rightarrow \text{IO} + \text{I}$	1.4×10^{-10}	0	1.4×10^{-10}	1.4	250	H1
$\text{O} + \text{IO} \rightarrow \text{O}_2 + \text{I}$			1.2×10^{-10}	2.0		H2
$\text{OH} + \text{I}_2 \rightarrow \text{HOI} + \text{I}$			1.8×10^{-10}	2.0		H3
$\text{OH} + \text{HI} \rightarrow \text{H}_2\text{O} + \text{I}$			3.0×10^{-11}	2.0		H4
$\text{OH} + \text{CH}_3\text{I} \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{I}$	2.9×10^{-12}	1100	7.2×10^{-14}	1.5	300	H5
$\text{OH} + \text{CF}_3\text{I} \rightarrow \text{HOI} + \text{CF}_3$	2.5×10^{-11}	2070	2.4×10^{-14}	1.3	200	H6
$\text{HO}_2 + \text{I} \rightarrow \text{HI} + \text{O}_2$	1.5×10^{-11}	1090	3.8×10^{-13}	2.0	500	H7
$\text{HO}_2 + \text{IO} \rightarrow \text{HOI} + \text{O}_2$			8.4×10^{-11}	1.5		H8
$\text{NO}_3 + \text{HI} \rightarrow \text{HNO}_3 + \text{I}$	(See Note)					H9
$\text{Cl} + \text{CH}_3\text{I} \rightarrow \text{CH}_2\text{I} + \text{HCl}$	2.9×10^{-11}	1000	1.0×10^{-12}	1.5	250	H10
$\text{I} + \text{O}_3 \rightarrow \text{IO} + \text{O}_2$	2.3×10^{-11}	870	1.2×10^{-12}	1.2	200	H11
$\text{I} + \text{NO} \xrightarrow{\text{M}} \text{INO}$	(See Table 2-1)					
$\text{I} + \text{NO}_2 \xrightarrow{\text{M}} \text{INO}_2$	(See Table 2-1)					
$\text{I} + \text{BrO} \rightarrow \text{IO} + \text{Br}$			1.2×10^{-11}	2.0		H12
$\text{IO} + \text{NO} \rightarrow \text{I} + \text{NO}_2$	9.1×10^{-12}	-240	2.0×10^{-11}	1.2	150	H13
$\text{IO} + \text{NO}_2 \xrightarrow{\text{M}} \text{IONO}_2$	(See Table 2-1)					
$\text{IO} + \text{ClO} \rightarrow \text{products}$	5.1×10^{-12}	-280	1.3×10^{-11}	2.0	200	H14
$\text{IO} + \text{BrO} \rightarrow \text{products}$			6.9×10^{-11}	1.5		H15
$\text{IO} + \text{IO} \rightarrow \text{products}$	1.5×10^{-11}	-500	8.0×10^{-11}	1.5	500	H16
$\text{INO} + \text{INO} \rightarrow \text{I}_2 + 2\text{NO}$	8.4×10^{-11}	2620	1.3×10^{-14}	2.5	600	H17

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{INO}_2 + \text{INO}_2 \rightarrow \text{I}_2 + 2\text{NO}_2$	2.9×10^{-11}	2600	4.7×10^{-15}	3.0	1000	H18
SO_x Reactions						
$\text{O} + \text{SH} \rightarrow \text{SO} + \text{H}$			1.6×10^{-10}	5.0		I1
$\text{O} + \text{CS} \rightarrow \text{CO} + \text{S}$	2.7×10^{-10}	760	2.1×10^{-11}	1.1	250	I2
$\text{O} + \text{H}_2\text{S} \rightarrow \text{OH} + \text{SH}$	9.2×10^{-12}	1800	2.2×10^{-14}	1.7	550	I3
$\text{O} + \text{OCS} \rightarrow \text{CO} + \text{SO}$	2.1×10^{-11}	2200	1.3×10^{-14}	1.15	150	I4
$\text{O} + \text{CS}_2 \rightarrow \text{CS} + \text{SO}$	3.2×10^{-11}	650	3.6×10^{-12}	1.2	150	I5
$\text{O} + \text{SO}_2 \xrightarrow{\text{M}} \text{SO}_3$	(See Table 2-1)					
$\text{O} + \text{CH}_3\text{SCH}_3 \rightarrow \text{CH}_3\text{SO} + \text{CH}_3$	1.3×10^{-11}	-410	5.0×10^{-11}	1.1	100	I6
$\text{O} + \text{CH}_3\text{SSCH}_3 \rightarrow \text{CH}_3\text{SO} + \text{CH}_3\text{S}$	3.9×10^{-11}	-290	1.03×10^{-10}	1.1	100	I7
$\text{O} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{products}$	2.0×10^{-12}	-440	8.8×10^{-12}	1.2	200	I8
$\text{O}_3 + \text{H}_2\text{S} \rightarrow \text{products}$			$< 2.0 \times 10^{-20}$			I9
$\text{O}_3 + \text{CH}_3\text{SCH}_3 \rightarrow \text{products}$			$< 1.0 \times 10^{-18}$			I10
$\text{O}_3 + \text{SO}_2 \rightarrow \text{SO}_3 + \text{O}_2$	3.0×10^{-12}	>7000	$< 2.0 \times 10^{-22}$			I11
$\text{OH} + \text{H}_2\text{S} \rightarrow \text{SH} + \text{H}_2\text{O}$	6.1×10^{-12}	75	4.7×10^{-12}	1.1	75	I12
$\text{OH} + \text{OCS} \rightarrow \text{products}$	1.1×10^{-13}	1200	1.9×10^{-15}	2.0	500	I13
$\text{OH} + \text{CS}_2 \rightarrow \text{SH} + \text{OCS}$			$< 2.0 \times 10^{-15}$			I14
$\text{OH} + \text{CS}_2 \rightarrow \text{CS}_2\text{OH} \xrightarrow{\text{O}_2} \text{products}$	(See Note)	(See Note)	1.2×10^{-12} at $P_{\text{air}} = 1 \text{ atm}$	1.25		I15
$\text{CS}_2\text{OH} + \text{O}_2 \rightarrow \text{products}$	2.8×10^{-14}	0	2.8×10^{-14}	1.2	100	I16
$\text{OH} + \text{CH}_3\text{SH} \rightarrow \text{CH}_3\text{S} + \text{H}_2\text{O}$	9.9×10^{-12}	-360	3.3×10^{-11}	1.07	75	I17
$\text{OH} + \text{CH}_3\text{SCH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{SCH}_3$	1.1×10^{-11}	240	4.9×10^{-12}	1.1	100	I18
$\text{OH} + \text{CH}_3\text{SCH}_3 \xrightarrow{\text{O}_2} (\text{CH}_3)_2\text{SOH} \xrightarrow{\text{O}_2} \text{products}$	(See Note)	(See Note)	1.6×10^{-12} at $P_{\text{air}} = 1 \text{ atm}$	1.2		I19
$(\text{CH}_3)_2\text{SOH} + \text{O}_2 \rightarrow \text{products}$	9.6×10^{-13}	0	9.6×10^{-13}	1.3	0	I20
$\text{OH} + \text{CH}_3\text{SSCH}_3 \rightarrow \text{products}$	6.0×10^{-11}	-400	2.3×10^{-10}	1.2	200	I21
$\text{OH} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{products}$	6.1×10^{-12}	-800	8.9×10^{-11}	1.2	500	I22

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CH ₃ S(O)OH → products			9.0×10 ⁻¹¹	1.4		123
OH + S → H + SO			6.6×10 ⁻¹¹	3.0		124
OH + SO → H + SO ₂	2.7×10 ⁻¹¹	-335	8.3×10 ⁻¹¹	1.2	150	125
OH + SO ₂ \xrightarrow{M} HOSO ₂	(See Table 2-1)					
HO ₂ + H ₂ S → products			<3.0×10 ⁻¹⁵			126
HO ₂ + CH ₃ SH → products			<4.0×10 ⁻¹⁵			126
HO ₂ + CH ₃ SCH ₃ → products			<5.0×10 ⁻¹⁵			126
HO ₂ + SO ₂ → products			<1.0×10 ⁻¹⁸			127
NO ₂ + SO ₂ → products			<2.0×10 ⁻²⁶			128
NO ₃ + H ₂ S → products			<8.0×10 ⁻¹⁶			129
NO ₃ + OCS → products			<1.0×10 ⁻¹⁶			130
NO ₃ + CS ₂ → products			<4.0×10 ⁻¹⁶			131
NO ₃ + CH ₃ SH → products		-210	8.9×10 ⁻¹³	1.25	210	132
NO ₃ + CH ₃ SCH ₃ → CH ₃ SCH ₂ + HNO ₃		-500	1.0×10 ⁻¹²	1.15	200	133
NO ₃ + CH ₃ SSCH ₃ → products		270	5.3×10 ⁻¹³	1.4	270	134
NO ₃ + CH ₃ S(O)CH ₃ → products			2.9×10 ⁻¹³	1.6		135
NO ₃ + SO ₂ → products			<7.0×10 ⁻²¹			136
N ₂ O ₅ + CH ₃ SCH ₃ → products			<1.0×10 ⁻¹⁷			137
CH ₃ O ₂ + SO ₂ → products			<5.0×10 ⁻¹⁷			138
F + CH ₃ SCH ₃ → products			2.4.×10 ⁻¹⁰	2.0		139
Cl + H ₂ S → HCl + SH	3.7×10 ⁻¹¹	-210	7.4×10 ⁻¹¹	1.2	100	140
Cl + OCS → products			<1.0×10 ⁻¹⁶			141
Cl + CS ₂ → products	(See Table 2-1)					
CS ₂ Cl + O ₂ → products			<2.5×10 ⁻¹⁶			142
Cl + CH ₃ SH → CH ₃ S + HCl	1.2×10 ⁻¹⁰	-150	2.0×10 ⁻¹⁰	1.1	100	143

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{Cl} + \text{CH}_3\text{SCH}_3 \rightarrow \text{CH}_3\text{SCH}_2 + \text{HCl}$	1.6×10^{-10}	0	1.6×10^{-10}	1.6	350	144
$\text{Cl} + \text{CH}_3\text{SCH}_3 \xrightarrow{\text{M}} (\text{CH}_3)_2\text{SCl}$	(See Table 2-1)					
$(\text{CH}_3)_2\text{SCl} + \text{O}_2 \rightarrow \text{products}$			$<4.0 \times 10^{-18}$			145
$(\text{CH}_3)_2\text{SCl} + \text{NO} \rightarrow \text{products}$			1.2×10^{-11}	1.25		145
$(\text{CH}_3)_2\text{SCl} + \text{NO}_2 \rightarrow \text{products}$			2.7×10^{-11}	1.25		145
$\text{Cl} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{CH}_3\text{S(O)CH}_2 + \text{HCl}$			1.7×10^{-11}	1.25		146
$\text{Cl} + \text{CH}_3\text{S(O)CH}_3 \xrightarrow{\text{M}} \text{CH}_3(\text{Cl})\text{S(O)CH}_3$	(See Table 2-1)					
$\text{CH}_3(\text{Cl})\text{S(O)CH}_3 + \text{O}_2 \rightarrow \text{products}$			$<1.0 \times 10^{-17}$			147
$\text{CH}_3(\text{Cl})\text{S(O)CH}_3 + \text{NO} \rightarrow \text{products}$			1.6×10^{-11}	1.5		147
$\text{CH}_3(\text{Cl})\text{S(O)CH}_3 + \text{NO}_2 \rightarrow \text{products}$			2.0×10^{-11}	1.5		147
$\text{ClO} + \text{OCS} \rightarrow \text{products}$			$<2.0 \times 10^{-16}$			148
$\text{ClO} + \text{CH}_3\text{SCH}_3 \rightarrow \text{products}$	2.1×10^{-15}	-340	6.6×10^{-15}	1.5	300	149
$\text{ClO} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{products}$			$<2.0 \times 10^{-14}$			150
$\text{ClO} + \text{SO} \rightarrow \text{Cl} + \text{SO}_2$	2.8×10^{-11}	0	2.8×10^{-11}	1.3	50	151
$\text{ClO} + \text{SO}_2 \rightarrow \text{Cl} + \text{SO}_3$			$<4.0 \times 10^{-18}$			148
$\text{Br} + \text{H}_2\text{S} \rightarrow \text{HBr} + \text{SH}$	1.4×10^{-11}	2750	1.4×10^{-15}	2.0	300	152
$\text{Br} + \text{CH}_3\text{SH} \rightarrow \text{CH}_3\text{S} + \text{HBr}$	9.2×10^{-12}	390	2.5×10^{-12}	2.0	100	152
$\text{Br} + \text{CH}_3\text{SCH}_3 \rightarrow \text{CH}_3\text{SCH}_2 + \text{HBr}$	9.0×10^{-11}	2390	3.0×10^{-14}	1.4	150	153
$\text{Br} + \text{CH}_3\text{SCH}_3 \xrightarrow{\text{M}} (\text{CH}_3)_2\text{SBr}$	(See Table 2-1)					
$\text{Br} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{products}$			1.2×10^{-14}	1.5		154
$\text{BrO} + \text{CH}_3\text{SCH}_3 \rightarrow \text{products}$	1.4×10^{-14}	-950	3.4×10^{-13}	1.25	200	155
$\text{BrO} + \text{CH}_3\text{SSCH}_3 \rightarrow \text{products}$			1.5×10^{-14}	2.0		156
$\text{BrO} + \text{CH}_3\text{S(O)CH}_3 \rightarrow \text{products}$			1.0×10^{-14}	2.0		157
$\text{BrO} + \text{SO} \rightarrow \text{Br} + \text{SO}_2$			5.7×10^{-11}	1.4		158
$\text{IO} + \text{CH}_3\text{SH} \rightarrow \text{products}$			6.6×10^{-16}	2.0		159

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
IO + CH ₃ SCH ₃ → products			1.2×10 ⁻¹⁴	1.3		160
S + O ₂ → SO + O	2.3×10 ⁻¹²	0	2.3×10 ⁻¹²	1.2	200	161
S + O ₃ → SO + O ₂			1.2×10 ⁻¹¹	2.0		162
SO + O ₂ → SO ₂ + O	1.25×10 ⁻¹³	2190	8.0×10 ⁻¹⁷	1.3	350	163
SO + O ₃ → SO ₂ + O ₂	3.4×10 ⁻¹²	1100	8.4×10 ⁻¹⁴	1.1	150	164
SO + NO ₂ → SO ₂ + NO	1.4×10 ⁻¹¹	0	1.4×10 ⁻¹¹	1.2	50	165
SO + OCIO → SO ₂ + ClO			1.9×10 ⁻¹²	3.0		166
SO ₃ + 2 H ₂ O → products	(See Note)	(See Note)	(See Note)	1.2	200	167
SO ₃ + NH ₃ → products	(See Table 2-1)					
SO ₃ + NO ₂ → products			1.0×10 ⁻¹⁹	10.0		168
SH + O ₂ → OH + SO			<4.0×10 ⁻¹⁹			169
SH + O ₃ → HSO + O ₂	9.0×10 ⁻¹²	280	3.5×10 ⁻¹²	1.2	200	170
SH + H ₂ O ₂ → products			<5.0×10 ⁻¹⁵			171
SH + NO \xrightarrow{M} HSNO	(See Table 2-1)					
SH + NO ₂ → HSO + NO	2.9×10 ⁻¹¹	-240	6.5×10 ⁻¹¹	1.2	50	172
SH + N ₂ O → HSO + N ₂			<5.0×10 ⁻¹⁶			173
SH + Cl ₂ → ClSH + Cl	1.4×10 ⁻¹¹	690	1.4×10 ⁻¹²	1.15	200	174
SH + BrCl → products	2.3×10 ⁻¹¹	-350	7.4×10 ⁻¹¹	2.0	200	175
SH + Br ₂ → BrSH + Br	6.0×10 ⁻¹¹	-160	1.0×10 ⁻¹⁰	2.0	160	175
SH + F ₂ → FSH + F	4.3×10 ⁻¹¹	1390	4.0×10 ⁻¹³	2.0	200	175
HSO + O ₂ → products			<2.0×10 ⁻¹⁷			176
HSO + O ₃ → products			1.0×10 ⁻¹³	1.3		177
HSO + NO → products			<1.0×10 ⁻¹⁵			178
HSO + NO ₂ → HSO ₂ + NO			9.6×10 ⁻¹²	2.0		178
HSO ₂ + O ₂ → HO ₂ + SO ₂			3.0×10 ⁻¹³	3.0		179

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{HOSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_3$	1.3×10^{-12}	330	4.3×10^{-13}	1.15	200	180
$\text{CS} + \text{O}_2 \rightarrow \text{OCS} + \text{O}$			2.9×10^{-19}	2.0		181
$\text{CS} + \text{O}_3 \rightarrow \text{OCS} + \text{O}_2$			3.0×10^{-16}	3.0		182
$\text{CS} + \text{NO}_2 \rightarrow \text{OCS} + \text{NO}$			7.6×10^{-17}	3.0		182
$\text{CH}_3\text{S} + \text{O}_2 \rightarrow \text{products}$			$<3.0 \times 10^{-18}$			183
$\text{CH}_3\text{S} + \text{O}_3 \rightarrow \text{products}$	1.5×10^{-12}	-360	5.0×10^{-12}	1.15	100	184
$\text{CH}_3\text{S} + \text{NO} \rightarrow \text{products}$			$<1.0 \times 10^{-13}$			185
$\text{CH}_3\text{S} + \text{NO} \xrightarrow{\text{M}} \text{products}$	(See Table 2-1)					
$\text{CH}_3\text{S} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO} + \text{NO}$	3.0×10^{-11}	-240	6.7×10^{-11}	1.2	150	186
$\text{CH}_2\text{SH} + \text{O}_2 \rightarrow \text{products}$			6.5×10^{-12}	2.0		187
$\text{CH}_2\text{SH} + \text{O}_3 \rightarrow \text{products}$			3.5×10^{-11}	2.0		188
$\text{CH}_2\text{SH} + \text{NO} \rightarrow \text{products}$			1.9×10^{-11}	2.0		189
$\text{CH}_2\text{SH} + \text{NO}_2 \rightarrow \text{products}$			5.2×10^{-11}	2.0		190
$\text{CH}_3\text{SO} + \text{O}_3 \rightarrow \text{products}$			4.0×10^{-13}	1.5		191
$\text{CH}_3\text{SO} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{NO}$			1.2×10^{-11}	1.2		192
$\text{CH}_3\text{SOO} + \text{O}_3 \rightarrow \text{products}$			$<8.0 \times 10^{-13}$			193
$\text{CH}_3\text{SOO} + \text{NO} \rightarrow \text{products}$	1.1×10^{-11}	0	1.1×10^{-11}	2.0	100	193
$\text{CH}_3\text{SO}_2 + \text{NO}_2 \rightarrow \text{products}$	2.2×10^{-11}	0	2.2×10^{-11}	2.0	100	194
$\text{CH}_3\text{SCH}_2 + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_3\text{SCH}_2\text{O}_2$	(See Table 2-1)					
$\text{CH}_3\text{SCH}_2 + \text{NO}_3 \rightarrow \text{products}$			3.0×10^{-10}	2.0		195
$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{S} + \text{CH}_2\text{O} + \text{NO}_2$	4.9×10^{-12}	-260	1.2×10^{-11}	1.3	200	196
$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{CH}_3\text{SCH}_2\text{O}_2 \rightarrow \text{products}$			1.0×10^{-11}	1.25		197
$\text{CH}_3\text{SS} + \text{O}_3 \rightarrow \text{products}$			4.6×10^{-13}	2.0		198
$\text{CH}_3\text{SS} + \text{NO}_2 \rightarrow \text{products}$			1.8×10^{-11}	2.0		199
$\text{CH}_3\text{SSO} + \text{NO}_2 \rightarrow \text{products}$			4.5×10^{-12}	2.0		199

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Sodium Reactions						
$\text{Na} + \text{O}_2 \xrightarrow{\text{M}} \text{NaO}_2$	(See Table 2-1)					
$\text{Na} + \text{O}_3 \rightarrow \text{NaO} + \text{O}_2$ $\rightarrow \text{NaO}_2 + \text{O}$	1.0×10^{-9}	95	7.3×10^{-10} $< 4.0 \times 10^{-11}$	1.2	50	J1 J1
$\text{Na} + \text{N}_2\text{O} \rightarrow \text{NaO} + \text{N}_2$	2.8×10^{-10}	1600	1.3×10^{-12}	1.2	400	J2
$\text{Na} + \text{Cl}_2 \rightarrow \text{NaCl} + \text{Cl}$	7.3×10^{-10}	0	7.3×10^{-10}	1.3	200	J3
$\text{NaO} + \text{O} \rightarrow \text{Na} + \text{O}_2$	4.4×10^{-10}	0	4.4×10^{-10}	1.5	200	J4
$\text{NaO} + \text{O}_2 \xrightarrow{\text{M}} \text{NaO}_3$	(See Table 2-1)					
$\text{NaO} + \text{O}_3 \rightarrow \text{NaO}_2 + \text{O}_2$ $\rightarrow \text{Na} + 2\text{O}_2$	1.1×10^{-9} 6.0×10^{-11}	570 0	1.6×10^{-10} 6.0×10^{-11}	1.5 3.0	300 800	J5 J5
$\text{NaO} + \text{H}_2 \rightarrow \text{NaOH} + \text{H}$	2.6×10^{-11}	0	2.6×10^{-11}	2.0	600	J6
$\text{NaO} + \text{H}_2\text{O} \rightarrow \text{NaOH} + \text{OH}$	4.3×10^{-10}	500	8.0×10^{-11}	1.5	200	J7
$\text{NaO} + \text{NO} \rightarrow \text{Na} + \text{NO}_2$	1.5×10^{-10}	0	1.5×10^{-10}	4.0	400	J8
$\text{NaO} + \text{CO}_2 \xrightarrow{\text{M}} \text{NaCO}_3$	(See Table 2-1)					
$\text{NaO} + \text{HCl} \rightarrow \text{products}$	2.8×10^{-10}	0	2.8×10^{-10}	3.0	400	J9
$\text{NaO}_2 + \text{O} \rightarrow \text{NaO} + \text{O}_2$	2.2×10^{-11}	0	2.2×10^{-11}	5.0	600	J10
$\text{NaO}_2 + \text{NO} \rightarrow \text{NaO} + \text{NO}_2$			$< 10^{-14}$			J11
$\text{NaO}_2 + \text{HCl} \rightarrow \text{products}$	2.3×10^{-10}	0	2.3×10^{-10}	3.0	400	J12
$\text{NaOH} + \text{HCl} \rightarrow \text{NaCl} + \text{H}_2\text{O}$	2.8×10^{-10}	0	2.8×10^{-10}	3.0	400	J13
$\text{NaHCO}_3 + \text{H} \rightarrow \text{Na} + \text{H}_2\text{O} + \text{CO}_2$	1.4×10^{-11}	1000	5×10^{-13}	2.0	100	J14
$\text{NaOH} + \text{CO}_2 \xrightarrow{\text{M}} \text{NaHCO}_3$	(See Table 2-1)					

Shaded areas indicate changes or additions since JPL 97-4/JPL 00-3. Italicized entries denote estimates.

^a Units are $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

^b $f(298 \text{ K})$ is the uncertainty factor at 298 K. To calculate the uncertainty at other temperatures, use the expression:

$$f(T) = f(298) \exp \left[g \left(\frac{1}{T} - \frac{1}{298} \right) \right]$$

Note that the exponent is absolute value.

1.3 Notes to Table 1

JPL Publication numbers for the most recent revision of the table entry and note are given at the end of each note.

- A1. $O + O_3$. The recommended rate expression is from Wine et al. [1468] and is a linear least squares fit of all data (unweighted) from Davis et al. [360], McCrumb and Kaufman [891], West et al. [1442], Arnold and Comes [32], and Wine et al. [1468]. (Table: 83-62, Note: 83-62) [Back to Table](#)
- A2. $O(^1D)$ Reactions. In general, the rate constants given in the table are for the disappearance of $O(^1D)$, which includes physical quenching or deactivation and chemical reaction. Where information is available, the rate coefficient for a specific channel is also given. The details of deriving a recommended rate coefficient are given in the note for that reaction. In deriving recommended values direct measurements are used whenever they are available. However, the rate coefficients measured via relative rate techniques have also been considered for checking consistency in measured elementary reaction rate coefficients.

The rate constant recommendations are based on the absolute rate constants reported by Streit et al. [1249], Davidson et al. [353] and Davidson et al. [352] for N_2O , H_2O , CH_4 , H_2 , N_2 , O_2 , O_3 , CCl_4 , $CFCl_3$, CF_2Cl_2 , NH_3 , and CO_2 ; by Amimoto et al. [21], Amimoto et al. [20], and Force and Wiesenfeld [467, 468] for N_2O , H_2O , CH_4 , N_2 , H_2 , O_2 , O_3 , CO_2 , CCl_4 , $CFCl_3$, CF_2Cl_2 , and CF_4 ; by Wine and Ravishankara [1469-1471] for N_2O , H_2O , N_2 , H_2 , O_3 , CO_2 , and CF_2O ; by Lee and Slanger [791, 792] for H_2O and O_2 ; by Gericke and Comes [491] for H_2O ; and by Shi and Barker [1180] for N_2 and CO_2 by Talukdar and Ravishankara [1289] for H_2 , by Dunlea and Ravishankara [419] or N_2 , O_2 , O_3 , CO_2 , N_2O , and H_2O ; by Strekowski et al. [1253] for N_2 and O_2 , and by Blitz et al. for N_2 , O_2 , N_2O , CH_4 , H_2 , and CO_2 [153]. Measurements for other reactions are specifically cited in the notes for those reactions. The weight of the evidence from the studies noted above indicates that the results of Heidner and Husain [565], Heidner et al. [564] and Fletcher and Husain [461, 462] contain a systematic error. (Note: 06-2) [Back to Table](#)

- A3. $O(^1D) + O_2$. The 298 K recommended rate coefficient is derived from the studies of Blitz et al., Amimoto et al., Lee and Slanger, Davidson et al., Dunlea and Ravishankara, Streit et al., and Strekowski et al. (See above for references) The temperature dependence was computed by normalizing the results of Strekowski et al., Dunlea and Ravishankara, and Streit et al. at 298 K to the value recommended here. The deactivation of $O(^1D)$ by O_2 leads to the production of $O_2(^1\Sigma)$ with an efficiency of $80 \pm 20\%$. (Noxon [1003], Biedenkapp and Bair [137], Snelling [1220], and Lee and Slanger [791]). The $O_2(^1\Sigma)$ is produced in the $v=0, 1$, and 2 vibrational levels in the amounts 60% , 40% , and $<3\%$, respectively (Gauthier and Snelling [487] and Lee and Slanger [791]). The fractional deactivation of $O(^1D)$ that leads to the excitation of $O_2(^3\Sigma)$ to $O_2(^1\Delta)$ is expected to be $\sim 20\%$. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A4. $O(^1D) + O_3$. $k(298\text{ K})$ was derived from results of Davidson et al., Streit et al., Amimoto et al., Wine and Ravishankara, Talukdar et al. and Dunlea and Ravishankara. The rate coefficients measured for this reaction by Husain's group (Gilpin et al., and Heidner and Husain) are not expected to be influenced by the possible systematic error(s) that affect their other rate coefficient determinations. Their results are consistent with the recommended values. The reaction of $O(^1D)$ with O_3 gives $O_2 + O_2$ or $O_2 + O + O$. Davenport et al. [347] and Amimoto et al. [21] reported that, on average, one ground state O is produced per $O(^1D)$ reacting with O_3 . Very recent results from Dunlea et al. [422] also show that the yield of $O(^3P)$ in this reaction is close to, but not exactly, unity. Also, Dunlea et al. suggest a small but significant temperature dependence to this yield. Further studies on this yield would be useful. A unity yield of $O(^3P)$ is recommended. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A5. $O(^1D) + H_2$. The recommended rate coefficient is based on the references noted in Note A2. Wine and Ravishankara [1470] have determined that the yield of $O(^3P)$ is less than 4.9% . The major products are $H + OH$. Koppe et al. [737] report a 2.7 times larger rate coefficient at a collisional energy of 0.12 eV . This does not agree with the observations of Davidson et al. [353], who reported that k is independent of temperature ($200\text{--}350\text{ K}$) and Matsumi et al. [886] who report no change in k when translationally hot $O(^1D)$ is moderated with Ar. (Table: 97-4, Note: 97-4) [Back to Table](#)

- A6. $O(^1D) + H_2O$. The recommended $k(298\text{ K})$ is based on the results of Davidson et al., Amimoto et al., Wine and Ravishankara, Gericke and Comes, and Dunlea and Ravishankara, [420] but is weighted towards the study of Dunlea and Ravishankara because the latter study used several different methods to quantify the water vapor concentration. The results of Lee and Slanger are consistent with the recommended value. The temperature dependence of this rate coefficient is derived from the data of Streit et al. and of Dunlea and Ravishankara, after normalizing the results from the two studies to $k(298\text{ K})$ recommended here. The $O_2 + H_2$ product yield was measured by Zellner et al. [1516] to be $(1 + 0.5 \text{ or } -1)\%$ and by Glinski and Birks [512] to be $(0.6 + 0.7 \text{ or } -0.6)\%$. The yield of $O(^3P)$ from $O(^1D) + H_2O$ is reported to be less than $(4.9 \pm 3.2)\%$ by Wine and Ravishankara [1470] and $(2 \pm 1)\%$ by Takahashi et al. [1276]. Therefore, we recommend the yield of OH in this reaction to be 2.0.

To calculate the rates of OH production via $O(^1D)$ reactions in the atmosphere, the quantities of interest are the ratios of the rate coefficients for the reaction of $O(^1D)$ with H_2O to those with N_2 and with O_2 . The ratios of the rate coefficients for $O(^1D)$ reactions measured using the same method (and often the same apparatus) are more accurate (and precise) than the individual rate constants that are quoted in Table 1. Ratio data are given in the original references for this reaction. (Table: 06-2, Note: 06-2) [Back to Table](#)

- A7. $O(^1D) + N_2$. The rate coefficient for this reaction is taken from the paper of Ravishankara et al., [1092] which includes results from three different groups (Strekowski et al., Blitz et al., and Dunlea and Ravishankara) (See Note A2). Strekowski et al., have reported the rate coefficient for $O(^1D)$ removal by air and their results are in excellent agreement with the value derived using the current recommendation for $O(^1D)$ removal by N_2 and O_2 . (Table: 06-2, Note: 06-2) [Back to Table](#)
- A8. $O(^1D) + N_2O$. This reaction has two channels, one producing $2NO$ and the other producing $N_2 + O_2$. For atmospheric calculations of NO_x production, the rate coefficient for the channel that produces NO is critical, while the overall rate coefficient is important for deriving the loss rate of N_2O . The procedure employed to derive the rate coefficients recommended here was as follows: (1) the overall rate coefficient at 298 K and as a function of temperature for the removal of $O(^1D)$ in the interaction with N_2O was evaluated; (2) the branching ratio for the two possible channels shown in the table was evaluated for 298 K, the only temperature at which such data are available; (3) the overall rate coefficient from step 1 was divided into the two channels derived in step 2 to obtain the $k(298\text{ K})$ for the two channels listed in the table at 298 K; (4) the individual rate coefficients for the two channels as a function of temperature was derived by assuming that the branching ratio for the two channels is invariant with temperature.

The branching ratio for the reaction of $O(^1D)$ with N_2O to give $N_2 + O_2$ or $NO + NO$ is an average of the values reported by Davidson et al. [350]; Volltrauer et al. [1381]; Marx et al. [885] and Lam et al. [763], with a spread in $R = k(NO + NO)/k(\text{Total}) = 0.52 - 0.62$. Cantrell et al. [229] reported a measurement of $R = 0.57$ and an analysis of all measurements from 1957–1994 led them to recommend a value of $R = 0.61 \pm 0.06$, where the uncertainty indicates their 95% confidence interval. The recommended branching ratio agrees well with earlier measurements of the quantum yield from N_2O photolysis (Calvert and Pitts [220]). Dependencies on $O(^1D)$ translational energy and temperature are not clearly resolved. Wine and Ravishankara [1470] have determined that the yield of $O(^3P)$ from $O(^1D) + N_2O$ is less than 4.0%. The uncertainty for this reaction includes factors for both the overall rate coefficient and the branching ratio. A direct measurement by Greenblatt and Ravishankara [524] of the NO yield from the $O(^1D) + N_2O$ reaction in synthetic air and a reanalysis of this data by Dunlea and Ravishankara [419] agrees very well with the value predicted using the recommended $O(^1D)$ rate constants for N_2 , O_2 , and N_2O and the $O(^1D) + N_2O$ product branching ratio to give $NO + NO$.

The overall rate coefficient for the removal of $O(^1D)$ by N_2O was derived from the results of Davidson et al., Amimoto et al., Wine and Ravishankara, Blitz et al., and Dunlea and Ravishankara. The temperature dependence of this rate coefficient was derived from the results of Davidson et al. and Dunlea and Ravishankara, after normalizing both data sets to the $k(298\text{ K})$ recommended here for the overall rate coefficient, i.e., the sum of the two channels. The ratios of the rate coefficients for $O(^1D)$ reactions measured using the same method (and often the same apparatus) may be more accurate and precise than the individual rate constants that are quoted in Table 1. The values of f

and g listed in Table 1 were derived from all the available information. Better branching ratio measurements at the stratospheric temperatures and/or measurements of NO yield in this reaction as a function of temperature below 298 K would be useful for stratospheric modeling. (Table: 06-2, Note: 06-2) [Back to Table](#)

- A9. $O(^1D) + NH_3$. Sanders et al. [1141] have detected the products $NH(a^1\Delta)$ and OH formed in the reaction. They report that the yield of $NH(a^1\Delta)$ is in the range 3–15% of the amount of OH detected. (Table: 82-57, Note: 82-57) [Back to Table](#)
- A10. $O(^1D) + CO_2$. $k(298\text{ K})$ was derived from the studies of Davidson et al., Streit et al., Amimoto et al., Blitz et al., Dunlea and Ravishankara, and Shi and Barker, Blitz et al. Temperature dependence was computed after normalizing the results of Dunlea and Ravishankara and Streit et al. (only the data in the range of 200 to 354 K) to the value of $k(298\text{ K})$ recommended here. The rate coefficient at 195 K reported by Blitz et al. is consistent with the recommendation.
- This reaction produces $O(^3P)$ and CO_2 , and is expected to proceed through the formation of a CO_2 complex (see for example DeMore and Dede, [378]). This complex formation leads to isotopic scrambling (See for example Perri et al. [1046]). There appears to be a small, but non-negligible, channel for $O(^1D)$ quenching. A reactive channel to give CO and O_2 has been reported ([1167]), but needs better quantification. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A11. $O(^1D) + CH_4$. The reaction products are (a) $CH_3 + OH$, (b) CH_3O or $CH_2OH + H$ and (c) $CH_2O + H_2$. Lin and DeMore [830] analyzed the final products of N_2O/CH_4 photolysis mixtures and concluded that (a) accounted for about 90% and that CH_2O and H_2 (c) accounted for about 9%. Addison et al. [9] reported an OH yield of 80%. Casavecchia et al. [233] used a molecular beam experiment to observe H and CH_3O (or CH_2OH) products. They reported that the yield of H_2 was less than 25% of the yield of H from (b). Satyapal et al. [1147] observed the production of H atoms in a pulsed laser experiment and reported a yield of H of $(25\pm 8)\%$. Matsumi et al. [886] measured the yields of H and $O(^3P)$ in low pressure gas mixtures and reported that the yield of H was $(15\pm 3)\%$ and the yield of $O(^3P)$ was $<5\%$. Wine and Ravishankara [1470] reported that the yield of $O(^3P)$ was less than 4.3%. Takahashi et al. [1276] reported that the $O(^3P)$ yield is less than 1%. We recommend the following branching ratios: (a) $(75\pm 15)\%$, (b) $(20\pm 7)\%$, (c) $(5\pm 5)\%$. (Table: 94-26, Note: 97-4) [Back to Table](#)
- A12. $O(^1D) + HCl$. The recommendation is based on the measurements by Davidson et al. [353], Wine et al. [1476] and Chichinin [262]. The temperature dependence is based on Davidson et al. Product studies by Wine et al. indicate: $O(^3P) + HCl$ $(9\pm 5)\%$; $H + ClO$ $(24\pm 5)\%$; and $OH + Cl$ $(67\pm 10)\%$. Takahashi et al. [1276] report that the $O(^3P)$ yield is $(15\pm 4)\%$. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A13. $O(^1D) + HF$. The recommended value of $k(298\text{ K})$ is based on the one reported value of Sorokin et al. [1223]. It is assumed that the rate coefficient is independent of temperature. The possible products of this reaction are: $HF + O(^3P)$ and $F + OH$. The channel to give $H + FO$ is endothermic and, hence, considered to be unimportant. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A14. $O(^1D) + NF_3$. The recommended value of $k(298\text{ K})$ is based on the results of Sorokin et al. [1223] and Barone et al. [85]. The temperature dependence of the rate coefficient is based on Barone et al., the only temperature dependence study. Sorokin et al. and Barone et al., respectively, report that 70 and 80% of the $O(^1D)$ - NF_3 collisions lead to removal of NF_3 , i.e., products other than $O(^3P) + NF_3$. The identities of the products are not known. Therefore, the rate coefficient for the removal of NF_3 by reaction with $O(^1D)$ is greater than 70% of the overall rate coefficient for $O(^1D)$ removal by NF_3 . NEW ENTRY [Back to Table](#)
- A15. $O(^1D) + HBr$. Rate coefficient and product yields at 298 K was reported by Wine et al. [1476]. There are no reports on the temperature dependence of this rate coefficient. Because it is close to a collisional rate coefficient, the rate coefficient is assumed to be temperature independent. Product yields: $HBr + O(^3P)$ $(20\pm 7)\%$, $H + BrO$ $<4.5\%$, and $OH + Br$ $(80\pm 12)\%$. (Table: 87-41, Note: 87-41) [Back to Table](#)
- A16. $O(^1D) + Cl_2$. The recommended $k(298\text{ K})$ is based on the reports of Wine et al. [1466], and Sorokin et al. [1223]. There are no reports on the temperature dependence of this rate coefficient. The rate

coefficient is assumed to be temperature independent because $k(298\text{ K})$ is close to a collisional rate coefficient. Both Sorokin et al. and Wine et al. report that the branching ratio to produce $\text{ClO} + \text{Cl}$ is 0.75, based on their measured $\text{O}(^3\text{P})$ yield. This value is in excellent agreement with the directly measured ClO yield of $(74\pm 15)\%$, by Takahashi et al. [1276]. An indirect study by Freudenstein and Biedenkapp [471] is in reasonable agreement on the yield of ClO . Though energetically allowed, the formation of Cl_2O is expected to be negligible under atmospheric conditions of pressure and temperature. (Table: 06-2, Note: 06-2) [Back to Table](#)

- A17. $\text{O}(^1\text{D}) + \text{COCl}_2$. The recommended value of $k(298\text{ K})$ is derived from the values reported by Chichinin [262] and Strekowski et al. [1251]. The value of Fletcher and Husain, reduced by a factor of 2 to account for the systematic errors in their measurement method, is in reasonable agreement with the recommended value. The relative rate study of Jayanty et al. [654] is also consistent with the recommended value. The temperature dependence is taken from Strekowski et al. There are three possible reactive channels: $\text{CO} + \text{ClO} + \text{Cl}$; $\text{CO}_2 + 2\text{Cl}$; $\text{CO}_2 + \text{Cl}_2$. In the stratosphere, all these processes will lead to CO_2 and ClO . Chichinin reports that the above 3 reactions account for 80% of $\text{O}(^1\text{D})$ loss with 20% leading to $\text{O}(^3\text{P})$. The rate coefficient for the loss of COCl_2 via reaction with $\text{O}(^1\text{D})$ is expected to be more than 80% for the overall rate coefficient recommended here. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A18. $\text{O}(^1\text{D}) + \text{COCIF}$ and COF_2 . For the reactions of $\text{O}(^1\text{D})$ with COCIF the recommended rate constants are derived from data of Fletcher and Husain [463]. For consistency, the recommended values for these rate constants were derived using a scaling factor (0.5) that corrects for the difference between rate constants from the Husain laboratory and the recommendations for other $\text{O}(^1\text{D})$ rate constants in this table. The recommendation for COF_2 is from the data of Wine and Ravishankara [1471]. Their result is preferred over the value of Fletcher and Husain [463] because it appears to follow the pattern of decreased reactivity with increased fluorine substitution observed for other halocarbons. These reactions have been studied only at 298 K. Based on consideration of similar $\text{O}(^1\text{D})$ reactions, it is assumed that E/R equals zero, and therefore the value shown for the A-factor has been set equal to $k(298\text{ K})$. (Table: 82-57, Note: 97-4) [Back to Table](#)
- A19. $\text{O}(^1\text{D}) + \text{Halocarbons}$. The halocarbon rate constants are for the total disappearance of $\text{O}(^1\text{D})$ and probably include physical quenching. Products of the reactive channels may include $\text{CX}_3\text{O} + \text{X}$, $\text{CX}_2\text{O} + \text{X}_2$ (or 2X), and $\text{CX}_3 + \text{XO}$, where $\text{X} = \text{H}, \text{F}, \text{Cl},$ or Br in various combinations. Bromine, chlorine and hydrogen are more easily displaced than fluorine from halocarbons. Some values have been reported for the fractions of the total rate of disappearance of $\text{O}(^1\text{D})$ proceeding through physical quenching and reactive channels. For CCl_4 : quenching = $(14\pm 6)\%$ and reaction = $(86\pm 6)\%$ (Force and Wiesenfeld [468]), ClO yield = $(90\pm 19)\%$ (Takahashi et al. [1276]); for CFCl_3 : quenching = $(25\pm 10)\%$, ClO formation = $(60\pm 15)\%$ (Donovan, private communication, 1980), ClO yield = $(88\pm 18)\%$ (Takahashi et al.); for CF_2Cl_2 : quenching = $(14\pm 7)\%$ and reaction = $(86\pm 14)\%$ (Force and Wiesenfeld [468]), quenching = $(20\pm 10)\%$, ClO formation = $(55\pm 15)\%$ (Donovan), quenching = $(19\pm 5)\%$ and ClO formation = $(87\pm 18)\%$ (Takahashi et al.). (Table: 82-57, Note: 97-4) [Back to Table](#)
- A20. $\text{O}(^1\text{D}) + \text{CH}_3\text{Br}$. The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $\text{O}(^3\text{P})$ from physical quenching is $0\pm 7\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A21. $\text{O}(^1\text{D}) + \text{CH}_2\text{Br}_2$. The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $\text{O}(^3\text{P})$ from physical quenching is $(5\pm 7)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A22. $\text{O}(^1\text{D}) + \text{CHBr}_3$. The recommendation is based on data from Thompson and Ravishankara [1298]. The rate coefficient is somewhat large compared to analogous compounds. They report that the yield of $\text{O}(^3\text{P})$ from physical quenching is $(32\pm 8)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A23. $\text{O}(^1\text{D}) + \text{CH}_3\text{F}$ (HFC-41). The recommendation is the average of measurements of Force and Wiesenfeld [468] and Schmoltner et al. [1159]. The $\text{O}(^3\text{P})$ product yield was reported to be $(25\pm 3)\%$ by Force and Wiesenfeld, $(11\pm 5)\%$ by Schmoltner et al., and $(19\pm 5)\%$ by Takahashi et al. [1276]. Burks and Lin [202] reported observing vibrationally excited HF as a product. Park and Wiesenfeld [1035] observed OH . (Table: 94-26, Note: 97-4) [Back to Table](#)

- A24. $O(^1D) + CH_2F_2$ (HFC-32). The recommendation is based upon the measurement of Schmoltnner et al. [1159], who reported that the yield of $O(^3P)$ is $(70 \pm 11)\%$. Green and Wayne [522] measured the loss of CH_2F_2 relative to the loss of N_2O . Their value when combined with our recommendation for $O(^1D) + N_2O$ yields a rate coefficient for reactive loss of CH_2F_2 that is about three times the result of Schmoltnner et al., Burks and Lin [202] reported observing vibrationally excited HF as a product. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A25. $O(^1D) + CHF_3$ (HFC-23). The recommendation is the average of measurements of Force and Wiesenfeld [468] and Schmoltnner et al. [1159]. The $O(^3P)$ product yield was reported to be $(77 \pm 15)\%$ by Force and Wiesenfeld and $(102 \pm 3)\%$ by Schmoltnner et al. Although physical quenching is the dominant process, detectable yields of vibrationally excited HF have been reported by Burks and Lin [202] and Aker et al. [17], which indicate the formation of HF + CF_2O products. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A26. $O(^1D) + CHCl_2F$ (HCFC-21). The recommendation is based upon the measurement by Davidson et al. [352] of the total rate coefficient (physical quenching and reaction). Takahashi et al. [1276] report that the yield of ClO is $(74 \pm 15)\%$. (Table: 90-1, Note: 94-26) [Back to Table](#)
- A27. $O(^1D) + CHClF_2$ (HCFC-22). The recommendation is based upon the measurements by Davidson et al. [352] and Warren et al. [1426] of the total rate coefficient. A measurement of the rate of reaction (halocarbon removal) relative to the rate of reaction with N_2O by Green and Wayne [522] agrees very well with this value when the $O(^1D) + N_2O$ recommendation is used to obtain an absolute value. A relative measurement by Atkinson et al. [46] gives a rate coefficient about a factor of two higher. Addison et al. [9] reported the following product yields: ClO $(55 \pm 10)\%$, CF_2 $(45 \pm 10)\%$, $O(^3P)$ $(28 + 10$ or $-15)\%$, and OH 5%, where the $O(^3P)$ comes from a branch yielding CF_2 and HCl. Warren et al. [1426] also report a yield of $O(^3P)$ of $(28 \pm 6)\%$, which they interpret as the product of physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A28. $O(^1D) + CHF_2Br$. The recommended $k(298\text{ K})$ and the temperature dependence are based on the study of Streckowski et al., [1252] which is the only available investigation of this reaction. They report a branching ratio for $O(^3P)$ production of $\sim 40\%$, independent of temperature and a branching ratio for H atom production of $\sim 2\%$ at 298 K. Therefore, 60% of the reaction is expected to lead to destruction of CHF_2Br . NEW ENTRY [Back to Table](#)
- A29. $O(^1D) + CClF_3$ (CFC-13). The recommendation is based on the measurement by Ravishankara et al. [1097] who report $(31 \pm 10)\%$ physical quenching. Takahashi et al. [1276] report the yields of $O(^3P)$ $(16 \pm 5)\%$ and ClO $(85 \pm 18)\%$. (Table: 92-20, Note: 97-4) [Back to Table](#)
- A30. $O(^1D) + CClBrF_2$ (Halon 1211). The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $O(^3P)$ from physical quenching is $(36 \pm 4)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A31. $O(^1D) + CBr_2F_2$ (Halon 1202). The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $O(^3P)$ from physical quenching is $(54 \pm 6)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A32. $O(^1D) + CBrF_3$ (Halon 1301). The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $O(^3P)$ from physical quenching is $(59 \pm 8)\%$. Lorenzen-Schmidt et al. [844] measured the Halon removal rate relative to the N_2O removal rate and report that the rate coefficient for the Halon destruction path is $(4.0 \pm 0.4) \times 10^{-11}$, which is in excellent agreement with Thompson and Ravishankara. (Table: 94-26, Note: 97-4) [Back to Table](#)
- A33. $O(^1D) + CF_4$ (CFC-14). The recommendation is based upon the measurement by Ravishankara et al. [1097], who report $(92 \pm 8)\%$ physical quenching. Force and Wiesenfeld [468] measured a quenching rate coefficient about 10 times larger. Shi and Barker [1180] report an upper limit that is consistent with the recommendation. The small rate coefficient for this reaction makes it vulnerable to interference from reactant impurities. For this reason the recommendation should probably be considered an upper limit. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A34. $O(^1D) + CH_3CH_2F$ (HFC 161). The recommendation is based on data from Schmoltnner et al. [1159]. They report that the yield of $O(^3P)$ from physical quenching is $(18 \pm 5)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)

- A35. $O(^1D) + CH_3CHF_2$ (HFC-152a). The recommendation is based on the measurements of Warren et al. [1426], who report (54±7)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A36. $O(^1D) + CH_3CCl_2F$ (HCFC-141b). The recommendation is based upon the measurement of Warren et al. [1426], who report (31±5)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A37. $O(^1D) + CH_3CClF_2$ (HCFC-142b). The recommendation is based upon the measurement of Warren et al. [1426], who report (26±5)% physical quenching. This agrees very well with Green and Wayne [522], who measured the loss of CH_3CF_2Cl relative to the loss of N_2O , when the recommendation for N_2O is used. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A38. $O(^1D) + CH_3CF_3$ (HFC-143a). The recommendation is based upon the relative rate measurement of Green and Wayne [522], who measured the loss of CH_3CF_3 relative to the loss of N_2O . The recommendation for N_2O is used to obtain the value given. It is assumed that there is no physical quenching, although the reported physical quenching by CH_2FCF_3 and CH_3CHF_2 suggests some quenching is possible. (Table: 90-1, Note: 90-1) [Back to Table](#)
- A39. $O(^1D) + CH_2ClCClF_2$ (HCFC-132b). The recommendation is based upon the relative rate measurement of Green and Wayne [522], who measured the loss of CH_2ClCF_2Cl relative to the loss of N_2O . The recommendation for N_2O is used to obtain the value given. It is assumed that there is no physical quenching. (Table: 90-1, Note: 90-1) [Back to Table](#)
- A40. $O(^1D) + CH_2ClCF_3$ (HCFC-133a). The recommendation is based upon the measurement of Warren et al. [1426], who report (20±5)% physical quenching. This agrees with Green and Wayne [522] who measured the loss of CH_2ClCF_3 relative to the loss of N_2O , when the recommendation for N_2O is used. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A41. $O(^1D) + CH_2FCF_3$ (HFC-134a). The recommendation is based on the measurement of Warren et al. [1426] who report (94+6/-1)% physical quenching. The predominance of physical quenching is surprising, considering the presence of C-H bonds, which are usually reactive toward $O(^1D)$. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A42. $O(^1D) + CHCl_2CF_3$ (HCFC-123). The recommendation is based upon measurements by Warren et al. [1426]. The relative rate measurement of Green and Wayne [522], who measured the loss of $CHCl_2CF_3$ relative to the loss of N_2O , agrees well with the recommendation when the recommendation for N_2O is used. Warren et al. report (21 ± 8)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A43. $O(^1D) + CHClFCF_3$ (HCFC-124). The recommendation is based upon the measurement of Warren et al. [1426], who report (31 ± 10)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A44. $O(^1D) + CHF_2CF_3$ (HFC-125). The recommendation is based upon the measurement of Warren et al. [1426], who report (85+15/-22)% physical quenching. Green and Wayne [522] measured the loss of CHF_2CF_3 relative to the loss of N_2O and report a loss corresponding to about 40% of the recommended rate coefficient. This reaction is much faster than one would predict by analogy to similar compounds, such as CH_2FCF_3 . (Table: 92-20, Note: 92-20) [Back to Table](#)
- A45. $O(^1D) + CCl_3CF_3$ (CFC-113a). The recommendation is an estimate based on analogy to similar compounds. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A46. $O(^1D) + CCl_2FCClF_2$ (CFC-113). The recommendation is an estimate based on analogy to similar compounds. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A47. $O(^1D) + CCl_2FCF_3$ (CFC-114a). The recommendation is an estimate based on analogy to similar compounds. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A48. $O(^1D) + CClF_2CClF_2$ (CFC-114). The recommendation is based on the measurement by Ravishankara et al. [1097], who report (25 ± 9)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A49. $O(^1D) + CClF_2CF_3$ (CFC-115). The recommendation is based on the measurement by Ravishankara et al. [1097], who report (70 ± 7)% physical quenching. (Table: 92-20, Note: 92-20) [Back to Table](#)

- A50. $O(^1D) + CBrF_2CBrF_2$ (Halon 2402). The recommendation is based on data from Thompson and Ravishankara [1298]. They report that the yield of $O(^3P)$ from physical quenching is $(25 \pm 7)\%$. Lorenzen-Schmidt et al. [844] measured the Halon removal rate relative to the N_2O removal rate and report that the rate coefficient for the Halon destruction path is $(8.8 \pm 1.2) \times 10^{-11}$, in fair agreement with the result of Thompson and Ravishankara. (Table: 94-26, Note: 97-4) [Back to Table](#)
- A51. $O(^1D) + C_2F_6$ (CFC-116). The recommendation is based on a measurement by Ravishankara et al. [1097], who report $(85 \pm 15)\%$ physical quenching. The small rate coefficient for this reaction makes it vulnerable to interference from reactant impurities. For this reason the recommendation should probably be considered an upper limit. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A52. $O(^1D) + CHF_2CF_2CF_2CHF_2$ (HFC 338 pcc). The recommendation is based on data from Schmoltner et al. [1159]. They report that the yield of $O(^3P)$ from physical quenching is $(97 \pm 9)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A53. $O(^1D) + c-C_4F_8$. The recommendation for perfluorocyclobutane is based upon the measurement by Ravishankara et al. [1097], who report $(100 +0 / -15)\%$ physical quenching. The small rate coefficient for this reaction makes it vulnerable to interference from reactant impurities. For this reason the recommendation should probably be considered an upper limit. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A54. $O(^1D) + CF_3CHFCHFCF_2CF_3$ (HFC 43-10 mee). The recommendation is based on data from Schmoltner et al. [1159]. The rate coefficients for this compound and CHF_2CF_3 do not follow the reactivity trend of other HFCs. Schmoltner et al. report that the yield of $O(^3P)$ from physical quenching is $(91 \pm 4)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A55. $O(^1D) + C_5F_{12}$ (CFC 41-12). The recommendation is based on data from Ravishankara et al. [1097]. They report that the yield of $O(^3P)$ from physical quenching is $(79 \pm 12)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A56. $O(^1D) + C_6F_{14}$ (CFC 51-14). The recommendation is based on data from Ravishankara et al. [1097]. They report that the yield of $O(^3P)$ from physical quenching is $(75 \pm 9)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A57. $O(^1D) + 1,2-(CF_3)_2c-C_4F_6$. The recommendation is based on data from Ravishankara et al. [1097]. They report that the yield of $O(^3P)$ from physical quenching is $(84 \pm 16)\%$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- A58. $O(^1D) + SF_6$. The recommendation is based upon measurements by Ravishankara et al. [1097] who report $(32 \pm 10)\%$ physical quenching. The small rate coefficient for this reaction makes it vulnerable to interference from reactant impurities. For this reason the recommendation should probably be considered an upper limit. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A59. $O_2(^1\Delta) + O$. The recommendation is based on the upper limit reported by Clark and Wayne [269]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A60. $O_2(^1\Delta) + O_2$. The recommendation is the average of eight room temperature measurements: Steer et al. [1235], Findlay and Snelling [454], Borrell et al. [163], Leiss et al. [796], Tachibana and Phelps [1270], Billington and Borrell [145], Raja et al. [1087], and Wildt et al. [1455]. The temperature dependence is derived from the data of Findlay and Snelling, and Billington and Borrell. Several other less direct measurements of the rate coefficient agree with the recommendation, including Clark and Wayne [270], Findlay et al. [453], and McLaren et al. [894]. Wildt et al. [1456] report observations of weak emissions in the near IR due to collision-induced radiation. Wildt et al. [1457] give rate coefficients for this process. (Table: 92-20, Note: 94-26) [Back to Table](#)
- A61. $O_2(^1\Delta) + O_3$. The recommendation is the average of the room temperature measurements of Clark et al. [268], Findlay and Snelling [455], Becker et al. [107], and Collins et al. [305]. Several less direct measurements agree well with the recommendation (McNeal and Cook [895], Wayne and Pitts [1438], and Arnold and Comes [33]). The temperature dependence is from Findlay and Snelling and Becker et al., who agree very well, although both covered a relatively small temperature range. An earlier study by Clark et al. covered a much larger range, and found a much smaller temperature coefficient. The reason for this discrepancy is not clear. The yield of $O + 2O_2$ products appears to

be close to unity, based on many studies of the quantum yield of O₃ destruction near the peak of the Hartley band. For example, measurements of the number of O₃ molecules destroyed per photon absorbed: Von Ellenrieder et al. [1382], Ravishankara et al. [1103], Lissi and Heicklen [836], and references cited therein and measurements of O₃ loss and O atom temporal profiles in pulsed experiments Klais et al. [720] and Arnold and Comes [33]. Anderson et al. [29] report that the rate coefficient for atom exchange between O₂(¹Δ) and O₃ is < 5×10⁻¹⁶ at 300 K. (Table: 92-20, Note: 94-26) [Back to Table](#)

- A62. O₂(¹Δ) + H₂O. The recommendation is the average of the measurements reported by Becker et al. [106] and Findlay and Snelling [454]. An earlier study by Clark and Wayne [270] reported a value about three times larger. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A63. O₂(¹Δ) + N. The recommendation is an upper limit based upon the measurement reported by Westenberg et al. [1450], who used ESR to detect O₂(X³Σ and a¹Δ), O(³P) and N(⁴S) with a discharge flow reactor. They used an excess of O₂(¹Δ) and measured the decay of N and the appearance of O at 195 and 300 K. They observed that the reaction of N with O₂(¹Δ) is somewhat slower than its reaction with O₂(³Σ). The recommended rate constant value for the latter provides the basis for the recommendation. Clark and Wayne [269, 271] and Schmidt and Schiff [1156] reported observations of an O₂(¹Δ) reaction with N that is about 30 times faster than the recommended limit. Schmidt and Schiff attribute the observed loss of O₂(¹Δ) in excess N to a rapid energy exchange with some constituent in discharged nitrogen, other than N. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A64. O₂(¹Δ) + N₂. The recommendation is based upon the measurements by Findlay et al. [453] and Becker et al. [106]. Other studies obtained higher values for an upper limit: Clark and Wayne [270] and Steer et al. [1235]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A65. O₂(¹Δ) + CO₂. The recommendation is based on the measurements reported by Findlay and Snelling [454] and Leiss et al. [796]. Upper limit rate coefficients reported by Becker et al. [106], McLaren et al. [894], and Singh et al. [1197] are consistent with the recommendation. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A66. O₂(¹Σ) + O. The recommendation is based on the measurement reported by Slanger and Black [1211]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A67. O₂(¹Σ) + O₂. The recommendation is the average of values reported by Martin et al. [881], Lawton et al. [775], and Lawton and Phelps [776], who are in excellent agreement. Measurements by Thomas and Thrush [1297], Chatha et al. [247], and Knickelbein et al. [726] are in reasonable agreement with the recommendation. Knickelbein et al. report an yield of O₂(¹Δ) product to be approximately unity. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A68. O₂(¹Σ) + O₃. The recommendation is based upon the room temperature measurements of Gilpin et al. [506], Gauthier and Snelling [488], Slanger and Black [1211], Choo and Leu [264], Shi and Barker [1180], Turnipseed et al. [1342], and Dunlea et al [423]. Measurements by Snelling [1220], Amimoto and Wiesenfeld [22], and Ogren et al. [1005] are in agreement with the recommendation. The value from the study of Biedenkapp and Baer [136] is lower than the recommended value. The temperature dependence is taken from the results of Dunlea et al., who measured the rate coefficient between 210 and 370 K. The results of Choo and Leu, which encompassed 295-362 K, are consistent with the recommended value. This reaction has multiple product channels. The yield of O + 2O₂ products is reported to be (70±20)% by Slanger and Black and Amimoto and Wiesenfeld. The remaining ~30% of the reaction is expected to lead to quenching to O₂(¹Δ or ³Σ) while leaving ozone intact; the electronic state of O₂ that is produced in all these channels are not known. (Table: 06-2, Note: 06-2) [Back to Table](#)
- A69. O₂(¹Σ) + H₂. The rate coefficient for this reaction at, or around 298 K, has been measured by Kohse-Hoinghaus and Stuhl [734], Braithwaite et al., [174], Choo and Leu, [264], Singh and Setser, [1197], Wildt et al., [1455], Michelangeli et al., [922], Borrell and Richards, [164], Hohmann et al. [594], and Talukdar et al. [1283]. k(298K) was derived from the results of all, but two, of the above studies.

Results of Singh and Setser and Borrell and Richards, which are clearly outside of the range of values obtained by others, were not used.

The temperature dependence of the rate coefficient was computed using the results of Braithwaite et al., Hohmann et al., and Talukdar et al. The results of Kohse-Hoinghaus and Stuhl were not included because it is assumed to be superseded by those of Hohmann et al. from the same group. It is suspected that the Kohse-Hoinghaus and Stuhl study was hampered by impurities in their system, as discussed in Talukdar et al.

The rate coefficient for the reaction to produce 2 OH radicals is listed separately as an upper limit at 298 K and is based on the results of Talukdar et al. The same upper limit is shown to be valid even at 209 K. Therefore, this upper limit is recommended for all atmospheric calculations.

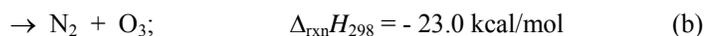
This reaction could also produce O(³P) + H₂O. However, there is no evidence for the formation of O(³P) (Dunlea et al.[418]). Therefore, it is assumed that O₂(¹Σ) is removed exclusively via quenching. The electronic state of O₂ that is produced is not known. NEW ENTRY [Back to Table](#)

- A70. O₂(¹Σ) + H₂O. The recommendation is the average of room temperature measurements reported by Stuhl and Niki [1256], Aviles et al., [57] Shi and Barker [1180], and Dunlea et al. [421]. Measurements reported by O'Brien and Myers [1004] are lower likely due to an interference from O₂(¹Σ) regeneration.. The results of Derwent and Thrush [385], and Thomas and Thrush [1297] are in agreement with the recommendation. The value reported by Gauthier and Snelling [488] has a very large uncertainty and hence overlaps with the recommendation. It is not clear why the results of Filseth et al. are lower than all the other reported values; perhaps, they had an error in measuring water vapor concentration. The temperature dependence of the reaction is taken from the only reported value of Dunlea et al. Wildt et al. [1455] report that the yield of O₂(¹Δ) greater than 90%. There are no thermodynamically allowed reactive channels for this reaction. Therefore, the reaction products are written as O₂ + H₂O [421].(Table: 06-2, Note: 06-2) [Back to Table](#)
- A71. O₂(¹Σ) + N. The recommendation is based on the limit reported by Slanger and Black [1211]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- A72. O₂(¹Σ) + N₂. The recommendation is the average of measurements reported by Izod and Wayne [646], Stuhl and Welge [1259], Filseth et al. [452], Martin et al. [881], Kohse-Hoinghaus and Stuhl [734], Choo and Leu [264], Wildt et al. [1455], Shi and Barker [1180], and Dunlea et al.[421]. Less direct measurements reported by Noxon [1003], Myers and O'Brien [940], and Chatha et al. [247] are consistent with the recommendation. The temperature dependence of the rate coefficient is derived from the results of Kohse-Hoinghaus and Stuhl between 203 and 349 K and of Dunlea et al. between 210 and 370 K.

There are no exothermic reaction channels. The channel to produce 2 NO molecules is endothermic by 5.6 kcal mol⁻¹ at 298 K. (Table: 06-2, Note: 06-2) [Back to Table](#)

- A73. O₂(¹Σ) + N₂O. The rate coefficient for the removal of O₂(¹Σ) by N₂O at 298 K is derived from the studies of Filseth et al., [452, 1297] Borrell et al., [162] and Dunlea et al. [424]. The results of Gauthier and Snelling has a very large error bar and overlaps with the recommended value within their quoted error bars. The temperature dependence of this rate coefficient is taken from Dunlea et al., who are the only ones to report this value.

There are many possible reactive channels for this reaction:





Dunlea et al. have placed upper limits of $<2 \times 10^{-4}$, $<1 \times 10^{-3}$, and $<3 \times 10^{-3}$ for channel (a+c), channel (c), and overall N_2O loss from this reaction at 298 K. Based on these results, we recommend the upper limit for the NO_x production process in the table. The upper limit for NO_x production from this reaction noted in the table is assumed to be valid for all atmospheric temperatures. NEW ENTRY [Back to Table](#)

- A74. $\text{O}_2(^1\Sigma) + \text{CO}_2$. The recommendation is the average of measurements reported by Filseth et al. [452], Davidson et al. [351], Avilés et al. [57], Muller and Houston [937], Choo and Leu [264], Wildt et al. [1455], Hohmann et al. [594], Dunlea and Ravishankara, and Shi and Barker [1180] at room temperature. The temperature dependence is from the work of Choo and Leu. Muller and Houston, and Singh and Setser [1197] give evidence that $\text{O}_2(^1\Delta)$ is a product. Wildt et al. report that the yield of $\text{O}_2(^1\Delta) \geq 90\%$. (Table: 92-20, Note: 06-2) [Back to Table](#)
- B1. $\text{O} + \text{OH}$. The rate constant for $\text{O} + \text{OH}$ is a fit to three temperature dependence studies: Westenberg et al. [1448], Lewis and Watson [817], and Howard and Smith [609]. This recommendation is consistent with earlier work near room temperature as reviewed by Lewis and Watson [817] and with the measurements of Brune et al. [185], Smith and Stewart [1215] and Robertson and Smith [1121]. The ratio $k(\text{O} + \text{HO}_2)/k(\text{O} + \text{OH})$ measured by Keyser [708] agrees with the rate constants recommended here. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B2. $\text{O} + \text{HO}_2$. The recommended values are based on the results of studies over a range of temperatures by Keyser [707] and Nicovich and Wine [971] and the room temperature studies of Sridharan et al. [1226], Ravishankara et al. [1103], and Brune et al. [185]. Earlier studies by Hack et al. [536] and Burrows et al. [203, 206] are not considered, because the $\text{OH} + \text{H}_2\text{O}_2$ reaction was important in these studies and the value used for its rate constant in their analyses has been shown to be in error. A study by Lii et al. [825] is also not considered because of the insensitivity of the observed to decays to $\text{O} + \text{HO}_2$. Data from Ravishankara et al. [1103] at 298 K show no dependence on pressure between 10 and 500 torr N_2 . The ratio $k(\text{O} + \text{HO}_2)/k(\text{O} + \text{OH})$ measured by Keyser [708] agrees with the rate constants recommended here. Sridharan et al. [1224] showed that the reaction products correspond to abstraction of an oxygen atom from HO_2 by the O reactant. Keyser et al. [712] reported $<1\%$ $\text{O}_2(^1\Delta)$ yield. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B3. $\text{O} + \text{H}_2\text{O}_2$. There are two direct studies of the $\text{O} + \text{H}_2\text{O}_2$ reaction: Davis et al. [361] and Wine et al. [1468]. The recommended value is a fit to the combined data. An indirect measurement of the E/R by Roscoe [1124] is consistent with the recommendation. The A-factor for both data sets is quite low compared to similar atom-molecule reactions. A somewhat higher activation barrier reported by Albers et al. [18] over the temperature range 370-800 K is suggestive of a non-linear temperature dependence. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B4. $\text{H} + \text{O}_3$. The recommendation is an average of the results of Lee et al. [783] and Keyser [703], which are in excellent agreement over the 200–400 K range. Results by Finlayson-Pitts, Seeley [1168] and Kleindienst [459] agree well with the present recommendations. An earlier study by Clyne and Monkhouse [290] is in very good agreement on the T dependence in the range 300–560 K but lies about 60% below the recommended values. Although we have no reason not to believe the Clyne and Monkhouse values, we prefer the two studies that are in excellent agreement, especially since they were carried out over the T range of interest. Reports of a channel forming $\text{HO}_2 + \text{O}$ (Finlayson-Pitts and Kleindienst [459]: ~25%, and Force and Wiesenfeld [467]: ~40%) have been contradicted by other studies (Howard and Finlayson-Pitts [608]: <3%; Washida et al. [1429]: <6%; Finlayson-Pitts et al. [460]: <2%; and Dodonov et al. [403]: <0.3%). Secondary chemistry is believed to be responsible for the observed O-atoms in this system. Washida et al. [1430] measured a low limit (<0.1%) for the production of singlet molecular oxygen in the reaction $\text{H} + \text{O}_3$. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B5. $\text{H} + \text{HO}_2$. There are five studies of this reaction: Hack et al. [540], Hack et al. [538], Thrush and Wilkinson [1304], Sridharan et al. [1226] and Keyser [710]. Related early work and combustion studies are referenced in the Sridharan et al. paper. All five studies used discharge flow systems. It is difficult to obtain a direct measurement of the rate constant for this reaction because both reactants

are radicals and the products OH and O are very reactive toward the HO₂ reactant. The recommendation is based on the kinetics and product data of Sridharan et al. and Keyser because their measurements were the most direct and required the fewest corrections. Keyser found the rate coefficient and product yields to be independent of temperature for 245 < T < 300 K. The other measurements, $(5.0 \pm 1.3) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by Thrush and Wilkinson [1304] and $(4.65 \pm 1) \times 10^{-11}$ by Hack et al. [538] are in reasonable agreement with the recommended value. Hislop and Wayne [585], Keyser et al. [712], and Michelangeli et al. [922] reported on the yield of O₂(b¹Σ) formed in the H₂ + O₂ channel as $(2.8 \pm 1.3) \times 10^{-4}$, $< 8 \times 10^{-3}$, and $< 2.1 \times 10^{-2}$, respectively as a fraction of the overall reaction. (Table: 06-2, Note: 06-2) [Back to Table](#)

- B6. OH + O₃. Recommended values are based on the results of studies over a range of temperatures by Anderson and Kaufman [26], Ravishankara et al. [1102], Smith et al. [1214] and Nizkorodov et al. [999] and the room temperature measurements of Kurylo [749], Zahniser and Howard [1508], and Kulcke et al. [744]. The recommended E/R and k(298 K) values are based on averages of the individual E/R and k(298 K) values obtained in the above-mentioned studies. The values reported by Kulcke et al. [744] and Nizkorodov et al. [1000] have been corrected for a minor contribution from k(HO₂ + O₃). (Table: 02-25, Note: 02-25) [Back to Table](#)
- B7. OH + H₂. The OH + H₂ reaction has been the subject of numerous studies. The recommendation is fixed to the average of eleven studies at 298 K: Greiner [525], Stuhl and Niki [1258], Westenberg and de Haas [1446], Smith and Zellner [1217], Atkinson et al. [48], Overend et al. [1028], Tully and Ravishankara [1332], Zellner and Steinert [1515], Ravishankara et al. [1095], Talukdar et al. [1284] and Orkin et al. [1019]. Temperature dependent studies of Orkin et al. Talukdar et al. and Ravishankara et al. find that the reaction does not follow a simple Arrhenius expression over a large range of temperature. The recommended temperature dependence is based on the average of E/R's determined in the above-mentioned studies for temperatures below 300 K. Accordingly, the recommended Arrhenius expression is only valid between 200 – 300 K. Even over this range the simple Arrhenius expression likely overestimates, near 250 K, and underestimates, near 200 K, the data by approximately 10%. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B8. OH + HD. The recommendation is based on direct measurements made by Talukdar et al. [1284] using pulsed photolysis-laser induced fluorescence over the temperature range 248–418 K. The recommendation is in excellent agreement with the ratio k(OH + H₂)/k(OH + HD) = 1.65±0.05 at 298 K reported by Ehhalt et al. [433] when combined with the recommended k(OH + H₂). (Table: 06-2, Note: 06-2) [Back to Table](#)
- B9. OH + OH. The recommendation for the OH + OH reaction is the average of seven measurements near 298 K: Westenberg and de Haas [1445], McKenzie et al. [893], Clyne and Down [279], Trainor and von Rosenberg [1319], Farquharson and Smith [446], Wagner and Zellner [1384], and Bedjanian et al. [110]. The rate constants for these studies all fall between $(1.4 \text{ and } 2.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. Temperature studies by Wagner and Zellner, which show a slight positive T-dependence, are in contrast with those of Bedjanian et al. which show a small negative T-dependence. The earlier work might have been complicated by an increased contribution of the OH + H reaction due to an underestimate of its reaction rate. However, theoretical calculations by Harding and Wagner [551] suggest that the reaction rate is substantially influenced by tunneling. In taking account of the tunneling contribution the rate constant is found to reach a minimum value near room temperature. In view of this predicted behavior and given that the experimental data are consistent with each other, within their stated uncertainties, we recommend a temperature independent value for the rate constant over the 200 – 300 K range. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B10. OH + HO₂. A study by Keyser [711] appears to resolve a discrepancy among low-pressure discharge flow experiments that all gave rate coefficients near $7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$: Keyser [706], Thrush and Wilkinson [1305], Sridharan et al. [1225], [1227], Temps and Wagner [1292], and Rozenshtein et al. [1128], and atmospheric pressure studies that gave rate coefficients near 11×10^{-11} : Lii et al. [824], Hochanadel et al. [592], DeMore [370], Cox et al. [317], Burrows et al. [205], and Kurylo et al. [755]. Laboratory measurements using a discharge flow experiment and a chemical model analysis of the results by Keyser [711] demonstrate that the previous discharge flow measurements were probably subject to interference from small amounts of O and H. In the presence

of excess HO₂ these atoms generate OH and result in a rate coefficient measurement that falls below the true value. The temperature dependence is from Keyser [711], who covered the range 254 to 382 K. A flow tube study by Schwab et al. [1164] reported $k = (8.0 \pm 3/-4) \times 10^{-11}$. These workers measured the concentrations of HO₂, OH, O, and H and used a computer model of the relevant reactions to test for interference. A flow tube study by Dransfeld and Wagner [413] employing an isotope labeled ¹⁸OH reactant obtained $k = (11 \pm 2) \times 10^{-11}$ in good agreement with the recommendation. They attributed about half of the reactive events to isotope scrambling because control experiments with ¹⁶OH gave $k = 6 \times 10^{-11}$. It should be noted that their control experiments were subject to the errors described by Keyser [711] due to the presence of small amounts of H and O, whereas their ¹⁸OH measurements were not. Kurylo et al. [755] found no evidence of significant scrambling in isotope studies of the OH and HO₂ reaction. An additional careful study of the reaction temperature dependence would be useful. Hippler and Troe [583] have analysed data for this reaction at temperatures up to 1250 K. In summary, this has historically been a difficult reaction to study. Earlier problems appear to have been resolved, as discussed above, and results now tend to converge on a central value, but the recommended value is still subject to a large uncertainty. (Table: 06-2, Note: 06-2) [Back to Table](#)

- B11. OH + H₂O₂. Data from a number of studies are in relatively good agreement between 300 and 500 K after revising some of the data to account for the H₂O₂ UV absorption cross section recommendations in this evaluation. Taken together the studies of Keyser [704], Sridharan et al. [1228], Wine et al. [1472], Kurylo et al. [759], Lamb et al. [764], and Vaghjiani et al. [1364] show that the reaction displays a small (~160 kcal/mole) positive temperature dependence over the 300 – 500 K range. Measurements at room temperature by Marinelli and Johnston [873], Turnipseed et al. [1342] and Vakhtin et al. [1365] agree well with the other studies. A value of $1.8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ is obtained by averaging all of the room temperature data. Below room temperature measurements by Lamb et al. and Vaghjiani diverge from the other studies, finding k to increase slightly with decreasing temperature. Vakhtin et al. have used a pulsed Laval nozzle technique to study the reaction at very low temperatures (165 K - 96 K). They measure a significant increase in k with decreasing temperature and suggest that the reaction mechanism includes formation of a hydrogen-bonded complex. Given the propensity of H₂O₂ for heterogeneous wall interactions at low temperatures, more studies are needed for this reaction, especially at low temperature and high pressures. Hippler and Troe [583] have analysed data for this reaction at temperatures up to 1250 K. At this time, we recommend a temperature independent value of 1.8×10^{-12} over the temperature range of 200 – 300 K. (Table: 06-2, Note: 06-2) [Back to Table](#)
- B12. HO₂ + O₃. The recommended values are based on results of studies over a range of temperatures by DeMore [368] at 231 to 334 K, Zahniser and Howard [1508] at 245 to 365 K, Manzanares et al. [864] at 298 K, Sinha et al. [1206] at 243 to 413 K, Wang et al. [1424] at 233 to 400 K and Herndon et al. [574] at 200 to 298 K. The data of Simonaitis and Heicklen [1192] and DeMore and Tschuikow-Roux [381] were not considered. The temperature dependence studies show varying degrees of curvature in the Arrhenius plots, with the E/R decreasing at lower temperature. This is especially evident in the low temperature data of Herndon et al. where a number of measures were taken to control potential kinetic complications. The recommended E/R and $k(298 \text{ K})$ values are based on averages of the individual E/R and $k(298 \text{ K})$ values. Furthermore, only data at temperatures less than 298 K were used for the E/R determination, accordingly the recommendation is not valid for $T > 298 \text{ K}$. Additional temperature dependence data are needed for this reaction over a larger range to more fully characterize the non-linear behavior of the rate constant. The mechanism of the reaction has been studied using ¹⁸O labeled HO₂ by Sinha et al. [1206], who reported that the reaction occurs 75±10% via H atom transfer at 297 K and by Nelson and Zahniser [951], who reported branching ratios for H transfer vs O transfer over the range 226–355 K. They report that the H atom transfer decreases from 94±5% at 226±11 K to 88±5% at 355±8 K. (Table: 00-3, Note: 00-3) [Back to Table](#)
- B13. HO₂ + HO₂. Two separate expressions are given for the rate constant for the HO₂ + HO₂ reaction. The effective rate constant is given by the sum of these two equations. This reaction has been shown to have a pressure-independent bimolecular component and a pressure-dependent termolecular component. Both components appear to have negative temperature coefficients. However, Christensen et al. [266] found that all of the previous temperature studies, which used CH₃OH as a

precursor, are complicated below 298 K by a reaction between CH_3OH and HO_2 . The bimolecular expression is obtained by fitting low pressure data of Cox and Burrows [316], Thrush and Tyndall [1301, 1302], Kircher and Sander [714], Takacs and Howard [1274, 1275], Sander [1134] and Kurylo et al. [761] above 298K so as to avoid possible complications due to CH_3OH chemistry. Data of Rozenshtein et al. [1128] are consistent with the low pressure recommendation, but they report no change in k with pressure up to 1 atm. Results of Thrush and Wilkinson [1303] and Dobis and Benson [401] are inconsistent with the recommendation. The termolecular expression is obtained from data of Sander et al. [1138], Simonaitis and Heicklen [1194], and Kurylo et al. [761] at room temperature and from Christensen [266] and Kircher and Sander [714] (only data above 298 K) for the temperature dependence. The recommended equation applies to $M = \text{air}$. The $\text{HO}_2 + \text{HO}_2$ reaction also exhibits a dependence on water vapor (Hamilton [544], Hochanadel et al. [591], Hamilton and Lii [545], Cox and Burrows [316], DeMore [368], Lii et al. [826], Sander et al. [1138], and Andersson et al. [30]) and H/D isotopic substitution (Hamilton and Lii [476] and Sander et al. [1138]). For systems containing water vapor, the multiplicative factor given by Lii et al. [826] and Kircher and Sander [714] can be used: $1 + 1.4 \times 10^{-21} [\text{H}_2\text{O}] \exp(2200/T)$. The major reaction products at 300 K have been identified as $\text{H}_2\text{O}_2 + \text{O}_2$ by Su et al. [1260], Niki et al. [988], Sander et al. [1138], and Simonaitis and Heicklen [1194]. Sahetchian et al. [1132, 1133] give evidence for the formation of a small amount of H_2 (~10%) at temperatures near 500 K, but Baldwin et al. [67] and Ingold [640] give evidence that the yield must be much less. Glinski and Birks [512] report an upper limit of 1% H_2 yield at a total pressure of about 50 torr and 298 K, but their experiment may have interference from wall reactions. A smaller limit to H_2 production (0.01%) was later determined in the same laboratory (Stephens et al. [1238]). The mechanism of the reaction has been studied using ^{18}O labelled HO_2 by Sinha et al. [1206], who reported that the reaction occurs 75±10% via H atom transfer at 297 K and by Nelson and Zahniser [951], who reported branching ratios for H transfer vs O transfer over the range 226–355 K. They report that the H atom transfer decreases from 94±5% at 226±11 K to 88±5% at 355±8 K. Lightfoot et al. [822] reported atmospheric pressure measurements over the temperature range 298–777 K that are in agreement with the recommended value at room temperature but indicate an upward curvature in the Arrhenius plot at temperatures above 500 K. A high temperature study by Hippler et al. [584] confirms the strong curvature, where a number of measures were taken to control potential kinetic complications. Because of this complex reaction behavior, the recommended rate expressions are only valid for temperatures below 500 K. Additional temperature dependence data are needed for this reaction over a larger range to more fully characterize the non-linear behavior of the rate constant. (Table: 06-2, Note: 06-2) [Back to Table](#)

- C1. $\text{O} + \text{NO}_2$. The recommended values are based on the results of studies over a range of temperatures by Estupiñán et al. [440], Gierczak et al. [492], Ongstad and Birks [1012], Slinger et al. [1212] and Geers-Muller and Stuhl [489] and the room temperature study of Paulson et al. [1040]. In the most recent studies of Estupiñán et al. [440] and Gierczak et al. [492], special emphasis was placed on accurate measurement of the NO_2 concentration and on measurements at low temperatures. The results of earlier studies by Davis et al. [356] and Bemand et al. [127] were not used in deriving the recommended values either because of possible complications from decomposition of NO_2 at higher temperatures or lack of direct NO_2 detection. (Table: 06-2, Note: 06-2) [Back to Table](#)
- C2. $\text{O} + \text{NO}_3$. The recommendation is based on the study of Graham and Johnston [520] at 298 K and 329 K. While limited in temperature range, the data indicate no temperature dependence. Furthermore, by analogy with the reaction of O with NO_2 , it is assumed that this rate constant is independent of temperature. Clearly, temperature-dependence studies are needed. (Table: 82-57, Note: 82-57) [Back to Table](#)
- C3. $\text{O} + \text{N}_2\text{O}_5$. The recommendation is based on the study by Kaiser and Japar [686]. (Table: 82-57, Note: 82-57) [Back to Table](#)
- C4. $\text{O} + \text{HNO}_3$. The upper limit reported by Chapman and Wayne [245] is accepted. (Table: 82-57, Note: 82-57) [Back to Table](#)
- C5. $\text{O} + \text{HO}_2\text{NO}_2$. The recommended value is based on the study of Chang et al. [243]. The large uncertainty in E/R and k at 298 K are due to the fact that the recommendation is based on a single study. (Table: 82-57, Note: 82-57) [Back to Table](#)

- C6. $\text{H} + \text{NO}_2$. The recommended value of k_{298} is derived from the studies of Wagner et al. [1386], Bemand and Clyne [125], Clyne and Monkhouse [290], Michael et al. [917] and Ko and Fontijn [732]. The temperature dependence is from the studies of Wagner et al. and Ko and Fontijn. The data from Wategaonkar and Setser [1433] and Agrawalla et al. [16] were not considered. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C7. $\text{OH} + \text{NO}_3$. The recommendation is derived from an average of the results of Boodaghians et al. [158], Mellouki et al. [904], Becker et al. [103] and Mellouki et al. [907]. There are no temperature dependence data. The reaction products are probably $\text{HO}_2 + \text{NO}_2$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- C8. $\text{OH} + \text{HONO}$. The recommended rate expression is derived from the work of Jenkin and Cox [660], which supersedes the earlier room temperature study of Cox et al. [323]. Results from the Burkholder et al. [200] suggest that the reaction may have a small negative temperature dependence. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C9. $\text{OH} + \text{HNO}_3$. The recent study of Brown et al. [184] furnishes the most comprehensive set of rate measurements for N_2 as the bath gas over a significant range of temperature (200–350 K) and pressure (20–500 torr). They analyzed their results in terms of the mechanism proposed by Smith et al. [1214], involving the formation of a bound, relatively long-lived $\text{HO}\cdot\text{HNO}_3$ complex, as well as the direct reaction channel. Studies of the effects of isotopic substitution on the reactions $\text{OD} + \text{DNO}_3$, $\text{OH} + \text{DNO}_3$, $\text{OD} + \text{HNO}_3$ and $^{18}\text{OH} + \text{HNO}_3$ by Brown et al. [183] support this mechanism and suggest that the structure of the intermediate consists of a H-bonded six-membered ring. Thus, the P dependence can be represented by combining a low pressure (bimolecular) limit, k_0 , with a Lindemann-Hinshelwood expression for the p-dependence:

$$k([\text{M}], T) = k_0 + \frac{k_3[\text{M}]}{1 + \frac{k_3[\text{M}]}{k_2}} \quad \left\{ \begin{array}{l} k_0 = 2.4 \times 10^{-14} \exp(460/T) \\ k_2 = 2.7 \times 10^{-17} \exp(2199/T) \\ k_3 = 6.5 \times 10^{-34} \exp(1335/T) \end{array} \right\}$$

The coefficients k_3 and k_2 are the termolecular and high pressure limits for the “association” channel. The value of k at high pressures is the sum $k_0 + k_2$.

This expression for $k([\text{M}], T)$ and the values of the Arrhenius parameters for k_0 , k_2 , and k_3 derived by Brown et al. [184] for N_2 as the bath gas constitute the recommended values for this rate coefficient. These recommended values are derived from a fit to the data of Brown et al. [184], Stachnik et al. [1230], Devolder et al. [386] and Margitan and Watson [868].

The reaction yield of NO_3 (per OH removed) is assumed to be unity at all temperatures for either reaction channel. These assumptions are supported by the isotopic studies of Brown et al. [183] and the theoretical calculations of Xia and Lin [1490]. (Table: 00-3, Note: 02-25) [Back to Table](#)

- C10. $\text{OH} + \text{HO}_2\text{NO}_2$. The recommendation for both k at 298 K and the Arrhenius expression is based upon the data of Trevor et al. [1321], Barnes et al. [73], C. A. Smith et al. [1214] and Barnes et al. [75]. Trevor et al. studied this reaction over the temperature range 246–324 K and reported a temperature invariant value of $4.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, although a weighted least squares fit to their data yields an Arrhenius expression with an E/R value of $(193 \pm 193) \text{ K}$. In contrast, Smith et al. studied the reaction over the temperature range 240–300 K and observed a negative temperature dependence with an E/R value of $-(650 \pm 30) \text{ K}$. The early Barnes et al. study [73] was carried out only at room temperature and 1 torr total pressure while their later study was performed in the pressure range 1–300 torr N_2 and temperature range 268–295 K with no rate constant variation being observed. In addition, k_{298} derived in Barnes et al. [73] was revised upward in the later study from 4.1×10^{-12} to 5.0×10^{-12} due to a change in the rate constant for the reference reaction. The values of k at 298 K from the four studies are in excellent agreement. An unweighted least squares fit to the data from the above-mentioned studies yields the recommended Arrhenius expression. The less precise value for k at 298 K reported by Littlejohn and Johnston [837] is in fair agreement with the recommended value. The error limits on the recommended E/R are sufficient to encompass the results of both Trevor et al. and Smith et al. It should be noted that the values of k at 220 K deduced

from the two studies differ by a factor of 2. Clearly, additional studies of k as a function of temperature and the identification of the reaction products are needed. (Table 02-25, Note: 02-25) [Back to Table](#)

- C11. OH + NH₃. The recommended value at 298 K is the average of the values reported by Stuhl [1254], Smith and Zellner [1218], Perry et al. [1048], Silver and Kolb [1184], Stephens [1237] and Diau et al. [388]. The values reported by Pagsberg et al. [1030] and Cox et al. [322] were not considered because these studies involved the analysis of a complex mechanism and the results are well outside the error limits implied by the above six direct studies. The results of Kurylo [749] and Hack et al. [534] were not considered because of their large discrepancies with the other direct studies (factors of 3.9 and 1.6 at room temperature, respectively). Because the Arrhenius plot displays considerable curvature, the temperature dependence is based only on the data below 300 K, i.e., the studies of Smith and Zellner [1218] and Diau et al. [388], and the A-factor has been selected to fit the recommended room temperature value. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C12. HO₂ + NO. The recommendation for HO₂ + NO is based on the average of eight measurements of the rate constant at room temperature and below: Howard and Evenson [607], Leu [812], Howard [604], Glaschick-Schimpf et al. [507], Hack et al. [537], Thrush and Wilkinson [1305] and Jemi-Alade Thrush [657], and Seeley et al. [1170]. All of these are in quite good agreement. The results of Imamura and Washida [638] were not considered due to the relatively large uncertainty limits reported in this study. An earlier study, Burrows et al. [203] has been disregarded because of an error in the reference rate constant, $k(\text{OH} + \text{H}_2\text{O}_2)$. The room temperature study of Rozenshtein et al. [1128] has also been disregarded due to an inadequate treatment of possible secondary reactions. The recommended Arrhenius parameters are obtained from a fit to all the data. The recommended value of $k(298 \text{ K})$ is obtained from the Arrhenius line. (Table: 97-4, Note: 97-4) [Back to Table](#)
- C13. HO₂ + NO₂. Tyndall et al. [1348] obtained an upper limit to the rate coefficient of $5 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ based on static photolysis experiments with FTIR analysis at 296 K and 760 torr of N₂. (Table: 97-4, Note: 97-4) [Back to Table](#)
- C14. HO₂ + NO₃. The recommendation for k_{298} is based on a weighted average of the data of Hall et al. [542], Mellouki et al. [904], Becker et al. [103] and Mellouki et al. [907]. There are insufficient data on which to base the temperature dependence of the rate coefficient. The measured branching ratios for the OH + NO₂ + O₂ channel range from 0.57 to 1.0. The most direct measurement is derived from the study of Mellouki et al. [907], which obtained a value of $1.0 \pm 0.0/-0.3$ at 298 K. (Table: 94-26, Note: 94-26) [Back to Table](#)
- C15. HO₂ + NH₂. There is a fairly good agreement on the value of k at 298 K between the direct study of Kurasawa and Lesclaux [748] and the relative studies of Cheskis and Sarkisov [260] and Pagsberg et al. [1030]. The recommended value is the average of the values reported in these three studies. The identity of the products is not known; however, Kurasawa and Lesclaux suggest that the most probable reaction channels give either NH₃ + O₂ or HNO + H₂O as products. (Table: 83-62, Note: 83-62) [Back to Table](#)
- C16. N + O₂. The recommended expression is derived from a least squares fit to the data of Kistiakowsky and Volpi [716], Wilson [1461], Becker et al. [105], Westenberg et al. [1450], Clark and Wayne [271], Winkler et al. [1479] and Barnett et al. [84]. $k(298 \text{ K})$ is derived from the Arrhenius expression and is in excellent agreement with the average of all of the room temperature determinations. (Table: 90-1, Note: 90-1) [Back to Table](#)
- C17. N + O₃. The recommendation is based on the results of Barnett et al. [84]. The value of $(1.0 \pm 0.2) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ reported by Barnett et al. should probably be considered an upper limit rather than a determination. The low values reported by Barnett et al., Stief et al. [1247] and Garvin and Broida [486] cast doubt on the much faster rates reported by Phillips and Schiff [1055], and Chen and Taylor [256]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- C18. N + NO. The recommended temperature dependence is based on the discharge flow-resonance fluorescence studies of Wennberg and Anderson [1441], and the discharge flow-resonance fluorescence and flash photolysis-resonance fluorescence studies of Lee et al. [785]. There is relatively poor agreement between these studies and the results of Clyne and McDermid [287],

- Kistiakowsky and Volpi [717], Herron [575], Phillips and Schiff [1055], Lin et al. [828], Ishikawa et al. [643], Sugawara et al. [1264], Cheah and Clyne [248], Husain and Slater [626], Clyne and Ono [294], Brunning and Clyne [186] and Jeoung et al. [670]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- C19. $\text{N} + \text{NO}_2$. The recommendation for k_{298} is from the discharge flow-resonance fluorescence study of Wennberg and Anderson [1441]. The latter study had significantly better sensitivity for $\text{N}(^4\text{S})$ than the discharge flow-resonance fluorescence study of Clyne and Ono [294], which obtained a value about four times smaller. The results of Husain and Slater [626] and Clyne and McDermid [287] are not considered. The temperature dependence is obtained from the study of Wennberg and Anderson. In the latter study, atomic oxygen was shown to be the principal reaction product, in agreement with Clyne and McDermid. A recent study by Iwata et al. [644] suggested an upper limit of $3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the corresponding reaction involving $\text{N}(^2\text{D})$ and $\text{N}(^2\text{P})$ atoms (sum of all reaction channels). (Table: 94-26, Note: 94-26) [Back to Table](#)
- C20. $\text{NO} + \text{O}_3$. The recommended values are based on the results of studies over a range of temperatures by Birks et al. [147], Lippmann et al. [833], Ray and Watson [1109], Michael et al. [912], Borders and Birks [160] and Moonen et al. [931] and the room temperature studies of Stedman and Niki [1233] and Bemand et al. [127]. The six temperature-dependent studies were given equal weighting in the recommendation by averaging over the E/R's from each individual data set. Following the Moonen et al. recommendation, the 200-K data point from their study has been excluded from the fit. All of the temperature dependence studies show some curvature in the Arrhenius plot at temperatures below 298 K. Increasing scatter between the data sets is evident at the lower temperatures. Clough and Thrush [275], Birks et al., Schurath et al. [1163], and Michael et al. have reported individual Arrhenius parameters for the two primary reaction channels producing ground and excited molecular oxygen. (Table: 00-3, Note: 00-3) [Back to Table](#)
- C21. $\text{NO} + \text{NO}_3$. The recommendation is based on the studies of Hammer et al. [546], Sander and Kircher [1137] and Tyndall et al. [1349], which are in excellent agreement. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C22. $\text{NO}_2 + \text{O}_3$. The recommended expression is derived from a least squares fit to the data of Davis et al. [359], Graham and Johnston [519], Huie and Herron [620], and Cox and Coker [318]. The data of Verhees and Adema [1373] and Stedman and Niki [1233] were not considered because of systematic discrepancies with the other studies. (Table: 90-1, Note: 90-1) [Back to Table](#)
- C23. $\text{NO}_2 + \text{NO}_3$. The existence of the reaction channel forming $\text{NO} + \text{NO}_2 + \text{O}_2$ has not been firmly established. However, studies of N_2O_5 thermal decomposition that monitor NO_2 (Daniels and Johnston [345]; Johnston and Tao [675]; Cantrell et al. [227]) and NO (Hjorth et al. [587], and Cantrell et al. [230]) require reaction(s) that decompose NO_3 into $\text{NO} + \text{O}_2$. The rate constant from the first three studies is obtained from the product kK_{eq} , where K_{eq} is the equilibrium constant for $\text{NO}_2 + \text{NO}_3 \rightarrow \text{N}_2\text{O}_5$, while for the latter two studies the rate constant is obtained from the ratio $k/k(\text{NO} + \text{NO}_3)$, where $k(\text{NO} + \text{NO}_3)$ is the rate constant for the reaction $\text{NO} + \text{NO}_3 \rightarrow 2\text{NO}_2$. Using K_{eq} and $k(\text{NO} + \text{NO}_3)$ from this evaluation, the rate expression that best fits the data from all five studies is $4.5 \times 10^{-14} \exp(-1260/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ with an overall uncertainty factor of 2. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C24. $\text{NO}_3 + \text{NO}_3$. The recommendation for $k(298 \text{ K})$ is from the studies of Graham and Johnston [520] and Biggs et al. [141]. The temperature dependence is from Graham and Johnston. (Table: 94-26, Note: 94-26) [Back to Table](#)
- C25. $\text{NH}_2 + \text{O}_2$. This reaction has several product channels which are energetically possible, including $\text{NO} + \text{H}_2\text{O}$ and $\text{HNO} + \text{OH}$. With the exception of the studies of Hack et al. [533] and Jayanty et al. [653] and several studies at high temperature, there is no evidence for a reaction. The following upper limits have been measured ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$): 3×10^{-18} (Lesclaux and Demissy [798]), 8×10^{-15} (Pagsberg et al. [1030]), 1.5×10^{-17} (Cheskis and Sarkisov [260]), 3×10^{-18} (Lozovsky et al. [852]), 1×10^{-17} (Patrick and Golden [1039]) and 7.7×10^{-18} (Michael et al. [913]) and 6×10^{-21} (Tyndall et al. [1351]). The recommendation is based on the study of Tyndall et al., which was sensitive to reaction paths leading to the products NO , NO_2 and N_2O . The reaction forming NH_2O_2

cannot be ruled out, but is apparently not important in the atmosphere. (Table: 92-20, Note: 92-20)
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- C26. $\text{NH}_2 + \text{O}_3$. There is poor agreement among the recent studies of Cheskis et al. [259], $k(298) = 1.5 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Patrick and Golden [1039], $k(298 \text{ K}) = 3.25 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Hack et al. [532], $1.84 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Bulatov et al. [193], $1.2 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, and Kurasawa and Lesclaux [747], $0.63 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$. The very low value of Kurasawa and Lesclaux may be due to regeneration of NH_2 from secondary reactions (see Patrick and Golden), and it is disregarded here. The discharge flow value of Hack et al. is nearly a factor of two less than the recent Patrick and Golden flash photolysis value. The large discrepancy between Bulatov et al. and Patrick and Golden eludes explanation. The recommendation is the $k(298 \text{ K})$ average of these four studies, and E/R is an average of Patrick and Golden (1151 K) with Hack et al. (710 K). (Table: 90-1, Note: 90-1) [Back to Table](#)
- C27. $\text{NH}_2 + \text{NO}$. The recommended value for k at 298 K is the average of the values reported by Lesclaux et al. [800], Hancock et al. [547], Sarkisov et al. [1145], Stief et al. [1245], Andresen et al. [31], Whyte and Phillips [1451], Dreier and Wolfrum [415], Atakan et al. [37], Wolf et al. [1480], Diau et al. [389] and Imamura and Washida [638]. The results of Gordon et al. [516], Gehring et al. [490], Hack et al. [539] and Silver and Kolb [1185] were not considered because they lie at least 2 standard deviations from the average of the previous group. The results tend to separate into two groups. The flash photolysis results average $1.8 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ (except for the pulse radiolysis study of Gordon et al.), while those obtained using the discharge flow technique average $0.9 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The apparent discrepancy cannot be due simply to a pressure effect as the pressure ranges of the flash photolysis and discharge flow studies overlapped and none of the studies observed a pressure dependence for k . Whyte and Phillips have suggested that the difference may be due to decomposition of the adduct NH_2NO , which occurs on the timescale of the flow experiments, but not the flash experiments. There have been many studies of the temperature dependence but most have investigated the regime of interest to combustion and only two have gone below room temperature (Hack et al. from 209–505 K and Stief et al. from 216–480 K. Each study reported k to decrease with increasing temperature. The recommended temperature dependence is taken from a fit to the Stief et al. data at room temperature and below. The reaction proceeds along a complex potential energy surface, which results in product branching ratios that are strongly dependent on temperature. *Ab initio* calculations by Walch [1389] show the existence of four saddle points in the potential surface leading to $\text{N}_2 + \text{H}_2\text{O}$ without a reaction barrier. Elimination to form $\text{OH} + \text{HN}_2$ can occur at any point along the surface. While results from early studies on the branching ratio for OH formation differ significantly, the most recent studies (Hall et al., Dolson [405], Silver and Kolb [1188], Atakan et al., Stephens et al. [1236], Park and Lin [1036]) agree on a value around 0.1 at 300 K, with $\text{N}_2 + \text{H}_2\text{O}$ making up the balance. (Table: 97-4, Note: 97-4) [Back to Table](#)
- C28. $\text{NH}_2 + \text{NO}_2$. There have been four studies of this reaction (Hack et al. [539]; Kurasawa and Lesclaux [746]; Whyte and Phillips [1451]; and Xiang et al. [1491]). There is very poor agreement among these studies both for k at 298 K (factor of 2.3) and for the temperature dependence of k ($T^{-3.0}$ and $T^{-1.3}$). The recommended values of k at 298 K and the temperature dependence of k are averages of the results reported in these four studies. Hack et al. have shown that the predominant reaction channel (>95%) produces $\text{N}_2\text{O} + \text{H}_2\text{O}$. Just as for the $\text{NH}_2 + \text{NO}$ reaction, the data for this reaction seem to indicate a factor of two discrepancy between flow and flash techniques, although the data base is much smaller. (Table: 85-37, Note: 87-41) [Back to Table](#)
- C29. $\text{NH} + \text{NO}$. The recommendation is derived from the room temperature results of Hansen et al. [550], Cox et al. [313] and Harrison et al. [553]. The temperature dependence is from Harrison et al. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C30. $\text{NH} + \text{NO}_2$. The recommendation is derived from the temperature-dependence study of Harrison et al. [553]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- C31. $\text{O}_3 + \text{HNO}_2$. Based on Kaiser and Japar [685] and Streit et al. [1250]. (Table: 82-57, Note: 82-57) [Back to Table](#)
- C32. $\text{N}_2\text{O}_5 + \text{H}_2\text{O}$. The recommended value at 298 K is based on the studies of Tuazon et al. [1327], Atkinson et al. [54] and Hjorth et al. [588]. Sverdrup et al. [1266] obtained an upper limit that is a factor of four smaller than that obtained in the other studies, but the higher upper limit is

recommended because of the difficulty of distinguishing between homogeneous and heterogeneous processes in the experiment. See the heterogeneous chemistry section of this evaluation for additional rate data for this reaction. (Table: 85-37, Note: 90-1) [Back to Table](#)

- C33. $\text{N}_2(\text{A},v) + \text{O}_2$. Rate constants for the overall reaction for the $v=0, 1$ and 2 vibrational levels of $\text{N}_2(\text{A})$ have been made by Dreyer et al. [416], Zipf [1530], Piper et al. [1059], Iannuzzi and Kaufman [636], Thomas and Kaufman [1296] and De Sousa et al. [365]. The results of these studies are in relatively good agreement. The recommended values are (2.5 ± 0.4) , (4.0 ± 0.6) and $(4.5 \pm 0.6) (\times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$, from the work of De Sousa et al. The only temperature dependence data are from De Sousa et al., who obtained $k(T,v) = k(v,298\text{K})(T/300)^{0.55}$ for $v=0,1,2$. The observation of high N_2O production initially reported by Zipf [1530] has not been reproduced by other groups, and the branching ratio for this channel is probably less than 0.02 (Iannuzzi et al. [635], Black et al. [150], De Sousa et al. [365], Fraser and Piper [469]). The branching ratios for the other channels are poorly established, although there is strong evidence for the formation of both $\text{O}(^3\text{P})$ and $\text{O}_2(\text{B}^3\Sigma_u^-)$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- C34. $\text{N}_2(\text{A},v) + \text{O}_3$. The only study is that of Bohmer and Hack [156], who obtained 298 K rate constants of 4.1 ± 1.0 , 4.1 ± 1.2 , 8.0 ± 2.3 , and $10 \pm 3.0 (\times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1})$ for the $v=0-3$ vibrational levels of $\text{N}_2(\text{A})$, respectively. This study determined that the NO channel accounts for about 20% of the reaction products. (Table: 94-26, Note: 94-26) [Back to Table](#)
- D1. $\text{O} + \text{CH}_3$. The recommended $k(298 \text{ K})$ is the weighted average of three measurements by Washida and Bayes [1431], Washida [1428], and Plumb and Ryan [1065]. The E/R value is based on the results of Washida and Bayes [1431], who found k to be independent of temperature between 259 and 341 K. (Table 83-62, Note: 83-62) [Back to Table](#)
- D2. $\text{O} + \text{HCN}$. Because it is a very slow reaction, there are no studies of this reaction below 450 K. Davies and Thrush [354] studied this reaction between 469 and 574 K while Perry and Melius [1051] studied it between 540 and 900 K. Results of Perry and Melius are in agreement with those of Davies and Thrush. Our recommendation is based on these two studies. The higher-temperature ($T > 1000 \text{ K}$) combustion-related studies of Roth et al. [1125], Szekely et al. [1267], and Louge and Hanson [845] have not been considered. This reaction has two reaction pathways: $\text{O} + \text{HCN} \rightarrow \text{H} + \text{NCO}$, $\Delta H = -2 \text{ kcal/mol}$ (k_a); and $\text{O} + \text{HCN} \rightarrow \text{CO} + \text{NH}$ (k_b), $\Delta H = -36 \text{ kcal/mol}$. The branching ratio k_a/k_b for these two channels has been measured to be ~ 2 at $T = 860 \text{ K}$. The branching ratio at lower temperatures, which is likely to vary significantly with temperature, is unknown. (Table 87-41, Note: 92-20) [Back to Table](#)
- D3. $\text{O} + \text{C}_2\text{H}_2$. The value at 298 K is an average of ten measurements (Arrington et al. [34], Sullivan and Warneck [1265], Brown and Thrush [181], Hoyermann et al. [610, 611], Westenberg and deHaas [1443], James and Glass [649], Stuhl and Niki [1257], Westenberg and deHaas [1447], and Aleksandrov et al. [19]). There is reasonably good agreement among these studies. Arrington et al. [34] did not observe a temperature dependence, an observation that was later shown to be erroneous by Westenberg and deHaas [1443]. Westenberg and deHaas [1443], Hoyermann et al. [611] and Aleksandrov et al. [19] are the only authors, who have measured the temperature dependence below 500 K. Westenberg and deHaas observed a curved Arrhenius plot at temperatures higher than 450 K. In the range 194–450 K, Arrhenius behavior provides an adequate description and the E/R obtained by a fit of the data from these three groups in this temperature range is recommended. The A-factor was calculated to reproduce $k(298 \text{ K})$. This reaction can have two sets of products, i.e., $\text{C}_2\text{HO} + \text{H}$ or $\text{CH}_2 + \text{CO}$. Under molecular beam conditions C_2HO has been shown to be the major product. The study by Aleksandrov et al. using a discharge flow-resonance fluorescence method (under undefined pressure conditions) indicates that the $\text{C}_2\text{HO} + \text{H}$ channel contributes no more than 7% to the net reaction at 298 K, while a similar study by Vinckier et al. [1379] suggests that both CH_2 and C_2HO are formed. (Table: 82-57, Note: 82-57) [Back to Table](#)
- D4. $\text{O} + \text{H}_2\text{CO}$. The recommended values for A, E/R and $k(298 \text{ K})$ are the averages of those determined by Klemm [722] (250 to 498 K) using flash photolysis-resonance fluorescence, by Klemm et al. [723] (298 to 748 K) using discharge flow-resonance fluorescence, and Chang and Barker [240] (296 to 436 K) using discharge flow-mass spectrometry techniques. All three studies are in good agreement. The $k(298 \text{ K})$ value is also consistent with the results of Niki et al. [984], Herron and

Penzhorn [577], and Mack and Thrush [854]. Although the mechanism for $O + H_2CO$ has been considered to be the abstraction reaction yielding $OH + HCO$, Chang and Barker suggest that an additional channel yielding $H + HCO_2$ may be occurring to the extent of 30% of the total reaction. This conclusion is based on an observation of CO_2 as a product of the reaction under conditions where reactions such as $O + HCO \rightarrow H + CO_2$ and $O + HCO \rightarrow OH + CO$ apparently do not occur. This interesting suggestion needs independent confirmation. (Table: 82-57, Note: 82-57) [Back to Table](#)

- D5. $O_2 + HOCO$. HOCO is produced by the association of OH with CO (See Table 2). The rate coefficient for the reaction of O_2 with HOCO has been measured by Petty et al. [1053] and Nolte et al. [1001] and the recommendation is based on these measurements. There are no reports on the temperature dependence of this reaction; however, the value at 298 K would be appropriate for all atmospheric conditions. The products of this reaction are HO_2 , as shown by Nolte et al., and CO_2 , as seen in numerous previous studies where it has been known to be the product of the reaction of OH with CO in air. NEW ENTRY [Back to Table](#)
- D6. $O + CH_3CHO$. The recommended $k(298\text{ K})$ is the average of three measurements by Cadle and Powers [215], Mack and Thrush [855], and Singleton et al. [1200], which are in good agreement. Cadle and Powers and Singleton et al. studied this reaction as a function of temperature between 298 and 475 K and obtained very similar Arrhenius parameters. The recommended E/R value was obtained by considering both sets of data. This reaction is known to proceed via H-atom abstraction (Mack and Thrush [855], Avery and Cvetanovic [56], and Singleton et al. [1200]). (Table 87-41, Note: 87-41) [Back to Table](#)
- D7. $O_3 + C_2H_2$. The database for this reaction is not well established. Room temperature measurements (Cadle and Schadt [216]; DeMore [366]; DeMore [367]; Stedman and Niki [1232]; Pate et al. [1038]; and Atkinson and Aschmann [39]) disagree by as much as an order of magnitude. It is probable that secondary reactions involving destruction of ozone by radical products resulted in erroneously high values for the rate constants in several of the previous measurements. The present recommendation for $k(298\text{ K})$ is based on the room temperature value of Atkinson and Aschmann [39], which is the lowest value obtained and therefore perhaps the most accurate. The temperature dependence is estimated, based on an assumed A-factor of $10^{-14}\text{ cm}^3\text{ s}^{-1}$ similar to that for the $O_3 + C_2H_4$ reaction and corresponding to the expected five-membered ring structure for the transition state (DeMore [366, 367]). Further studies, particularly of the temperature dependence, are needed. Major products in the gas phase reaction are CO, CO_2 , and HCOOH, and chemically-activated formic anhydride has been proposed as an intermediate of the reaction (DeMore [367], and DeMore and Lin [379]). The anhydride intermediates in several alkyne ozonations have been isolated in low temperature solvent experiments (DeMore and Lin [379]). (Table: 90-1, Note: 90-1) [Back to Table](#)
- D8. $O_3 + C_2H_4$. The rate constant of this reaction is well established over a large temperature range, 178 to 360 K. The present recommendation is based on the data of DeMore [366], Stedman et al. [1234], Herron and Huie [576], Japar et al. [650, 651], Toby et al. [1310], Su et al. [1262], Adeniji et al. [10], Kan et al. [692], Atkinson et al. [44], and Bahta et al. [64]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- D9. $O_3 + C_3H_6$. The rate constant of this reaction is well established over the temperature range 185 to 360 K. The present recommendation is based largely on the data of Herron and Huie [576], in the temperature range 235–362 K. (Note that a typographical error in Table 2 of that paper improperly lists the lowest temperature as 250 K, rather than the correct value, 235 K.) The recommended Arrhenius expression agrees within 25% with the low temperature (185–195 K) data of DeMore [366], and is consistent with, but slightly higher (about 10%) than Treacy et al. [1320] and slightly lower (about 40%) than the data of Adeniji et al. [10] in the temperature range 260–294 K. Room temperature measurements of Cox and Penkett [328], Stedman et al. [1234], Japar et al. [650, 651], and Atkinson et al. [44] and Neeb and Moorgat [948] are in good agreement (10% or better) with the recommendation. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D10. $OH + CO$. The recommendation allows for an increase in k with pressure. The zero pressure value was derived by averaging direct low pressure determinations (those listed in Baulch et al. [100]) and the values reported by Dreier and Wolfrum [414], Husain et al. [624], Ravishankara and Thompson

[1098], Paraskevopoulos and Irwin [1033], Hofzumahaus and Stuhl [593]. The results of Jonah et al. [677] are too high and were not included. An increase in k with pressure has been observed by a large number of investigators (Overend and Paraskevopoulos [1027], Perry et al. [1050], Chan et al. [239], Biermann et al. [139], Cox et al. [323], Butler et al. [214], Paraskevopoulos and Irwin [1032, 1033], DeMore [371], Hofzumahaus and Stuhl [593], Hynes et al. [633]). In addition, Niki et al. [992] have measured k relative to $\text{OH} + \text{C}_2\text{H}_4$ in one atmosphere of air by following CO_2 production using FTIR. The recommended 298 K value was obtained by using a weighted nonlinear least squares analysis of all pressure-dependent data in N_2 (Paraskevopoulos and Irwin [1033], DeMore [371], Hofzumahaus and Stuhl [593], and Hynes et al. [633]) as well as those in air (Niki et al. [994], Hynes et al. [633]), to the form $k = (A+BP)/(C+DP)$, where P is pressure in atmospheres. The data were best fit with $D = 0$ and therefore a linear form is recommended. Previous controversy regarding the effect of small amounts of O_2 (Biermann et al. [139]) has been resolved and is attributed to secondary reactions (DeMore [371], Hofzumahaus and Stuhl [593]). The results of Butler et al. [214] have to be re-evaluated in the light of refinements in the rate coefficient for the $\text{OH} + \text{H}_2\text{O}_2$ reaction. The corrected rate coefficient is in approximate agreement with the recommended value. Currently, there are no indications to suggest that the presence of O_2 has any effect on the rate coefficient other than as a third body. The E/R value in the pressure range 50–760 torr has been shown to be essentially zero between 220 and 298 K by Hynes et al. [633]. Further substantiation of the temperature independence of k at 1 atm. may be worthwhile. Beno et al. [128] observe an enhancement of k with water vapor, which is in conflict with the flash photolysis studies; e.g., Ravishankara and Thompson [1098], Paraskevopoulos and Irwin [1033], and Hynes et al. [633]. The uncertainty factor is for 1 atm. of air.

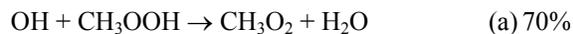
The bimolecular channel yields $\text{H} + \text{CO}_2$ while the addition leads to HOCO . In the presence of O_2 , the HOCO intermediate is converted to $\text{HO}_2 + \text{CO}_2$ (DeMore [371], Miyoshi et al. [924]). Miyoshi et al. report a rate constant for the reaction of HOCO with O_2 of $\sim 1.5 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K). Therefore, for atmospheric purposes, the products can be taken to be HO_2 and CO_2 . (Table: 06-2, Note: 06-2) [Back to Table](#)

- D11. $\text{OH} + \text{CH}_4$. This reaction has been extensively studied. The most recent data are from Vaghjiani and Ravishankara [1363], Saunders et al. [1149], Finlayson-Pitts et al. [458], Dunlop and Tully [426], Mellouki et al. [910], and Gierczak et al. [498], who measured the absolute rate coefficients for this reaction using discharge flow and pulsed photolysis techniques. Sharkey and Smith [1179] have reported a high value ($7.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for $k(298 \text{ K})$, and this value has not been considered here. The current recommendation for $k(298 \text{ K})$ was derived from the results of Vaghjiani and Ravishankara, Dunlop and Tully, Saunders et al., Mellouki et al., Finlayson-Pitts et al., and Gierczak et al. The temperature dependence of this rate coefficient has been measured by Vaghjiani and Ravishankara (223–420 K), Dunlop and Tully (above 298 K), Finlayson-Pitts et al. (278–378 K), and Mellouki et al. (233–343 K). Gierczak et al. have extended the measurements of k to 195 K, and it appears that the rate coefficient does not strictly follow an Arrhenius expression. The recommended E/R was obtained from these results using data below 300 K. A more accurate representation of the rate constant as a function of temperature is obtained by using the three-parameter expression: $k = 2.80 \times 10^{-14} T^{0.667} \exp(-1575/T)$. This three-parameter fit may be preferred for lower stratosphere and upper troposphere calculations. A very recent report on this rate coefficient by Bonard et al. [157] agrees extremely with the value recommended here. (Table: 97-4, Note: 06-2) [Back to Table](#)
- D12. $\text{OH} + {}^{13}\text{CH}_4$. This reaction has been studied relative to the $\text{OH} + \text{CH}_4$ reaction, since the ratio of the rate coefficients is the quantity needed for quantifying methane sources. Rust and Stevens [1129], Davidson et al. [349], and Cantrell et al. [231] have measured k_{12}/k_{13} at 298 K to be 1.003, 1.010, and 1.0055, respectively. Cantrell et al.'s data supersede the results of Davidson et al. The recommended value of 1.005 ± 0.002 is based on the results of Rust and Stevens and Cantrell et al. Cantrell et al. find k_{12}/k_{13} to be independent of temperature between 273 and 353 K. (Table: 92-20, Note: 92-20) [Back to Table](#)
- D13. $\text{OH} + \text{CH}_3\text{D}$. The rate coefficient for this reaction has been measured between 249 and 422 K using a pulsed laser photolysis-laser induced fluorescence system by Gierczak et al. [497]. The recommended values of k (298 K) and E/R are from this study. The recommendation agrees within

about 10% at 298 K with the rate constant measured by DeMore [375] in a relative rate study over the temperature range 298–360 K. The difference, while small in an absolute sense, is nevertheless significant for the isotopic fractionation of atmospheric CH₃D and CH₄ by OH. An earlier result of Gordon and Mulac at 416 K [517] is in good agreement with the extrapolated data of both of these determinations. However, that measurement has not been explicitly included in this recommendation because the experiments were carried out at higher temperatures and therefore are less applicable to the atmosphere. The rate coefficients for the reactions of OH with other deuterated methanes have also been measured (Dunlop and Tully [426], Gierczak et al. [1284], Gordon and Mulac [517]). (Table: 94-26, Note: 94-26) [Back to Table](#)

- D14. OH + H₂CO. The value for k(298 K) is the average of those determined by Niki et al. [993], Atkinson and Pitts [51], Stief et al. [1246], Yetter et al. [1498], Temps and Wagner [1293], and Sivakumaran et al. [1207]. The value reported by Morris and Niki [934] is expected to be superseded by the later report of Niki et al. [993]; but, it agrees within the stated uncertainty. There are two relative values that are not in agreement with the recommendations. The value of Niki et al. [986] relative to the OH + C₂H₄ reaction is higher, while the value of Smith [1219] relative to the OH + OH reaction is lower. The later report of Niki et al. [993] is assumed to supersede the earlier rate constant. The rate coefficient reported by Zabarnick et al. [1503] at and above 298 K are consistently higher than those recommended here, but overlap within the combined uncertainty. The temperature dependence was calculated from the data of Stief et al. obtained below 298 K and from the data of Sivakumaran et al. below 330 K after normalizing the results of both studies to k(298 K) recommended here. There is a clear indication that the Arrhenius plot of this rate coefficient is curved with a positive activation energy at temperatures above ~330 K. It is therefore important that the recommended rate coefficients be used only in the 200-300K temperature range. The abstraction reaction shown in the table is the major channel (Temps and Wagner [1293], Niki et al. [992]); other channels may contribute to a small extent (Horowitz et al. [601]). There is no indication that this rate coefficient is pressure dependent under atmospheric pressures and temperatures. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D15. OH + CH₃OH. The recommended value for k(298 K) is the average of direct studies by Overend and Paraskevopoulos [1026], Ravishankara and Davis [1090], Hagele et al. [541], Meier et al. [897], McCaulley et al. [890], Wallington and Kurylo [1410], Hess and Tully [579], Jimenez et al. [673], and Dillon et al. [392]. When these measurements were not at exactly 298 K, their values were recalculated for 298 K by using the E/R recommended here. Indirect measurements by Campbell et al. [221], Barnes et al. [74], Tuazon et al. [1328], Picquet et al. [1056], and Klopffer et al. [725] are in good agreement with the recommended value. The temperature dependence of k has been measured by Hagele et al., Meier et al., Greenhill and O'Grady, Wallington and Kurylo, Hess and Tully, Jimenez et al., and Crowley et al. The recommended value of E/R was calculated using the results obtained at temperature below 330 K by Wallington and Kurylo, Meier et al., Hess and Tully, Jimenez et al., and Crowley et al. The results of Greenhill and O'Grady is in reasonable agreement with the recommendation at and above 298 K, but it is clearly lower than the recommendation below 298 K. Hess and Tully report a curved Arrhenius plot over the temperature range 298 – 1000 K, while Meier et al. do not observe such a curvature. This reaction has two pathways: abstraction of the H-atom from the methyl group to give CH₂OH + H₂O or from the OH group to give CH₃O + H₂O. The results of Hagele et al., Meier et al., and Hess and Tully suggest that H abstraction from the methyl group to give CH₂OH + H₂O is the dominant channel below room temperature. At 298 K, for example, the branching ratio for the formation of CH₂OH is about 0.85 and increases as the temperature decreases. In the Earth's atmosphere, the eventual products of OH + CH₃OH reaction are the same: CH₂O and HO₂. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D16. OH + CH₃OOH. The recommended value for k(298 K) is the average of the rate coefficients measured by Niki et al. [991] and Vaghjiani and Ravishankara [1362], which differ by nearly a factor of two. Niki et al. measured the rate coefficient relative to that for OH with C₂H₄ ($= 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) by monitoring CH₃OOH disappearance using an FTIR system. Vaghjiani and Ravishankara monitored the disappearance of OH, OD, and ¹⁸OH in excess CH₃OOH in a pulsed photolysis-LIF system. They measured k between 203 and 423 K and report a negative activation energy with E/R = -190 K; the recommended E/R is based on their results. The reaction of OH with CH₃OOH occurs via abstraction of H from the oxygen end to produce the CH₃OO radical and from

the CH₃ group to produce the CH₂OOH radical, as originally proposed by Niki et al. and confirmed by Vaghjiani and Ravishankara. CH₂OOH is unstable and falls apart to CH₂O and OH within a few microseconds. The possible reaction of CH₂OOH with O₂ is unimportant under atmospheric conditions (Vaghjiani and Ravishankara). The recommended branching ratios are,



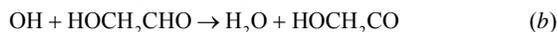
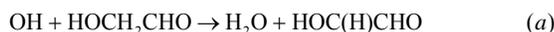
(from Vaghjiani and Ravishankara) and are nearly independent of temperature. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D17. OH + HC(O)OH. The recommended value of k(298 K) is the average of those measured by Zetzsch and Stuhl [1518], Wine et al. [1462], Jolly et al. [676], Dagaut et al. [344], and Singleton et al. [1205]. The temperature dependence of k has been studied by Wine et al. and by Singleton et al., who observed k to be essentially independent of T.

Wine et al. found the rate coefficient for the OH + HC(O)OH reaction to be the same as that for OH + DC(O)OH reaction. Jolly et al. found the formic acid dimer to be unreactive toward OH, i.e., abstraction of the H atom attached to C was not the major pathway for the reaction. A comprehensive study of Singleton et al. showed that reactivity of HC(O)OH is essentially the same as that of DC(O)OH, but DC(O)OD reacts much slower than HC(O)OH and DC(O)OH. These observations show that the reaction proceeds via abstraction of the acidic H atom. Wine et al. and Jolly et al. also found that H atoms are produced in the reaction, which is consistent with the formation of HC(O)O, which would rapidly fall apart to CO₂ and H. End product studies are also consistent with the formation of CO₂ and H₂O in this reaction (Singleton et al. [1205]). The products of this reaction would be mostly HC(O)O and H₂O. The fate of HC(O)O in the atmosphere will be to give HO₂ either directly via reaction with O₂ or via thermal decomposition to H atom, which adds to O₂.

Wine et al. have suggested that, in the atmosphere, the formic acid could be hydrogen bonded to a water molecule and its reactivity with OH could be lowered because the hydrogen bonded water would obstruct the abstraction of the H atom. This suggestion needs to be checked. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D18. OH + HC(O)C(O)H. The only available data are from the 298 K relative rate study of Plum et al. [1064] and the results are recommended here. Because the rate coefficient is so large, it is unlikely to have a substantial temperature dependence and an E/R of zero is recommended. This reaction is expected to proceed via H-abstraction to yield H₂O, CO and HCO. NEW ENTRY [Back to Table](#)
- D19. OH + HOCH₂CHO. The available data are from relative rate studies at 298 K (Bacher et al. [61], Niki et al. [995], and Mellouki et al. [900]). The recommendation is based on all these studies, which are in good agreement. Because the rate coefficient is very large, it is unlikely to have a substantial temperature dependence. Therefore, we recommend an E/R of zero. There are three possible sites for H-abstraction: the alcohol group, the CH₂ group and the carbonyl group. Of these, the likely pathways for abstraction are from the latter two sites:



Niki et al. have shown that the branching ratio for channel (b) is 0.8 and for channel (a) is 0.2. It is unlikely that the branching ratio changes significantly with temperature. NEW ENTRY [Back to Table](#)

- D20. OH + HCN. This reaction is pressure dependent. The recommended value is the high pressure limit measured by Fritz et al. [476] using a laser photolysis-resonance fluorescence apparatus. Phillips [1054] studied this reaction using a discharge flow apparatus at low pressures and found the rate coefficient to have reached the high pressure limit at ~10 torr at 298 K. Fritz et al.'s results contradict this finding. They agree with Phillip's measured value, within a factor of two, at 7 torr, but they find k to increase further with pressure. The products of the reaction are unknown. (Table 83-62, Note: 83-62) [Back to Table](#)

- D21. OH + C₂H₆. There are nineteen studies of this reaction at 298 K (Greiner [526], Howard and Evenson [605], Overend et al. [1028], Lee and Tang [787], Leu [812], Tully et al. [1333], Jeong et al. [667], Tully et al. [1331], Nielsen et al. [979], Zabarnick et al. [1503], Wallington et al. [1412], Smith et al. [1214], Baulch et al. [99], Bourmada et al. [168], Abbatt et al. [2], Schiffman et al. [1152], Talukdar et al. [1287], Sharkey and Smith [1179] and Anderson and Stephens [27]). The recommended value is obtained by averaging the results of the recent investigations by Tully et al., Wallington et al., Abbatt et al., Schiffman et al., Talukdar et al. and Anderson and Stephens. The results of Sharkey and Smith are approximately 20% higher than those recommended here. When the measurements were not carried out at exactly 298 K, we have recalculated k using an E/R of 1070 K. The temperature dependence of the rate coefficient below 298 K has been measured only by Jeong et al., Wallington et al., Talukdar et al. and Anderson and Stephens. The last three studies are in good agreement. The recommended E/R is obtained from an analysis of the data of these three studies. The ratio of the rate coefficients for OH reactions with C₂H₆ and C₃H₈ has been measured by Finlayson-Pitts [458]. Our recommendations are in reasonable agreement with this ratio. Crowley et al. [335] have measured k at 247, 294, and 303 K, and the results are in agreement with the recommendations. (Table: 92-20, Note: 94-26) [Back to Table](#)
- D22. OH + C₃H₈. There are many measurements of the rate coefficients at 298 K. In this evaluation we have considered only the direct measurements (Greiner [526], Tully et al. [1333], Droege and Tully [417], Schmidt et al. [1157], Baulch et al. [99], Bradley et al. [171], Abbatt et al. [2], Schiffman et al. [1152], Talukdar et al. [1287], Mellouki et al. [910], Donahue et al. [410], Clarke et al. [273] and Kozlov et al. [738]). The 298 K value is the average of these thirteen studies. Greiner, Tully et al. [1330], Droege and Tully, Talukdar et al., Mellouki et al., Donahue et al., Clarke et al. and Kozlov et al. [738] have measured the temperature dependence of this reaction. Donahue and Clark [411] have shown that there is outstanding agreement between all of the data sets after correcting some of them for small offsets due to systematic calibration errors. Due to the significant curvature in the Arrhenius behavior over the studied temperature range, the recommended Arrhenius expression is only valid between 190 – 300 K. The recommended E/R is obtained from a composite fit to the four data sets (Kozlov et al., Clarke et al., Talukdar et al, and Mellouki et al.) at temperature below 300 K. Each data set was normalized to the recommended k(298). This reaction has two possible channels, i.e., abstraction of the primary and the secondary H-atom. Observations of both channels by Tully et al. and Droege and Tully indicate that the reaction exhibits non-Arrhenius behavior over a wide temperature range. The branching ratios were estimated from the latter study:
- $$k_{\text{primary}} = 6.3 \times 10^{-12} \exp(-1050/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
- $$k_{\text{secondary}} = 6.3 \times 10^{-12} \exp(-580/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$
- These numbers are in reasonable agreement with the older data of Greiner. The ratio of the rate coefficients for OH reactions with C₂H₆ and C₃H₈ has been measured by Finlayson-Pitts et al. [458] and DeMore and Bayes [377]. Our recommendations are in reasonable agreement with their ratios. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D23. OH + C₂H₅CHO. The recommended value at 298 K is an average of the results from Niki et al., Niki et al. [986], Audley et al. [55], Kerr and Sheppard [700], Semmes et al. [1177], Papagni [1031], Thevenet [1295], and D'Anna [339]. The temperature dependence has been measured by Thevenet. The E/R is taken from Thevenet and the A-factor is adjusted to reproduce k(298 K). Vandenberk and Peeters [1367] measured unity yields of H₂O from the reaction and conclude that the reaction proceeds exclusively by H-abstraction of the aldehydic H-atom. NEW ENTRY [Back to Table](#)
- D24. OH + 1-C₃H₇OH. There have been a number of room temperature measurements that are in excellent agreement. The recommended value is an average of the results from absolute kinetics studies by Overend and Paraskevopoulos [1026], Wallington and Kurylo [1410], Nelson et al. [955], and Yujing and Mellouki [1501]. Relative rate studies of Nelson et al., Oh and Andino [1007], Wu et al. [1488], and Cheema et al. [249] are in excellent agreement with the recommended value. The indirect study of Campbell [221] is consistent with but 30% lower than the recommended value. The reaction is observed to be nearly temperature independent; Yujing and Mellouki find a slight positive temperature dependence while Cheema et al. find a small negative temperature dependence. The recommended E/R value is based on the direct study of Yujing and Mellouki. End product

studies carried out by Azad and Andino [60] support predictions based on the structure-activity relationship that identify the primary reaction channels as hydrogen abstraction by the OH radical from the α (~75%) and β (~20) carbons. NEW ENTRY [Back to Table](#)

- D25. OH + 2-C₃H₇OH. The recommended value at 298 K is an average of the absolute measurements by Overend and [1026], Wallington and Kurylo [1410], Nelson et al. [955], Dunlop and Tully [425], and Yujing and Mellouki [1501]. A relative rate study by Lloyd et al. [840] is, within its wide error limits, consistent with the recommendation. The temperature dependence is observed to vary little with temperature below 400 K. Measurements over the range 293-745 K by Dunlop and Tully revealed a “bowl” shaped temperature dependence, with a minimum in the rate coefficient observed at 378 K. The recommended E/R is based on the measurements of Yujing and Mellouki and, on account of the complex reaction behavior, is valid only for temperatures below 400 K. Temperature dependent data of Dunlop and Tully and Wallington and Kurylo are, within the experimental uncertainties, consistent with the recommendation. By using isotopic substitution, Dunlop and Tully determined that the primary reaction channel below 400K involves H atom abstraction by OH from the α -site. This result is in agreement with estimates based on the structure-activity relationship (Yujing and Mellouki). NEW ENTRY [Back to Table](#)
- D26. OH + C₂H₅C(O)OH. Studies of this reaction have been confined to 298 K and above on account of the tendency of propionic acid to dimerize at lower temperatures and higher concentrations. Kinetic isotope effects measured by Singleton et al. [1204] are consistent with a two channel mechanism proposed previously for OH reaction with acetic acid. In the propionic acid case, the channel involving direct abstraction of an alkyl hydrogen is predominant, thus accounting for the observed temperature independence of the rate constant. The recommended temperature independent rate constant, is based on an average of the results of Singleton et al. and Dagout et al. [344] taken at a variety of temperatures between 298 K and 446 K. An earlier study room temperature measurement by Zetsch and Stuhl [1518] is ~30% higher, but consistent with the recommendation. Further studies below 298 K would be desirable in order to investigate possible non-Arrhenius behavior. NEW ENTRY [Back to Table](#)
- D27. OH + CH₃C(O)CH₃. The rate coefficient for this reaction has been measured at temperatures close to 298 K by Cox et al. [325], Zetsch [1517], Chiorboli et al. [263], Kerr and Stocker [701], Wallington and Kurylo [1411], LeCalve et al. [780], Wollenhaupt et al. [1481], Gierczak et al. [493] and Yamada et al. [1496]. Cox reported only an upper limit of $<5 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, which is consistent with this recommendation. The primary aim of Chiorboli et al. was to examine the atmospheric degradation of styrene, which produces acetone. They employed a relative rate measurement and reported a value of k(298 K) that is almost three times faster than the recommended value. Because of possible complications in their system, we have not included their results in arriving at the recommended value. Wallington and Kurylo, LeCalve et al., Wollenhaupt et al., Gierczak et al., and Yamada et al. have reported k as a function of temperature; all these studies directly measured the rate constant using the pulsed photolysis method where the temporal profile of OH was measured using resonance fluorescence or laser induced fluorescence. The extensive data of Wollenhaupt et al. and Gierczak et al. seem to show that this rate coefficient does not follow an Arrhenius expression. The results of LeCalve et al. and Wallington et al. are in general agreement with the results of Wollenhaupt et al. and Gierczak et al. The non-Arrhenius behavior was not evident in the results of Wallington et al. and LeCalve et al. because they measured the rate constant at a few temperatures and did not explore temperature below 240 K, where the curvature becomes increasingly evident. Yamada et al. measured k only above room temperature and their values are consistently lower than those of all the others noted above. As they noted in their paper, Yamada et al. did not measure the acetone concentration in the reactor and, thus, could have overestimated its concentration leading to consistently lower values of k. We have not included data of Yamada et al. (2003) in deriving the fit because of this possible systematic error and because they did not report k under atmospheric temperatures. The following recommendation reproduces all reported data, except that of Chiorboli et al. within the recommended uncertainty of 25% at all temperatures:

$$k(T) = 1.33 \times 10^{-13} + 3.82 \times 10^{-11} \exp(-2000/T)$$

This reaction can proceed via the abstraction of an H atom or via the formation of a complex that decomposes to give many different products, which include $\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{OH}$, $\text{CH}_3\text{OH} + \text{CH}_3\text{C}(\text{O})$, $\text{CH}_4 + \text{CH}_3\text{CO}_2$, $\text{H}_2\text{O} + \text{CH}_3\text{C}(\text{O})\text{CH}_2$. The branching ratios for the formation of different sets of products could vary with temperature. Wollenhaupt and Crowley (2000) have deduced that CH_3 radicals are produced with a yield of ~50% at 298 K and ~30% at 233 K. A similar branching ratio has also been reported by Vasvari et al. [1372]. The results of Gierczak et al. on $\text{OH} + \text{CD}_3\text{C}(\text{O})\text{CD}_3$ reaction, whose rate coefficient nearly obeys an Arrhenius expression between 240 and 400 K and is nearly an order of magnitude smaller than the non-deuterated analog at 250 K, suggests that H abstraction may be the dominant channel. Vandenberg et al. [1369], Tyndall et al. [1344], and Talukdar et al. [1285], clearly show that $\text{CH}_3\text{C}(\text{O})\text{OH}$ is a minor, if not negligible, product of this reaction and that the reaction proceeds to abstract an H atom. The results of Yamada et al. are consistent with this finding. Theoretical calculations of Henon et al. [571], and Vandenberg et al. [1368] also suggest that formation of acetic acid is negligible. We recommend that the products of this reaction be taken as H_2O and $\text{CH}_3\text{C}(\text{O})\text{CH}_2$. (Table: 06-2, Note: 06-2) [Back to Table](#)

- D28. $\text{OH} + \text{CH}_3\text{CN}$. This rate coefficient has been measured as a function of temperature by Harris et al. [552] between 298 and 424 K, Kurylo and Knable [756] between 250 and 363 K, Rhasa [1116] between 295 and 520 K, and Hynes and Wine [630] between 256 and 388 K. In addition, the 298 K value has been measured by Poulet et al. [1071]. The 298 K results of Harris et al. are in disagreement with all other measurements and therefore have not been included. The recommended 298 K value is a weighted average of all other studies. The temperature dependence was computed using the results of Kurylo and Knable, the lower temperature values (i.e., 295–391 K) of Rhasa, and the data of Hynes and Wine. Three points are worth noting: (a) Rhasa observed a curved Arrhenius plot even in the temperature range of 295 to 520 K, and therefore extrapolation of the recommended expression could lead to large errors; (b) Hynes and Wine observed a pressure dependent increase of $k(298\text{ K})$ that levels off at about 1 atmosphere, and this observation is contradictory to the results of other investigations; (c) Hynes and Wine have carried out extensive pressure, temperature, O_2 concentration, and isotope variations in this reaction. Hynes and Wine postulate that the reaction proceeds via addition as well as abstraction pathways. They observe OH regeneration in the presence of O_2 . The recommended $k(298\text{ K})$ and E/R are applicable for only lower tropospheric conditions. Because of the unresolved questions of pressure dependence and reaction mechanism, the recommended value may not be applicable under upper tropospheric and stratospheric conditions. (Table: 92-20, Note: 92-20) [Back to Table](#)
- D29. $\text{OH} + \text{CH}_3\text{ONO}_2$. The rate coefficient for this reaction at 298 K has been measured by Kerr and Stocker [701], Nielsen et al. [981], Gaffney et al. [479], Talukdar et al. [479], Kakesu et al. [690] and Shallcross et al. [1178]. The results of Kerr and Stocker and of Nielsen et al. are a factor of ten higher than those reported by the other groups. There are no obvious reasons for the reported differences but the lower values are preferred for a number of reasons. Firstly, Talukdar et al. have carried out a large number of checks which ruled out possible effects in their system due to the regeneration of OH via secondary reactions, to bath gas pressure, and to formation of an adduct that could undergo further reaction in the presence of oxygen. Secondly, the lower values are more consistent with reactivity predictions of Atkinson and Aschmann [42], who assumed that the series of nitrate reactions proceed by H-atom abstraction pathways. Kinetic measurements of Talukdar et al. performed with isotopically substituted hydroxyl radical (OH , ^{18}OH , and OD) and methyl nitrate (CH_3ONO_2 and CD_3ONO_2) are consistent with this reaction proceeding via an H-atom abstraction pathway. Accordingly, the recommended value of $k(298\text{ K})$ is based on an average of the values given by Gaffney et al., Talukdar et al., Kakesu et al. and Shallcross et al. Further verification of the reaction mechanism by identification of the products of the reaction is needed. The temperature dependence of the rate coefficient has been measured by Nielsen et al., Talukdar et al., and Shallcross et al. While Nielsen et al. report a negative activation energy, Talukdar et al. and Shallcross et al. report positive values. For the reasons given above, the temperature dependence recommended here is based on an average of Talukdar et al. and Shallcross et al. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D30. $\text{OH} + \text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2$ (PAN). This reaction has been studied by four groups, Winer et al. [1477], Wallington et al. [1393], Tsalkani et al. [1322], and Talukdar et al. [1282]. Winer et al. obtained only

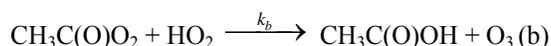
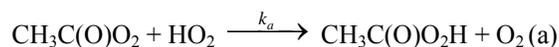
an upper limit for the rate coefficient. Tsalkani et al. noted that their system was very ill-behaved and obtained a value of $k(298\text{ K})$ that is a factor of ~ 2 lower than that obtained by Wallington et al. The pulsed photolysis study of Wallington et al. yielded consistent results, but PAN was not directly measured and photodissociation of H_2O in the vacuum UV, where PAN absorbs strongly, was used as the OH source. The recent study of Talukdar et al. [1282] yielded much lower rate coefficients. These investigators measured the PAN concentration directly in their system, minimized secondary reactions due to the photodissociation of PAN, and carried out extensive tests for decomposition of PAN, impurities, and secondary reactions. The recommended upper limit is a factor of two higher than the highest value measured by Talukdar et al. at 298 K and at 272 K. The quoted upper limit is expected to be valid at all atmospheric temperatures. The products of the reaction are not known. Further measurements of the rate coefficients and information on the reaction pathways are needed. (Table: 94-26, Note: 94-26) [Back to Table](#)

- D31. $\text{OH} + \text{C}_2\text{H}_5\text{ONO}_2$. The rate constant for this reaction at 298 K has been measured by Kerr and Stocker [701], Nielsen et al. [981], Talukdar et al. [1286], Kakesu et al. [690], and Shallcross et al. [1178]. As in the case of the reaction of OH with CH_3ONO_2 , the results of Kerr and Stocker and of Nielsen et al. are larger (by a factor of 3) than those of the more recent studies. The reasons for the differences are not clear. Because of the exhaustive tests carried out (see the note for the $\text{OH} + \text{CH}_3\text{ONO}_2$ reaction), the values of Talukdar et al., Kakesu et al., and Shallcross et al. are recommended. Nielsen et al., Talukdar et al., and Shallcross et al. have measured the rate constant as a function of temperature. As with the $\text{OH} + \text{CH}_3\text{ONO}_2$ reaction, Nielsen et al. report a negative activation energy while Talukdar et al. and Shallcross et al. have observed a small positive activation energy. Talukdar et al. note that the rate coefficient for this reaction does not strictly follow Arrhenius behavior, consistent with the abstraction of both the primary and the secondary H atoms. Above 298 K, E/R values measured by Shallcross et al. and Talukdar et al. are in excellent agreement. Only Talukdar et al. have kinetics data below 298 K and the recommended E/R value was obtained by fitting the rate coefficients measured by Talukdar et al. at or below 298 K. The large uncertainty encompasses the results of Kerr and Stocker and Nielsen et al. (Table: 06-2, Note: 06-2) [Back to Table](#)
- D32. $\text{OH} + 1\text{-C}_3\text{H}_7\text{ONO}_2$. The reaction has been studied by Kerr and Stocker [701] and Atkinson and Aschmann [42] at room temperature and by Nielsen et al. [981] between 298 and 368 K. The results of the three studies are in good agreement at room temperature. Nielsen et al. find that the reaction is temperature independent within the measurement uncertainty over the range studied. However as discussed above, the Nielsen et al. results for the analogous reactions of OH with CH_3ONO_2 and $\text{C}_2\text{H}_5\text{ONO}_2$, yield negative activation energies that disagree with the positive activation energies obtained by others. Judging from the E/R's for the analogous reactions, one might expect the E/R for this reaction to be on the order of 300 kcal/mole. Accordingly, we place a large uncertainty on the recommended temperature dependence. A thorough investigation of the temperature dependence of this reaction is needed. (Table: 02-25, Note: 02-25) [Back to Table](#)
- D33. $\text{OH} + 2\text{-C}_3\text{H}_7\text{ONO}_2$. The reaction has been studied by Atkinson and Aschmann [42], Atkinson et al. [43] and Becker and Wirtz [109] at room temperature and by Talukdar et al. [1286] over the range 233 and 395 K. The results of Atkinson and Aschmann supersede those of Atkinson et al. There is fair agreement between the results of the three studies at room temperature, with roughly a factor of two spread in the values. The recommendation is based on an average of the room temperature values and the E/R measured by Talukdar et al. (Table: 02-25, Note: 02-25) [Back to Table](#)
- D34. $\text{HO}_2 + \text{CH}_2\text{O}$. There is sufficient evidence to suggest that HO_2 adds to CH_2O (Su et al. [1261, 1263], Veyret et al. [1376], Zabel et al. [1504], Barnes et al. [80], and Veyret et al. [1375]). The recommended $k(298\text{ K})$ is the average of values obtained by Su et al. [1261], Veyret et al. [1376], and Veyret et al. [1375]. The temperature dependence observed by Veyret et al. [1375] is recommended. The value reported by Barnes et al. at 273 K is consistent with this recommendation. The adduct $\text{HO}_2\cdot\text{CH}_2\text{O}$ seems to isomerize to HOCH_2OO reasonably rapidly and reversibly. There significant discrepancies between measured values of the equilibrium constants for this reaction. (Table: 90-1, Note: 90-1) [Back to Table](#)
- D35. $\text{HO}_2 + \text{CH}_3\text{O}_2$. This recommendation is taken from the evaluated review of Tyndall et al. [1346]. The kinetics of this reaction has been studied by using UV absorption following pulsed photolytic

production of the radicals. These authors first analyzed the available data for the products of the reaction and concluded that the major products are CH₃OOH and O₂. They used this product yield information with their evaluated UV absorption cross sections for HO₂ and CH₃O₂ to reanalyze the UV absorption profiles measured in kinetics experiments by Dagaut et al. [343] and by Lightfoot et al. [823], the two groups that carried out the most extensive studies. They found that rate coefficients reported by these two groups need to be increased by ~20%. The recommended value is based on the average of the corrected data from these two groups. The temperature dependence was evaluated by Tyndall et al. by assuming that the absorption cross sections of CH₃O₂ and HO₂ are independent of temperature at the wavelengths used for the kinetics studies. The products of this reaction are shown as CH₃OOH + O₂ in the table. However, Elrod et al. [436] have determined that the reaction also yields CH₂O + H₂O + O₂ with yields that range from 0.1 at 298 K and 0.3 at 220 K. In anticipation of further work, the recommended product yield for the CH₂O channel is zero..(Table: 02-25, Note: 06-2) [Back to Table](#)

D36. HO₂ + C₂H₅O₂. The recommended value is the weighted average of those measured by Cattell et al. [237], Dagaut et al. [342], Fenter et al. [451], and Maricq and Szenté [870]. In all experiments the rate coefficient was obtained by modeling the reaction system. Also, the calculated rate coefficients depended on the UV absorption cross sections of both C₂H₅O₂ and HO₂. The absorption cross section of C₂H₅O₂ is not well-defined. The value reported by Dagaut et al. would be ~30% higher if the cross sections used by Maricq and Szenté were used. The recommended E/R is derived from the measurements of Dagaut et al., Fenter et al., and Maricq and Szenté. Wallington and Japar [1409] have shown that C₂H₅O₂H and O₂ are the only products of this reaction. (Table: 94-26, Note: 94-26) [Back to Table](#)

D37. HO₂ + CH₃C(O)O₂. This recommendation is taken from the evaluated review of Tyndall et al. [1346]. This reaction has two sets of products:



The majority of the reaction proceeds via channel (a), but there is clear evidence for channel (b). Tyndall et al. reevaluated the available data on end products of this reaction, particularly those of Crawford et al. [333], Moortgat et al. [932], and Horie and Moortgat [598], and concluded that channel (a) contributes ~80% while channel (b) contributes ~20% at 298 K. They also concluded that $k_a/k_b = 37 \times \exp(-660/T)$ with a large uncertainty in this value. They derived the overall rate coefficient for this reaction, which has been measured only by following the radical concentrations via UV absorption. They based their recommendation mostly on the results of Moortgat et al. [932] and Tomas et al. [1314]. (Table: 02-25, Note: 02-25) [Back to Table](#)

D38. HO₂ + CH₃C(O)CH₂O₂. This recommendation is from Tyndall et al. [1346]. This reaction has been studied by only Bridier et al. [177] and Tyndall et al. based their recommendation on this one study. (Table: 02-25, Note: 02-25) [Back to Table](#)

D39. NO₃ + CO. The upper limit is based on the results of Hjorth et al. [589], who monitored isotopically labeled CO loss in the presence of NO₃ by FTIR. Burrows et al. [207] obtained an upper limit of $4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, which is consistent with the Hjorth et al. study. Products are expected to be NO₂ + CO₂, if the reaction occurs. (Table 87-41, Note: 92-20) [Back to Table](#)

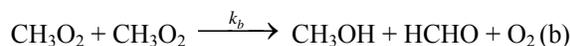
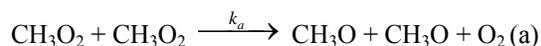
D40. NO₃ + CH₂O. There are three measurements of this rate coefficient at 298 K: Atkinson et al. [53], Cantrell et al. [232], and Hjorth et al. [590]. The value reported by Atkinson et al. [53], $k = (3.23 \pm 0.26) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, is corrected to $5.8 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to account for the different value of the equilibrium constant for the NO₃ + NO₂ → N₂O₅ reaction that was measured subsequent to this study by the same group using the same apparatus. This correction is in accordance with their suggestion (Tuazon et al. [1329]). The values reported by Cantrell et al. and Hjorth et al., $k = 6.3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $(5.4 \pm 1.1) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, respectively, are in good agreement with the corrected value of Atkinson et al. The recommended value is the average of these three studies. Cantrell et al. have good evidence to suggest that HNO₃ and CHO are the products of this reaction. The temperature dependence of this rate coefficient is

unknown, but comparison with the analogous $\text{NO}_3 + \text{CH}_3\text{CHO}$ reaction suggests a large E/R. (Table: 90-1, Note: 90-1) [Back to Table](#)

- D41. $\text{NO}_3 + \text{CH}_3\text{CHO}$. There are four measurements of this rate constant: Morris and Niki [935], Atkinson et al. [53], Cantrell et al. [226], and Dlugokencky and Howard [394]. The value reported by Atkinson et al. [53], $k = (1.34 \pm 0.28) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, is corrected to $2.4 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ as discussed for the $\text{NO}_3 + \text{H}_2\text{CO}$ reaction above and as suggested by Tuazon et al. [1329]. The recommended value is the average of the values obtained by Atkinson et al., Cantrell et al., and Dlugokencky and Howard. The results of Morris and Niki agree with the recommended value when their original data is re-analyzed using a more recent value for the equilibrium constant for the reaction $\text{NO}_2 + \text{NO}_3 \leftrightarrow \text{N}_2\text{O}_5$ as shown by Dlugokencky and Howard. Dlugokencky and Howard have studied the temperature dependence of this reaction. Their measured value of E/R is recommended. The A-factor has been calculated to yield the $k(298 \text{ K})$ recommended here. Morris and Niki, and Cantrell et al. observed the formation of HNO_3 and PAN in their studies, which strongly suggests that HNO_3 and CH_3CO are the products of this reaction. (Table 87-41, Note: 87-41) [Back to Table](#)
- D42. $\text{CH}_3 + \text{O}_2$. This bimolecular reaction is not expected to be important, based on the results of Baldwin and Golden [66], who found $k < 5 \times 10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for temperatures up to 1200 K. Klais et al. [719] failed to detect OH (via $\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$) at 368 K and placed an upper limit of $3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for this rate coefficient. Bhaskaran et al. [133] measured $k = 1 \times 10^{-11} \exp(-12,900/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for $1800 < T < 2200 \text{ K}$. The latter two studies thus support the results of Baldwin and Golden. Studies by Selzer and Bayes [1176] and Plumb and Ryan [1065] confirm the low value for this rate coefficient. Previous studies of Washida and Bayes [1431] are superseded by those of Selzer and Bayes. Plumb and Ryan have placed an upper limit of $3 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ based on their inability to find HCHO in their experiments. A study by Zellner and Ewig [1514] suggests that this reaction is important at combustion temperature but is unimportant for the atmosphere. (Table 83-62, Note: 83-62) [Back to Table](#)
- D43. $\text{CH}_3 + \text{O}_3$. The recommended A-factor and E/R are those obtained from the results of Ogryzlo et al. [1006]. The results of Simonaitis and Heicklen [1193], based on an analysis of a complex system, are not used. Washida et al. [1430] used $\text{O} + \text{C}_2\text{H}_4$ as the source of CH_3 . Studies on the $\text{O} + \text{C}_2\text{H}_4$ reaction (Schmoltner et al. [1158], Kleinermanns and Luntz [721], Hunziker et al. [621], and Inoue and Akimoto [641]) have shown this reaction to be a poor source of CH_3 . Therefore, the results of Washida et al. are also not used. (Table 83-62, Note: 83-62) [Back to Table](#)
- D44. $\text{HCO} + \text{O}_2$. The value of $k(298 \text{ K})$ is the average of the determinations by Washida et al. [1432], Shibuya et al. [1182], Veyret and Lesclaux [1374], Langford and Moore [769], Nesbitt et al. [959], Temps et al. [1293], and Ninomiya et al. [996]. There are three measurements of k where HCO was monitored via the intracavity dye laser absorption technique (Reilly et al. [1110], Nadtochenko et al. [941], and Gill et al. [499]). Even though these studies agree with the recent measurements of Nesbitt et al., the only recent measurement to obtain a low value, they have not been included in deriving the recommended value of $k(298 \text{ K})$. However, the uncertainty has been increased to overlap with those measurements. The main reason for not including them in the average is the possible depletion of O_2 in those static systems (as suggested by Veyret and Lesclaux). Also, these experiments were designed more for the study of photochemistry than kinetics. The temperature dependence of this rate coefficient has been measured by Veyret and Lesclaux, Timonen et al. [1309], and Nesbitt et al. While Timonen et al. obtain a slightly positive activation energy, Veyret and Lesclaux, and Nesbitt et al. measure slightly negative activation energy. It is very likely that the Arrhenius expression is curved. We recommend an E/R value of zero, with an uncertainty of 100 K. Veyret and Lesclaux preferred a T^n form ($k = 5.5 \times 10^{-11} T^{-(0.4 \pm 0.3)} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$). Hsu et al. [612] suggest that this reaction proceeds via addition at low temperature and abstraction at higher temperatures. (Table: 02-25, Note: 02-25) [Back to Table](#)
- D45. $\text{CH}_2\text{OH} + \text{O}_2$. The rate coefficient was first measured directly by Radford [1083] by detecting the HO_2 product in a laser magnetic resonance spectrometer. The wall loss of CH_2OH could have introduced a large error in this measurement. Radford also showed that the previous measurement of Avramenko and Kolesnikova [58] was in error. Wang et al. [1422] measured a value of $1.4 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by detecting the HO_2 product. Recently, Dobe et al. [397], Grotheer et al. [529],

Payne et al. [1042], Grotheer et al. [530] and Nesbitt et al. [962] have measured $k(298\text{ K})$ to be close to $1.0 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ under conditions where wall losses are small. This reaction appears to exhibit a very complex temperature dependence. Based on the recent data of Grotheer et al. [530], and Nesbitt et al. [962], k appears to increase from 200 K to approximately 250 K in an Arrhenius fashion, levels off at approximately 300 K, decreases from 300 to 500 K, and finally increases as temperature is increased. This complex temperature dependence is believed to be due to the formation of a $\text{CH}_2(\text{OH})\cdot\text{O}_2$ adduct which can isomerize to $\text{CH}_2\text{O}\cdot\text{HO}_2$ or decompose to reactants. The $\text{CH}_2\text{O}\cdot\text{HO}_2$ isomer can also decompose to CH_2O and HO_2 or reform the original adduct. At temperatures less than 250 K, the data of Nesbitt et al. suggests an E/R value of $\sim 1700\text{ K}$. For atmospheric purposes, the value $E/R = 0$ is appropriate. (Table: 90-1, Note: 90-1) [Back to Table](#)

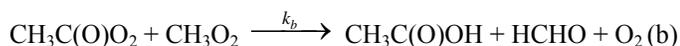
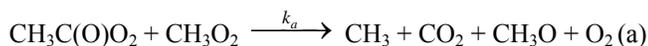
- D46. $\text{CH}_3\text{O} + \text{O}_2$. The recommended value for $k(298\text{ K})$ is the average of those reported by Lorenz et al. [843] and Wantuck et al. [1425]. The recommended E/R was obtained using the results of Gutman et al. [531] (413 to 608 K), Lorenz et al. [843] (298 to 450 K), and Wantuck et al. [1425] (298 to 498 K). These investigators have measured k directly under pseudo-first order conditions by following CH_3O via laser induced fluorescence. Wantuck et al. measured k up to 973 K and found the Arrhenius plot to be curved; only their lower temperature data are used in the fit to obtain E/R. The A factor has been adjusted to reproduce the recommended $k(298\text{ K})$. The previous high temperature measurements (Barker et al. [71] and Batt and Robinson [96]) are in reasonable agreement with the derived expression. This value is consistent with the 298 K results of Cox et al. [324], obtained from an end product analysis study, and with the upper limit measured by Sanders et al. [1142]. The A-factor appears low for a hydrogen atom transfer reaction. The reaction may be more complicated than a simple abstraction. At 298 K, the products of this reaction are HO_2 and CH_2O , as shown by Niki et al. [989]. (Table 87-41, Note: 87-41) [Back to Table](#)
- D47. $\text{CH}_3\text{O} + \text{NO}$. The reaction of CH_3O with NO proceeds mainly via addition to form CH_3ONO (Batt et al. [95], Wiebe and Heicklen [1454], Frost and Smith [477], and Ohmori et al. [1008]). However, a fraction of the energized CH_3ONO adducts decompose to $\text{CH}_2\text{O} + \text{HNO}$, and appear to be a bimolecular channel. This reaction has been investigated recently by direct detection of CH_3O via laser-induced fluorescence (Zellner [1512]; Frost and Smith [477]; Ohmori et al. [1008]). The previous end-product studies (Batt et al. [95], Wiebe and Heicklen [1454]) are generally consistent with this conclusion. Since the fraction of the CH_3ONO adduct that falls apart to $\text{CH}_2\text{O} + \text{HNO}$ decreases with increases in pressure and decreases in temperature, it is not possible to derive a "bimolecular" rate coefficient. A value of $k < 8 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ can be deduced from the work of Frost and Smith [477] and Ohmori et al. [1008] for lower atmospheric conditions. (Table: 97-4, Note: 97-4) [Back to Table](#)
- D48. $\text{CH}_3\text{O} + \text{NO}_2$. The reaction of CH_3O with NO_2 proceeds mainly via the formation of CH_3ONO_2 . However, a fraction of the energized adducts fall apart to yield $\text{CH}_2\text{O} + \text{HNO}_2$. The bimolecular rate coefficient reported here is for the fraction of the reaction that yields CH_2O and HNO_2 . It is not meant to represent a bimolecular metathesis reaction. The recommended value was derived from the study of McCaulley et al. [890] and is discussed in the section on association reactions. (Table: 97-4, Note: 97-4) [Back to Table](#)
- D49. $\text{CH}_3\text{O}_2 + \text{O}_3$. This recommendation is from Tyndall et al. [1346]. Their recommendation is based mostly on the recent study by Tyndall et al. [1357]. The temperature dependence is based on the assumption that the only possible reaction which can occur is the O atom transfer from the CH_3O_2 radical and that the activation energy of $\sim 2 \text{ kcal mol}^{-1}$ for this O-atom transfer is similar to that in the $\text{HO}_2 + \text{O}_3$ reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- D50. $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2$. This recommendation is from Tyndall et al. [1346]. There are two confirmed sets of products for this reaction.



The relative product yield, k_a/k_b , was evaluated by Tyndall et al. to be $(26.2 \pm 6.6) \times \exp((-1130 \pm 240)/T)$. They concluded that there was no evidence for the formation of the CH_3OOCH_3 . The

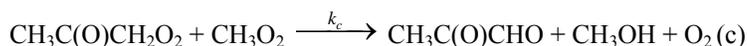
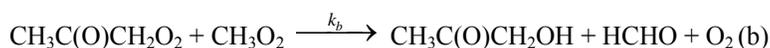
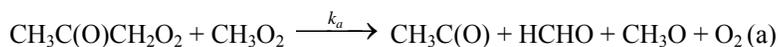
kinetics of this reaction has been studied by using UV absorption following pulsed photolytic production of the radicals. Tyndall et al. used the values of k/σ measured by a large number of groups along with the σ values from their evaluation to calculate k . (σ is the absorption cross section of the radical at the wavelength at which it was monitored.) They only used the kinetics data obtained at wavelengths larger than 240 nm, since the absorption by HO_2 radicals that are unavoidably produced in these measurements can significantly contribute to the measure UV profiles at shorter wavelengths. They noted that the values of k/σ measured by various groups were much more accurate than the values of σ measured by the same groups. The value of k obtained by this method was then corrected using the above branching ratio for the production of CH_3O that leads to the unavoidable occurrence of the $\text{CH}_3\text{O}_2 + \text{HO}_2$ side reaction; this side reaction consumes another CH_3O_2 radical. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D51. $\text{CH}_3\text{O}_2 + \text{NO}$. This recommendation is from Tyndall et al. [1346]. They evaluated the available information to deduce that the main set of products under atmospheric conditions is $\text{CH}_3\text{O} + \text{NO}_2$. They noted, however, that a very small yield, <0.5%, of CH_3ONO_2 is also possible. The rate coefficient for the reaction at 298 K and its temperature dependence is based on numerous direct studies of this reaction that have been reported. (Table: 02-25, Note: 02-25) [Back to Table](#)
- D52. $\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2$. This recommendation is from Tyndall et al. [1346]. This reaction has two sets of products:



Tyndall et al. reanalyzed the previously available data on the branching ratios for this reaction and concluded that the branching ratio for channel (a) was $k_a/k = 0.9 \pm 0.1$ and $k_b/k = 0.1 \pm 0.1$ at 298 K. They also concluded that branching ratios could not be derived for other temperatures from the existing data and therefore did not make a recommendation for the temperature dependence. The recommendation from Tyndall et al. is based on the work of Roehl et al. [1123] and Villenave et al. [1377]. Their recommended temperature dependence for the overall rate coefficient is based on analogy with other RO_2 reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D53. $\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2$. This recommendation is from Tyndall et al. [1346]. This reaction has three possible sets of products:



The branching ratios for these channels, $k_a/k = 0.3 \pm 0.1$, $k_b/k = 0.2 \pm 0.1$, and $k_c/k = 0.5 \pm 0.1$, are based on the work of Bridier et al. [177] and Jenkin et al. [661]. The overall rate coefficient for this reaction has been studied only at 298 K by Bridier et al. and the recommendation is based on this value. The recommended values of E/R and g are based on analogy with other RO_2 reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D54. $\text{C}_2\text{H}_5 + \text{O}_2$. This is a complex reaction that involves the formation of an $\text{C}_2\text{H}_5\text{O}_2$ adduct, which can either be stabilized by collisions or fall apart to HO_2 and C_2H_4 (Wagner et al. [1383], Bozzelli and Dean [170], and Kaiser et al. [687]). The fraction of the energized adducts that fall apart to give HO_2 and C_2H_4 will decrease with increasing pressure and decreasing temperature, i.e., as the $\text{C}_2\text{H}_5\text{O}_2$ formation increases. The C_2H_4 -formation channel cannot be separated from the addition reaction. We recommend a conservative upper limit as a guide to the extent of this reaction. This upper limit is applicable only for lower atmospheric pressure and temperature conditions. (Table: 94-26, Note: 94-26) [Back to Table](#)
- D55. $\text{C}_2\text{H}_5\text{O} + \text{O}_2$. The recommendation is based on the pulsed laser photolysis studies of Gutman et al. [531] and Hartmann et al. [554]. In both these studies, removal of $\text{C}_2\text{H}_5\text{O}$ in an excess of O_2 was

directly monitored via laser induced fluorescence. Gutman et al. measured k at only two temperatures, while Hartmann et al. measured k at 5 temperatures between 295 and 411 K. The E/R is from Hartmann et al. The 298 K value deduced from an indirect study by Zabarnick and Hecklen [1502] is in reasonable agreement with the recommended value. (Table: 92-20, Note: 92-20) [Back to Table](#)

- D56. $C_2H_5O_2 + C_2H_5O_2$. $k(298\text{ K})$ has been studied by Adachi et al. [7], Anastasi et al. [25], Munk et al. [938], Cattell et al. [237], Anastasi et al. [24], Wallington et al. [1399], Bauer et al. [98], and Fenter et al. [451]. All the above determinations used only UV absorption to monitor $C_2H_5O_2$ and hence measured k/σ , where σ is the absorption cross section of $C_2H_5O_2$ at the monitoring wavelength. These investigators also measured the σ that was used in evaluating the rate coefficient. There are large discrepancies in the measured values of σ . For this evaluation, we have used the cross sections recommended here and recalculated the values of k from each investigation. The recommended k is based on the results of Cattell et al., Wallington et al., Bauer et al., and Fenter et al. In all these experiments the observed rate coefficient is higher than the true rate coefficient because of secondary reactions involving HO_2 . HO_2 is formed by the reaction of CH_3CH_2O with O_2 and it reacts with $C_2H_5O_2$ to enhance the observed rate coefficient (see Wallington et al. [1401] or Lightfoot et al. [821] for further discussion). Based on product branching ratios discussed below, which determine the magnitude of the necessary correction, the recommended rate coefficient is 0.6 times the average observed rate coefficient. The recommended value of E/R was obtained from the results of Anastasi et al., Wallington et al., Cattell et al., Bauer et al., and Fenter et al. The observed products (Niki et al. [990]), suggest that at 298 K the channel to yield $2 C_2H_5O + O_2$ accounts for about 60% of the reaction; the channel to yield $CH_3CHO + C_2H_5OH + O_2$ accounts for about 40% of the reaction; and the channel to yield $C_2H_5O_2C_2H_5 + O_2$ accounts for less than 5% of the reaction. These branching ratios were used above to obtain the true rate coefficient from the observed rate coefficient. (Table: 94-26, Note: 94-26) [Back to Table](#)
- D57. $C_2H_5O_2 + NO$. The recommended $k(298\text{ K})$ is obtained from the results of Plumb et al. [1067], Sehested et al. [1174], Daele et al. [341], Eberhard and Howard [427], and Maricq and Sente [871]. The value reported by Adachi and Basco [6], which is a factor of three lower than the recommended value, was not used. The rate coefficient for the $CH_3O_2 + NO$ reaction measured by Basco and co-workers (Adachi et al. [7]), using the same apparatus, is also much lower than the value recommended here. The recommended temperature dependence is derived from Eberhardt and Howard, and Maricq and Sente, which are in good agreement. (Table: 97-4, Note: 97-4) [Back to Table](#)
- D58. $CH_3C(O)O_2 + CH_3C(O)O_2$. This reaction has been studied by Addison et al. [8], Basco and Parmar [94], Moortgat et al. [932], Maricq and Sente [871], and Roehl et al. [1123], using UV absorption techniques. The recommended value is obtained from the data of Moortgat et al., Maricq and Sente, and Roehl et al. As pointed out by Moortgat et al., the six times lower value of k obtained by Addison et al. is likely due to the use of incorrect UV absorption cross sections for the peroxy radical. The k obtained by Basco and Parmar is ~ 2 times lower than the recommended value. This discrepancy is possibly due to neglecting the UV absorption of CH_3O_2 and other stable products in their data analysis (Moortgat et al., Maricq and Sente). The recommended temperature dependence was calculated from the data of Moortgat et al. and Maricq and Sente. Addison et al. reported the formation of O_3 , which was attributed to the reaction channel which produces $CH_3C(O)OCH_3C(O) + O_3$. Moortgat et al. place an upper limit of 2% for this channel. The main products of this reaction appear to be $CH_3C(O)O + O_2$. The $CH_3C(O)O$ radicals rapidly decompose to give CH_3 and CO_2 . (Table: 97-4, Note: 97-4) [Back to Table](#)
- D59. $CH_3C(O)O_2 + NO$. This recommendation is from Tyndall et al. [1346]. These authors have argued that the only set of products of importance in the atmosphere is the production of $CH_3 + CO_2 + NO_2$. This is because the alkoxy radical produced upon O abstraction from the peroxy radical by NO will be unstable towards decomposition to give CH_3 and CO_2 . The rate coefficient for the reaction was deduced primarily from direct studies, but was found to be consistent with the relative rate studies. In the relative rate studies, this rate coefficient was measured relative to the rate coefficient for the reaction of $CH_3C(O)O_2$ with NO_2 . The temperature dependence of this rate coefficient was derived

from a set of direct measurement and kept consistent with the observed temperature dependence of the rate coefficient for the $\text{CH}_3\text{C}(\text{O})\text{O}_2 + \text{NO}_2$ reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)

- D60. $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2 + \text{NO}$. This recommendation is from Tyndall et al. [1346]. They deduced, based on the results of Sehested et al. [1171], Jenkin et al. [661], and Orlando et al. [1023], that the products of this reaction are $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O} + \text{NO}_2$. The $\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}$ radical decomposes rapidly to give $\text{CH}_3\text{C}(\text{O}) + \text{CH}_2\text{O}$. The only kinetics study of this reaction by Sehested et al. forms the basis for the rate coefficient at 298 K. This value is uncertain because of the corrections that had to be made in the study of Sehested et al. to account for the production of NO_2 , the monitored species, via the reaction of peroxy radicals (such as $\text{CH}_3\text{C}(\text{O})\text{O}_2$ and CH_3O_2) with NO . The temperature dependence of the reaction is derived based on analogy with other peroxy radical reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E1. $\text{O} + \text{FO}$. The recommended value is based on results of the room temperature study of Bedzhanyan et al. [123]. The temperature dependence of the rate constant is expected to be small, as it is for the analogous ClO reaction. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E2. $\text{O} + \text{FO}_2$. No experimental data. The rate constant for such a radical-atom process is expected to approach the gas collision frequency, and is not expected to exhibit a strong temperature dependence. (Table: 82-57, Note: 82-57) [Back to Table](#)
- E3. $\text{OH} + \text{CH}_3\text{F}$ (HFC-41). The recommended values for $k(298 \text{ K})$ and E/R are averages of these parameters derived from fits to the data of Schmoltner et al. [1159], Nip et al [998], Hsu and DeMore [615], and DeMore [376] (with the relative rate constants from the last two studies recalculated based on the current recommendations for the rate constants for the $\text{OH} + \text{CH}_3\text{CHF}_2$ and $\text{OH} + \text{CH}_3\text{Cl}$ reference reactions respectively.) The A factor was then calculated. The renormalization procedure for relative rate measurements referenced to the $\text{OH} + \text{CH}_3\text{CHF}_2$ reaction is discussed in the note for that reaction. The results of Howard and Evenson [606], Jeong and Kaufman [669], and Wallington and Hurley [1405] appear to be systematically lower than those of the other studies over the temperature region of interest and were not used to derive the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E4. $\text{OH} + \text{CH}_2\text{F}_2$ (HFC-32). The recommended value of $k(298 \text{ K})$ is an average from the studies of Nip et al. [998], Jeong and Kaufman [669], Talukdar et al. [1281], Hsu and DeMore [615] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_3\text{CHF}_2$ reference reaction, as described in the note for that reaction), and Szilagyi et al. [1268]. The recommended value for E/R is derived from an Arrhenius fit to the data from these same five studies below 400 K. The results of Howard and Evenson [606], Clyne and Holt [282], and Bera and Hanrahan [130] were not used in deriving the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E5. $\text{OH} + \text{CHF}_3$ (HFC-23). The recommended values for $k(298 \text{ K})$ and E/R are averages of the values Schmoltner et al. [1159], and Hsu and DeMore [615] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CHF}_2\text{CF}_3$ reference reaction). The results of Jeong and Kaufman [669], and Medhurst et al. [896], being predominantly above room temperature, were not used in deriving the recommended parameters. The results from Clyne and Holt [282] and Bera and Hanrahan [130] were also not used due to their inconsistency with the other studies. The room temperature values of Howard and Evenson [606] and Nip et al. [998] are encompassed within the 2σ confidence limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E6. $\text{OH} + \text{CH}_3\text{CH}_2\text{F}$ (HFC-161). The recommended value for $k(298 \text{ K})$ is an average of the values from Nip et al. [998], Schmoltner et al. [1159], and Kozlov et al. [738]. The value of E/R is based on a fit to the data from these three studies from room temperature and below. The relative rate study by Hsu and DeMore [615] reports a temperature dependence that is markedly different from those of Schmoltner et al. [1159] and Kozlov et al. [738], which are in excellent agreement. This difference is due to significantly lower rate constant values being obtained in the Hsu and DeMore study in the region near room temperature. Given the most recent results for the reaction of $\text{OH} + \text{CH}_3\text{CHF}_2$ (HFC-152a), it seems likely that the HFC-161 reaction also has two channels with different activation energies and that the temperature dependence below room temperature should be less than that recommended for HFC-152a, consistent with the present recommendation. Curvature in the Arrhenius plot is evident from the study by Kozlov et al. [738], which was conducted over an

extended temperature range above and below room temperature. Singleton et al. [1202] determined that $85 \pm 3\%$ of the abstraction by OH is from the fluorine substituted methyl group at room temperature. Hence this curvature is quite possibly due to the increasing importance of hydrogen abstraction from the unsubstituted methyl group with increasing temperature. Due to such occurrence, the recommended parameters should not be used for calculating rate constants above room temperature. (Table: 02-25, Note: 02-25) [Back to Table](#)

- E7. OH + CH₃CHF₂ (HFC-152a). The recommended value for k(298 K) is an average of the values from Howard and Evenson [605], Handwerk and Zellner [549], Nip et al. [998], Gierczak et al. [495] (two different absolute determinations), Hsu and DeMore [615] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₄ and OH + CH₃CCl₃ reference reactions), and Kozlov et al [738]. There are systematic differences in the temperature dependencies determined in the absolute studies (particularly below room temperature) and relative studies (conducted at room temperature and above). Curvature in the Arrhenius plot (as suggested by the data of Gierczak et al. [495]) has been more clearly demonstrated by the study of Kozlov et al. [738] and seems to explain the earlier cited differences between the relative and absolute rate data. This curvature is likely due to the presence of two hydrogen-abstraction reaction channels. Hence, care must be taken in deriving a recommended rate expression suitable for atmospheric modeling (in the temperature region below room temperature).

In spite of the noticeable Arrhenius curvature over the temperature range from 480 K to 210 K, the data below 300 K can be well represented by a two-parameter Arrhenius expression. Thus, the recommended value for E/R is derived from a fit to the data (T ≤ 300 K) of Gierczak et al. and Kozlov et al. The results from Clyne and Holt [282], Brown et al. [179], Nielsen [975], and Liu et al. [839] (superceded by the study of Kozlov et al.) were not used in deriving the recommended parameters.

Clearly, in light of the observed Arrhenius curvature, the above procedure for deriving our recommendation for E/R below 300 K does not yield a parameter suitable for use in recalculating rate constants from relative rate studies in which the OH + CH₃CHF₂ reaction was the reference and which were conducted at temperatures above 300 K. Use of the below-room-temperature value for E/R for such purposes results in rate constant values that are systematically different from those determined relative to other reactions or determined by absolute techniques. For such renormalization purposes, one should use an Arrhenius expression derived from data over the appropriate temperature range. A fit to the absolute rate data of Gierczak et al. [495] and Kozlov et al. [738] between room temperature and 400 K yields the Arrhenius expression

$$k_{\text{abs}} = 2.36 \times 10^{-12} \exp\{-1255/T\}$$

This is in good agreement with the expression derived from the relative rate data of Hsu and DeMore [615]

$$k_{\text{rel}} = 2.1 \times 10^{-12} \exp\{-1265/T\}$$

The small difference in the pre-exponential factors results from a slight systematic difference in the actual rate constants determined in these three studies that is probably within the combined uncertainties of the determinations. Thus, the following expression derived from the above room temperature E/R value and the recommended k(298 K) has been used for renormalization purposes in this evaluation.

$$k_{T \geq 300\text{K}} = 2.33 \times 10^{-12} \exp\{-1260/T\}$$

However, this expression should not be used below 298 K, as erroneous values for OH + CH₃CHF₂ reaction rate constants would be obtained. (Table: 02-25, Note: 02-25) [Back to Table](#)

- E8. OH + CH₂FCH₂F (HFC-152). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [880], Kozlov et al. [738], and DeMore et al. [384] (three relative rate studies using HFC-152a, cyclopropane, and ethane as reference reactants). The value for E/R is from a fit to the data of Kozlov et al. [738] at room temperature and below. The A factor was then calculated to yield the recommended value for k(298 K). The data above room temperature from Kozlov et al. [738] are in excellent agreement with the three relative rate data sets of DeMore et al.

[384]. Together, they show a pronounced curvature in the Arrhenius plot, which may indicate the existence of different conformers for HFC-152, each with differing temperature populations and reactivities. (Table: 02-25, Note: 02-25) [Back to Table](#)

- E9. OH + CH₃CF₃ (HFC-143a). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [880], Orkin et al. [1013], Talukdar et al. [1281] (two different determinations), and Hsu and DeMore [615] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₄ and OH + CHF₂CF₃ reference reactions). The value for E/R is an average of the E/R values from the last three of these studies which are in excellent agreement (Martin and Paraskevopoulos having made measurements only at room temperature). The data of Clyne and Holt [282] were not used due to their inconsistency with the other studies. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E10. OH + CH₂FCHF₂ (HFC-143). The recommended temperature dependence is based on results of the relative rate study of Barry et al. [90] normalized to the value of the rate constant for the reference reaction (OH + CH₃CCl₃) recommended in this evaluation. The value for k(298 K) is an average of the room temperature values of Martin and Paraskevopoulos [880] and Barry et al. The significantly higher values reported by Clyne and Holt [282] were not used in the derivation of the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E11. OH + CH₂FCF₃ (HFC-134a). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [880], Bednarek et al. [118], Orkin and Khamaganov [1015], Leu and Lee [801], Gierczak et al. [495] (two different determinations), Liu et al. [839], and DeMore [374] (three determinations which have been recalculated based on the current recommendations for the rate constants for the reference reactions OH + CH₄, OH + CH₃CCl₃, and OH + CHF₂CF₃). The value for E/R is an average of the E/R values from the last five of these investigations (the studies by Martin and Paraskevopoulos and by Bednarek et al. being conducted only at room temperature). The 270 K result of Zhang et al. [1521] is in excellent agreement with the recommendation. The data of Jeong et al. [667], Brown et al. [179], and Clyne and Holt [282] were not used in deriving the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E12. OH + CHF₂CHF₂ (HFC-134). The preferred rate expression is based on results of the three relative rate measurements by DeMore [374] (which have been recalculated based on the current rate constant recommendations for the OH + CH₃CCl₃, OH + CH₂FCF₃, and OH + CHF₂CF₃ reference reactions). The room temperature value of Clyne and Holt [282] agrees within the 2σ confidence limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E13. OH + CHF₂CF₃ (HFC-125). The recommended rate expression is derived from a combined fit to the temperature dependence data of Talukdar et al. [1281] and DeMore [374] and the room temperature data of Martin and Paraskevopoulos [880]. The data of Brown et al. [179] and Clyne and Holt [282] were not used in deriving the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E14. OH + CH₃CHFCH₃ (HFC-281ea). The recommended parameters were derived from a fit to the data of DeMore and Wilson [383] who conducted five independent relative rate determinations. Using infrared detection, these investigators based their determinations on the reference reactions of OH with C₂H₆, C₃H₈, and C₂H₅Cl. Using gas chromatographic detection, they based their determinations on the reference reactions of OH with C₂H₆ and C₃H₈. All of the data were recalculated based on the current recommendations for the reference rate constants. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E15. OH + CH₃CH₂CF₃ (HFC-263fb). Based on room temperature measurement of Nelson et al. [953]. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E16. OH + CH₂FCF₂CHF₂ (HFC-245ca). The absolute rate constant results of Zhang et al. [1524] differ from the relative rate data (Hsu and DeMore [615]) by approximately 30 to 40% over the temperature region of measurement overlap. Both studies, however, derive nearly identical T-dependencies. The recommended rate expression, hence, averages both the k(298 K) and E/R values from these studies (with the results of Hsu and DeMore [615] recalculated using the current recommendation for the rate constant of the OH + CH₄ reference reaction). (Table: 02-25, Note: 02-25) [Back to Table](#)

- E17. OH + CHF₂CHFCHF₂ (HFC-245ea). Based on room temperature measurement of Nelson et al. [953]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E18. OH + CH₂FCHF₂CF₃ (HFC-245eb). Based on room temperature measurement of Nelson et al. [953]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E19. OH + CHF₂CH₂CF₃ (HFC-245fa). The recommended room temperature value is the mean of the values reported by Orkin et al. [1013] and Nelson et al. [953], which are in good agreement. The temperature dependence is from Orkin et al. The A-factor has been calculated to fit the recommended room temperature value. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E20. OH + CH₂FCF₂CF₃ (HFC-236cb). The recommended rate expression is estimated as being the same as that for the reaction of OH with CH₂FCF₃ (HFC-134a), since these reactions are expected to have very similar Arrhenius parameters. This estimate is preferred over the results reported by Garland et al. [483], the only published experimental study. The A-factor reported in that study is much lower than expected and the value reported for E/R (1107 K) is lower than that reported for any similar halocarbon reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E21. OH + CHF₂CHF₂CF₃ (HFC-236ea). The recommended value for k(298 K) averages the values reported by Hsu and DeMore [615] by a relative rate method (recalculated based on the current recommendation for the rate constant of the OH + CH₄ reference reaction) and by Nelson et al. [953] by an absolute technique. The temperature dependence is from Hsu and DeMore [615], with the A-factor adjusted to fit the recommended room temperature value. The higher and somewhat more scattered values of Garland et al. [483] and Zhang et al. [1524] were not used in deriving the recommended expression. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E22. OH + CF₃CH₂CF₃ (HFC-236fa). The recommended rate expression is derived from a combined fit to the data from the relative rate study of Hsu and DeMore [615] (recalculated based on the current recommendation for the rate constant for the reference reaction OH + CHF₂CF₃) and the absolute rate study of Gierczak et al. [496]. The higher results of Nelson et al. [953] and of Garland and Nelson [484], which superseded the earlier results of Garland et al. [484], were not used. A relative rate determination at room temperature by Barry et al. [88] yields a rate constant in excellent agreement with the recommended value. However, the extremely small rate constant ratio measured (relative to OH + CH₃CF₂CH₂CF₃) resulted in fairly large uncertainties. Hence this determination was not directly used in the evaluation. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E23. OH + CF₃CH₂CF₃ (HFC-227ea). The recommended rate expression is derived from a combined fit to the data (below 400 K) from the absolute studies of Nelson et al. [949], Zellner et al. [1513], and Zhang et al. [1524] and the relative rate studies of Hsu and DeMore [615] (two determinations which have been recalculated based on the current recommendations for the rate constants for the reference reactions OH + CH₄ and OH + CHF₂CF₃). (Table: 02-25, Note: 02-25) [Back to Table](#)
- E24. OH + CH₃CF₂CH₂CF₃ (HFC-365mfc). The recommended value of k(298 K) is an average of the values obtained from the individual rate expressions by Mellouki et al. [911] and Barry et al. [88] (renormalized to the current recommendation for the rate constant for the reference reaction OH + CH₃CCl₃). The value for E/R is an average of the values for this parameter from the same two studies. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E25. OH + CF₃CH₂CH₂CF₃ (HFC-356mff). The recommended value of k(298 K) is an average of the values from Nelson et al. [953] and Zhang et al. [1524]. The temperature dependence is from a fit to the data of Zhang et al. excluding the lowest temperature points (at 260 K), which are somewhat higher than an extrapolation from their other data would indicate. The A-factor has been calculated to fit the recommended room temperature value. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E26. OH + CH₂FCH₂CF₂CF₃ (HFC-356mcf). The recommended parameters are based on a fit to the data of Nelson et al. [953]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E27. OH + CHF₂CF₂CF₂CHF₂ (HFC-338pcc). The recommended values for both k(298 K) and E/R are averages of these values taken from the individual fits to the data of Schmoltner et al. [1159] and Zhang et al. [1527]. (Table: 02-25, Note: 02-25) [Back to Table](#)

- E28. $\text{OH} + \text{CF}_3\text{CH}_2\text{CF}_2\text{CH}_2\text{CF}_3$ (HFC-458mfcf). The recommended values for both $k(298\text{ K})$ and E/R are from a fit to the data of Nelson et al. [953]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E29. $\text{OH} + \text{CF}_3\text{CHFCHFCF}_2\text{CF}_3$. (HFC-43-10mee). The recommended rate expression is derived from a combined fit to the data from Schmoltner et al. [1159] and Zhang et al. [1527]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E30. $\text{OH} + \text{CF}_3\text{CF}_2\text{CH}_2\text{CH}_2\text{CF}_2\text{CF}_3$ (HFC-55-10mcf). The recommended value for $k(298\text{ K})$ is based on Nelson et al. [953]. As expected, the rate constant is similar to that for $\text{CF}_3\text{CH}_2\text{CH}_2\text{CF}_3$. Hence the recommendation for E/R is estimated as being approximately the same as for this reaction, with the A -factor calculated to yield $k(298\text{ K})$. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E31. $\text{OH} + \text{CH}_2=\text{CHF}$. The recommended parameters were derived from a fit to the data of Perry et al. [1047]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E32. $\text{OH} + \text{CH}_2=\text{CF}_2$. The recommended value for $k(298\text{ K})$ is from Howard [603]. The value of E/R was estimated as being similar to that for the reactions of OH with $\text{CH}_2=\text{CHF}$ and with $\text{CF}_2=\text{CF}_2$, and the value for A was then calculated. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E33. $\text{OH} + \text{CF}_2=\text{CF}_2$. The recommended value for $k(298\text{ K})$ is an average of the values determined in the studies of Acerboni et al. [5] (two relative rate determinations referenced to the rate constants for the reactions of OH with propene and cyclohexane) and the absolute rate studies of Orkin et al. [1014], and Orkin et al. [1020]. The value for E/R is from a fit to the data of Orkin et al. [1020], with the value for A calculated to yield the recommended value for $k(298\text{ K})$. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E34. $\text{OH} + \text{CF}_3\text{OH}$. There are no measurements of the rate coefficient of this reaction. The recommendation is based on the recommended limit for the reverse reaction rate coefficient and an estimated equilibrium constant. The thermochemistry of CF_3O and CF_3OH are taken from *ab initio* calculations (Montgomery et al. [930] and Schneider and Wallington [1160]) and laboratory measurements (Huey et al. [619]) to estimate $\Delta G^\circ_{298}(\text{OH} + \text{CF}_3\text{OH} \rightarrow \text{CF}_3\text{O} + \text{H}_2\text{O})$ to be about $(2\pm 4)\text{ kcal mol}^{-1}$. In considering the large uncertainty in the free energy change, the estimated rate coefficient limit is based on the assumption that the reaction is approximately thermoneutral. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E35. $\text{OH} + \text{CH}_2(\text{OH})\text{CF}_3$. The recommended value for $k(298\text{ K})$ is an average of the values reported by Wallington et al. [1400], Inoue et al. [642], and Tokuhashi et al. [1311] (two independent studies). The recommended value for E/R is derived from the data of Tokuhashi et al. [1311]. The A factor was calculated to agree with the recommended value for $k(298\text{ K})$. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E36. $\text{OH} + \text{CH}_2(\text{OH})\text{CF}_2\text{CF}_3$. The recommended parameters were derived from a combined fit to the data of Tokuhashi et al. [1311] (two independent absolute measurement studies) and the relative rate study of Chen et al. [255] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Cl}_2$ reference reaction). (Table: 02-25, Note: 02-25) [Back to Table](#)
- E37. $\text{OH} + \text{CF}_3\text{CH}(\text{OH})\text{CF}_3$. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1311] (two independent absolute measurement studies). (Table: 02-25, Note: 02-25) [Back to Table](#)
- E38. $\text{OH} + \text{CH}_3\text{OCHF}_2$ (HFOC-152a). The recommended rate expression is derived from a fit to the data of Orkin et al. [1017] below 400 K. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E39. $\text{OH} + \text{CH}_3\text{OCF}_3$ (HFOC-143a). The preferred rate expression is derived from a combined fit to the data of Orkin et al. [1017] and Hsu and DeMore [616] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the $\text{OH} + \text{CH}_3\text{CHF}_2$ and $\text{OH} + \text{CH}_2\text{F}_2$ reference reactions). The renormalization procedure for relative rate measurements referenced to the $\text{OH} + \text{CH}_3\text{CHF}_2$ reaction is discussed in the note for that reaction. The room temperature result of Zhang et al. [1526] was not used in the derivation since it is significantly higher than the values of the other studies and may be influenced by the presence of reactive impurities. (Table: 97-4, Note: 02-25) [Back to Table](#)

- E40. OH + CHF₂OCHF₂ (HFOC-134). The recommended values of k(298 K) and E/R were derived from a combined fit to the data of Hsu and DeMore [616] (a relative rate study whose results have been recalculated using the current recommendation for the rate constant of the OH + CH₃CCl₃ reference reaction), Orkin et al. [1021], and Wilson et al. [1460]. The more scattered measurements of Garland et al. [483] were not used in derivation of the preferred value. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E41. OH + CHF₂OCF₃ (HFOC-125). The recommended rate expression is based on results of the relative rate study of Hsu and DeMore [616] (recalculated using the rate constant for the CHF₃ reference reaction given in this evaluation). Additional measurements by Hsu and DeMore [616] relative to CHF₂CF₃ and CH₄ are encompassed well within the 2σ limits, but were not used for assigning the recommended rate expression due to the large differences in reactivity between these two species and the target molecule. The room temperature result of Zhang et al. [1526] lies significantly higher than the recommended value, possibly due to the presence of reactive impurities in the sample. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E42. OH + CHF₂OCH₂CF₃ (HFOC-245fa). The recommended rate expression is derived from a fit to the data of Orkin et al. [1017] below 400 K. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E43. OH + CH₃OCF₂CHF₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1313] (two independent absolute measurement studies). A room temperature measurement by Heathfield et al. [561] is nearly an order of magnitude higher than recommended and may be affected by reactive impurities. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E44. OH + CH₃OCF₂CF₃. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1312] (two independent absolute measurement studies). The expression, as expected, is similar to those for the OH + CH₃OCF₃ and OH + CH₃OCF₂CF₂CF₃ reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E45. OH + CH₃OCF₂CF₂CF₃. The recommended value for k(298 K) is an average of the values reported by Tokuhashi et al. [1312] (two independent absolute measurement studies) and Nonomiya et al. [996] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₄ and OH + CH₃Cl reference reactions). The value for E/R was determined from a fit to the data (below 400 K) of Tokuhashi et al. and the A factor calculated to agree with the value for k(298 K). The expression, as expected, is similar to those for the OH + CH₃OCF₃ and OH + CH₃OCF₂CF₃ reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E46. OH + CH₃OCF(CF₃)₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1312] (two independent absolute measurement studies). The rate constants from this study are surprisingly somewhat larger than those for the similar OH + CH₃OCF₃ and OH + CH₃OCF₂CF₃ reactions. (Table: 02-25, Note: 02-25) [Back to Table](#)
- E47. OH + CHF₂OCH₂CF₂CHF₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1313] (two independent absolute measurement studies). (Table: 02-25, Note: 02-25) [Back to Table](#)
- E48. OH + CHF₂OCH₂CF₂CF₃. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1313] (two independent absolute measurement studies). (Table: 02-25, Note: 02-25) [Back to Table](#)
- E49. F + O₃. The recommended value is based on results of the room temperature study of Bedzhanyan et al. [120] and the temperature-dependent study of Wagner et al. [1387]. The value appears to be quite reasonable in view of the well-known reactivity of atomic chlorine with O₃. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E50. F + H₂. The value of k at 298 K seems to be well established with the results reported by Zhitneva and Pshezhetskii [1529], Heidner et al. [562, 563], Wurzburg and Houston [1489], Dodonov et al. [402], Clyne et al. [288], Bozzelli [169], Igoshin et al. [637], Clyne and Hodgson [281] and Stevens et al. [1241] being in excellent agreement (range of k being 2.3–3.0 × 10⁻¹¹ cm³ molecule⁻¹ s⁻¹). The preferred value at 298 K is taken to be the mean of the values reported in these references. Values of

E/R range from 433–595 K (Heidner et al.; Wurzberg and Houston; Igoshin et al.; and Stevens et al.). The preferred value of E/R is derived from a fit to the data in these studies. The A-factor was chosen to fit the recommended room temperature value. (Table: 90-1, Note: 90-1) [Back to Table](#)

- E51. F + H₂O. The recommended temperature-independent value is based on results reported in the study by Stevens et al. [1241] over the temperature range 240–373 K using a discharge flow system with chemical conversion of fluorine atoms to deuterium atoms and detection of the latter by resonance fluorescence. This value is in excellent agreement with the room temperature results of Frost et al. [478] and Walther and Wagner [1414]. The latter authors in a limited temperature-dependent study reported an E/R value of 400 K. Although these data have not been included in the derivation of the preferred value, with the exception of the one low temperature data point, they are encompassed within the indicated uncertainty limits. (Table: 90-1, Note: 90-1) [Back to Table](#)
- E52. F + HNO₃. The recommendation is based on results of the temperature-dependent study of Wine et al. [1475] and the room temperature results of Mellouki et al. [903], Rahman et al. [1085] and Becker et al. [102]. The values at room temperature are in good agreement. The study of Wine et al. [1475] was over the temperature range 260–373 K. Below 320 K the data were fitted with the Arrhenius expression recommended here, whereas at higher temperatures a temperature-independent value was found, suggesting the occurrence of different mechanisms in the two temperature regimes. (Table: 90-1, Note: 90-1) [Back to Table](#)
- E53. F + CH₄. The recommended room temperature value is the mean of the results of Wagner et al. [1385], Clyne et al. [288], Kompa and Wanner [736], Foon and Reid [466], Fasano and Nogar [448], and Persky et al. [1052]. The temperature dependence is that reported by Persky et al. in a competitive study using the reaction F + D₂ as the reference reaction. These results are preferred over the temperature dependences reported in the earlier studies of Wagner et al. and Foon and Reid. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E54. FO + O₃. Recommended upper limit is based on the results of Li et al. [819] in a study using a discharge flow-mass spectrometric technique. FO was produced in the reaction of F atoms with excess O₃. No appreciable decay of FO, and only a small increase in FO₂, was detected, allowing an upper limit to the rate constant of 10⁻¹⁴ cm³ molecule⁻¹s⁻¹ to be derived. A two orders of magnitude higher upper limit was derived by Sehested et al. [1175]. A lower value of the upper limit was derived by Colussi and Grela [307] from a re-analysis of data on the quantum yields for ozone destruction in F₂/O₃ mixtures reported by Starrico et al. [1231]. The results of the recent, more direct, study of Li et al. [819] are preferred over the earlier results of Starrico et al. There are two possible pathways which are exothermic, resulting in the production of F + 2O₂ or FO₂ + O₂. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E55. FO + NO. The recommended value is based on results of the temperature-dependent study of Bedzhanyan et al. [121] and the value reported by Ray and Watson [1108] for k at 298 K using the discharge flow-mass spectrometric technique. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E56. FO + FO. The recommended value is based on the results of Bedzhanyan et al. [122] and Clyne and Watson [299]. Wagner et al. [1387], in a less direct study, report a higher value. The results of Bedzhanyan et al. indicate the predominant reaction channel is that to produce 2F + O₂. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E57. FO₂ + O₃. Recommended value is based on results of Sehested et al. [1175]. A higher upper limit has been reported by Li et al. [819]. (Table: 94-26, Note: 97-4) [Back to Table](#)
- E58. FO₂ + NO. Recommended values are based on results of Li et al. [819], the only temperature-dependent study. The room temperature value is nearly a factor of 2 less than the previous recommendation, which was based on the results of Sehested et al. [1175]. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E59. FO₂ + NO₂. Recommended values are based on results of Li et al. [819], the only temperature-dependent study. The room temperature value is a factor of 2.5 less than the previous recommendation, which was based on the results of Sehested et al. [1175]. This discrepancy might be attributable to a small NO impurity in the NO₂ sample used in the Sehested et al. study. (Table: 97-4, Note: 97-4) [Back to Table](#)

- E60. $\text{FO}_2 + \text{CO}$. Recommended value is based on results of Sehested et al. [1175], the only published study of this reaction. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E61. $\text{FO}_2 + \text{CH}_4$. Recommended value is based on results of Li et al. [819]. This upper limit is a factor of 20 less than the previously recommended upper limit, which was based on the results of Sehested et al. [1175]. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E62. $\text{CF}_3\text{O} + \text{O}_2$. The recommendation is based upon the results of Turnipseed et al. [1336] who reported $k(373 \text{ K}) \leq 4 \times 10^{-17}$. Assuming an E/R of 5000 K, which is equal to the reaction endothermicity, yields the recommended A and $k(298 \text{ K})$ limits. By comparison to other reactions involving abstraction by O_2 the A- factor is likely to be much smaller. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E63. $\text{CF}_3\text{O} + \text{O}_3$. The recommendation is based on the average of room temperature measurements reported by Turnipseed et al. [1336], Wallington and Ball [1396], and Bourbon et al. [165]. Turnipseed et al. and Bourbon et al. made direct measurements using LIF detection of CF_3O with pulsed photolysis and flow tube reactors, respectively. Wallington and Ball used a competitive reaction scheme with IR absorption detection and $\text{CF}_3\text{O} + \text{CH}_4$ as the reference reaction. The recommended A factor is estimated by comparison to other CF_3O reactions, and the E/R is calculated to give the recommended $k(298 \text{ K})$. Upper limits reported by Maricq and Szenté [869], Nielsen and Sehested [980], and Wallington et al. [1406] are consistent with the $k(298 \text{ K})$ recommendation. Measurements reported by Fockenberg et al. [464] and Meller and Moortgat [898] gave rate coefficients about an order of magnitude less than the recommended value. Although the reason for this discrepancy is not known, both studies appear to have the possibility of significant secondary chemistry. The reaction products have not been observed. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E64. $\text{CF}_3\text{O} + \text{H}_2\text{O}$. The recommendation is based upon the measurement $k(381) \leq 2 \times 10^{-16}$ reported by Turnipseed et al. [1334]. The A factor is estimated and the E/R is calculated to fit $k(381)$. The limits $k = (0.2\text{--}40) \times 10^{-17}$ at $296 \pm 2 \text{ K}$ given by Wallington et al. [1407] are consistent with the recommendation. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E65. $\text{CF}_3\text{O} + \text{NO}$. The recommendation is based upon the room temperature rate coefficients reported by Sehested and Nielsen [1173], Turnipseed et al. [1336], and Jensen et al. [664] which are in very good agreement. An earlier low value given by Bevilacqua et al. [132] is superseded by Jensen et al. The temperature-dependence is derived from measurements by Turnipseed (233–360 K) and Jensen et al. (231–393 K). Room temperature results from Bourbon et al. [166] and Bhatnagar and Carr [134] and a temperature dependence study by Dibble et al. [391] are in good agreement with the recommendation. The reaction products have been reported by Chen et al. [252] Bevilacqua et al. [132], Bhatnagar and Carr and Dibble et al. (Table: 94-26, Note: 97-4) [Back to Table](#)
- E66. $\text{CF}_3\text{O} + \text{NO}_2$. There are no published measurements of the rate coefficient for this reaction. The reaction products have been reported by Chen et al. [251] who used photolysis of CF_3NO to prepare CF_3O_2 and subsequently CF_3O in 700 torr of air at $297 \pm 2 \text{ K}$. They considered two product channels: (a) CF_3ONO_2 obtained via three-body recombination and (b) $\text{CF}_2\text{O} + \text{FNO}_2$ obtained via fluorine transfer. Products from both channels were observed and found to be thermally stable in their reactor. They report $k_a/(k_a + k_b) \geq 90\%$ and $k_b/(k_a + k_b) \leq 10\%$, thus the formation of CF_3ONO_2 is the dominant channel at 700 torr and 297 K. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E67. $\text{CF}_3\text{O} + \text{CO}$. The kinetics of this reaction were studied by Turnipseed et al. [1334], who used pulsed laser photolysis with pulsed laser-induced fluorescence detection and a flow tube reactor with chemical ionization detection to obtain data at temperatures from 233 to 332 K and at pressures from 0.8 to about 300 torr in He and at about 300 torr in SF_6 . The reaction was found to be predominantly a three-body recombination, presumably producing CF_3OCO as described in Table 2. The bimolecular reaction has at least two product channels: (a) $\text{CF}_2\text{O} + \text{CFO}$ and (b) $\text{CF}_3 + \text{CO}_2$. The recommended bimolecular rate coefficient limit is derived from the low pressure results of Turnipseed et al., where the reaction was in the fall-off region. Their low pressure data indicate that $k_b < 4 \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K. The fate of the CF_3OCO adduct is uncertain, and it may lead to the regeneration of CF_3 or CF_3O radicals in the atmosphere. Wallington and Ball [1397]

report a yield of $96 \pm 8\%$ CO_2 at one atmosphere and 296 ± 2 K. (Table: 94-26, Note: 97-4) [Back to Table](#)

- E68. $\text{CF}_3\text{O} + \text{CH}_4$. The absolute rate coefficients reported by Saathoff and Zellner [1131], Barone et al. [86], Jensen et al. [664], Bourbon et al. [167], and Bednarek et al. [119] at room temperature are in excellent agreement. Kelly et al. [697] used a relative method with FTIR detection to determine the ratio $k(\text{CF}_3\text{O} + \text{CH}_4)/k(\text{CF}_3\text{O} + \text{C}_2\text{H}_6) = R = 0.01 \pm 0.001$ at 298 ± 2 K. This does not agree with the ratio of our recommended values, which is 0.017. A relative rate measurement reported by Chen et al. [253] using FTIR methods also gives a low result for the rate coefficient. A relative rate measurement reported by Wallington and Ball [1397], $R = 0.0152 \pm 0.0023$ at 296 K, is in good agreement with the recommended rate coefficients. The temperature dependence is from the data of Barone et al. (247–360 K), Jensen et al. (231–385 K), and Bednarek et al. (235–401 K), who agree very well. Measurements at higher temperatures by Bourbon et al. (296–573 K) gave a higher E/R (1606 K). The $k(298 \text{ K})$ is the average of the three absolute studies. The CF_3OH product was observed by Jensen et al. and Bevilacqua et al. [132]. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E69. $\text{CF}_3\text{O} + \text{C}_2\text{H}_6$. The room temperature recommendation is based on results reported by Saathoff and Zellner [1131], Barone et al. [86], and Bourbon et al. [167]. These studies are in excellent agreement. Chen et al. [253] measured the rate coefficient relative to that for the $\text{CF}_3\text{O} + \text{NO}$ reaction in 700 torr of air at 297 K. Their ratio is in good agreement with the values recommended in this evaluation. Kelly et al. [697] used a relative method with FTIR detection to determine the ratio $k(\text{CF}_3\text{O} + \text{CH}_4)/k(\text{CF}_3\text{O} + \text{C}_2\text{H}_6) = 0.01 \pm 0.001$ at 298 ± 2 K. This does not agree with the ratio of our recommended values, which is 0.017. A relative rate measurement reported by Wallington and Ball [1397], $R = 0.0152 \pm 0.0023$ at 296 K is in good agreement with the recommended rate coefficients. The temperature dependence is from the work of Barone et al., who studied the reaction over the temperature range from 233 to 360 K. Measurements by Bourbon et al. (295–573 K) gave a higher E/R (642 K). The products are inferred by analogy to other reactions of CF_3O with organic compounds. (Table: 97-4, Note: 97-4) [Back to Table](#)
- E70. $\text{CF}_3\text{O}_2 + \text{O}_3$. The recommended upper limit is given by the measurements reported by Ravishankara et al. [1099] who used chemical ionization detection of CF_3O_2 with a flow tube reactor. No measurable reaction was observed in their study. The less direct studies of Nielsen and Sehested [980], Maricq and Szente [869] and Turnipseed et al. [1336] report somewhat larger upper limits to the rate coefficient. An observable reaction was reported in an indirect measurement by Meller and Moortgat [898]. Their result for the $\text{CF}_3\text{O} + \text{O}_3$ reaction is not consistent with the value recommended above. Their study may have interference from unknown reactions. The products are assumed to be $\text{CF}_3\text{O} + 2\text{O}_2$. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E71. $\text{CF}_3\text{O}_2 + \text{CO}$. The recommended upper limit is reported by Turnipseed et al. [1334] who used chemical ionization mass spectrometric detection of CF_3OO with a flow tube reactor at 296 K. This result is at odds with an earlier study by Czarnowski and Schumacher [338], who deduced a "fast reaction" when they observed the thermal decomposition of $\text{CF}_3\text{OOOCF}_3$ to accelerate in the presence of CO at 315–343K. It is possible that the reaction of CF_3O with CO could account for their observations. (Table: 94-26, Note: 94-26) [Back to Table](#)
- E72. $\text{CF}_3\text{O}_2 + \text{NO}$. The recommendation is an average of the room temperature rate coefficients reported by Plumb and Ryan [1066], Dognon et al. [404], Peeters et al. [1044], Bevilacqua et al. [132], Sehested and Nielsen [1173], Turnipseed et al. [1336], Bourbon et al. [166], and Bhatnagar and Carr [134], all of whom are in excellent agreement. The temperature dependence is derived from the results of Dognon et al. Several studies have confirmed the identity of the products. (Table: 97-4, Note: 97-4) [Back to Table](#)
- F1. $\text{O} + \text{ClO}$. There have been five studies of this rate constant over an extended temperature range using a variety of techniques: Leu [815]; Margitan [866]; Schwab et al. [1165]; Ongstad and Birks [1012]; Nicovich et al. [973] and Goldfarb et al. [513]. The recommended value is based on a least squares fit to the data reported in these studies and in the earlier studies of Zahniser and Kaufman [1509] and Ongstad and Birks [1011]. Values reported in the early studies of Bemand et al. [126] and Clyne and Nip [292] are significantly higher and were not used in deriving the recommended value. Leu and Yung [810] were unable to detect $\text{O}_2(^1\Delta)$ or $\text{O}_2(^1\Sigma)$ and set upper limits to the

branching ratios for their production of 4.4×10^{-4} and 2.5×10^{-2} respectively. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F2. O + OCIO. The recommended value is based on results of the DF-RF study of Gleason et al. [510]. Over the temperature range from 400 K down to 240 K their data are well fitted by this Arrhenius expression, but at lower temperatures down to 200 K their data show an abrupt change to a negative temperature dependence. At 200 K the value measured is a factor of 3 higher than that calculated from the Arrhenius expression. Similar results were obtained in a recent study (Toohey, Avallone, and Anderson, private communication). Over the temperature range 413–273 K their data showed a temperature dependence very similar to that reported by Gleason et al. over the same temperature range. Moreover, as the temperature was lowered further their rate constant values also levelled off and then increased at the lowest temperature. Their rate constant values were nearly 50% lower than the values of Gleason et al. from 400 K down to 273 K and 30% lower at 253 K. Colussi [306], using a laser-flash photolysis–resonance fluorescence technique over an extended pressure range, reported a value of the bimolecular rate coefficient at room temperature 50% higher than the recommended value. Colussi et al. [308] extended these measurements down to 248 K; in contrast to the positive temperature dependence over this temperature range reported by Gleason et al., these authors report a negative temperature dependence. The bimolecular rate constants reported by Colussi et al. are not directly measured but are derived quantities which are consistent with fall-off curves fitted to the experimental data over the pressure range 20–600 torr. It appears that the experiments of Bemand et al. [126], were complicated by secondary chemistry. The results of Colussi and Colussi et al. over an extended pressure range demonstrate the importance of the termolecular reaction $O + OCIO + M \rightarrow ClO_3 + M$ (see entry for this reaction in Table 2). It should be noted that the termolecular rate constants derived by Gleason et al. on the basis of their low temperature data are not consistent with the termolecular rate constant expression recommended in this evaluation (factor of 3 difference). The recommended expression is based on the results of Colussi [306] and Colussi et al. [308]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F3. O + Cl₂O. Recommended value is based on the results of Stevens and Anderson [1240] and Miziolek and Molina [925], which are in good agreement. The significantly lower values of Wecker et al. [1439] are not included, nor are earlier results by Basco and Dogra [92] and Freeman and Phillips [470] due to data analysis difficulties in both studies. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F4. O + HCl. Fair agreement exists between the results of Brown and Smith [182], Wong and Belles [1482], Ravishankara et al. [1096], Hack et al. [535] and Singleton and Cvetanovic [1199] at 300 K (some of the values for k(300 K) were obtained by extrapolation of the experimentally determined Arrhenius expressions), but these are a factor of ~7 lower than that of Balakhnin et al. [65]. Unfortunately, the values reported for E/R are in complete disagreement, ranging from 2260–3755 K. The preferred value was based on the results reported by Brown and Smith, Wong and Belles, Ravishankara et al., Hack et al. and Singleton and Cvetanovic, but not on those reported by Balakhnin et al. (Table: 82-57, Note: 82-57) [Back to Table](#)
- F5. O + HOCl. Recommended value is based on results of Schindler et al. [1154]. In this study the rate constant was found to be practically independent of temperature in the range 213–298 K. Product analysis indicated that Cl atom abstraction is the predominant primary reaction channel. (Table: 97-4, Note: 97-4) [Back to Table](#)
- F6. O + ClONO₂. The results reported by Molina et al. [928] and Kurylo [750] are in good agreement, and these data have been used to derive the preferred Arrhenius expression. The value reported by Ravishankara et al. [1091] at 245 K is a factor of 2 greater than those from the other studies, and this may possibly be attributed to (a) secondary kinetic complications, (b) the presence of NO₂ as a reactive impurity in the ClONO₂, or (c) formation of reactive photolytic products. None of the studies reported identification of the reaction products. The room temperature result of Adler-Golden and Wiesenfeld [11] is in good agreement with the recommended value. (Table: 82-57, Note: 82-57) [Back to Table](#)
- F7. O₃ + OCIO. The recommended value is based on results over the temperature range 262–296 K reported by Wongdontri-Stuper et al. [1483]. Within the indicated uncertainty limits it also

encompasses the somewhat lower room temperature result of Birks et al. [146]. (Table: 90-1, Note: 90-1) [Back to Table](#)

- F8. $O_3 + Cl_2O_2$. The recommended upper limit is taken from the study of DeMore and Tschuikow-Roux [382] measured at 195 K. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F9. $OH + Cl_2$. The recommended room temperature value is the average of the results reported by Boodaghians et al. [159], Loewenstein and Anderson [841], Ravishankara et al. [1093], and Leu and Lin [806]. The temperature dependence is from Boodaghians et al. Loewenstein and Anderson determined that the exclusive products are $Cl + HOCl$. (Table 87-41, Note: 87-41) [Back to Table](#)
- F10. $OH + ClO$. The reaction has two known product channels under atmospheric conditions: $OH + ClO \rightarrow Cl + HO_2$ and $OH + ClO \rightarrow HCl + O_2$. Most studies measure the rate coefficients for the overall reaction ($OH + ClO \rightarrow$ products) that is presumably the sum of the two channels. The recommendation for the $Cl + HO_2$ channel is obtained from the difference between a critical assessment of the measurements of the overall reaction and the recommendation for the $HCl + O_2$ channel as discussed below. The assessment of the overall reaction ($OH + ClO \rightarrow$ products) is based on a fit to the 219–373 K data of Hills and Howard [582], the 208–298 K data of Lipson et al. [835], the 234–356 K data of Kegley-Owen et al. [696] and the 298 K data of Poulet et al. [1075]. Data reported in the studies of Burrows et al. [208], Ravishankara et al. [1093], and Leu and Lin [806] were not used in deriving the recommended value because ClO was not measured directly in these studies and the concentration of ClO was determined by an indirect method. Recent measurements of the overall rate constant by Wang and Keyser (218–298 K) [1416], Bedjanian et al. (230–360 K) [113] and Tyndall et al. (298 K) [1347] are consistent with the recommendation.

The minor reaction channel forming HCl poses significant experimental difficulties due to the complications associated with the measurement of the HCl reaction product. Early studies inferred the HCl branching ratio without measuring HCl . These included the 298 K measurements of Leu and Lin [806] (>0.65); Burrows et al. [208] (0.85 ± 0.2) and Hills and Howard [582] (0.86 ± 0.14). Poulet et al. [1075] measured the HCl product yield to be 0.98 ± 0.12 using mass spectroscopy but their HCl sensitivity was marginal. These studies were not considered in the evaluation. Later studies using mass spectroscopy [834] and diode laser spectroscopy [1417] improved the precision of the HCl product channel measurements. Lipson et al. measured rate constants for the HCl channel over the temperature range 207–298 K while Wang and Keyser [1417] measured the HCl yield between 218–298 K, obtaining (9.0 ± 4.8) %, independent of temperature. The recommendation for the HCl channel is based on an average of the results of Lipson et al. and the rate expression obtained from the product of the HCl yield of Wang and Keyser and the evaluated overall rate constant as discussed above. Recent measurements by Tyndall et al. [1347] and Bedjanian et al. [113] are noted but are not considered in this evaluation. (Table 00-3, Note: 00-3) [Back to Table](#)

- F11. $OH + OClO$. The recommended value is that reported by Poulet et al. [1079], the only reported study of this rate constant, using a discharge flow system in which OH decay was measured by LIF or EPR over the temperature range 293–473 K. Product $HOCl$ was detected by modulated molecular beam mass spectrometry. The branching ratio for the channel to produce $HOCl + O_2$ was determined to be close to unity, but experimental uncertainty would allow it to be as low as 0.80. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F12. $OH + HCl$. The recommended value is based on a least squares fit to the data over the temperature range 240–300 K reported in the studies by Molina et al. [929], Keyser [709], Ravishankara et al. [1105] and Battin-Leclerc et al. [97]. In these studies particular attention was paid to the determination of the absolute concentration of HCl by UV and IR spectrophotometry. Earlier studies by Takacs and Glass [1271], Zahniser et al. [1510], Smith and Zellner [1217], Ravishankara et al. [1096], Hack et al. [535], Husain et al. [624], Cannon et al. [222], Husain et al. [625], and Smith and Williams [1216] had reported somewhat lower room temperature values. The data of Sharkey and Smith [1179] over the temperature range 138–216 K and Battin-Leclerc et al. [97] below 240 K depart from normal Arrhenius behavior. It is unknown whether this is due to an effect such as tunneling at low temperature or a systematic experimental error. Additional work at low temperature is needed. (Table 00-3, Note: 00-3) [Back to Table](#)

- F13. OH + HOCl. In the only reported study of this system Ennis and Birks [439] reported the value of this rate constant at room temperature to lie in the range $(1.7 - 9.5) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. A temperature-dependent expression has been estimated by choosing a pre-exponential factor by analogy with the OH + H₂O₂ reaction and selecting the midpoint of the experimental range for the room temperature rate constant. The large uncertainty factor is needed to encompass the entire range. (Table 87-41, Note: 87-41) [Back to Table](#)
- F14. OH + ClNO₂. The recommended value is based on results of the direct study of Ganske et al. [480, 481] using the discharge flow-resonance fluorescence technique. Mass spectrometric studies showed HOCl to be the major chlorine-containing product, with no evidence for a channel to produce HONO₂ + Cl. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F15. OH + ClONO₂. The results reported by Zahniser et al. [1507] and Ravishankara et al. [1091] are in good agreement at ~245 K (within 25%), considering the difficulties associated with handling ClONO₂. The preferred value is that of Zahniser et al. Neither study reported any data on the reaction products. (Table: 82-57, Note: 82-57) [Back to Table](#)
- F16. OH + CH₃Cl. The recommended rate expression is derived from a combined fit (for T ≤ 400 K) to the data from the relative rate study by Hsu and DeMore [614] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CHF₂ reference reaction, as described in the note for that reaction) and the absolute rate studies of Orkin et al. [1017] and Herndon et al. [573]. Data from the earlier studies of Howard and Evenson [606], Perry et al. [1049], Davis et al. [358], Paraskevopoulos et al. [1034], Taylor et al. [1290], and Jeong and Kaufman [669] are reasonably well encompassed within the 2σ limits. The room temperature value from Taylor et al. [1290] is inconsistent with the higher temperature results in the same study and with the other investigations and lies outside of the 2σ band, as do the higher room temperature values of Cox et al. [320] and Brown et al. [180]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F17. OH + CH₂Cl₂. The recommended values for k(298 K) and E/R are averages of the values from the absolute rate studies of Villenave et al. [1378] and Herndon et al. [573] and the relative rate study of Hsu and DeMore [614] (two determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₃CHF₂ and OH + CH₃CH₂F reference reactions). The renormalization procedure for relative rate measurements referenced to the OH + CH₃CHF₂ reaction is discussed in the note for that reaction. The rate constant determined relative to the rate constant of the OH + CH₃CH₂F was recalculated using a rate constant of the reference reaction obtained from the data of Schmoltner et al. [1159] and Kozlov et al. [738] above room temperature. The results of Cox et al. [320] and Davis et al. [358] support this recommendation. The results from Taylor et al. [1291], Jeong and Kaufman [669], Perry et al. [1049] and Howard and Evenson [606] lie considerably higher and were not used in deriving the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F18. OH + CHCl₃. The recommended value for k(298 K) is an average of the values from the relative rate study of Hsu and DeMore [614] (which has been recalculated based on the current recommendation for the rate constant of the OH + CH₃CHF₂ reference reaction, as described in the note for that reaction) and the absolute rate studies of Taylor et al. [1291] (which superseded Taylor et al. [1290]), Jeong and Kaufman [669], Davis et al. [358], and Howard and Evenson [606]. The recommended value of E/R is an average of values for this parameter derived in the first four of the above studies. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F19. OH + CCl₄. The recommended upper limit at 298 K is based on the upper limit reported in the competitive study by Cox et al. [320]. The value given there has been increased by a factor of four to allow for uncertainties in the number of NO molecules oxidized. The recommendation is compatible with the less sensitive upper limits reported by Howard and Evenson [606] and Clyne and Holt [283]. None of these investigators reported any evidence for reaction between these species. The A-factor was estimated and a lower limit for E/R was derived. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F20. OH + CH₂FCl (HCFC-31). The recommended value for k(298 K) is an average of the values from the relative rate study of DeMore [376] (which has been recalculated based on the current recommendation for the rate constant of the OH + CH₂Cl₂ reference reaction) and the absolute rate

studies of Howard and Evenson [606], Paraskevopoulos et al. [1034], Watson et al. [1434], Handwerk and Zellner [549] and Jeong and Kaufman [669]. The recommended value for E/R is an average of the values for this parameter determined by DeMore and by Watson et al., Handwerk and Zellner, and Jeong and Kaufman below 400 K. (Table: 02-25, Note: 02-25) [Back to Table](#)

- F21. OH + CHFCl₂ (HCFC-21). The recommended rate expression is derived from a combined fit to the data of Howard and Evenson [606], Perry et al. [1049], Watson et al. [1434], Chang and Kaufman [241], Paraskevopoulos et al. [1034], Jeong and Kaufman [669], and Fang et al. [444]. The rate constants reported by Clyne and Holt [282] are significantly higher than those from the other seven studies and were not used in deriving the recommended parameters. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F22. OH + CHF₂Cl (HCFC-22). Results for this compound show very good agreement among both absolute and relative rate constant measurements. The recommended rate expression is derived from a combined fit to the relative rate data of Hsu and DeMore [615] (which has been recalculated based on the current recommendation for the rate constant of the OH + CH₄ reference reaction), and the absolute rate studies of Orkin and Khamaganov [1015], Fang et al. [444], Atkinson et al. [48], Watson et al. [1434], Chang and Kaufman [241], Paraskevopoulos et al. [1034] and Jeong and Kaufman [669]. The more scattered results of Handwerk and Zellner [549] are in general agreement. The results from the studies of Howard and Evenson [606] and Clyne and Holt [282] are significantly different from those of the other studies and were not used in the derivation. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F23. OH + CFCl₃ (CFC-11). The A-factor was estimated, and a lower limit for E/R was derived by using the upper limit for the rate constant reported by Chang and Kaufman [242] at about 480 K. This expression is compatible with the upper limits reported by Atkinson et al. [48], Howard and Evenson [606], Cox et al. [320] and Clyne and Holt [283]. None of the investigators reported any evidence for reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F24. OH + CF₂Cl₂ (CFC-12). The A-factor was estimated, and a lower limit for E/R was derived by using the upper limit for the rate constant reported by Chang and Kaufman [242] at about 480 K. This expression is compatible with the upper limits reported by Atkinson et al. [48], Howard and Evenson [606], Cox et al. [320], and Clyne and Holt [283]. None of the investigators reported any evidence for reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F25. OH + CH₂ClCH₃. The recommended value for k(298 K) is an average of the values reported by Howard and Evenson [605], Paraskevopoulos et al. [1034], Kasner et al. [694], and Herndon et al. [573]. The recommended value for E/R is an average of the values for this parameter determined by Kasner et al. and Herndon et al. with the value for A calculated to yield the recommended value for k(298 K). Data from the study by Markert and Nielsen [874] were not used to derive the recommended parameters, as they are somewhat more scattered. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F26. OH + CH₃CCl₃. The recommended value for k(298 K) is an average of the values from the absolute rate studies of Talukdar et al. [1288] and Finlayson-Pitts et al. [457], and a relative rate study of DeMore [373] (recalculated based on the current recommendation for the rate constant of the OH + CH₄ reference reaction). The temperature dependence is a fit to the data between 243 K and 379 K of Talukdar et al. [1288]. These studies indicate both a lower k(298 K) and E/R than was reported in earlier studies: Nelson et al. [956], Jeong and Kaufman [668], and Kurylo et al. [753]. More recent measurements by Jiang et al. [671] and Lancar et al. [766] yield rate constants that are slightly higher at 298 K than this recommendation. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F27. OH + CH₃CFCl₂ (HCFC-141b). Both absolute and relative rate measurements are in excellent agreement for this compound, and the data are linear over a wide temperature range. The recommended rate expression is derived from a combined fit to the data of Huder and DeMore [618] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants for the reference reactions OH + CH₄ and OH + CH₃CCl₃), Lancar et al. [766], Zhang et al. [1521] (together with the data at 330 K and above from Liu et al. [839], Talukdar et al. [1281] above 253 K (two studies), and Mors et al. [936]). The temperature-dependence data of Brown et al. [179] were not considered because the relatively large rate constants

and Arrhenius curvature are suggestive of sample impurities. (Table: 02-25, Note: 02-25) [Back to Table](#)

- F28. $\text{OH} + \text{CH}_3\text{CF}_2\text{Cl}$ (HCFC-142b). The recommended value for $k(298 \text{ K})$ is an average of the values from Howard and Evenson [605], Cox et al. [320], Paraskevopoulos et al. [1034], Mors et al. [936], Watson et al. [1434], Handwerk and Zellner [549], Liu et al. [839], Gierczak et al. [495], and Fang et al. [445]. The recommended value of E/R is an average of values for this parameter derived in the last five of these studies. The data from Brown et al. [179] and Clyne and Holt [282] were not used to derive the recommended parameters. The 270 K data of Zhang et al. [1521] are in reasonable agreement with the recommendation. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F29. $\text{OH} + \text{CH}_2\text{ClCF}_2\text{Cl}$ (HCFC-132b). The recommended rate expression was derived from the data of Watson et al. [1436], which were corrected by these authors for the presence of alkene impurities. The data of Jeong et al. [667], indicating faster rate constants, may have been affected by such impurities; hence they were not included in deriving the recommendation. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F30. $\text{OH} + \text{CH}_2\text{ClCF}_3$ (HCFC-133a). The recommended value of k_{298} is the average of the values of Howard and Evenson [605] and Handwerk and Zellner [549] adjusted to 298 K. The recommended temperature dependence was derived from the data of Handwerk and Zellner [549]. The data of Clyne and Holt [282] were not used in deriving the recommended parameters but (below 400 K) are encompassed within the 2σ limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F31. $\text{OH} + \text{CHCl}_2\text{CF}_2\text{Cl}$ (HCFC-122). The recommended rate expression is derived from a combined fit to the data of Orkin and Khamaganov [1015] (below 400 K) and DeMore [376] (two determinations which have been recalculated based on the current recommendations for the rate constants of the $\text{OH} + \text{CH}_2\text{Cl}_2$ and $\text{OH} + \text{CHCl}_2\text{CF}_3$ reference reactions). (Table: 02-25, Note: 02-25) [Back to Table](#)
- F32. $\text{OH} + \text{CHFClCFCl}_2$ (HCFC-122a). The recommended rate expression was derived from the relative rate data of Hsu and DeMore [615] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_3\text{CHF}_2$ reference reaction, as discussed in the note for that reaction). (Table: 02-25, Note: 02-25) [Back to Table](#)
- F33. $\text{OH} + \text{CHCl}_2\text{CF}_3$ (HCFC-123). The recommended value of k_{298} is the average of the values from the absolute studies of Gierczak et al. [495] (two determinations) Liu et al. [839], and Yamada et al. [1494], and from the relative rate study by Hsu and DeMore [615] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_3\text{CHF}_2$ reference reaction, as discussed in the note for that reaction). The recommendation for the temperature dependence is derived from a fit to the data of these same five investigations. The temperature dependence data of Nielsen [975], Watson et al. [1436], Clyne and Holt [282], and Brown et al. [179] and the room temperature data of Howard and Evenson [605] were not used in the derivations. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F34. $\text{OH} + \text{CHFClCF}_2\text{Cl}$ (HCFC-123a). The recommended rate expression is based on the data of Orkin and Khamaganov [1015]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F35. $\text{OH} + \text{CHFClCF}_3$ (HCFC-124). The recommended value for $k(298 \text{ K})$ is an average of the values from the studies of Watson et al. [1436], Gierczak et al. [495] (2 studies), Yamada et al. [1494], and Hsu and DeMore [615] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the $\text{OH} + \text{CH}_4$ and $\text{OH} + \text{CHF}_2\text{CHF}_2$ reference reactions). The room temperature rate constant of Howard and Evenson [605] is considerably higher than these other values and was not included in the average. The recommended temperature dependence is an average of the dependencies derived from these same studies (but using only data below 400 K from Gierczak et al. [495] and Yamada et al. [1494]). (Table: 02-25, Note: 02-25) [Back to Table](#)
- F36. $\text{OH} + \text{CH}_3\text{CF}_2\text{CFCl}_2$ (HCFC-243cc). The recommended rate expression is derived from the temperature-dependence data of Nelson et al. [952]. Although there is only a single study of this reaction, the uncertainties have been assigned to reflect our belief that the rate constant for this reaction should be less than that for $\text{OH} + \text{CH}_3\text{CF}_2\text{Cl}$. (Table: 02-25, Note: 02-25) [Back to Table](#)

- F37. $\text{OH} + \text{CHCl}_2\text{CF}_3\text{CF}_2$ (HCFC-225ca). The recommended value for $k(298\text{ K})$ is an average of the values from Nelson et al. [952] and Zhang et al. [1522]. The recommendation for E/R is taken from Nelson et al. [952]. The temperature-dependence data of Brown et al. [178] were not considered because the relatively large rate constants at and below room temperature and the Arrhenius curvature are suggestive of sample impurities. The temperature dependence results of Zhang et al. [1522] are in reasonable agreement with those of Nelson et al. [952] over the temperature range of measurement overlap. However, the complete Zhang et al. [1522] data set yields a value for E/R much larger than currently recommended for the $\text{OH} + \text{CHCl}_2\text{CF}_3$ (HFC-123) reaction, for which the activation energy should be similar. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F38. $\text{OH} + \text{CF}_2\text{ClCF}_2\text{CHCl}$ (HCFC-225cb). The recommended rate expression is derived from a combined fit to the temperature-dependence data of Nelson et al. [952] and Zhang et al. [1522], which are in excellent agreement. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F39. $\text{OH} + \text{CH}_2=\text{CHCl}$. The recommended value for $k(298\text{ K})$ is an average of the values reported by Howard [603], Perry et al. [1047], Liu et al. [838] and [1495]. The recommended value for E/R is an average of the values for this parameter derived from fits to the data of Perry et al., Liu et al. and Yamada et al. at temperatures below about 400 K. In the 400–500 K region the rate constant levels off before increasing at higher temperatures, suggesting the stronger importance of an abstraction mechanism at the higher temperatures. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F40. $\text{OH} + \text{CH}_2=\text{CCl}_2$. The recommended value for $k(298\text{ K})$ is an average of the values reported by Edney et al. [431], Tuazon et al. [1325], Abbatt and Anderson [1], Zhang et al. [1523], Canosa-Mas et al. [224], and [1493]. The recommended value for E/R comes from a combined fit to the data of Abbatt and Anderson, Zhang et al., and Yamada et al. The data of Kirchner et al. [715] were not used in deriving the recommended parameters since they were obtained at very low pressure and the much stronger temperature dependence obtained may be indicative of a pressure dependence above room temperature. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F41. $\text{OH} + \text{CHCl}=\text{CCl}_2$. The recommended value for $k(298\text{ K})$ is the mean of the values reported by Howard [603], Chang and Kaufman [241], Kirchner et al. [715], Klopffer et al. [725], Edney et al. [431] and Tichenor et al. [1306]. The recommended value of E/R is an average of values for this parameter derived by Chang and Kaufman [241], Kirchner et al. [715], and Tichenor et al. [1306]. The value for $k(298\text{ K})$ derived from a relative rate study by Winer et al. [1478] is a factor of ~ 2 greater than the other values and is not considered in deriving the preferred value. An absolute study by Jiang et al. [672] yielding a significantly higher value for $k(298\text{ K})$ as well as a considerably stronger temperature dependence ($E/R = -970\text{ K}$) is assumed to be superseded by Tichenor et al. [1306]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F42. $\text{OH} + \text{CCl}_2=\text{CCl}_2$. The recommended value for $k(298\text{ K})$ is the mean of the values reported by Howard [603], Chang and Kaufman [241], and Kirchner et al. [715]. The room temperature value reported by Winer et al. [1478] is more than a factor of 10 greater and was not used in deriving the recommendation. The recommended value for E/R is an average of values for this parameter derived by Chang and Kaufman [241] and Kirchner et al. [715]. A study by Tichenor et al. [1307] yields a value for $k(298\text{ K})$ slightly lower than these other studies, but a temperature dependence less than half of that recommended. While these latest results were not used in deriving the recommendations, they are encompassed within the 95% confidence limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F43. $\text{OH} + \text{CH}_3\text{OCl}$. The recommended rate expression is derived from a fit to the data of Crowley et al. [335], the only reported study of this reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F44. $\text{OH} + \text{CCl}_3\text{CHO}$. The recommended value for $k(298\text{ K})$ is an average of the values reported by Barry et al. [89] (using three independent techniques), Dobe et al. [395], Nelson et al. [956], Ballestra-Garcia et al. [68], and Scollard et al. [1166]. The temperature dependence is derived from a fit to the data of Dobe et al. [395]. The A factor was then calculated to agree with the recommended value for $k(298\text{ K})$. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F45. $\text{HO}_2 + \text{Cl}$. The recommendations for the two reaction channels are based upon the results by Lee and Howard [793] using a discharge flow system with laser magnetic resonance detection of HO_2 ,

OH, and ClO. The total rate constant is temperature independent with a value of $(4.2 \pm 0.7) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ over the temperature range 250–420 K. This value for the total rate constant is in agreement with the results of indirect studies relative to $\text{Cl} + \text{H}_2\text{O}_2$ (Leu and DeMore [802], Poulet et al. [1077], Burrows et al. [203] or to $\text{Cl} + \text{H}_2$ (Cox [314])). The contribution of the reaction channel producing OH + ClO (21% at room temperature) is much higher than the upper limit reported by Burrows et al. (1% of total reaction). Cattell and Cox [238], using a molecular modulation-UV absorption technique over the pressure range 50–760 torr, report results in good agreement with those of Lee and Howard both for the overall rate constant and for the relative contribution of the two reaction channels. A study by Dobis and Benson [400] reports a total rate constant in good agreement with this recommendation but a much lower contribution ($5 \pm 3\%$) of the channel producing OH + ClO. The rate constant for the channel producing ClO + OH can be combined with that for the reaction $\text{ClO} + \text{OH} \rightarrow \text{Cl} + \text{HO}_2$ to give an equilibrium constant from which a value of the heat of formation of HO_2 at 298 K of 3.0 kcal/mol can be derived. (Table: 82-57, Note: 94-26) [Back to Table](#)

- F46. $\text{HO}_2 + \text{ClO}$. Three new studies by Nickolaisen et al [965], Knight et al. [727], and Laszlo et al. [771] have been added to the previous five studies of this rate constant (Reimann and Kaufman, [1111]; Stimpfle et al. [1248]; Leck et al. [781]; Burrows and Cox [204]; Cattell and Cox [238]). The studies span a wide variety of pressure conditions and detection techniques. The studies of Cattell and Cox and Nickolaisen et al. were performed over extended pressure ranges and indicate that the reaction is pressure independent. However, the room temperature rate constant obtained by averaging the five low pressure (< 10 torr) studies is slightly lower (5.1 ± 1.5 vs. 6.5 ± 1.2 in units of $10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) than that obtained by averaging the higher pressure measurements (> 50 torr). Although within the combined uncertainty, this offset may suggest possible systematic experimental complications (e.g. unknown secondary reactions) in the low or high pressure experiments. The recommended value for $k(298 \text{ K})$ is the mean of the eight studies. Temperature-dependence data has been obtained by Stimpfle et al., Nickolaisen et al., Knight et al., and Laszlo et al. The earliest study (Stimpfle et al.) observed nonlinear Arrhenius behavior. The data were best described by a four parameter equation of the form $k = A \exp(-B/T) + CT^n$, possibly suggesting that two different mechanisms may be occurring. The more recent studies find the T-dependence to display linear Arrhenius behavior over the entire temperature range. Moreover, they derive much smaller E/R values (17 to 312) than that obtained by Stimpfle ($E/R \approx 700$ for $T < 300 \text{ K}$). The recommended value for E/R is based on an average of the four studies over their entire temperature ranges. The two most probable pairs of reaction products are, (1) $\text{HOCl} + \text{O}_2$ and (2) $\text{HCl} + \text{O}_3$. Leu [814], Leck et al., Knight et al., and Laszlo et al. used mass spectrometric detection of ozone to place upper limits on channel 2 of 1.5%, 2%, 1%, and 2%, respectively at 298 K. In addition, Leck et al. and Laszlo set upper limits of 3.0% (248 K); and 5.0% (243 K), respectively, on k_2/k . Burrows and Cox report an upper limit of 0.3% for k_2/k at 300 K. Finkbeiner et al. [456], using matrix-isolation/FTIR spectroscopy, studied product formation between 210 and 300 K at 700 torr. HOCl was observed as the dominant product ($> 95\%$ at all temperatures). The branching ratio values for k_2/k were determined to be $< 1\%$ at 300 K and 270 K, $2 \pm 1\%$ at 240 K, and $5 \pm 2\%$ at 210 K. No evidence for any other product channel was found. Theoretical calculations by Nickolaisen et al. suggest that the reaction to channel (1) proceeds mainly through the ClO- HO_2 complex on the triplet potential surface. However, these calculations also suggest that collisionally stabilized HOOCl formed on the singlet surface will possess an appreciable lifetime. Further studies on possible formation of HOOCl are warranted. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F47. $\text{H}_2\text{O} + \text{ClONO}_2$. This recommendation is based on the upper limits to the homogeneous bimolecular rate constant reported by Atkinson et al. [54], and by Hatakeyama and Leu [558, 559]. Atkinson et al. observed by FTIR analysis the decay of ClONO_2 in the presence of H_2O in large-volume (2500 and 5800 liters) Teflon or Teflon-coated chambers. Their observed decay rate gives an upper limit to the homogeneous gas phase rate constant, and they conclude that the decay observed is due to heterogeneous processes. Hatakeyama and Leu, using a static photolysis system with FTIR analysis, derive a similar upper limit. Rowland et al. [1126] concluded that the decay they observed resulted from rapid heterogeneous processes. The homogeneous reaction is too slow to have any significant effect on atmospheric chemistry. (Table 87-41, Note: 87-41) [Back to Table](#)

- F48. NO + OClO. The Arrhenius expression was estimated based on 298 K data reported by Bemand, Clyne and Watson [126]. (Table: 82-57, Note: 82-57) [Back to Table](#)
- F49. NO + Cl₂O₂. The recommended upper limit is that determined by Friedl (private communication) in a study using a DF-MS technique. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F50. NO₃ + HCl. The recommended upper limit is that reported by Mellouki et al. [905] in a study using DF-EPR techniques. This upper limit shows that this reaction is of negligible importance in stratospheric chemistry. Somewhat lower upper limits have been reported by Cantrell et al. [228] and Canosa-Mas et al. [225]; the latter study also reports Arrhenius parameters at higher temperatures (333–473 K). (Table: 90-1, Note: 90-1) [Back to Table](#)
- F51. HO₂NO₂ + HCl. This upper limit is based on results of static photolysis-FTIR experiments reported by Leu et al. [805]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F52. Cl + O₃. The results reported for k(298 K) by Watson et al. [1435], Zahniser et al. [1511], Kurylo and Braun [754], Clyne and Nip [293], Nicovich et al. [968], Seeley et al. [1169] and Beach et al. [101] are in good agreement, and have been used to determine the preferred value at this temperature. The values reported by Leu and DeMore [802] (due to the wide error limits) and Clyne and Watson [298] (the value is inexplicably high) are not considered. The six Arrhenius expressions are in fair agreement within the temperature range 205–300 K. In this temperature range, the rate constants at any particular temperature agree to within 30–40%. Although the values of the activation energy obtained by Watson et al. and Kurylo and Braun are in excellent agreement, the value of k in the study of Kurylo and Braun is consistently (~17%) lower than that of Watson et al. This may suggest a systematic underestimate of the rate constant, as the values from the other three agree so well at 298 K. Two recent studies (Nicovich et al. and Seeley et al.) obtained significantly smaller temperature dependences than those observed in the earlier studies. There is no reason to prefer any one set of data to any other; therefore, the preferred Arrhenius expression shown above was obtained by computing the mean of the six results between 205 and 298 K. DeMore [372] directly determined the ratio k(Cl + O₃)/k(Cl + CH₄) at 197–217 K to be within 15% of that calculated from the absolute rate constant values recommended here.

Vanderzanden and Birks [1370] have interpreted their observation of oxygen atoms in this system as evidence for some production (0.1–0.5%) of O₂ (¹Σ_g⁺) in this reaction. The possible production of singlet molecular oxygen in this reaction has also been discussed by DeMore [369], in connection with the Cl₂ photosensitized decomposition of ozone. However Choo and Leu [265] were unable to detect O₂(¹Σ) or O₂(¹Δ) in the Cl + O₃ system and set upper limits to the branching ratios for their production of 5 × 10⁻⁴ and 2.5 × 10⁻², respectively. They suggested two possible mechanisms for the observed production of oxygen atoms, involving reactions of vibrationally excited ClO radicals with O₃ or with Cl atoms, respectively. Burkholder et al. [199], in a study of infrared line intensities of the ClO radical, present evidence in support of the second mechanism. In their experiments with excess Cl atoms, the vibrationally excited ClO radicals produced in the Cl + O₃ reaction can react with Cl atoms to give Cl₂ and oxygen atoms, which can then remove additional ClO radicals. These authors point out the possibility for systematic error from assuming a 1:1 stoichiometry for [Cl]:[O₃]₀ when using the Cl + O₃ reaction as a quantitative source of ClO radicals for kinetic and spectroscopic studies. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F53. Cl + H₂. The recommended value for k(298 K) is an average of the values measured by Westenberg and De Haas [1449], Lee et al. [784], Miller and Gordon [923], and Kita and Stedman [718]. The value of k(298 K) derived in the flash photolysis resonance fluorescence study of Davis et al. [355] agrees with these studies but was probably overestimated by ~10% (the authors assumed that the fluorescence signal, I_f was proportional to [Cl]^{0.9}, whereas a linear relationship between I_f and [Cl] probably held under their experimental conditions). Room temperature determinations by Kumaran et al. [745] (focused primarily on high temperature measurements) and Eberhard et al. [428] (focused on obtaining yields of HCl product in different vibrational levels) are both in reasonable agreement with the recommendation as are the results from the relative rate studies by Su et al. [1260] and by Rodebush and Klingelhofer [1122]. The value for E/R is derived from a fit to the data at temperatures below 300 K reported by Westenberg and De Haas [1449], Lee et al. [784], and

Miller and Gordon [923]. The value is in good agreement with that determined by Adusei and Fontijn [12], although these data lie systematically lower than the results from other studies. The Arrhenius A-factor was calculated from $k(298\text{ K})$ and E/R . Extrapolation above room temperature using the recommended Arrhenius parameters is in reasonable agreement with the data of Benson et al. [129] and Kita and Stedman [718]. For a discussion of the large body of rate data at high temperatures, see the review by Baulch et al. [100]. Miller and Gordon [923] and Kita and Stedman [718] also measured the rate of the reverse reaction, and found the ratio to be in good agreement with equilibrium constant data. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F54. $\text{Cl} + \text{H}_2\text{O}_2$. The absolute rate coefficients determined at $\sim 298\text{ K}$ by Watson et al. [1435], Leu and DeMore [802], Michael et al. [921], Poulet et al. [1077] and Keyser [705] range in value from $(3.6\text{--}6.2) \times 10^{-13}$. The studies of Michael et al., Keyser, and Poulet et al. are presently considered to be the most reliable. The preferred value for the Arrhenius expression is taken to be that reported by Keyser. The A-factor reported by Michael et al. is considerably lower than that expected from theoretical considerations and may possibly be attributed to decomposition of H_2O_2 at temperatures above 300 K . The data of Michael et al. at and below 300 K are in good agreement with the Arrhenius expression reported by Keyser. More data are required before the Arrhenius parameters can be considered to be well-established. Heneghan and Benson [569], using mass spectrometry, confirmed that this reaction proceeds only by the abstraction mechanism giving HCl and HO_2 as products. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F55. $\text{Cl} + \text{NO}_3$. The recommended value at room temperature is based on the discharge flow-EPR study of Mellouki et al. [903] and the discharge flow-mass spectrometric study of Becker et al. [104]. The results of these direct absolute rate studies are preferred over results of the earlier relative rate studies of Cox et al. [315], Burrows et al. [207], and Cox et al. [326], in all of which NO_3 was monitored in the photolysis of $\text{Cl}_2\text{-ClONO}_2\text{-N}_2$ mixtures. Complications in the chemistry of the earlier systems probably contributed to the spread in reported values. This radical-radical reaction is expected to have negligible temperature dependence, which is consistent with the results from the study of Cox et al. [326] in which the complications must have been temperature independent. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F56. $\text{Cl} + \text{N}_2\text{O}$. This rate coefficient has been determined in a study of the halogen-catalyzed decomposition of nitrous oxide at about 1000 K by Kaufman et al. [695]. The largest value reported was $10^{-17}\text{ cm}^3\text{ molecule}^{-1}\text{ s}^{-1}$, with an activation energy of 34 kcal/mol . Extrapolation of these results to low temperature shows that this reaction cannot be of any significance in atmospheric chemistry. (Table 87-41, Note: 87-41) [Back to Table](#)
- F57. $\text{Cl} + \text{HNO}_3$. The recommended upper limit at room temperature is that reported in the study of Wine et al. [1475], in which long-path laser absorption spectroscopy was used to look for the appearance of NO_3 following the pulsed laser photolysis of $\text{Cl}_2\text{-HNO}_3$ mixtures with no evidence for NO_3 production was observed. In the same study a less sensitive upper limit was derived from monitoring Cl atom decay by resonance fluorescence. A less sensitive upper limit was also found in the discharge flow-EPR study of Zagogianni et al. [1505]. Higher values obtained in earlier studies (Leu and DeMore [802], Kurylo et al. [760], and Clark et al. [272]) as well as the higher temperature results of Poulet et al. [1077] are not used. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F58. $\text{Cl} + \text{HO}_2\text{NO}_2$. The only study of this reaction is by Simonaitis and Leu [1195] using the low pressure discharge flow technique coupled with resonance fluorescence detection of Cl and mass spectrometric detection of HO_2NO_2 ion fragments. Consistent results were obtained monitoring either Cl or HO_2NO_2 decays and retrieved rate constants were less than $1 \times 10^{-13}\text{ cm}^3\text{ molecule}^{-1}\text{ s}^{-1}$ for all conditions. Impurities in the HO_2NO_2 sample (especially H_2O_2) complicated the measurements. A limited temperature study over the $298\text{--}399\text{ K}$ range suggests that E/R is in the range of $500\text{--}1500$. Given the experimental difficulties, only an upper limit is recommended for the reaction rate. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F59. $\text{Cl} + \text{CH}_4$. The recommended value for $k(298\text{ K})$ is based on the values reported in the absolute rate constant studies of Manning and Kurylo [862], Whytock et al. [1452], Michael and Lee [914], Lin et al. [831], Zahniser et al. [1506], Keyser [702], Baghal-Vayjoee et al. [63], Ravishankara and Wine [1100], Heneghan et al. [570], Dobis and Benson [398], Sawerysyn et al. [1150], Lazarou et al.

[777], Beichert et al. [124], Seeley et al. [1169], Pilgrim et al. [1058], Mellouki et al. [899], Wang and Keyser [1415], and Bryukov et al. [189], all of which fall in the range $(0.9 - 1.13) \times 10^{-13}$. Other absolute studies by Davis et al. [355], Clyne and Walker [297], Poulet et al. [1076], Leu and DeMore [802], Watson et al. [1435], and Schlyer et al. [1155] give rate constant values slightly higher than those of the aforementioned studies. In some cases, this may be due to uncertainties in correcting the data for OH loss via reaction with trace levels of ethane and propane in the methane samples used. Nevertheless, these results were not used in deriving the recommended value for $k(298\text{ K})$. The values derived for k at 298 K from the competitive chlorination studies of Pritchard et al. [1080], Pritchard et al. [1081], Knox [729], Knox and Nelson [731], Lee and Rowland [782], and Lin et al. [831] range from $(0.8-1.6) \times 10^{-13}$ when the original data are referenced to the presently recommended rate constant values for the reference reactions of Cl with H_2 and C_2H_6 . The recommended value $k(298\text{ K}) = 1.0 \times 10^{-13}$ is derived as an unweighted average of the rate constants from the thirteen preferred absolute studies and the most recent and comprehensive relative rate study of Lin et al. [831].

There have been nine absolute studies of the temperature dependence of k in which the measurements extend below 300 K (Watson et al. [1435], Manning and Kurylo [862], Whytock et al. [1452], Lin et al. [831], Zahniser et al. [1506], Keyser [702], Ravishankara and Wine [1100], Heneghan et al. [570], and Seeley et al. [1169]). In general, the agreement among most of these studies is quite good. However, systematic differences in activation energies are apparent when calculated using data obtained below 300 K versus data from above 300 K. Three resonance fluorescence studies have been performed over the temperature region between 200 and 500 K (Whytock et al. [1452], Zahniser et al. [1506] and Keyser [702]), and in each case a non-linear Arrhenius behavior was observed. Ravishankara and Wine [1100] also noted nonlinear Arrhenius behavior over a more limited temperature range. This behavior tends to partially explain the variance in the values of E/R reported between those investigators who mainly studied this reaction below 300 K (Watson et al. [1435], Manning and Kurylo [862], and Seeley et al. [1169]) and those who only studied it above 300 K (Clyne and Walker [297], Poulet et al. [1076], and Lin et al. [831]). The agreement between all studies below 300 K is reasonably good, with values of E/R ranging from 1060 K to 1320 K. There have not been any absolute studies at stratospheric temperatures other than those that utilized the resonance fluorescence technique. Ravishankara and Wine [1100] have suggested that the results obtained using the discharge flow and competitive chlorination techniques may be in error at the lower temperatures ($<240\text{ K}$) due to a non-equilibration of the $^2\text{P}_{1/2}$ and $^2\text{P}_{3/2}$ states of atomic chlorine. They observed that at temperatures below 240 K the apparent bimolecular rate constant was dependent upon the chemical composition of the reaction mixture; i.e., if the mixture did not contain an efficient spin equilibrator, e.g., Ar or CCl_4 , the bimolecular rate constant decreased at high CH_4 concentrations. The chemical composition in each of the flash photolysis studies contained an efficient spin equilibrator, whereas this was not the case in the discharge flow studies. However, the reactor walls in the discharge flow studies could have been expected to have acted as an efficient spin equilibrator. Consequently, until the hypothesis of Ravishankara and Wine is proven, it is assumed that the discharge flow and competitive chlorination results are reliable. A composite unweighted Arrhenius fit to all of the temperature dependent absolute studies with data in the temperature region $\leq 300\text{ K}$ (with the exception of the data of Watson et al. [1435], which appear to be systematically high due to reactive impurities) yields $E/R = 1280\text{ K}$ and $k(298\text{ K}) = 1.0 \times 10^{-13}$. The Arrhenius A-factor was calculated from recommended $k(298\text{ K})$ and E/R . (Table: 06-2, Note: 06-2) [Back to Table](#)

- F60. $\text{Cl} + \text{CH}_3\text{D}$. The recommended value for $k(298\text{ K})$ is an average of the relative rate determinations by Saueressig et al. [1148] (two independent measurements) and by Tyler et al. [1343]. It agrees with the value determined by Wallington and Hurley [1404] after the latter is corrected as per a personal communication from the authors. The value for E/R is an average of the values determined by Saueressig et al. and Tyler et al. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F61. $\text{Cl} + \text{H}_2\text{CO}$. The results from five of the six published studies (Michael et al. [918], Anderson and Kurylo [28], Niki et al. [985], Fasano and Nogar [447] and Poulet et al. [1072]) are in good agreement at $\sim 298\text{ K}$, but are $\sim 50\%$ greater than the value reported by Foon et al. [465]. The preferred value at 298 K was obtained by combining the absolute values reported by Michael et al.,

Anderson and Kurylo, and Fasano and Nogar, with the values obtained by combining the ratio of $k(\text{Cl} + \text{H}_2\text{CO})/k(\text{Cl} + \text{C}_2\text{H}_6)$ reported by Niki et al. (1.3 ± 0.1) and by Poulet et al. (1.16 ± 0.12) with the preferred value of 5.7×10^{-11} for $k(\text{Cl} + \text{C}_2\text{H}_6)$ at 298 K. The preferred value of E/R was obtained from a least squares fit to all the data reported in Michael et al. and in Anderson and Kurylo. The A-factor was adjusted to yield the preferred value at 298 K. (Table: 82-57, Note: 82-57) [Back to Table](#)

- F62. $\text{Cl} + \text{HC}(\text{O})\text{OH}$. The room temperature kinetics of this reaction have been studied by Wallington et al. [1390] and Li et al. [818]. Wallington et al. used a relative rate technique at atmospheric pressure while Li et al. employed flash photolysis and operated at 10 torr. The results of the two studies are in excellent agreement and have been averaged together to derive the recommended value. Reaction products have been investigated by Tyndall et al. [1358] at room temperature and 700 torr pressure. They measured the CO_2 yield to be $96 \pm 5\%$ and suggested that the HOCO complex reacted with either O_2 or Cl_2 in their experiment to give the observed product. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F63. $\text{Cl} + \text{CH}_3\text{O}_2$. Recommended value is based on results of Maricq et al. [872], Jungkamp et al. [683], and Daele and Poulet [340]. All three studies agree that this overall reaction is very fast. However, there is a discrepancy in the reported values of the branching ratios for the two pathways producing $\text{ClO} + \text{CH}_3\text{O}$ (a) and $\text{HCl} + \text{CH}_2\text{O}_2$ (b). The branching ratio for the reaction channels producing $\text{HCl} + \text{CH}_2\text{O}_2$ (b) has been reported to be 50% by both Maricq et al. [872] and Jungkamp et al., but has been reported to be 90% by Daele and Poulet. Because of this large discrepancy no branching ratios are recommended. (Table: 97-4, Note: 97-4) [Back to Table](#)
- F64. $\text{Cl} + \text{CH}_3\text{OH}$. This recommendation at 298 K) is based on results of the absolute rate studies of Michael et al. [919], Payne et al. [1042], Dobe et al. [396], Pagsberg et al. [1029] and Tyndall et al. [1350], and results obtained in the competitive chlorination studies of Wallington et al. [1413], Lightfoot et al. [823], Nelson et al. [955] and Tyndall et al. The temperature independence of the rate constant was reported by Michael et al. in a direct study. This is consistent with the indirect results of Lightfoot et al. who deduced the rate coefficient for this reaction relative to that for methane as a function of temperature. This reaction can have two sets of products: $\text{CH}_2\text{OH} + \text{HCl}$, channel (a) and $\text{CH}_3\text{O} + \text{HCl}$, channel (b). Product analysis and isotopic substitution have established that the reaction proceeds via channel (a) rather than via channel (b). See Radford [1083], Radford et al. [1084], Meier et al. [897], and Payne et al. [1042]. This reaction has been used in the laboratory as a source of CH_2OH and as a source of HO_2 by the reaction of CH_2OH with O_2 . (Table: 02-25, Note: 02-25) [Back to Table](#)
- F65. $\text{Cl} + \text{CH}_3\text{OOH}$. The only study of this reaction was by Wallington et al. [1390], who measured the rate relative to $\text{Cl} + \text{C}_2\text{H}_6$ at 295 K and atmospheric pressure. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F66. $\text{Cl} + \text{CH}_3\text{ONO}_2$. This reaction has been studied at 298 K by Nielsen et al [981] using a relative rate technique. The reference compound was ethane. The recommended value is adjusted from that given by Nielsen et al. using the currently recommended value for $k(\text{Cl} + \text{C}_2\text{H}_6)$. The temperature dependence is estimated by assuming an A-factor equal to approximately 20 times that of $\text{OH} + \text{CH}_3\text{ONO}_2$. This is consistent with observed OH/Cl A-factor ratios for primary H-abstraction from alkanes. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F67. $\text{Cl} + \text{C}_2\text{H}_6$. The recommended value for $k(298 \text{ K})$ is an average of the absolute rate coefficients reported in the studies of Manning and Kurylo [862], Lewis et al. [816], Dobis and Benson [399], Beichert et al. [124], Pilgrim et al. [1058], Tyndall et al. [1352], Hitsuda et al. [586], Bryukov et al. [190], and Hickson and Keyser [580], all of which fall in the range $(5.3 - 6.1) \times 10^{-11}$. The value derived by Ray et al. [1107] in a study whose primary focus was not the determination of the rate constant for the target reaction, lies in the same range. A somewhat higher value reported by Davis et al. [355], was probably overestimated by $\sim 10\%$ (the authors assumed that the fluorescence signal, I_f was proportional to $[\text{Cl}]^{0.9}$, whereas a linear relationship between I_f and $[\text{Cl}]$ probably held under their experimental conditions). The rate constant reported by Schlyer et al. [1155] lies significantly lower than those from all other absolute studies while the values from Mellouki et al. [899] and from Kaiser et al. [688] lie slightly higher. Room temperature rate constants derived from the relative rate

experiments of Pritchard et al. [1081], Knox and Nelson [731], Atkinson and Aschmann [40], Atkinson and Ashmann [41], Tschuikow-Roux et al. [1323], Wallington et al. [1413], Beichert et al. [124], Hooshiyar and Niki [597], and Lin et al. [831] exhibit considerably more scatter even when recalculated based on the same current recommendation for the rate constant of the reference reactions. Nevertheless, most are encompassed within the 95% uncertainty limits recommended for the value of $k(298\text{ K})$. The relative rate results of Kelly et al. [698] and Lee and Rowland [782] are significantly lower than other room temperature measurements. The recommended value for E/R is taken from a combined fit to the data of Manning and Kurylo [862], Dobis and Benson [399], and Hickson and Keyser [580] after normalizing all three data sets to the recommended value of $k(298\text{ K})$. The data from Lewis et al. [816] and Lin et al. [831] below 300 K are encompassed by the 95% uncertainty bands. The temperature dependent studies by Pilgrim et al. [1058] and Bryukov et al. did not extend below room temperature. An extrapolation of the recommended Arrhenius parameters and the 95% uncertainty bands above room temperature encompasses the data of Pilgrim et al. but not those of Bryukov et al., which are characterized by a much stronger temperature dependence. The Arrhenius A-factor was calculated from recommended $k(298\text{ K})$ and E/R. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F68. $\text{Cl} + \text{C}_2\text{H}_5\text{O}_2$. Recommended value is based on results of Maricq et al. [872]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F69. $\text{Cl} + \text{CH}_3\text{CH}_2\text{OH}$. The rate coefficient for this reaction has been studied at 298 K by four groups using a relative rate technique: Nelson et al. [955] (relative to $\text{Cl} + \text{cyclohexane}$), Wallington et al. [1413] (relative to $\text{Cl} + \text{C}_2\text{H}_6$), Edelbuttel-Einhaus et al. [429] (relative to $\text{Cl} + \text{C}_2\text{H}_6$), and Taatjes et al. [1269]. Nelson et al. measured this rate constant relative to the $\text{Cl} + \text{cyclohexane}$ while the others used the $\text{Cl} + \text{C}_2\text{H}_6$ reaction. Taatjes et al. also measured this rate coefficient by measuring the temporal profile of the HCl product. The agreement between these five measurements is quite good, yielding an average value that is recommended. The temperature dependence of this rate coefficient is based on the results of Taatjes et al., who studied this reaction above 298 K and found it to be essentially independent of temperature. We recommend the same independence of temperature at atmospheric temperatures.
- This reaction can have three sets of products: $\text{CH}_2\text{CH}_2\text{OH} + \text{HCl}$, channel (a); CH_3CHOH , channel (b); and $\text{CH}_3\text{CH}_2\text{O}$ channel (c). Taatjes et al. have deduced that channel (c) is negligible and that channel (a) is about 8% at 298 K. Therefore, the majority of reaction is expected to occur via channel (b). It is very unlikely that these branching ratios will change significantly at lower atmospheric temperatures. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F70. $\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{OH}$. Koch and Moortgat [733] have studied this reaction at room temperature using the relative rate technique. Deuterium substitution of the methyl hydrogens decreased the observed rate by a factor of 3.75. In addition, CO and CO_2 reaction products were observed in a stoichiometric ratio of 1:1. These observations were interpreted in terms of methyl hydrogen abstraction from acetic acid to form the $\text{CH}_2\text{C}(\text{O})\text{OH}$ radical followed by reaction with O_2 to form a peroxy radical. Thermal decomposition of the peroxy radical produces HCHO, CO_2 , and atomic H. In the laboratory system, the HCHO reacts with atomic chlorine to yield CO. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F71. $\text{Cl} + \text{CH}_3\text{CN}$. The recommendation is based on results of the study of Tyndall et al. [1353]. The results of this study, using both relative and absolute methods and measured over a wide range of experimental conditions are preferred over the results of earlier studies of Kurylo and Knable [756], Poulet et al. [1071], and Olbregts et al. [1009]. Product studies reported by Tyndall et al. show that reaction proceeds predominantly by hydrogen atom abstraction. (Table: 97-4, Note: 97-4) [Back to Table](#)
- F72. $\text{Cl} + \text{C}_2\text{H}_5\text{ONO}_2$. Wallington et al. [1403] and Nielsen et al. [981] have measured the rate of this reaction at room temperature relative to atomic chlorine reactions with ethyl chloride and ethane, respectively. The two studies are in excellent agreement and the recommended value is based on an average of the two. The values given in Wallington et al. and Nielsen et al. were adjusted based on the currently accepted values of the reference rate constants. The temperature dependence is estimated by assuming an A-factor equal to approximately 20 times that of $\text{OH} + \text{CH}_3\text{ONO}_2$. This is

consistent with observed OH/Cl A-factor ratios for primary H-abstraction from alkanes. (Table: 02-25, Note: 02-25) [Back to Table](#)

- F73. Cl + CH₃CO₃NO₂ (PAN). The recommended value is based on results of the relative rate study of Wallington et al. [1390]. In this study no reaction of PAN was observed in the presence of Cl atoms. These results are preferred over the results of the direct study of Tsalkani et al. [1322] using a discharge flow system with EPR detection of Cl atom decay (in which study the authors reported a rate constant of $(3.7 \pm 1.7) \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$). In both studies the major impurity in the PAN samples would be the alkane solvent. The presence of 0.1% tridecane in the PAN sample used by Tsalkani et al. could account for the observed Cl atom decay; however, solvent impurities in the PAN sample would be of no consequence in the relative rate study of Wallington et al. (Table: 92-20, Note: 92-20) [Back to Table](#)
- F74. Cl + C₃H₈. The recommended value for k(298 K) is the mean of results of the competitive chlorination studies of Pritchard et al. [1081], Knox and Nelson [731], Kelly et al. [698], Tschuikow-Roux et al. [1324], Atkinson and Aschmann [40], Wallington et al. [1413], Beichert et al. [124], Hooshiyar and Niki [597], Tyndall et al. [1352] (two determinations), and Sarzynski and Sztuba [1146] and the absolute rate studies of Lewis et al. [816], Beichert et al. [124], Pilgrim et al. [1058], Mellouki [899], and Hitsuda et al. [586]. The recommended E/R = 0 is based on the data obtained between 300 K and 400 K in the most recent and comprehensive study of Sarzynski and Sztuba. The recommended k(298 K) values for both reaction channels are the means of the results from the competitive chlorination studies by Knox and Nelson [731], Kelly et al. [698], Tschuikow-Roux et al. [1324], Tyndall et al. [1352], and Sarzynski and Sztuba [1146]. The recommended E/R values are based on the data of Sarzynski and Sztuba obtained between 300 K and 400 K. The Arrhenius A-factors were calculated from recommended k(298 K) and E/R. A sum of the recommended rate constant expressions for the two channels gives the same values as the rate constant expression recommended for the total reaction (A-factor: 1.45×10^{-10} , E/R: 0, k(298 K): 1.4×10^{-10} , f(298 K): 1.07 g: 20). (Table: 06-2, Note: 06-2) [Back to Table](#)
- F75. Cl + CH₃C(O)CH₃. The rate coefficient for this reaction has only been reported at 298 K. Wallington et al. [1413] and Olsson et al. [1010] report values of 2.37×10^{-12} and $1.69 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K measured via relative rate methods. The only direct measurement of this rate constant is by Notario et al. [1002] who report a value of $(3.06 \pm 0.38) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 298 K. Because of the reasons noted by Wallington et al. [1413], the value reported by Olsson et al. is suspect and is not considered here. The average of the results from Wallington et al. and Notario et al. is recommended for k(298 K). In the absence of temperature dependent measurements, based on analogy with other Cl atom reactions with halogenated hydrocarbons whose rate coefficients at 298 K are close to that for Cl + CH₃C(O)CH₃, we recommend an E/R value of 1000 K with a g value of 500 K. Such a temperature dependence is consistent with this reaction proceeding via H atom abstraction. This E/R and k(298 K) lead to an A factor of $7.7 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. This A factor is the same as that for the reaction of Cl atom with ethane, which also contains six primary C-H bonds. End product studies clearly show that the products of this reaction are CH₃C(O)CH₂ and HCl. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F76. Cl + C₂H₅CO₃NO₂. Wallington et al. [1390] have measured this rate constant relative to Cl + CH₃Cl. The recommended value is adjusted from that given by Wallington et al. using the currently recommended value for the reference reaction rate constant. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F77. Cl + 1-C₃H₇ONO₂. Wallington et al. [1403] and Nielsen et al. [981] have measured the rate of this reaction at room temperature relative to atomic chlorine reactions with ethyl chloride and ethane, respectively. The two studies are in excellent agreement and the recommended value is based on an average of the two. The values given in Wallington et al. and Nielsen et al. were adjusted based on the currently accepted values of the reference rates. The temperature dependence is estimated by assuming an A-factor equal to approximately 20 times that of OH + CH₃ONO₂. This is consistent with observed OH/Cl A-factor ratios for primary H-abstraction from alkanes. (Table: 02-25, Note: 02-25) [Back to Table](#)

- F78. $\text{Cl} + 2\text{-C}_3\text{H}_7\text{ONO}_2$. This reaction has been measured by Wallington et al [1403] at 295 K relative to $\text{Cl} + \text{C}_2\text{H}_5\text{Cl}$. The reported ratio of 0.46 ± 0.03 has been converted to an absolute rate using the currently recommended value for the ethyl chloride reaction rate. The temperature dependence is estimated by assuming an A-factor equal to approximately 20 times that of $\text{OH} + \text{CH}_3\text{ONO}_2$. This is consistent with observed OH/Cl A-factor ratios for primary H-abstraction from alkanes. (Table: 02-25, Note: 02-25) [Back to Table](#)
- F79. $\text{Cl} + \text{OCIO}$. The data of Toohey [1315] are in good agreement with the results of Bemand et al. [126] at room temperature, and the recommended value at room temperature is the mean of the values reported in these two studies. The slight negative temperature dependence reported by Toohey [1315] is accepted but with error limits that encompass the temperature independence reported in the earlier study. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F80. $\text{Cl} + \text{ClOO}$. The recommended value is based on the results of studies by Mauldin et al. [887] and Baer et al. [62], in which ClOO was formed by the pulsed photolysis of Cl_2/O_2 mixtures and its overall loss rate was monitored by UV absorption. In both studies k was found to be independent of temperature. These results are preferred over the results of the earlier, indirect studies of Johnston et al. [674], Cox et al. [321], and Ashford et al. [36]. The earlier studies did show that the predominant reaction pathway is that yielding $\text{Cl}_2 + \text{O}_2$ as products. From the branching ratio data of Cox et al., Ashford et al., and Nicholas and Norrish [963], it can be estimated that this reaction channel constitutes 95% of the overall reaction with ClO + ClO the products of the minor (5%) reaction channel. (Table: 92-20, Note: 92-20) [Back to Table](#)
- F81. $\text{Cl} + \text{Cl}_2\text{O}$. The preferred value was determined from results of the temperature-dependent study of Stevens and Anderson [1240] and the results of two independent absolute rate coefficient studies reported by Ray et al. [1107], which used the discharge flow-resonance fluorescence and discharge flow-mass spectrometric techniques. This value has been confirmed by Burrows and Cox [204], who determined the ratio $k(\text{Cl} + \text{Cl}_2\text{O})/k(\text{Cl} + \text{H}_2) = 6900$ in modulated photolysis experiments. The earlier value reported by Basco and Dogra [93] has been rejected. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F82. $\text{Cl} + \text{Cl}_2\text{O}_2$. The recommended value is that determined by Friedl (private communication) in a study using a DF-MS technique. It is in agreement with the value reported by Cox and Hayman [327] in a study using a static photolysis technique with photodiode array UV spectroscopy. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F83. $\text{Cl} + \text{HOCl}$. This recommendation is based on results over the temperature range 243–365 K reported by Cook et al. [309] and the room temperature result of Vogt and Schindler [1380]. There is a significant discrepancy in the reported values of the product branching ratios. Ennis and Birks [438] reported that the major reaction channel is that to give the products $\text{Cl}_2 + \text{OH}$ with a yield of $91 \pm 6\%$, whereas Vogt and Schindler report this yield to be $24 \pm 11\%$, with the major reaction channel giving $\text{HCl} + \text{ClO}$ as products. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F84. $\text{Cl} + \text{ClNO}$. The discharge flow-resonance fluorescence study of Abbatt et al. [4] provides the first reliable data on the temperature dependence. The laser photolysis-LMR study of Chasovnikov et al. [246] provides rate data for each Cl atom spin state, and they attribute the low value reported by Nelson and Johnston [954] in a laser flash photolysis-resonance fluorescence study to reaction of the $\text{Cl } ^2\text{P}_{1/2}$ state. Adsorption and decomposition of ClNO on the walls of their static system may account for the very low value of Grimley and Houston [528]. The results of Clyne and Cruse [278] in a discharge flow-resonance fluorescence study are significantly lower than all recent results. The recommended value at room temperature is the mean of the values reported by Abbatt et al. [4], Chasovnikov et al. [246], Nesbitt et al. [961], and Kita and Stedman [718]. The recommended temperature dependence is from the study of Abbatt et al. [4]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- F85. $\text{Cl} + \text{ClONO}_2$. Recommended value is based on the results of Yokelson et al. [1499] and those of Margitan [865]. These results are in excellent agreement; the slightly higher values of Kurylo et al. [757] are encompassed within the stated uncertainties. Yokelson et al. report that at 298 K, more than 95% of this reaction proceeds by the reaction channel giving $\text{Cl}_2 + \text{NO}_3$ as products. (Table: 97-4, Note: 97-4) [Back to Table](#)

- F86. $\text{Cl} + \text{CH}_3\text{Cl}$. The recommended value for $k(298 \text{ K})$ is the mean of results of the absolute rate study of Manning and Kurylo [862] and the relative rate studies of Wallington et al. [1390], Beichert et al. [124], and Orlando [1022] (two independent determinations). The recommended temperature dependence is derived from a fit to the data from Manning and Kurylo [862] and from the two relative rate studies of Orlando [1022]. The Arrhenius A-factor was calculated from $k(298 \text{ K})$ and E/R. While the 298 K results reported by Clyne and Walker [297] are in good agreement, the value of the activation energy derived by these researchers is significantly higher than that recommended, similar to the situation encountered for the $\text{Cl} + \text{CH}_4$ reaction. Hence, it is assumed that the discharge flow-mass spectrometric studies of these authors were subject to a systematic error. Both the room temperature measurements and E/R obtained between 300 K and 400 K by Bryukov et al. [190], from a study primarily focused at higher temperatures, are in good agreement with the recommendations. The early relative rate studies by Pritchard et al. [1081], Goldfinger et al. [514], Knox [729], and Tschuikow-Roux et al. [1323], were not used to derive the recommended parameters since they were performed at temperatures above 298 K and, with the exception of Pritchard et al., yield somewhat higher values for E/R. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F87. $\text{Cl} + \text{CH}_2\text{Cl}_2$. The recommended value for $k(298 \text{ K})$ is an average of the values measured in the relative rate studies of Niki et al. [987], Beichert et al. [124], Catoire et al. [236], and Orlando [1022] (two independent determinations) and in the absolute rate study of Bryukov et al. [190]. For this evaluation all of the relative rate measurements were recalculated based on the current recommendations for the rate constant of the reference reactions. The recommended value for E/R is taken from a fit to the data of Orlando and agrees with a fit to the data of Bryukov et al. (obtained at room temperature and above) up to 400 K. Above 400K, these latter data increase more rapidly with temperature. The relative rate studies of Goldfinger et al. [514], Knox [730], Tschuikow-Roux et al. [1323] were performed at temperatures above 298 K and yield significantly higher values for E/R, with the exception of one of the Knox et al. determinations (relative to CH_4), which gives a value of E/R in good agreement with that recommended. The results of Clyne and Walker [297] are higher than those from any other study and were not used in deriving the recommended parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F88. $\text{Cl} + \text{CHCl}_3$. The recommended $k(298 \text{ K})$ is an average of the values measured in the relative rate studies of Beichert et al. [124], Brahan et al. [172] (two independent determinations), Catoire et al. [236], and Orlando [1022] (two independent determinations). The recommended temperature dependence is derived from a fit to the two determinations by Orlando and agrees with a fit to the absolute rate data of Bryukov et al. [190] (obtained at room temperature and above) up to 400 K. Above 400 K, these latter data increase more rapidly with temperature. The room temperature value determined in the relative rate study by Yu and Wijnen [1500] is a factor of 50 greater than recommended and was not considered in the recommendation. The results of the absolute investigation of Clyne and Walker [297] are also higher and more scattered than those from most other studies and were not used, nor was the room temperature value derived from the study by Jeoung et al. [670], which is more than a factor of two lower than recommended. The relative rate study by Goldfinger et al. [514] performed near 500 K also resulted in values higher than those in more recent investigations. The relative rate study of Knox [730] yields a similar temperature dependence to that recommended but with rate constant values systematically lower than other studies. The absolute study by Talhaoui et al. [1278] yielded a 298 K rate constant somewhat lower than recommended and a temperature dependence somewhat higher. For this evaluation all of the relative rate measurements were recalculated based on the current recommendations for the rate constant of the reference reactions. The Arrhenius A-factor has been derived from the recommended parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F89. $\text{Cl} + \text{CH}_3\text{F}$ (HFC-41). The recommended value for $k(298 \text{ K})$ is an average of the values from the absolute rate study of Manning and Kurylo [862] and Hitsuda et al. [586] and the relative rate studies of Tschuikow-Roux et al. [1323], Tuazon et al. [1326], and Wallington et al. [1398]. The recommended value for E/R is based on the study of Tschuikow-Roux et al. conducted at room temperature and above. However, in formulating this recommendation, their reported value for the temperature dependence was reduced slightly (by approximately 100 K) to account for what appears to be a small systematic difference between the activation energies obtained in their similar

investigations of the Cl + CH₃Cl and Cl + CH₃Br reactions above room temperature and the recommendations that are based on data at 300 K and below. The temperature dependence reported by Manning and Kurylo is significantly lower, seemingly due to a shift in their data below 250 K. This lower value of E/R is not consistent with the recommended values of E/R for Cl + CH₃Cl and Cl + CH₃Br when compared with those for OH + CH₃F, OH + CH₃Cl, and OH + CH₃Br. Hence, it appears that the Manning and Kurylo data may have been influenced by some systematic error at the lower temperatures. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F90. Cl + CH₂F₂ (HFC-32). The recommended value for k(298 K) is from the relative rate study of Nielsen et al. [976], calculated using the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation. The room temperature value from the relative rate study of Tschuikow-Roux et al. [1324] is encompassed within the recommended 95% uncertainty limits. The temperature dependence is estimated from a comparison among the Cl and OH reactions with CH₂F₂, CH₂Cl₂, and CH₂FCl. The recommended value of E/R (identical to that for the OH + CH₂F₂ reaction) is slightly lower than that determined by Tschuikow-Roux et al. from data at room temperature and above. However, as discussed for other Cl + halomethane reactions, there appears to be a small systematic overestimation in the temperature dependencies determined by these authors. The A-factor has been calculated from the recommended parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F91. Cl + CF₃H (HFC-23). The recommended upper limit for k(298 K) is based on results from the absolute rate study by Jourdain et al. [682] and from the relative rate study by Coomber and Whittle [310], which gives a room temperature value a factor of 50 smaller. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F92. Cl + CH₂FCl (HCFC-31). The recommended value for k(298 K) is an average of the room temperature results from the absolute rate study by Jourdain et al. [682] and the relative rate studies by Tuazon et al. [1326] and Wallington et al. [1408]. The temperature dependence is estimated from a comparison among the Cl and OH reactions with CH₂F₂, CH₂Cl₂, and CH₂FCl. The recommended value of E/R (essentially the same as that for the OH + CH₂FCl reaction) is slightly lower than that determined by Tschuikow-Roux et al. [1323], recalculated based on the current recommendation for the rate constant of the reference reaction (Cl + CH₄). However, as discussed for other Cl + halomethane reactions, there appears to be a small systematic overestimation in the temperature dependences determined by these authors. The A-factor has been calculated from the recommended parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F93. Cl + CHFCl₂ (HCFC-21). The recommended value for k(298 K) is the average of the results from the relative rate study of Tuazon et al. [1326] and the absolute rate study of Talhaoui et al. [1278]. These results are preferred over the earlier room temperature results of Glavas and Heicklen [508]. The room temperature value of Jourdain et al. [682] is approximately 50% higher than the recommendation. The recommended value for E/R was obtained from a fit to the data of Talhaoui et al. The A-factor has been calculated from the recommended k(298 K) and E/R. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F94. Cl + CHF₂Cl (HCFC-22). The recommended value for k(298 K) is the mean of the values derived in the relative rate study by Tuazon et al. [1326] and in the absolute rate studies of Jourdain et al. [682] and Talhaoui et al. [1278] (which is assumed to supercede the earlier study by Sawerysyn et al. [1151]). The temperature dependence is from Talhaoui et al. The A-factor from that study has been adjusted to fit the recommended room temperature value. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F95. Cl + CH₃CCl₃. The recommended value for k(298 K) is an average of the results from the absolute rate study by Talhaoui et al. [1279] and the relative rate study by Platz et al. [1063]. The recommended value for E/R is derived from a fit to the data of Talhaoui et al. It is reasonably consistent with the value derived by Cillien et al. [267] in a relative rate study conducted over a very narrow temperature range above room temperature, but is somewhat smaller than the value derived in the relative rate study of Tschuikow-Roux et al. [1324]. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F96. Cl + CH₃CH₂F (HFC-161). The recommended values for both k(298 K) and E/R for each of the two reaction channels are averages of the individual values derived in the relative rate studies of Cadman et al. [217], Martens et al. [875], and Tschuikow-Roux et al. [1324], with each recalculated based on

the current recommendation for the rate constant of the reference reaction. The value for $k(298\text{ K})$ of the total reaction obtained from a sum of the two channels is in excellent agreement with the value obtained in the absolute rate study by Hitsuda et al. [586]. The parameters for the total reaction are: A-factor: 2.28×10^{-11} , E/R: 370, $k(298\text{ K})$: 6.6×10^{-12} , $f(298\text{ K})$: 1.1, g: 100. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F97. $\text{Cl} + \text{CH}_3\text{CHF}_2$ (HFC-152a). The recommended values for both $k(298\text{ K})$ and E/R for each of the two reaction channels are averages of the individual values derived in the relative rate studies of Cadman et al. [217], Martens et al. [875], and Yano and Tschuikow-Roux [1497], with each recalculated based on the current recommendation for the rate constant of the appropriate reference reaction. The value for $k(298\text{ K})$ for the overall reaction obtained by summing the values from the two channels is in excellent agreement with results of the room temperature relative rate studies of Wallington and Hurley [1404], and Tuazon et al. [1326]. The parameters for the overall reaction ($\text{Cl} + \text{CH}_3\text{CHF}_2 \rightarrow \text{products}$) are: A-Factor: 6.0×10^{-12} , E/R: 960, $k(298\text{ K})$: 2.4×10^{-13} , $f(298\text{ K})$: 1.1, g: 100) (Table: 06-2, Note: 06-2) [Back to Table](#)
- F98. $\text{Cl} + \text{CH}_2\text{FCH}_2\text{F}$ (HFC-152). The recommended value for $k(298\text{ K})$ is an average of the values derived in the relative rate studies of Yano and Tschuikow-Roux [1497] and Wallington et al. [1408] (two determinations), after recalculating each one based on the current recommendation for the rate constant of the appropriate reference reaction. The recommended temperature dependence was determined from a fit to the data of Yano and Tschuikow-Roux, which were obtained at room temperature and above. The temperature dependence may exhibit curvature below room temperature, similar to that for $\text{OH} + \text{CH}_2\text{FCH}_2\text{F}$. Such curvature is most probably encompassed by the assigned uncertainty parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F99. $\text{Cl} + \text{CH}_3\text{CFCl}_2$ (HCFC-141b). The recommended value for $k(298\text{ K})$ is an average of the values derived in the absolute rate studies of Talhaoui et al. [1279] by the discharge flow - mass spectrometric and the relative rate studies of Wallington and Hurley [1404] and Tuazon et al. [1326]. The room temperature results of Talhaoui et al. are assumed to supercede those of Sawerysyn et al. [1151]. The recommended E/R was obtained from a fit to the data of Talhaoui et al. The data of Warren and Ravishankara [1427] at room temperature agree with the recommendation. However, at higher temperatures the data exhibit considerable scatter apparently due to Cl atom regeneration from decomposition of the radical product ($\text{CH}_2\text{-CFCl}_2$). Hence, this study was not used in deriving the recommended parameters. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F100. $\text{Cl} + \text{CH}_3\text{CF}_2\text{Cl}$ (HCFC-142b). The recommended value for $k(298\text{ K})$ is an average of the results of the relative rate studies of Wallington and Hurley [1404], and Tuazon et al. [1326], and the absolute rate studies of Jourdain et al. [682] and Talhaoui et al. [1279], which is assumed to supercede the earlier study by Sawerysyn et al. [1151]. The recommended temperature dependence is a fit to the data of Talhaoui et al. The A-factor from that study has been adjusted to fit the recommended room temperature value. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F101. $\text{Cl} + \text{CH}_3\text{CF}_3$ (HFC-143a). The recommended values for $k(298\text{ K})$ and E/R are based on results of the relative rate study of Tschuikow-Roux et al. [1324], recalculated based on the current recommendation for the rate constant of the reference reaction ($\text{Cl} + \text{CH}_4$). An upper limit for $k(298\text{ K})$ more than two orders of magnitude larger than the recommended value was derived by Hitsuda et al. [586]. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F102. $\text{Cl} + \text{CH}_2\text{FCHF}_2$ (HFC-143). The recommended values for $k(298\text{ K})$ and E/R for each of the two reaction channels are based on results of the relative rate study of Tschuikow-Roux et al. [1324] recalculated based on the current recommendation for the rate constant of the reference reaction ($\text{Cl} + \text{CH}_4$). The recommended parameters for the total reaction are derived from the sum of the recommended rate expressions for the two reaction channels. The parameters for the total reaction are: A-factor: 1.57×10^{-11} , E/R: 1720, $k(298\text{ K})$: 4.9×10^{-14} , $f(298\text{ K})$: 1.3, g: 200. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F103. $\text{Cl} + \text{CH}_2\text{ClCF}_3$ (HCFC-133a). The recommended value for $k(298\text{ K})$ is an average of the results from the absolute rate study of Jourdain et al. [679] and the relative rate study of Mogelberg et al. [926] (two determinations). The recommended value for E/R is a fit to the data of Jourdain et al. (Table: 06-2, Note: 06-2) [Back to Table](#)

- F104. $\text{Cl} + \text{CH}_2\text{FCF}_3$ (HFC-134a). The recommended value for $k(298\text{ K})$ is an average of the results from the relative rate studies of Wallington and Hurley [1404], Tuazon et al. [1326], and Kaiser [684] and from the absolute rate study of Louis et al. [846], which is assumed to supersede the earlier study by Sawerysyn et al. [1151]. The recommended value for E/R is an average of the values determined by Kaiser et al. and Louis et al. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F105. $\text{Cl} + \text{CHF}_2\text{CHF}_2$ (HFC-134). The recommended value for $k(298\text{ K})$ is an average of the results from the relative rate studies of Nielsen et al. [977] and Yano and Tschuikow-Roux [1497], each recalculated based on the current recommendation for the rate constant of the appropriate reference reaction. The recommended value of E/R is determined from a fit to the data of Yano and Tschuikow-Roux. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F106. $\text{Cl} + \text{CHCl}_2\text{CF}_3$ (HCFC-123). The recommended value for $k(298\text{ K})$ is an average of the results from the absolute rate study of Warren and Ravishankara [1427] and the relative rate studies of Wallington and Hurley [1404] and Tuazon et al. [1326] each recalculated based on the current recommendation for the rate constant of the appropriate reference reaction. The recommended value of E/R is derived from a fit to the data of Warren and Ravishankara. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F107. $\text{Cl} + \text{CHFClCF}_3$ (HCFC-124). The recommended value for $k(298\text{ K})$ is an average of the results from the absolute rate study by Warren and Ravishankara [1427] and the relative rate study by Tuazon et al. [1326]. The recommended value for E/R is based on a fit to the data of Warren and Ravishankara. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F108. $\text{Cl} + \text{CHF}_2\text{CF}_3$ (HFC-125). The recommended value for $k(298\text{ K})$ is an average of the results from the relative rate studies of Tuazon et al. [1326], Sehested et al. [1172], and Edney and Driscoll [430], all conducted only at room temperature. The temperature dependence is estimated from a comparison among the Cl and OH reactions with CH_2FCF_3 , CHF_2CHF_2 , and CHF_2CF_3 . The relative rate study by Coomber and Whittle [310] conducted between 303 K and 399 K corresponds to a value for $k(298\text{ K})$ a factor of 2.5 greater than that recommended. However, the value for E/R derived by these authors is only slightly lower than that estimated. (Table: 06-2, Note: 06-2) [Back to Table](#)
- F109. $\text{ClO} + \text{O}_3$. There are two possible channels for this reaction: $\text{ClO} + \text{O}_3 \rightarrow \text{ClOO} + \text{O}_2$ (k_1); and $\text{ClO} + \text{O}_3 \rightarrow \text{OCIO} + \text{O}_2$ (k_2). The recommended upper limit for k_1 at 298 K is based on results of the recent study by Stevens and Anderson [1239]. These authors also report that $k_1 = (4 \pm 2) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ at 413 K. These data can be combined to derive the Arrhenius parameters $A = 2 \times 10^{12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $E/R > 3600 \text{ K}$. The upper limit for k_2 is based on results reported by DeMore et al. [380] and Wongdontri-Stuper et al. [1483], the Arrhenius parameters for k_2 were estimated. (Table: 92-20, Note: 92-20) [Back to Table](#)
- F110. $\text{ClO} + \text{H}_2$. The Arrhenius expression was estimated based on the $\sim 600 \text{ K}$ data of Walker (reported in Clyne and Watson [298]). (Table: 82-57, Note: 82-57) [Back to Table](#)
- F111. $\text{ClO} + \text{NO}$. The absolute rate coefficients determined in the four discharge flow-mass spectrometric studies (Clyne and Watson [298], Leu and DeMore [804], Ray and Watson [1108] and Clyne and MacRobert [284]) and the discharge flow laser magnetic resonance study of Lee et al. [794] are in excellent agreement at 298 K, and are averaged to yield the preferred value. The value reported by Zahniser and Kaufman [1509] from a competitive study is not used in the derivation of the preferred value as it is about 33% higher. The magnitudes of the temperature dependences reported by Leu and DeMore [804] and Lee et al. are in excellent agreement. Although the E/R value reported by Zahniser and Kaufman [1509] is in fair agreement with the other values, it is not considered as it is dependent upon the E/R value assumed for the $\text{Cl} + \text{O}_3$ reaction. The Arrhenius expression was derived from a least squares fit to the data reported by Clyne and Watson, Leu and DeMore, Ray and Watson, Clyne and MacRobert, and Lee et al. (Table: 82-57, Note: 82-57) [Back to Table](#)
- F112. $\text{ClO} + \text{NO}_3$. The recommended value is based on results reported by Cox et al. [315], Cox et al. [326] Biggs et al. [142], and Kukui et al. [741]. Biggs et al. report the rate constant to be independent of temperature, consistent with the results of Cox et al. [326]. This recent study of Kukui et al. supersedes the earlier study of Becker et al. [104] from the same laboratory, which had

indicated the major products to be OCIO + NO₂. There is now agreement among all studies that the major reaction channel forms ClOO + NO₂ (see Biggs et al. [142] Cox et al. [326], and Kukui et al. From a study of the OCIO/NO₃ system Friedl et al. [475] conclude that at 220 K the formation of ClOO + NO₂ is favored. (Table: 82-57, Note: 82-57) [Back to Table](#)

- F113. ClO + N₂O. The Arrhenius expression was estimated based on the ~600 K data of Walker (reported in Clyne and Watson [298]). (Table: 82-57, Note: 82-57) [Back to Table](#)
- F114. ClO + CO. The Arrhenius expression was estimated based on the ~600 K data of Walker (reported in Clyne and Watson [298]). (Table: 82-57, Note: 82-57) [Back to Table](#)
- F115. ClO + CH₄. The Arrhenius expression was estimated based on the ~600 K data of Walker (reported in Clyne and Watson [298]). (Table: 82-57, Note: 82-57) [Back to Table](#)
- F116. ClO + H₂CO. Poulet et al. [1078] have reported an upper limit of 10⁻¹⁵ cm³ molecule⁻¹ s⁻¹ for k at 298 K using the discharge flow-EPR technique. (Table: 81-3, Note: 81-3) [Back to Table](#)
- F117. ClO + CH₃O₂. The recommended expressions for the overall rate constant is based on the results of Helleis et al. [566]. It is consistent with the room temperature measurements of Simon et al. [1190] and Kenner et al. [699]. The results of Kukui et al. [743] for the overall reaction are in agreement with the recommendation at room temperature, but these values show a slight negative temperature dependence in contrast with the slight positive temperature dependence recommended here. There is general agreement that the only important reaction channels are the two channels resulting in the production of ClOO + CH₃O (a) and CH₃OCl + O₂ (b). However, there is severe disagreement on their relative importance; at room temperature reaction channel (a) is reported to be the major channel by Helleis et al. [566], Simon et al. [1190], Kukui et al. and Helleis et al. [567] but it is reported to be the minor channel by Biggs et al. [140] and Daele and Poulet [340]. Because of this large discrepancy, no branching ratios are recommended. The branching ratio studies that go down to low temperatures (Helleis et al. [566], Kukui et al. , and Helleis et al. [567]) report that reaction channels (a) and (b) are both significant down to lower polar stratospheric temperatures. (Table: 97-4, Note: 97-4) [Back to Table](#)
- F118. ClO + ClO. There are three bimolecular channels for this reaction: ClO + ClO → Cl₂ + O₂ (k₁); ClO + ClO → ClOO + Cl (k₂); and ClO + ClO → OCIO + Cl (k₃). The recommended values for the individual reaction channels are from the study of Nickolaisen et al. [964]. This study, using a flash photolysis/long path ultraviolet absorption technique, is the most comprehensive study of this system, covering a wide range of temperature and pressure. These results are preferred over the results of earlier studies of the total bimolecular rate coefficient at low pressures by Clyne and Coxon [276], Clyne and White [302], and Clyne et al. [289], and those of other studies reported by Hayman et al. [560], Cox and Derwent [319], Simon et al. [1191], Horowitz et al. [599], and Horowitz et al. [600]. The room temperature branching ratio are k₁:k₂:k₃ = 0.29:0.50:0.21. The reaction exhibits both bimolecular and termolecular reaction channels (see entry in Table 2). The termolecular reaction dominates at pressures higher than about 10 torr. The equilibrium constant for formation of the Cl₂O₂ dimer is given in Table 3. (Table: 94-26, Note: 97-4) [Back to Table](#)
- F119. HCl + ClONO₂. Results of four studies of the kinetics of this system have been published, in which the following upper limits to the homogeneous bimolecular rate constant were reported: 10⁻¹⁹ cm³ molecule⁻¹ s⁻¹ by a static wall-less long-path UV absorption technique and a steady-state flow FTIR technique (Molina et al. [927]); 5 × 10⁻¹⁸ using a flow reactor with FTIR analysis (Friedl et al. [473]); and 8.4 × 10⁻²¹ using a static photolysis system with FTIR analysis (Hatakeyama and Leu [558] and Leu et al. [805]), and 1.5 × 10⁻¹⁹ by FTIR analysis of the decay of ClONO₂ in the presence of HCl in large-volume (2500 and 5800 liters) Teflon or Teflon-coated chambers (Atkinson et al. [41]). Earlier, Birks et al. [146] had reported a higher upper limit. All studies found this reaction to be catalyzed by surfaces. The differences in the reported upper limits can be accounted for in terms of the very different reactor characteristics and detection sensitivities of the various studies. The homogeneous reaction is too slow to have any significant effect on atmospheric chemistry. (Table 87-41, Note: 87-41) [Back to Table](#)
- F120. CH₂ClO + O₂. The CH₂ClO radical is reported to be resistant to unimolecular dissociation into Cl + CH₂O products, according to chain reaction/product analysis studies by Sanhueza and Heicklen

- [1143] and Niki et al. [987] and kinetics studies by Catoire et al. [235]. The recommendation is based on the work of Kaiser and Wallington [689] who studied the competition between reaction with O₂ and HCl elimination in a complex photochemical reaction system using FTIR detection of stable products. The recommendation is a factor of 5 higher than estimated using the empirical relationship given by Atkinson and Carter [47]. The fate of CH₂ClO in the atmosphere is this reaction with O₂. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F121. CH₂ClO₂ + HO₂. The recommendation is based on the measurement reported by Catoire et al. [235], who used pulsed photolysis with UV absorption detection at 1 atm pressure and 251–588 K. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F122. CH₂ClO₂ + NO. The recommendation is based on the value reported by Sehested et al. [1174], who used pulsed radiolysis and UV absorption detection of NO₂ to measure the rate coefficient. The temperature dependence is estimated by analogy to similar RO₂ + NO reactions. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F123. CCl₃O₂ + NO. The recommendation is based upon the measurements of Ryan and Plumb [1130] and Dognon et al. [404], who agree well at room temperature. The temperature dependence is derived from the data of Dognon et al., who covered the temperature range 228–413 K. The CCl₃O primary product of the reaction of CCl₃O₂ with NO decomposes rapidly to eliminate Cl, according to Lesclaux et al. [799]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F124. CCl₂FO₂ + NO. The recommendation is based on the measurements made by Dognon et al. [404] using pulsed photolysis with mass spectrometry detection at 1–10 torr and 228–413 K. These results supersede the earlier study of Lesclaux and Caralp [797]. The CCl₂FO radical primary product of the CCl₂FO₂ + NO reaction is reported by Lesclaux et al. [799] and Wu and Carr [1487] to rapidly decompose to eliminate Cl and to give the products indicated. (Table: 94-26, Note: 94-26) [Back to Table](#)
- F125. CClF₂O₂ + NO. The recommendation is based on the measurements made by Dognon et al. [404], who used pulsed photolysis with mass spectrometry detection at 1–10 torr and 228–413 K, and Sehested et al. [1174], who used pulsed radiolysis with UV absorption detection of the NO₂ product at one atm and 298 K. Wu and Carr [1487] observed the CClF₂O radical primary product to rapidly dissociate to CF₂O and Cl. (Table: 94-26, Note: 94-26) [Back to Table](#)
- G1. O + BrO. The preferred value is based on the value reported by Thorn et al. [1300] using a dual laser flash photolysis/long path absorption/resonance fluorescence technique. Clyne et al. [291] reported a value approximately 40% lower. (Table: 97-4, Note: 97-4) [Back to Table](#)
- G2. O + HBr. Results of the flash photolysis-resonance fluorescence study of Nava et al. [945] for 221–455 K and the laser flash photolysis-resonance fluorescence study of Nicovich and Wine [972] for 250–402 K provide the only data at stratospheric temperatures. Results reported include those of Singleton and Cvetanovic [1198] for 298–554 K by a phase-shift technique, and discharge flow results of Brown and Smith [182] for 267–430 K and Takacs and Glass [1272] at 298 K. The preferred value is based on the results of Nava et al., as well as those of Nicovich and Wine and those of Singleton and Cvetanovic over the same temperature range, since these results are less subject to complications due to secondary chemistry than are the results using discharge flow techniques. The uncertainty at 298 K has been set to encompass these latter results. (Table: 90-1, Note: 90-1) [Back to Table](#)
- G3. O + HOBr. Recommended room temperature value is the mean of results of Monks et al. [1300] and Kukui et al. [742]. The temperature dependence is from Nesbitt et al. [960]. The A-factor from that study has been adjusted to fit the recommended room temperature value. Kukui et al. determined that the Br atom abstraction channel is the only pathway at room temperature. (Table: 97-4, Note: 97-4) [Back to Table](#)
- G4. O + BrONO₂. The recommendation is based on the study of Soller et al. [1221] that employed the laser flash photolysis – resonance fluorescence technique and covered the temperature range 227 – 339 K. The recommended uncertainty parameters are larger than those reported by Soller et al. pending independent confirmation of their results. Burkholder [198] has coupled laser flash

photolysis with detection of NO_3 by long path absorption spectroscopy to show that the NO_3 yield is >0.85 at 298 K. NEW ENTRY. [Back to Table](#)

- G5. $\text{OH} + \text{Br}_2$. The recommended room temperature value is the average of the values reported by, Poulet et al. [1073], Loewenstein and Anderson [841], Gilles et al. [501] and Bedjanian et al. [111]. The temperature dependence is from an average of the E/R values of Gilles et al. and Bedjanian et al. The results of Boodaghians et al. [159] were not considered. Loewenstein and Anderson determined that the exclusive products are $\text{Br} + \text{HOBr}$. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G6. $\text{OH} + \text{BrO}$. The preferred value of k_{298} is from an average of the results of Gilles et al. [502] and Bedjanian et al. [116]. The only temperature dependence study is from Bedjanian et al. The recommendation is based on their results. The likely products of this reaction are $\text{Br} + \text{HO}_2$. Bedjanian et al. attempted to measure the branching ratio for HBr formation but there were significant problems from secondary chemistry. An upper limit of 3% was reported for the HBr yield. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G7. $\text{OH} + \text{HBr}$. The preferred value at room temperature is the average of the values reported by Ravishankara et al. [1101] using FP-RF, by Jourdain et al. [681] using DF-EPR, by Cannon et al. [222] using FP-LIF, by Ravishankara et al. [1104] using LFP-RF and LFP-LIF and Bedjanian et al. [114]. Values reported by Takacs and Glass [1273] and by Husain et al. [624] as well as the preliminary value of Smith and Zellner [1217] are a factor of 2 lower and were not included in the derivation of the preferred value. The recommendation for the temperature dependence is derived from the data of Bedjanian et al. [114]. This study obtained a small negative temperature dependence which is in qualitative agreement with the Laval nozzle studies of Sims et al. [1196], Atkinson et al. [38] and Jaramillo et al. [652] over the 200-300 K temperature range. The data of Ravishankara et al. [1101] show no dependence on temperature over the range 249–416 K. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G8. $\text{OH} + \text{CH}_3\text{Br}$. The recommended rate expression is derived from a combined fit to the data from the relative rate study of Hsu and DeMore [614] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_3\text{CHF}_2$ reference reaction, as discussed in the note for that reaction) and the absolute determinations by Chichinin et al. [261], Mellouki et al. [909] and Zhang et al. [1525]. The results of these extensive studies are in excellent agreement and are preferred over the higher values reported in the earlier studies of Davis et al. [358] and Howard and Evenson [606]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G9. $\text{OH} + \text{CH}_2\text{Br}_2$. The recommended value for $k(298 \text{ K})$ is an average of the values from the absolute studies of Mellouki et al. [909] and Zhang et al. [1519] and from the relative rate measurements of DeMore [376] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Cl}_2$ reference reaction) and Orlando et al. [1025] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_3(\text{CO})\text{CH}_3$ reference reaction). The recommended value of E/R is from the study of Mellouki et al. [909]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G10. $\text{OH} + \text{CHBr}_3$. The recommended rate expression is derived from a fit to the data from the relative rate study of DeMore [376] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Cl}_2$ reference reaction). The results of Orkin et al. [1017] are higher by a factor of 2 but have the same temperature dependence. They are encompassed within the 2σ confidence limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G11. $\text{OH} + \text{CHF}_2\text{Br}$. The recommended values for $k(298 \text{ K})$ and E/R are derived from a fit to the data of Talukdar et al. [1280] (two studies), Orkin and Khamaganov [1016], and Hsu and DeMore [615] (a relative rate measurement recalculated using the current recommendation for the rate constant for the $\text{OH} + \text{CH}_4$ reference reaction). These data are preferred over the consistently higher results reported by Brown et al. [178]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G12. $\text{OH} + \text{CH}_2\text{ClBr}$. The recommended value for $k(298 \text{ K})$ is an average of the values from two relative rate studies by DeMore [376] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Cl}_2$ reference reaction) and Bilde et al. [144] (recalculated using the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Br}_2$ reference reaction) and two

absolute determinations by Orkin et al. [1018], all of which are in good agreement. The recommended E/R is obtained from a fit to the data of DeMore and Orkin et al. The A factor was then calculated. (Table: 02-25, Note: 02-25) [Back to Table](#)

- G13. OH + CF₂ClBr. The A-factor was estimated, and a lower limit for E/R was derived using the upper limit for the rate constant at 298 K reported by Burkholder et al. [201] in a study using pulsed photolysis-LIF and DF-LMR techniques. A less sensitive upper limit was reported by Clyne and Holt [283]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G14. OH + CF₂Br₂. The A-factor was estimated, and a lower limit for E/R was derived by using the upper limit for the rate constant at 298 K reported by Burkholder et al. [201] in a study using pulsed photolysis-LIF and DF-LMR techniques. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G15. OH + CF₃Br. The A-factor was estimated and a lower limit for E/R was derived by using the upper limit for the rate constant at 460 K reported by Orkin and Khamaganov [1016]. These parameters were then used to calculate an upper limit for k(298 K). The upper limit for k(298 K) determined by Burkholder et al. [201] in a study using pulsed photolysis-LIF and DF-LMR techniques at room temperature is understandably higher. A less sensitive upper limit was also reported by Le Bras and Combourieu [778]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G16. OH + CH₂BrCH₃. The recommended values for k(298 K) and E/R are derived from a fit to the data (T ≤ 300 K) of Herndon et al. [573]. These data suggest a curvature of the Arrhenius plot similar to that found for the OH reaction with CH₃CH₂F. The data of Qiu et al. [1082] (which include earlier data reported by the same research group in Xing et al. [1492]) were not used because they were obtained mainly at above room temperature and exhibit a very steep temperature dependence resulting in a value for E/R that is larger than the E/R value obtained from data at T > 298 K for the OH reaction with CH₃CH₂F. The k(300 K) value reported by Donaghy et al. [409] seems too low for this reaction when compared with the recommendation for presumably slower (and better studied) OH reaction with CH₃CH₂F. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G17. OH + CH₂BrCF₃. The recommended values for k(298 K) and E/R are from a combined fit to the data of Nelson et al. [949] and Orkin and Khamaganov [1016]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G18. OH + CHFBrCF₃. The recommended rate expression is derived from a combined fit to the data (below 400°K) of Orkin and Khamaganov [1016] and Brown et al. [178]. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G19. OH + CHClBrCF₃. The recommended rate expression is derived from a fit to the data of Orkin and Khamaganov [1016] (for T ≤ 400 K). The room temperature value measured by Brown et al. [179] lies somewhat higher than this recommendation but is encompassed within the 2σ confidence limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G20. OH + CHFClCF₂Br. The recommended rate expression is derived from a fit to the data from the relative rate study of DeMore [376] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CCl₃ reference reaction). (Table: 02-25, Note: 02-25) [Back to Table](#)
- G21. OH + CF₂BrCF₂Br. The A-factor was estimated and a lower limit for E/R was derived by using the upper limit for the rate constant at 460 K reported by Orkin and Khamaganov [1016]. These parameters were then used to calculate an upper limit for k(298 K). The upper limit for k(298 K) determined by Burkholder et al. [201] in a study using pulsed photolysis-LIF and DF-LMR techniques at room temperature is understandably higher. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G22. OH + CH₂BrCH₂CH₃. The recommended values for k(298 K) and E/R are derived from a fit to the data (T ≤ 300 K) from Donaghy et al. [409], Teton et al. [1294], Nelson et al. [950], Herndon et al. [573], Gilles et al. [500], and Kozlov et al. [738]. Significant curvature in the Arrhenius plot has been observed over the 480 to 210 K temperature range, due to the three different hydrogen-abstraction reaction channels that occur. These channels have been quantified in the study of Gilles et al. In spite of the noticeable Arrhenius curvature, the data below 300 K can be well represented by a two-parameter Arrhenius fit. (Table: 02-25, Note: 02-25) [Back to Table](#)

- G23. $\text{OH} + \text{CH}_3\text{CHBrCH}_3$. The recommended values for $k(298 \text{ K})$ and E/R are averages of the parameters derived from a fit to the data ($T \leq 300 \text{ K}$) of Herndon et al. [573] and Kozlov et al. [738] which are in excellent agreement. The A factor was then calculated. The room temperature relative rate determination by Donaghy et al. [409] and the absolute temperature dependent data of Teton et al. [1294] lie systematically higher than those from these two more recent studies. Significant curvature in the Arrhenius plot has been observed over the 480 K to 210 K temperature range by Kozlov et al., presumably due to the two different hydrogen-abstraction reaction channels that occur. In spite of the noticeable Arrhenius curvature, the data below 300 K can be well represented by a two-parameter Arrhenius fit. (Table: 02-25, Note: 02-25) [Back to Table](#)
- G24. $\text{HO}_2 + \text{Br}$. The room temperature rate constant is obtained from an average of the results of Laverdet et al. [774], Toohey et al. [1317] and Bedjanian et al. [115]. The results of Posey et al. [1069] were not considered because of problems with the experimental method. The results of Poulet et al. [1074] were not considered because of complications associated with secondary reactions. The recommendation for the temperature dependence is based on the results of Bedjanian et al. [115]. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G25. $\text{HO}_2 + \text{BrO}$. The recommendation is based on results of the temperature-dependent studies of Elrod et al. [435], Li et al. [820] and Bedjanian et al. [117]. It is assumed that the Bedjanian et al. results supercede those of Larichev et al. [770] since the same experimental technique was used, and the same research group was involved in both studies. The recommended room temperature value is the mean of the values reported in these studies, as well as those of Cronkhite et al. [334] and Bloss et al. [155]. The room temperature value of Bridier et al. [176], which was not obtained under pseudo-first-order decay conditions, was not included in derivation of the recommendation. Bedjanian et al. have determined an upper limit of 0.4% for production of HBr and O_3 at 298 K. From a study of the reverse reaction above room temperature, Mellouki et al. [908] determined by extrapolation that the yield of $\text{HBr} + \text{O}_3$ is an insignificant fraction ($<0.01\%$) of the total reaction down to 200 K. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G26. $\text{NO}_3 + \text{HBr}$. The recommended upper limit is the upper limit reported by Mellouki et al. [905] in a study using DF-EPR techniques. This upper limit shows that this reaction is of negligible importance in stratospheric chemistry. Canosa-Mas et al. [225] reported a value that is consistent, within experimental error, with the upper limit of Mellouki et al. (Table: 90-1, Note: 92-20) [Back to Table](#)
- G27. $\text{Cl} + \text{CH}_2\text{ClBr}$. The recommended value for $k(298 \text{ K})$ is an average of two relative rate determinations by Bilde et al. [144] (recalculated based on the current recommendation for the rate constants of the reference). The temperature dependence is estimated from a comparison with the reactions of Cl with CH_2Cl_2 and CH_2Br_2 . The relative rate investigation by Tschuikow-Roux et al. [1323] gives a value for $k(298 \text{ K})$ only slightly larger than recommended, but a temperature dependence that is significantly stronger and inconsistent with the that recommended for the $\text{Cl} + \text{CH}_2\text{Cl}_2$ and $\text{Cl} + \text{CH}_2\text{Br}_2$ reactions. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G28. $\text{Cl} + \text{CH}_3\text{Br}$. The recommended value for $k(298 \text{ K})$ is an average of the results from the absolute rate studies of Gierczak et al. [494], Kambanis et al. [691] and Piety et al. [1057] and from the relative rate study of Orlando et al. [1025]. The recommended value for E/R is based on a combined fit to these same four studies restricted to temperatures of 300 K and below. Results of the relative rate study Tschuikow-Roux et al. [1323] were not used in derivation of the recommended values since they appear to be systematically higher than the results of the other investigations. The products of this reaction are expected to be primarily CH_2Br and HCl. The possible production of $\text{CH}_3\text{Cl} + \text{Br}$ is very small in the atmosphere [515]. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G29. $\text{Cl} + \text{CH}_2\text{Br}_2$. The recommended value for $k(298 \text{ K})$ is an average of the results from the absolute rate studies of Gierczak et al. [494] and Kambanis et al. [691] and from the three relative rate experiments of Orlando et al. [1025]. The recommended value for E/R is based on a combined fit to the data ($T < 300 \text{ K}$) from these same studies after normalizing each one to the recommended value for $k(298 \text{ K})$. Results of the relative rate study of Tschuikow-Roux et al. [1323] were not used in derivation of the recommended parameters since they are significantly greater at 298 K and

correspond to a temperature dependence substantially stronger than derived from the data of other investigations. (Table: 06-2, Note: 06-2) [Back to Table](#)

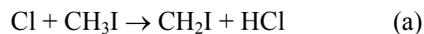
- G30. Cl + CHBr₃. The recommended parameters are based on the only reported study of this reaction by Kambanis et al. [691], who employed a very low pressure reactor and monitored reactants and products using mass spectrometry. (Table: 06-2, Note: 06-2) [Back to Table](#)
- G31. Br + O₃. The results reported for k(298 K) by Clyne and Watson [300], Leu and DeMore [803], Michael et al. [915], Michael and Payne [920], and Toohey et al. [1318] are in excellent agreement. The preferred value at 298 K is derived by taking a simple mean of these five values. The temperature dependences reported for k by Leu and DeMore and by Toohey et al. are in good agreement, but they can only be considered to be in fair agreement with those reported by Michael et al. and Michael and Payne. The preferred value was synthesized to best fit all the data reported from these five studies. The results of Nicovich et al. [968] are in excellent agreement with this recommendation. (Table 87-41, Note: 90-1) [Back to Table](#)
- G32. Br + H₂O₂. The recommended upper limit to the value of the rate constant at room temperature is based on results reported in the study by Toohey et al. [1317] using a discharge flow-resonance fluorescence/laser magnetic resonance technique. Their upper limit determined over the temperature range 298–378 K is consistent with less sensitive upper limits determined by Leu [813] and Posey et al. [1069] using the discharge flow-mass spectrometric technique. The much higher value reported by Heneghan and Benson [569] may result from the presence of excited Br atoms in the very low pressure reactor. The pre-exponential factor was chosen to be consistent with that for the Cl + H₂O₂ rate constant, and the E/R value was fitted to the upper limit at 298 K. Mellouki et al. [908] have measured the rate of the reverse reaction. (Table 87-41, Note: 94-26) [Back to Table](#)
- G33. Br + NO₃. The recommended value is that reported by Mellouki et al. [905] in a study using DF-DPR techniques. (Table: 90-1, Note: 92-20) [Back to Table](#)
- G34. Br + H₂CO. There have been two studies of this rate constant as a function of temperature: Nava et al. [947], using the flash photolysis–resonance fluorescence technique, and Poulet et al. [1072], using the discharge flow-mass spectrometric technique. These results are in reasonably good agreement. The Arrhenius expression was derived from a least squares fit to the data reported in these two studies. The higher room temperature value of Le Bras et al. [779], using the discharge flow–EPR technique, has been shown to be in error due to secondary chemistry (Poulet et al.). (Table: 82-57, Note: 82-57) [Back to Table](#)
- G35. Br + OCIO. The recommended value at room temperature is the mean of the values reported by Clyne and Watson [301] and Toohey [1315]. In the study of Clyne and Watson, correction for the effect of the rapid reverse reaction was required. The temperature dependence reported by Toohey [1315] is accepted but with increased error limits. (Table: 90-1, Note: 90-1) [Back to Table](#)
- G36. Br + Cl₂O. The recommended value is based on results reported by Stevens and Anderson [1240] and by Sander and Friedl [1136], which are in good agreement. (Table: 94-26, Note: 94-26) [Back to Table](#)
- G37. Br + Cl₂O₂. The recommended value is that determined by Friedl (private communication) in a study using a DF-MS technique. (Table: 90-1, Note: 90-1) [Back to Table](#)
- G38. BrO + O₃. There have been two recent studies of this reaction. Rattigan et al. [1088] report an overall rate constant of $\sim 10^{-17}$ cm³ molecule⁻¹s⁻¹ over the temperature range 318–343 K. Rowley et al. [1127] report a room temperature upper limit of 2×10^{-17} cm³ molecule⁻¹s⁻¹. Both papers report a value of $\sim 2 \times 10^{-18}$ cm³ molecule⁻¹s⁻¹ for the channel to produce OBrO + O₂. The recommended upper limit of 2×10^{-17} cm³ molecule⁻¹s⁻¹ is a factor of 2.5 less than the previously recommended upper limit of 5×10^{-17} , which was based on Mauldin et al. [888]. The pre-exponential factor was estimated, and E/R was calculated. (Table: 97-4, Note: 97-4) [Back to Table](#)
- G39. BrO + NO. The results of the three low pressure mass spectrometric studies (Clyne and Watson [300]; Ray and Watson [1108]; Leu [811]) and the high pressure UV absorption study (Watson et al. [1437]), which all used pseudo–first-order conditions, are in excellent agreement at 298 K and are thought to be much more reliable than the earlier low pressure UV absorption study (Clyne and Cruse [277]). The results of the two temperature-dependence studies are in good agreement and

both show a small negative temperature dependence. The preferred Arrhenius expression was derived from a least squares fit to all the data reported in the four recent studies. By combining the data reported by Watson et al. with those from the three mass spectrometric studies, it can be shown that this reaction does not exhibit any observable pressure dependence between 1 and 700 torr total pressure. The temperature dependences of k for the analogous ClO and HO₂ reactions are also negative and are similar in magnitude. (Table: 82-57, Note: 82-57) [Back to Table](#)

- G40. BrO + NO₃. The recommended value is the geometric mean of the lower and upper limits reported by Mellouki et al. [905] in a study using DF-DPR techniques. These reported limits are encompassed within the indicated uncertainty limits. (Table: 90-1, Note: 92-20) [Back to Table](#)
- G41. BrO + ClO. Friedl and Sander [474], using DF/MS techniques, measured the overall rate constant over the temperature range 220–400 K and also over this temperature range determined directly branching ratios for the reaction channels producing BrCl and OCIO. The same authors in a separate study using flash photolysis–ultraviolet absorption techniques (Sander and Friedl [1136]) determined the overall rate constant over the temperature range 220–400 K and pressure range 50–750 torr and also determined at 220 K and 298 K the branching ratio for OCIO production. The results by these two independent techniques are in excellent agreement, with the overall rate constant showing a negative temperature dependence. Toohey and Anderson [1316], using DF/RF/LMR techniques, reported room temperature values of the overall rate constant and the branching ratio for OCIO production. They also found evidence for the direct production of BrCl in a vibrationally excited Π state. Poulet et al. [1070], using DF/MS techniques, reported room temperature values of the overall rate constant and branching ratios for OCIO and BrCl production. Overall room temperature rate constant values reported also include those from the DF/MS study of Clyne and Watson [301] and the very low value derived in the flash photolysis study of Basco and Dogra [91] using a different interpretation of the reaction mechanism. The recommended Arrhenius expressions for the individual reaction channels are taken from the study of Friedl and Sander [474] and Turnipseed et al. [1339]. These studies contain the most comprehensive sets of rate constant and branching ratio data. The overall rate constants reported in these two studies are in good agreement (20%) at room temperature and in excellent agreement at stratospheric temperatures. Both studies report that OCIO production by channel (1) accounts for 60% of the overall reaction at 200 K. Both studies report a BrCl yield by channel (3) of about 8%, relatively independent of temperature. The recommended expressions are consistent with the body of data from all studies except those of Hills et al. [581] and Basco and Dogra [91]. (Table 00-3, Note: 00-3) [Back to Table](#)
- G42. BrO + BrO. Measurements of the overall rate constant can be divided into categories—those in which BrO was monitored by UV absorption and those in which BrO was monitored by mass spectrometer. Gilles et al. [504] have re-analyzed the results of the UV absorption studies and scaled the reported values of the rate constant to the UV absorption cross sections reported in their paper. When scaled in this manner, the room temperature rate constant values reported in the UV absorption studies (Sander and Watson [1139], Mauldin et al. [888], Bridier et al. [176], Rowley et al. [1127], Laszlo et al. [772], and Gilles et al.) come into very good agreement among themselves and also with results of the mass spectrometric studies of Clyne and Watson [300] and Lancar et al. [765]. This provides the basis for the recommended room temperature value. The temperature dependence is based on results of Sander and Watson, Turnipseed et al. [1338] and Gilles et al. The results of Harwood et al. [556] are in good agreement with the recommendation.

There are two possible bimolecular channels for this reaction: $\text{BrO} + \text{BrO} \rightarrow 2\text{Br} + \text{O}_2$ (k_1) and $\text{BrO} + \text{BrO} \rightarrow \text{Br}_2 + \text{O}_2$ (k_2). The partitioning of the total rate constant into its two components, k_1 and k_2 , has been measured at room temperature by Sander and Watson [1139], Turnipseed et al. [1338] and Lancar et al. [765], by Jaffe and Mainquist [648] from 258 to 333 K, by Cox et al. [330] from 278 to 348 K and by Mauldin et al. [888] from 220 to 298 K. All are in agreement that $k_1/k_2 = 0.85 \pm 0.03$ at 298 K. From the values of $k_1/k_2 = 0.85$ at 298 K (all studies) and 0.68 at 220 K (Mauldin et al. and Cox et al. extrapolated), one can derive the temperature-dependent expression $k_1/k_2 = 1.60 \exp(-190/T)$. From the recommended Arrhenius expression for the overall rate constant $k = k_1 + k_2$ and the expression for the branching ratio k_1/k_2 , one can derive the following Arrhenius expressions for the individual reaction channels: $k_1 = 2.4 \times 10^{-12} \exp(40/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ and $k_2 = 2.8 \times 10^{-14} \exp(860/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. (Table: 97-4, Note: 97-4) [Back to Table](#)

- G43. $\text{CH}_2\text{BrO}_2 + \text{NO}$. The recommendation is based on the 298 K measurement of Sehested et al. [1174], who used pulsed radiolysis with UV absorption detection of the NO_2 product formation rate. The temperature dependence is estimated based on analogy to similar $\text{RO}_2 + \text{NO}$ reactions. The CH_2BrO product has been shown to undergo rapid unimolecular decomposition to yield $\text{CH}_2\text{O} + \text{Br}$ by Chen et al. [250] and Orlando et al. [1024]. The domination of this channel over the reaction of CH_2BrO with O_2 is consistent with the fate of other alkoxy radicals (Chen et al. and Orlando et al.), but contradicts the earlier result of Nielson et al. [978]. [Back to Table](#)
- H1. $\text{O} + \text{I}_2$. Based on the room temperature data of Ray and Watson [1108] and Laszlo et al. [773]. The molecular beam study of Parrish and Herschbach [1037] suggests a zero activation energy, consistent with the near gas kinetic value of k at 298 K. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H2. $\text{O} + \text{IO}$. Based on results of Laszlo et al. [773], the only reported study of this rate constant. This value was derived from modeling a system in which the concentrations of I_2 and IO were monitored simultaneously. This rate constant is a factor of 4 greater than the values for the corresponding reactions of O with ClO and BrO . (Table: 97-4, Note: 97-4) [Back to Table](#)
- H3. $\text{OH} + \text{I}_2$. Based on the data of Loewenstein and Anderson [842] and Jenkin et al. [658]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H4. $\text{OH} + \text{HI}$. Based on the data of Lancar et al. [767] and MacLeod et al. [857]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H5. $\text{OH} + \text{CH}_3\text{I}$. The recommended rate expression is derived from a fit to the data of Brown et al. [180], the only reported study of this reaction. (Table: 02-25, Note: 02-25) [Back to Table](#)
- H6. $\text{OH} + \text{CF}_3\text{I}$. The recommended rate expression is derived from a fit to the data of Gilles et al. [503]. The results from the studies by Garraway and Donovan [485] and Berry et al. [131] were not used in deriving the recommendation as the results were possibly influenced by reactant photolysis. The room temperature value from the discharge flow/resonance fluorescence study of Brown et al. [180] agrees within the 2σ limits. (Table: 02-25, Note: 02-25) [Back to Table](#)
- H7. $\text{HO}_2 + \text{I}$. Based on the data of Jenkin et al. [663], the only reported study of this reaction. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H8. $\text{HO}_2 + \text{IO}$. The recommended value is the average of the values reported by Jenkin et al. [662] and Maguin et al. [860]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H9. $\text{NO}_3 + \text{HI}$. No recommendation is given, based on the potential for severe complications resulting from secondary chemistry in the only reported study of the reaction (Lancar et al. [767]). (Table: 94-26, Note: 94-26) [Back to Table](#)
- H10. $\text{Cl} + \text{CH}_3\text{I}$. This reaction, thought to be a simple H abstraction reaction, has been shown by Ayhens et al. [59] to be quite complex. At low temperatures, Cl atom reversibly adds to CH_3I to form CH_3ICl . Thus, there are at least two channels for this reaction,



The rate coefficient for channel (a) has been measured by Ayhens et al. above 364 K, Kambanis et al. [691] between 273 and 363 K, Bilde and Wallington [143] at 298 K, and Cotter et al. [312] at 298 K. The recommendation is based on these studies.

Under atmospheric conditions reaction (b) to form the adduct is about two orders of magnitude faster than reaction (a). However, the fate of the CH_3ICl adduct in the atmosphere is unclear. Its lifetime, based on the studies of Ayhens et al., can be as long as a few seconds at 200 K and a few hundred Torr pressure. Therefore, it is possible that it could react with O_2 or be photolyzed. At 298 K, in one atmosphere of O_2 , it appears that the overall fate of the CH_3ICl is to decompose back to the reactants, based on the work of Bilde and Wallington [143]. Therefore, if O_2 were to react with CH_3ICl , this rate coefficient has to be less than about $10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, using the rate coefficient for its decomposition measured by Ayhens et al. If the rate coefficient for $\text{CH}_3\text{ICl} + \text{O}_2$ were to remain approximately the same, i.e., $10^{-17} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, at lower temperatures, the

possible loss of CH₃ICl via reaction with O₂ cannot be ignored. Further, the possible atmospheric photolysis of CH₃ICl may be important if it has a J-value greater than 0.1 s⁻¹.

There is a third possible product channel for this reaction to yield CH₃Cl + I (Goliff and Rowland [515]). Based on the results of Bilde and Wallington and Goliff and Rowland, we recommend that the rate coefficient for the Cl + CH₃I → CH₃Cl + I reaction to be less than 0.2k_a at 298 K. Since such a reaction is likely to have a significant barrier in the gas phase, even though it is exothermic by ~14 kcal mol⁻¹ at 298 K, the branching ratio for the production of CH₃Cl and I in the atmosphere will be likely less than that at 298 K. (Table: 02-25, Note: 02-25) [Back to Table](#)

- H11. I + O₃. Based on the room temperature data of Jenkin and Cox [659] and Sander [1135], and the temperature dependent data of Buben et al. [191] and Turnipseed et al. [1340]. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H12. I + BrO. Based on results of Laszlo et al. [772], the only reported study of this rate constant. This value was derived from modeling the simultaneous decay of BrO and IO in a Br₂/I₂/N₂O system. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H13. IO + NO. Based on the data of Ray and Watson [1108], Daykin and Wine [364], Buben et al. [192], and Turnipseed et al. [1340]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H14. IO + ClO. Based on results of Turnipseed et al. [1341], the only reported study of this reaction. These authors also reported the product yield for channel(s) yielding an I atom to be 0.8 ± 0.2. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H15. IO + BrO. Based primarily on results of Laszlo et al. [772]. Gilles et al. [505] reported the following Arrhenius expression for non-iodine atom producing channels: $2.5 \times 10^{-11} \exp(260/T)$ cm³ molecule⁻¹s⁻¹. They also reported a branching ratio of <0.35 for channels producing I atoms. From their data they could constrain the value of the overall rate constant to be: $6 \times 10^{-11} < k < 10 \times 10^{-11}$ cm³ molecule⁻¹s⁻¹, the range of which is consistent with the results of Laszlo et al. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H16. IO + IO. Changed from the previous recommendation, which was based on the results of Sander [1135]. In that study, over the temperature range 250–373 K, a negative temperature dependence was reported for the overall rate constant and for the absorption cross section at 427.2 nm. In the recent study of Harwood et al. [555], the overall rate constant and the absorption cross section were found to be independent of temperature from 253 to 320 K. The recommended room temperature value is the average of the values reported by Sander, Harwood et al., and Laszlo et al. [773]. The recommended temperature dependence is the average of the values reported by Sander and by Harwood et al., with an uncertainty sufficient to encompass the two reported values. The A-factor has been fitted to the recommended room temperature rate constant and the recommended temperature dependence. The overall rate constant for the decay of IO in the absence of ozone has been found to be independent of pressure by Sander, Laszlo et al., and Harwood et al. A comparison of the overall rate observed in excess ozone to that in the absence of ozone was interpreted by Sander and by Harwood et al. to imply that formation of the dimer I₂O₂ is the dominant reaction channel in the IO self-reaction. (Table: 97-4, Note: 97-4) [Back to Table](#)
- H17. INO + INO. Based on the data of Van den Bergh and Troe [1366]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- H18. INO₂ + INO₂. Based on the data of Van den Bergh and Troe [1366]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I1. O + SH. This recommendation accepts the results of Cupitt and Glass [336]. The large uncertainty reflects the absence of any confirming investigation. (Table: 82-57, Note: 82-57) [Back to Table](#)
- I2. O + CS. The room temperature recommendation is an average of the rate constants determined by Slagle et al. [1210], Bida et al. [135], Lilenfeld and Richardson [827], and Hancock and Smith [548]. The temperature dependence is that of Lilenfeld and Richardson, with the A-factor adjusted to yield the recommended value of k(298 K). (Table: 94-26, Note: 94-26) [Back to Table](#)
- I3. O + H₂S. This recommendation is derived from an unweighted least squares fit of the data of Singleton et al. [1201] and Whytock et al. [1453]. The results of Slagle et al. [1208] show very good

agreement for E/R in the temperature region of overlap (300 – 500 K) but lie systematically higher at every temperature. The uncertainty factor at 298 K has been chosen to encompass the room temperature rate constant values of Slagle et al. [1208] and Hollinden et al. [595]. Other than the 263 K data point of Whytock et al. and the 281 K point of Slagle et al., the main body of rate constant data below 298 K comes from the study of Hollinden et al., which indicates a dramatic change in E/R in this temperature region. Thus, the parameter g was set to account for these observations. Such a nonlinearity in the Arrhenius plot might indicate a change in the reaction mechanism from abstraction (as written) to addition. An addition channel (resulting in H atom displacement) has been proposed by Slagle et al. [1208], Singleton et al. [1201], and Singleton et al. [1203]. In the latter two studies, an upper limit of 20% was placed on the displacement channel. Direct observations of product HSO were made in the reactive scattering experiments of Clemo et al. [274] and Davidson et al. [348]. A threshold energy of 3.3 kcal/mole was observed (similar to the activation energy measured in earlier studies), suggesting the importance of this direct displacement channel. Addition products from this reaction have been seen in a matrix by Smardzewski and Lin [1213]. Further kinetic studies in the 200–300-K temperature range, as well as quantitative direct mechanistic information, could clarify these issues. However, this reaction is thought to be of limited importance in atmospheric chemistry. (Table: 82-57, Note: 82-57) [Back to Table](#)

14. O + OCS. The value of $k(298\text{ K})$ is the average of the determinations by Westenberg and de Haas [1444], Klemm and Stief [724], Wei and Timmons [1440], Manning et al. [863], and Breckenridge and Miller [175]. The recommended value of E/R is the average value taken from the first three listed studies. Hsu et al. [613] report that this reaction proceeds exclusively by a stripping mechanism. The vibrational and rotational state distributions in the SO and CO products have been reported by Chen et al. [257] and Nickolaisen et al. [966] respectively. (Table: 06-2, Note: 06-2) [Back to Table](#)
15. O + CS₂. The value of $k(298\text{ K})$ is an average of the rate constants determined by Wei and Timmons [1440], Westenberg and de Haas [1444], Slagle et al. [1209], Callear and Smith [219], Callear and Hedges [218], Homann et al. [596], Borissenko et al. [161] and Graham and Gutman [518]. The E/R value is an average of the determinations by Wei and Timmons and Graham and Gutman. The g value has been set to encompass the limited temperature-dependent data of Westenberg and de Haas. The principal reaction products are thought to be CS + SO. However, Hsu et al. [613] report that 1.4% of the reaction at 298 K proceeds through a channel yielding CO + S₂ and calculate a rate constant for the overall process in agreement with that recommended. Graham and Gutman [518] have found that 9.6% of the reaction proceeds to yield OCS + S at room temperature. Using time-resolved diode laser spectroscopy, Cooper and Hershberger [311] determined the branching ratios for the CO- and OCS-producing channels to be (3.0±1.0)% and (8.5±1.0)% respectively. (Table: 82-57, Note: 82-57) [Back to Table](#)
16. O + CH₃SCH₃. This recommendation is based on a fit of the data from Nip et al. [997], Lee et al. [790], and Lee et al. [789]. Product studies by Cvetanovic et al. [337] indicate that the reaction proceeds almost entirely by addition followed by rapid fragmentation to the products as written. Pavanaja et al. [1041] examined the pressure and reactant ratio dependencies of OH(A²Σ⁺) and SO₂(³B, ¹B) emissions in this reaction system. Their observations are consistent with initial product formation as written, followed by secondary generation of both OH and SO₂. (Table: 94-26, Note: 97-4) [Back to Table](#)
17. O + CH₃SSCH₃. This recommendation averages the 298 K rate constants of Nip et al. [997] and Borissenko et al. [161], which are in good agreement with each other, but are about a factor of 2 slower than the value reported by Lee et al. [786]. The recommendation for E/R has been obtained from an unweighted Arrhenius fit that employs all available data, but scales the data of Lee et al. downward by a factor of 2.04 to bring their data into agreement with the other data at room temperature. Product studies by Cvetanovic et al. [337] indicate that the reaction proceeds mainly by addition followed by rapid fragmentation to the products as written. Pavanaja et al. [1041] examined the pressure and reactant ratio dependencies of OH(A²Σ⁺) and SO₂(³B, ¹B) emissions in this reaction system. Their observations are consistent with initial product formation as written, followed by secondary generation of both OH and SO₂. (Table: 06-2, Note: 06-2) [Back to Table](#)

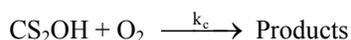
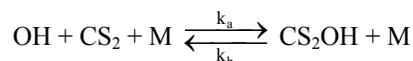
18. $O + CH_3S(O)CH_3$. The recommended 298 K rate constant is the average of values reported from a laser flash photolysis – resonance fluorescence study by Pope et al. [1068], and from a discharge flow – mass spectrometry study by Riffault et al. [1119]. A rate constant reported by Barnes et al. [76] (with no details about how the rate constant was obtained) is somewhat faster than the recommendation, but in agreement to within the recommended uncertainty factor. The recommended value for E/R is from Pope et al. The recommended value for the parameter g is larger than the value reported by Pope et al. to reflect the fact that only a single temperature dependence study has been reported. In their study at one Torr total pressure, Riffault et al. found that the products $SO_2 + 2 CH_3$ are produced with near unit yield. NEW ENTRY [Back to Table](#)
19. $O_3 + H_2S$. This upper limit was determined by Becker et al. [108] from measurements of the rates of SO_2 production and O_3 consumption. The heterogeneous reaction between H_2S and O_3 is far more efficient in most laboratory systems. (Table: 92-20, Note: 92-20) [Back to Table](#)
110. $O_3 + CH_3SCH_3$. This rate constant upper limit is based on the measurements of Martinez and Herron [884], which represent the only reported study of this reaction. (Table: 94-26, Note: 94-26) [Back to Table](#)
111. $O_3 + SO_2$. This recommendation is based on the limited data of Davis et al. [359] at 300 K and 360 K in a stopped flow investigation using mass spectrometric and UV spectroscopic detection. (Table: 85-37, Note: 85-37) [Back to Table](#)
112. $OH + H_2S$. The values of $k(298 K)$ and E/R are derived from a composite unweighted least squares fit to the individual data points of Perry et al. [1048], Cox and Sheppard [329], Wine et al. [1464], Leu and Smith [808], Michael et al. [916], Lin [829], Lin et al. [832], Wang and Lee [1419], Barnes et al. [72], and Lafage et al. [762]. The studies of Leu and Smith [808], Lin et al. [832], Lin [829], and Lafage et al. [762] show a slight parabolic temperature dependence of k with a minimum occurring near room temperature. However, with the error limits stated in this evaluation, all data are fit reasonably well by an Arrhenius expression. Lafage et al. and Michael et al. discuss the results in terms of a two-channel reaction scheme involving direct H atom abstraction and complex (adduct) formation. Lafage et al. analyzed their results above room temperature to yield an apparent E/R = 400 K for the abstraction channel, in good agreement with the E/R value determined above room temperature by Westenberg and de Haas [1445]. The results of these latter workers lie systematically higher (by about 70%), presumably due to secondary reactions. The room temperature value measured by Stuhl [1255] lies just outside the 2σ error limit set for $k(298 K)$. Butkovskaya and Setser [211] have observed infrared emission from vibrationally excited levels of the expected reaction product H_2O . (Table: 06-2, Note: 06-2) [Back to Table](#)
113. $OH + OCS$. The value of $k(298 K)$ is an average of the determinations by Wahner and Ravishankara [1388] and Cheng and Lee [258]. The room temperature rate constants from these studies are a factor of 3 higher than the earlier determination by Leu and Smith [807]. As discussed in the later studies, this difference may be due to an overcorrection of the Leu and Smith data to account for OH reaction with H_2S impurities and also to possible regeneration of OH. Nevertheless, the uncertainty factor at 298 K has been set to encompass the earlier study within 2σ . The work by Wahner and Ravishankara [1388] supersedes the study of Ravishankara et al. [1094], which minimized complications due to secondary and/or excited state reactions that presumably were interfering with the experiments of Atkinson et al. [50] and of Kurylo [751]. The upper limit for $k(298 K)$ reported by Cox and Sheppard [329] is too insensitive to permit comparison with the more recent studies. The room temperature measurements of Wahner and Ravishankara demonstrate the lack of an effect of total pressure (or O_2 partial pressure) on the rate constant and are supported by the more limited pressure- and O_2 -dependent studies of Cheng and Lee. The recommendation for E/R is based on the study of Cheng and Lee who determined a value considerably lower than reported by Leu and Smith, although this difference may be due in part to the earlier mentioned overcorrection of the data by the latter authors.

Product observations by Leu and Smith indicate that SH is a primary product of this reaction and tentatively confirm the suggestion of Kurylo and Laufer [758] that the predominant reaction pathway is to produce $SH + CO_2$ through a complex (adduct) mechanism similar to that observed for the OH

+ CS₂ reaction. However, the absence of an O₂/pressure effect for OH + OCS is in marked contrast with the strong dependence seen in studies of OH + CS₂ (see note for the latter reaction).

Experiments by Greenblatt and Howard [523] have shown that oxygen atom exchange in the reaction of ¹⁸OH with OCS is relatively unimportant, leading to an upper limit of 10⁻¹⁵ being set on the rate constant of the exchange reaction. (Table 87-41, Note: 92-20) [Back to Table](#)

- I14. OH + CS₂ → SH + OCS. There is a consensus of experimental evidence that this reaction proceeds very slowly as a direct bimolecular process. Wine et al. [1473] set an upper limit on k(298 K) of 1.5 × 10⁻¹⁵ cm³molec⁻¹s⁻¹. A consistent upper limit is also reported by Iyer and Rowland [645] for the rate of direct production of OCS, suggesting that OCS and SH are primary products of the bimolecular process. This mechanistic interpretation is further supported by the studies of Leu and Smith [809] and Biermann et al. [138], which set somewhat higher upper limits on k(298 K). The more rapid reaction rates measured by Atkinson et al. [50], Kurylo [751], and Cox and Sheppard [329] may be attributable to severe complications arising from excited state and secondary chemistry in their photolytic systems. The Cox and Sheppard study in particular may have been affected by the reaction of electronically excited CS₂ (produced via the 350 nm photolysis) with O₂ (in the 1-atm synthetic air mixture) as well as by the accelerating effect of O₂ on the OH + CS₂ reaction itself, which has been observed by other workers as summarized below. The possible importance of electronically excited CS₂ reactions in the tropospheric oxidation of CS₂ to OCS has been discussed by Wine et al. [1463]. (Table: 06-2, Note: 06-2) [Back to Table](#)
- I15. OH + CS₂ → CS₂OH $\xrightarrow{O_2}$ products. An accelerating effect of O₂ on the OH + CS₂ reaction rate has been observed by Jones et al. [678], Barnes et al. [79], and Hynes et al. [632], along with a near unity product yield for SO₂ and OCS. In the latter two studies the effective bimolecular rate constant was found to be a function of total pressure (O₂ + N₂), and exhibited an appreciably negative temperature dependence. These observations are consistent with the formation of a long-lived adduct as postulated by Kurylo [751] and Kurylo and Laufer [758] followed by its reaction with O₂:



The effective second order rate constant for CS₂ or OH removal in the above reaction scheme can be expressed as

$$1/k_{\text{eff}} = (k_b/k_a k_c)(1/P_{O_2}) + (1/k_a)(1/P_M)$$

where P_{O₂} is the partial pressure of O₂ and P_M equals P_{O₂} + P_{N₂}. The validity of this expression requires that k_a and k_b are invariant with the P_{O₂}/P_{N₂} ratio. A 1/k vs 1/P_{O₂} plot of the data of Jones et al. [678] taken at atmospheric pressure exhibits marked curvature, suggesting a more complex mechanistic involvement of O₂, whereas the data of Barnes et al. [79] and Hynes et al. [632] are more satisfactorily represented by this analytical expression. Nevertheless, while the qualitative features of the data from all three laboratories agree, there are some quantitative inconsistencies. First, under similar conditions of O₂ and N₂ pressures, the Barnes et al. rate constants lie approximately 60% higher than those of Jones et al. and up to a factor of 2 higher than those derived by Hynes et al. Secondly, two fits each of both the Barnes et al. and Hynes et al. data can be made: one at fixed P_M and varying P_{O₂}, and the other at fixed P_{O₂} and varying P_M (i.e., varying added N₂). Within each data set, rate constants calculated from both fits agree reasonably well for mole fractions of O₂ near 0.2 (equivalent to air) but disagree by more than a factor of 2 for measurements in a pure O₂ system. Finally, the temperature dependence (from 264–293 K) of the k_{eff} values from Barnes et al. varies systematically from an E/R of –1300 K for experiments in pure O₂ (at 700 torr total pressure) to –2900 K for experiments in a 50 torr O₂ plus 650 torr N₂ mixture. An Arrhenius fit of the Hynes et al. data (from 251–348 K) recorded in synthetic air at 690 torr yields an E/R = –3300 K, although the data show marked curvature over the temperature range of study. These observations suggest that k_a and k_b may not be independent of the identity of M. For this reason, we limit our recommendation to air mixtures (i.e., P_{O₂}/P_{N₂} = 0.25) at atmospheric pressure. Since most

CS₂ is oxidized within the atmospheric boundary layer, such restriction does not limit the applicability of this recommendation in atmospheric modeling.

The present recommendation accepts the measurements of Hynes et al. [632], which appear to be the most sensitive of the three investigations. Thus, $k(298\text{ K})$ is derived from the Arrhenius fit of the data near room temperature.

$$k(298\text{ K}) = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$$

To compute values of k below 298 K, we have accepted the analysis of Hynes et al.:

$$k(T) = \{1.25 \times 10^{-16} \exp(4550/T)\} / \{T + 1.81 \times 10^{-3} \exp(3400/T)\} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}.$$

This recommendation is only valid for one atmosphere pressure of air. It is interesting to note that measurements by Hynes et al. [632] at approximately 250 K and 700 Torr total pressure result in k_{eff} values that are independent of the amount of O₂ for partial pressures between 145 and 680 Torr. This suggests that the adduct is quite stable with respect to dissociation into the reactants (OH + CS₂) at this low temperature and that the effective rate constant for reactant removal approaches the elementary rate constant for adduct formation. NEW ENTRY [Back to Table](#)

- I16. CS₂OH + O₂. Three groups have obtained kinetic information about this reaction by observing either the perturbation of OH/CS₂OH equilibration kinetics upon addition of O₂, or by modeling the dependence of the observed rate constant for OH loss on [O₂]. Hynes et al. [632], Murrells et al. [939], and Diau and Lee [387] agree quite well on the value of k , with an average value of $2.8 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ independent of temperature and pressure being recommended. Diau and Lee also report rate constants for the reactions of the adduct (CS₂OH) with NO and NO₂ to be 7.3×10^{-13} and $4.2 \times 10^{-11} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, respectively.

From a mechanistic viewpoint, the primary products of this reaction determine the products of CS₂ oxidation in air. Lovejoy et al. [849] have shown that the yields of HO₂ and SO₂ are equal and near unity. Further insight is provided by the mechanistic study of Stickel et al. [1242], who observe OCS and CO product yields of (0.83±0.08) and (0.16±0.03), respectively. The results from this study are interpreted to imply that OCS and CO are formed either as primary products of the CS₂OH + O₂ reaction or as products of a secondary reaction between a primary product and O₂. These same authors report an SO₂ yield of (1.15±0.10), with the results suggesting that only about 75% of the SO₂ is formed as a prompt product, with the remainder generated via a slow reaction of SO (generated as a prompt product of the CS₂OH + O₂ reaction) with O₂. Insight into the specific reaction pathways can be gleaned from the study of Lovejoy et al. [848] in which the rate constant for the reaction of CS₂OD + O₂ was found to be the same as that for CS₂OH + O₂, indicating that simple H atom abstraction is not the likely process. Rather, HO₂ production most likely involves complex formation followed by HO₂ elimination. Lovejoy et al. [850] found that the ¹⁸O atom in the ¹⁸OH reactant is transferred predominantly (90 ± 20)% to the SO₂ product. These findings are consistent with an S–O–bonded CS₂–OH adduct and preservation of the S–O bond in the steps leading to SO₂ formation.

Theoretical studies by Zhang and Qin [1520] and by McKee and Wine [892] have provided further insight into the reaction mechanism. The initial step is, indeed, formation of SCS–OH followed by addition of O₂ to the carbon atom. A key subsequent step appears to be an O atom transfer to the sulfur bearing the hydroxyl group which leads directly to HOSO + OCS. The reaction HOSO + O₂ → HO₂ + SO₂ is expected to occur rapidly under atmospheric conditions. One remaining problem is identification of the pathway for generation of CO, which is observed as a minor product. NEW ENTRY [Back to Table](#)

- I17. OH + CH₃SH. This recommendation is based on a composite fit to the data of Atkinson et al. [49], Wine et al. [1464], Wine et al. [1474], and Hynes and Wine [629], which are in excellent agreement. The results from the relative rate study of Barnes et al. [72] are in agreement with this recommendation and indicate that the higher value of Cox and Sheppard [329] is due to complications resulting from the presence of O₂ and NO in their reaction system. MacLeod et al. [858, 859] and Lee and Tang [788] obtained rate constants at 298 K approximately 50% lower than recommended here. These authors also obtained lower values for the ethanethiol reaction in comparison with results from studies upon which the methanethiol recommendation is made. Wine

et al. [1474] present evidence that this reaction proceeds via adduct formation to produce a species that is thermally stable over the temperature range and time scales of the kinetic measurements. Tyndall and Ravishankara [1355] have determined the yield of CH₃S (via laser-induced fluorescence) to be unity, indicating that any adduct must be short lived (less than 100 μs). Longer lifetimes would have led to anomalies in the OH decay kinetics used for the rate constant determinations. Butkovskaya and Setser [213], based on observations of IR emissions from the products of the reactions of OH and OD with CH₃SH and CH₃SD, conclude that H-abstraction from the methyl group occurs with a yield of 24±8% for the OH reactions and 11±4% for the OD reactions. Hynes and Wine [629] observed that the rate constant is independent of O₂ partial pressure. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I18. OH + CH₃SCH₃ → H₂O + CH₂SCH₃. The OH + CH₃SCH₃ reaction is complex, proceeding by both H-abstraction and reversible addition pathways. In the presence of atmospheric levels of O₂, adduct reaction with O₂ makes the addition pathway partially irreversible. Only kinetic data obtained in the absence of O₂ and at low enough CH₃SCH₃ concentrations for the adduct to be a negligible reservoir for OH are considered in evaluation of the H-abstraction rate constant. This recommendation is based on the results of Hynes et al. [634], Wine et al. [1464], Hsu et al. [617], Abbatt et al. [3], Barone et al. [87], Turnipseed et al. [1337], and Williams et al. [1458]. The earlier higher rate constant values of Atkinson et al. [50] and Kurylo [752] are presumably due to reactive impurities, while those of MacLeod et al. [859] were most likely overestimated because of heterogeneous reactions. Absolute determinations lower than those recommended were obtained by Martin et al. [878], Wallington et al. [1392], and Nielsen et al. [983]. The reasons for these differences are not readily apparent. Confirmation that H-abstraction is the dominant pathway under the experimental conditions specified above comes from the studies of Stickel et al. [1244] and Turnipseed et al. [1337]. Stickel et al. used tunable diode laser spectroscopy to measure an HDO product yield of 0.84±0.15 for the OD + CH₃SCH₃ reaction in 10-30 Torr N₂, while Turnipseed et al. used laser induced fluorescence observations of CH₃S production from OH + CH₃SCH₃ to show that the branching ratio for the CH₃S elimination channel is <0.04 and the direct H-abstraction yield is 0.84±0.26. Further support for the dominance of the H-abstraction pathway comes from the work of Zhao et al. [1528], who obtained an upper limit yield of 0.07 for the methyl elimination channel in the OD + CH₃SCH₃ reaction. Barnes et al. [82, 83], Turnipseed et al., and Urbanski et al. [1360] all report that the abstraction product CH₃SCH₂ is converted predominantly to CH₃S under atmospheric conditions. Barnes et al. [82] measure a 0.7% yield of OCS under low NO_x conditions, which they attribute to further oxidation of CH₃S. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I19. OH + CH₃SCH₃ → (CH₃)₂SOH $\xrightarrow{O_2}$ products. The OH + CH₃SCH₃ reaction is complex, proceeding by both direct H-abstraction and reversible addition pathways. Much of the kinetic data available for evaluating this reaction were obtained for OH + CD₃SCD₃. Since the methyl hydrogens are not directly involved in the reaction, the rate constant is virtually the same for CH₃SCH₃ as for CD₃SCD₃; hence, data for both reactants are used in the evaluation. The recommended expression (units are cm³molec⁻¹s⁻¹),

$$k(T, [O_2]) = 1.0 \times 10^{-39} [O_2] \exp(+5820/T) / \{1 + 5.0 \times 10^{-30} [O_2] \exp(+6280/T)\}$$

is the best representation of the data of Hynes et al. [634] and Williams et al. [1458], and represents the rate constant for irreversible addition of OH to CH₃SCH₃ as a function of temperature and [O₂]. Both studies employed the laser flash photolysis – pulsed laser induced fluorescence technique, and obtained kinetic information by monitoring the decay of OH. The recommended expression is applicable at pressures near 1 atm over the temperature range 240 – 320 K, and can be used over the pressure range 0.1 – 1 atm at T = 298 K. Since the kinetic data of Hynes et al. and Williams et al. were obtained by monitoring OH loss, the overall rate constant for removal of CH₃SCH₃ would be underestimated if the adduct + O₂ reaction generated OH + dimethylsulfone (CH₃(O)S(O)CH₃) with a significant yield; the available data cannot rule out a small but significant branching ratio for this channel. Recommended rate constants for the elementary steps leading to OH loss and product formation (adduct formation, adduct dissociation, and adduct + O₂ reaction) are also provided in this document. NEW ENTRY [Back to Table](#)

120. $(\text{CH}_3)_2\text{SOH} + \text{O}_2$. All available kinetic data for this reaction were obtained by measuring k_{obs} for the $\text{OH} + \text{CH}_3\text{SCH}_3$ reaction as a function of O_2 partial pressure ($k_{\text{obs}} \equiv$ the sum of the rate constants for H-abstraction and irreversible addition). Most of the available data were obtained for $\text{OH} + \text{CD}_3\text{SCD}_3$. Since the methyl hydrogens are not directly involved in the reaction, the rate constant is expected to be virtually the same for CH_3SCH_3 as for CD_3SCD_3 ; hence, data for both reactants are used in the evaluation. The recommendation is based on the data of Hynes et al. [628] and Barone et al. [87]. The Hynes et al. study supercedes an earlier report of a considerably faster rate constant [634]. Over the range of experimental conditions where data are available (222 – 267 K and 30 – 200 Torr), the rate constant is essentially independent of temperature and pressure. By monitoring the regeneration of OH in the presence of NO, Hynes et al. [627] and Turnipseed et al. [1337] have determined the yield for the $\text{HO}_2 + \text{CH}_3\text{S(O)CH}_3$ (DMSO) channel to be ~ 0.5 . NEW ENTRY [Back to Table](#)
121. $\text{OH} + \text{CH}_3\text{SSCH}_3$. This recommendation is based on the temperature-dependent studies of Wine et al. [1464] and Abbatt et al. [3] and the room temperature relative rate study of Cox and Sheppard [329]. Domine and Ravishankara [407] have observed both CH_3S (via laser-induced fluorescence) and CH_3SOH (via photo-ionization mass spectrometry) as products of this reaction. At 298 K, the yield of CH_3S alone was quantified at approximately 30%. An FTIR product study of the photooxidation of dimethyl disulfide by Barnes et al. [81] presents evidence that oxidation of the CH_3SOH product is the principal source of the methane sulfonic acid observed. Butkovskaya and Setser [212] have observed that HDO and D_2O are produced from $\text{OD} + \text{CH}_3\text{SSCH}_3$ in the same proportion and with the same vibrational state distributions as the products observed by the same investigators in a similar study of the $\text{OD} + \text{CH}_3\text{SD}$ reaction [213], leading these authors to suggest that the major product channel for $\text{OD} + \text{CH}_3\text{SSCH}_3$ is $\text{CH}_3\text{SD} + \text{CH}_3\text{SO}$. (Table: 94-26, Note: 94-26) [Back to Table](#)
122. $\text{OH} + \text{CH}_3\text{S(O)CH}_3$. The recommended 298 K rate constant is the average of the direct studies of Hynes and Wine [631], Urbanski et al. [1359], and Kukui et al. [739], which employed three different experimental approaches and are in excellent agreement. Competitive kinetics studies by Barnes et al. [76] and Falbe-Hanson et al. [443] in 1 atm. of air report rate constants about a factor of 1.5 slower than those obtained in the direct studies. The recommended value for E/R is based on the only study of the temperature dependence [631], where a significant negative activation energy was observed. The large uncertainty in E/R reflects the availability of very limited data (none below room temperature). The experimental studies of Urbanski et al., Kukui et al. and Arsene et al. [35], as well as the theoretical study of Wang and Zhang [1418], provide strong evidence that the dominant reaction channel is production of $\text{CH}_3 + \text{CH}_3\text{S(O)OH}$ (MSIA, methanesulfonic acid). Arsene et al. attribute the failure to observe MSIA production in the chamber study of Sorensen et al. [1222] to loss via secondary gas phase and condensed phase oxidation before sampling. NEW ENTRY [Back to Table](#)
123. $\text{OH} + \text{CH}_3\text{S(O)OH}$. The recommendation is based on a turbulent flow reactor – chemical ionization mass spectrometry study by Kukui et al. [739], which was carried out with OH in excess over $\text{CH}_3\text{S(O)OH}$ at total pressures of 200–400 Torr N_2 . The large uncertainty factor results from the facts that (1) only a single room temperature study is reported in the literature and (2) $\text{CH}_3\text{S(O)OH}$ is a difficult species to study in the gas phase because of its low vapor pressure. Kukui et al. found that SO_2 was produced as a reaction product with near unit yield, suggesting that the dominant reaction channel (at least in the absence of O_2) is production of $\text{CH}_3 + \text{SO}_2 + \text{H}_2\text{O}$. NEW ENTRY [Back to Table](#)
124. $\text{OH} + \text{S}$. This recommendation is based on the study by Jourdain et al. [680]. Their measured value for $k(298 \text{ K})$ compares favorably with the recommended value of $k(\text{O} + \text{OH})$ when one considers the slightly greater exothermicity of the present reaction. (Table: 82-57, Note: 82-57) [Back to Table](#)
125. $\text{OH} + \text{SO}$. The value recommended for $k(298 \text{ K})$ is an average of the determinations by Fair and Thrush [441], Jourdain et al. [680], and Blitz et al. [154]. The result reported by Fair and Thrush is corrected using the present recommendation for the $\text{O} + \text{OH}$ reaction. The recommended value for E/R is taken from the temperature dependent data of Blitz et al. over the range 295–453 K. Higher temperature data of Blitz et al. are not used because significant curvature in the Arrhenius plot is

observed at $T > 500$ K. The recommended value for g is conservative because only one temperature dependence study has been reported. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I26. $\text{HO}_2 + \text{H}_2\text{S}$, $\text{HO}_2 + \text{CH}_3\text{SH}$, $\text{HO}_2 + \text{CH}_3\text{SCH}_3$. These upper limits are taken from the discharge flow laser magnetic resonance study of Mellouki and Ravishankara [906]. The H_2S value disagrees with the rate constant reported by Bulatov et al. [197] by approximately three orders of magnitude. The reason for this difference is not readily apparent. However, the recommended upper limit is consistent with the values for CH_3SH and CH_3SCH_3 , which respectively agree with upper limits from the work of Barnes et al. [72] and Niki (reported as a private communication in the Mellouki and Ravishankara paper). (Table: 94-26, Note: 94-26) [Back to Table](#)
- I27. $\text{HO}_2 + \text{SO}_2$. This upper limit is based on the atmospheric pressure study of Graham et al. [521]. A low pressure laser magnetic resonance study by Burrows et al. [203] places a somewhat higher upper limit on $k(298 \text{ K})$ of $4 \times 10^{-17} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ (determined relative to $\text{OH} + \text{H}_2\text{O}_2$). Their limit is based on the assumption that the products are OH and SO_3 . The weight of evidence from both studies suggests an error in the earlier determination by Payne et al. [1043]. (Table: 82-57, Note: 82-57) [Back to Table](#)
- I28. $\text{NO}_2 + \text{SO}_2$. This recommendation is based on the study of Penzhorn and Canosa [1045] using second derivative UV spectroscopy. While these authors actually report a measured value for $k(298 \text{ K})$, their observations of strong heterogeneous and water vapor catalyzed effects prompt us to accept their measurement as an upper limit. This value is approximately two orders of magnitude lower than that for a dark reaction observed by Jaffe and Klein [647], much of which may have been due to heterogeneous processes. Penzhorn and Canosa suggest that the products of this reaction are $\text{NO} + \text{SO}_3$. (Table: 85-37, Note: 85-37) [Back to Table](#)
- I29. $\text{NO}_3 + \text{H}_2\text{S}$. This recommendation accepts the upper limit set by Dlugokencky and Howard [393] based on experiments in which NO_3 loss was followed in the presence of large concentrations of H_2S . Less sensitive upper limits for the rate constant have been reported by Wallington et al. [1394] and Cantrell et al. [228]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- I30. $\text{NO}_3 + \text{OCS}$. This upper limit is based on the relative rate data of MacLeod et al. [856]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- I31. $\text{NO}_3 + \text{CS}_2$. This upper limit is based on the study of Burrows et al. [207]. A somewhat higher upper limit was derived in the relative rate study of MacLeod et al. [856]. (Table: 90-1, Note: 90-1) [Back to Table](#)
- I32. $\text{NO}_3 + \text{CH}_3\text{SH}$. The recommended values are derived from a composite fit to the data of Wallington et al. [1394], Rahman et al. [1085], and Dlugokencky and Howard [393]. The room temperature rate constant derived in the relative rate experiments of MacLeod et al. [856] is in good agreement with the recommended value. The suite of investigations shows the rate constant to be pressure independent over the range 1–700 torr. Dlugokencky and Howard place an upper limit of 5% on the production of NO_2 via this reaction at low pressure. Based on the product distribution observed in their investigation, Jensen et al. [666] propose a reaction mechanism initiated by abstraction of the hydrogen atom from the SH group, possibly after formation of an initial adduct as suggested by Wallington et al. and Dlugokencky and Howard. (Table: 90-1, Note: 94-26) [Back to Table](#)
- I33. $\text{NO}_3 + \text{CH}_3\text{SCH}_3$. The recommended values are derived from a composite fit to the data of Wallington et al. [1394], Tyndall et al. [1345], and Dlugokencky and Howard [393]. The relative rate study of Atkinson et al. [52] yields a rate constant at room temperature in good agreement with that recommended. The experimental data from all investigations demonstrate the pressure independence of the rate constant over the range 1–740 torr. Room temperature investigations by Daykin and Wine [362] and Wallington et al. [1395] are also in agreement with the recommended value. Jensen et al. [665] propose a mechanism that involves hydrogen abstraction as the first step to explain their observed product distribution. In a later study, Jensen et al. [666] measured a kinetic isotope effect for the rate constant for CH_3SCH_3 vs. that for CD_3SCD_3 of $k_{\text{H}}/k_{\text{D}} = (3.8 \pm 0.6)$, in agreement with the kinetic isotope effect reported by Daykin and Wine; this provides further confirmation of the H-abstraction mechanism. Butkovskaya and Le Bras [209] utilized chemical titration of the primary radical produced from $\text{NO}_3 + \text{CH}_3\text{SCH}_3$ in a discharge flow – mass

spectrometry system to show that the reaction produces predominantly $\text{CH}_3\text{SCH}_2 + \text{HNO}_3$. An upper limit of 2% was placed on the reaction channel yielding $\text{CH}_3 + \text{CH}_3\text{SONO}_2$. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I34. $\text{NO}_3 + \text{CH}_3\text{SSCH}_3$. The recommended values were derived from a composite fit to the data of Wallington et al. [1394] and Dlugokencky and Howard [393]. The investigation by Atkinson et al. [45] indicates that the relative rate technique cannot be considered as yielding reliable rate data for this reaction due to chemical complexities. Thus, the much lower room temperature results from the study of MacLeod et al. [856] can be considered to be erroneous. Based on their observations of intermediate and end products, Jensen et al. [666] proposed a reaction mechanism in which the initial addition of NO_3 to one of the sulfur atoms results in formation of $\text{CH}_3\text{S} + \text{CH}_3\text{SO} + \text{NO}_2$. (Table: 90-1, Note: 94-26) [Back to Table](#)
- I35. $\text{NO}_3 + \text{CH}_3\text{S(O)CH}_3$. The recommendation is the geometric mean of the rate constants reported by Barnes et al. [76] and Falbe-Hansen et al. [443] from similar competitive kinetics studies; the reported rate constants and associated 2σ uncertainties in units of $10^{-13} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ are 1.7 ± 0.6 (Barnes et al.) and 5.0 ± 3.8 (Falbe-Hansen et al.). In both studies, the only observed sulfur-containing end product was dimethylsulfone ($\text{CH}_3(\text{O})\text{S}(\text{O})\text{CH}_3$). Barnes et al. suggest that reaction proceeds via formation of an adduct that rapidly decomposes to $\text{NO}_2 + \text{CH}_3(\text{O})\text{S}(\text{O})\text{CH}_3$. NEW ENTRY [Back to Table](#)
- I36. $\text{NO}_3 + \text{SO}_2$. This recommended upper limit for $k(298 \text{ K})$ is based on the study by Daubendiek and Calvert [346]. Considerably higher upper limits have been derived by Burrows et al. [207], Wallington et al. [1394], Canosa-Mas et al. [223], and Dlugokencky and Howard [393]. (Table 87-41, Note: 90-1) [Back to Table](#)
- I37. $\text{N}_2\text{O}_5 + \text{CH}_3\text{SCH}_3$. This recommendation is based on the value estimated by Tyndall and Ravishankara [1356] from the study by Atkinson et al. [52]. (Table: 92-20, Note: 92-20) [Back to Table](#)
- I38. $\text{CH}_3\text{O}_2 + \text{SO}_2$. This recommendation accepts the results from the study of Sander and Watson [1140]. These authors conducted experiments using much lower CH_3O_2 concentrations than employed in the earlier investigations of Sanhueza et al. [1144] and Kan et al. [693], both of which resulted in $k(298 \text{ K})$ values approximately 100 times greater. A later report by Kan et al. [692] postulates that these differences are due to the reactive removal of the $\text{CH}_3\text{O}_2\text{SO}_2$ adduct at high CH_3O_2 concentrations prior to its reversible decomposition into CH_3O_2 and SO_2 . They suggest that such behavior of $\text{CH}_3\text{O}_2\text{SO}_2$ or its equilibrated adduct with O_2 ($\text{CH}_3\text{O}_2\text{SO}_2\text{O}_2$) would be expected in the studies yielding high k values, while decomposition of $\text{CH}_3\text{O}_2\text{SO}_2$ into reactants would dominate in the Sander and Watson experiments. It does not appear likely that such secondary reactions involving CH_3O_2 , NO , or other radical species would be rapid enough, if they occur under normal atmospheric conditions to compete with the adduct decomposition. This interpretation, unfortunately, does not explain the high rate constant derived by Cocks et al. [304] under conditions of low $[\text{CH}_3\text{O}_2]$. (Table: 81-3, Note: 81-3) [Back to Table](#)
- I39. $\text{F} + \text{CH}_3\text{SCH}_3$. This recommendation is based on the discharge flow mass spectrometric study by Butkovskaya et al. [210]. The uncertainty placed on this recommendation has been increased over that estimated by the authors to reflect the lack of any confirming investigations. Titration of the primary organic radical products indicated that the reaction proceeds via two channels to produce $\text{HF} + \text{CH}_3\text{SCH}_2$ and $\text{CH}_3 + \text{CH}_3\text{SF}$ with a branching ratio of approximately 0.8/0.2 respectively. (Table: 97-4, Note: 97-4) [Back to Table](#)
- I40. $\text{Cl} + \text{H}_2\text{S}$. This recommendation is based on the study by Nicovich et al. [970], who conducted an elaborate study with attention to sources of possible systematic error. The rate constant at 298 K is in good agreement with that determined by Nesbitt and Leone [957], who refined the data of Braithwaite and Leone [173], but is significantly greater than the values reported by Clyne and Ono [295], Clyne et al. [286], Nava et al. [946], and Chen et al. [254]. The small, but clearly observed, negative activation energy determined by Nicovich et al. contrasts with the lack of a temperature dependence observed by Nava et al. In fact, at the lowest temperature of overlap, the results from these two studies differ by 50%. Nevertheless, the Nicovich et al. study yields consistent results for both H_2S and CH_3SH as well as for D_2S and CD_3SD . In addition, Hossenlopp et al. [602] report a

room temperature rate constant for Cl + D₂S that is in excellent agreement with the value reported by Nicovich et al. While the reason for these differences remains to be determined, the full range of reported values is encompassed within the 2σ error limits recommended. Lu et al. [853] also measured a temperature-independent rate constant but report a value at 298 K that is about 40% greater than that of Nicovich et al. However, the presence of 4000 Torr of CF₃Cl bath gas in the Lu et al. study may suggest a slight pressure dependence of the reaction, although Nicovich et al. observed no pressure dependence for pressures ranging up to 600 Torr N₂. A theoretical study by Wilson and Hirst [1459] suggests the dominance of an addition-elimination pathway with a small but significant fraction of reactive events occurring via a direct hydrogen abstraction mechanism. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I41. Cl + OCS. This upper limit is based on the minimum detectable decrease in atomic chlorine measured by Eibling and Kaufman [434]. Based on the observation of product SCl, these authors set a lower limit on k(298 K) of 10⁻¹⁸ cm³molec⁻¹s⁻¹ for the SCl + CO reaction channel. Considerably higher upper limits on k(298 K) were determined in the studies of Clyne et al. [286] and Nava et al. [946]. (Table 83-62, Note: 87-41) [Back to Table](#)
- I42. CS₂Cl + O₂. This recommendation is based on the study of Nicovich et al. [969] who employed a laser flash photolysis – resonance fluorescence technique to observe the effect of added O₂ on the kinetics of the Cl + CS₂ ↔ CS₂Cl equilibration reactions. Martin et al. [876] report competitive kinetics results which they interpret as suggesting a fast CS₂Cl + O₂ reaction, but Wallington et al. [1391] have suggested that secondary production of OH in the photochemical system employed by Martin et al. is responsible for the observed dependence of the CS₂ loss rate on [O₂]. [Back to Table](#)
- I43. Cl + CH₃SH. This recommendation is based on the results of Nicovich et al. [970], who used laser photolysis with resonance fluorescence detection to study the reactions of Cl with H₂S, D₂S, CH₃SH, and CD₃SD. The room temperature determination by Nesbitt and Leone [957] is in good agreement with the recommended value. The k(298 K) value from the study of Mellouki et al. [902] is nearly a factor of 2 lower. However, the low sensitivity of EPR detection of Cl atoms did not permit these latter authors to conduct a precise determination of k under pseudo first-order conditions, and a more complex analysis of experiments conducted under second-order conditions was required. Nesbitt and Leone [958] report that 2±1% of the reaction occurs via abstraction of an H atom from the CH₃ group. A theoretical study by Wilson and Hirst [1459] predicts a Cl–S adduct bond strength (298 K) of 13.6 kcal mol⁻¹, but is unable to deduce the relative importance of addition-elimination vs. direct hydrogen abstraction pathways. (Table: 06-2, Note: 06-2) [Back to Table](#)
- I44. Cl + CH₃SCH₃. Stickel et al. [1243] have used laser photolysis – resonance fluorescence to measure the rate constant between 240 and 421 K, over the pressure range 3–700 Torr. The rate constant is near collisional but increases with increasing pressure from a low pressure limit of 1.8×10⁻¹⁰ to a value of 3.3×10⁻¹⁰ cm³molec⁻¹s⁻¹ at 700 Torr. The yield of HCl at 297 K, measured by diode laser spectroscopy, decreased from near unity at low pressure to a value of approximately 0.5 at 203 Torr, suggesting that stabilization of a (CH₃)₂SCl adduct becomes competitive with hydrogen atom abstraction with increasing pressure. These investigators also observed a negative temperature dependence for the reaction. Butkovskaya et al. [210] conducted a discharge flow – mass spectrometry study at 298 K, in which they determined that the reaction proceeds to form HCl + CH₃SCH₂ almost exclusively at 1 Torr total pressure. The sum of all other possible channels was estimated at less than 3%. Zhao et al. [1528] used laser photolysis coupled with CH₃ detection by time-resolved tunable diode laser absorption spectroscopy to determine an upper limit yield of 0.02 for CH₃ elimination at 298 K and pressures in the range 10–30 Torr. Langer et al. [768] coupled cw photolysis with gas chromatographic detection of products to show that the yield of CH₃Cl is (1.34 ± 0.07) × 10⁻³. Theoretical studies by Wilson and Hirst [1459], Resende and De Almeida [1114] and Thompson et al. [1299] support the experimentally-observed dominance of the H-abstraction pathway at low pressure. Diaz-de-Mera et al. [390] have employed a discharge flow – mass spectrometry technique to measure rate constants at pressures of 0.5 – 1.0 Torr He over the temperature range 259 – 364 K. The 298 K rate constant reported by Diaz-de-Mera et al. is nearly a factor of 3 slower than the low-temperature limit value reported by Stickel et al. Furthermore, Diaz-de-Mera et al. report a small positive activation energy whereas Stickel et al. report a small negative activation energy. The present recommendation for the H-abstraction pathway is based on an

extrapolated low pressure limit rate constant obtained from the data of Stickel et al., with the uncertainty adjusted to encompass the result of Diaz-de-Mera et al. Until additional temperature dependence data become available, a temperature-independent rate constant is recommended. The data of Stickel et al. suggest that a high pressure limit is reached at $P \sim 150$ Torr. Urbanski and Wine [1361] have observed the UV-visible absorption spectrum of $(\text{CH}_3)_2\text{SCl}$ in 155 Torr O_2 and used absorbance rise-time data to derive a rate constant that agrees well with those measured by Stickel et al. at pressures of 150–750 Torr N_2 . Enami et al. [437] have observed the kinetics of adduct formation using cavity ring down spectroscopy, and derived rate constants over the temperature and pressure ranges 278–318 K and 20–300 Torr N_2 that also agree well with those reported by Stickel et al. Room temperature competitive kinetics measurements by Nielsen et al. [982] at 740 Torr and Kinnison et al. [713] at 760 Torr agree quite well with the results of Stickel et al., Urbanski and Wine, and Enami et al. Kinnison et al. also observed the rate constant to increase from 3.6×10^{-10} to $4.2 \times 10^{-10} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ when the bath gas was changed from pure N_2 to synthetic air, suggesting that the $(\text{CH}_3)_2\text{SCl}$ adduct reacts with O_2 ; however, the results of Urbanski and Wine, and Enami et al. argue against the occurrence of such a reaction. Based on available data, a temperature-independent rate constant of $3.5 \times 10^{-10} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ in air at $P > 150$ Torr is recommended. NEW ENTRY [Back to Table](#)

- I45. $(\text{CH}_3)_2\text{SCl} + \text{O}_2, \text{NO}, \text{NO}_2$. The recommendations are based on the study of Urbanski and Wine [1361] which combined laser flash photolytic production of $(\text{CH}_3)_2\text{SCl}$ with kinetic observations by time-resolved absorption spectroscopy. The recommended uncertainties for the NO and NO_2 reactions are larger than those reported by Urbanski and Wine pending independent confirmation of their results. As in the Urbanski and Wine study, Enami et al. [437] report no observable reaction between $(\text{CH}_3)_2\text{SCl}$ and O_2 . NEW ENTRY [Back to Table](#)
- I46. $\text{Cl} + \text{CH}_3\text{S}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{S}(\text{O})\text{CH}_2 + \text{HCl}$. The recommended value of $k(298 \text{ K})$ for H-abstraction is based on the low pressure discharge flow – mass spectrometry studies of Martinez et al. [883] and Riffault et al. [1118]. Riffault et al. measured a yield of 91% for HCl production in 1.0 Torr of helium bath gas. The total rate constants reported by Martinez et al. at helium pressures of 0.5 – 3.0 Torr are scaled downward by 5–20% to account for the estimated contribution of an addition channel to the observed reactivity. The temperature dependence studies of Martinez et al. [883] (273–335 K) and Wine et al. (438–603 K) [1465] suggest the possibility of curvature in the Arrhenius plot. No recommendation is made for E/R pending the availability of additional data. Vandresen and Resende [1371] report a theoretical rate coefficient of $1.2 \times 10^{-10} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, i.e., a factor of seven faster than the value suggested by experimental results. NEW ENTRY [Back to Table](#)
- I47. $\text{CH}_3(\text{Cl})\text{S}(\text{O})\text{CH}_3 + \text{O}_2, \text{NO}, \text{NO}_2$. The recommendations are based on the study of Wine et al. [1465] which combined laser flash photolytic production of $\text{CH}_3(\text{Cl})\text{S}(\text{O})\text{CH}_3$ with kinetic observations by time-resolved absorption spectroscopy. The recommended uncertainties for the NO and NO_2 reactions are larger than those reported by Wine et al. pending independent confirmation of their results. NEW ENTRY [Back to Table](#)
- I48. $\text{ClO} + \text{OCS}; \text{ClO} + \text{SO}_2$. These recommendations are based on the discharge flow mass spectrometric data of Eibling and Kaufman [434]. The upper limit on $k(298 \text{ K})$ for $\text{ClO} + \text{OCS}$ was set from the minimum detectable decrease in ClO . No products were observed. The upper limit on $k(298 \text{ K})$ for $\text{ClO} + \text{SO}_2$ is based on the authors' estimate of their SO_3 detection limit. The upper limit for this same reaction based on the minimum detectable decrease in ClO was not used due to the potential problem of ClO reformation from the $\text{Cl} + \text{O}_3$ source reaction. (Table 83-62, Note: 83-62) [Back to Table](#)
- I49. $\text{ClO} + \text{CH}_3\text{SCH}_3$. The 298 K recommendation is the average of the values reported in discharge flow – mass spectrometry studies by Barnes et al. [77] and Diaz-de-Mera et al. [390]. Barnes et al. prefer their more recent rate constant to one a factor of 4 higher that they determined in an earlier version of their apparatus. The recommendation for E/R is based on the temperature dependence observed by Diaz-de-Mera et al. over the range 259 – 335 K. The uncertainty factors reflect the fact that the two reported values for $k(298 \text{ K})$ differ by more than a factor of two and that the activation energy is defined by data from a single study over a moderately narrow temperature range. (Table: 06-2, Note: 06-2) [Back to Table](#)

150. $\text{ClO} + \text{CH}_3\text{S(O)CH}_3$. The recommendation is based on the results of a low-pressure discharge flow – mass spectrometry study by Riffault et al. [1118]. These investigators were also able to establish an even lower upper limit of $2 \times 10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ for the channel that produces Cl atoms. NEW ENTRY [Back to Table](#)
151. $\text{ClO} + \text{SO}$. The value of $k(298 \text{ K})$ is an average of the determinations by Clyne and MacRobert [285] and Brunning and Stief [187]. The temperature independence is taken from the latter study with the A-factor recalculated to fit the $k(298 \text{ K})$ recommendation. (Table 87-41, Note: 87-41) [Back to Table](#)
152. $\text{Br} + \text{H}_2\text{S}$, $\text{Br} + \text{CH}_3\text{SH}$. These recommendations are based on the study by Nicovich et al. [967] who measured both the forward and reverse reactions by time-resolved resonance fluorescence detection of Br atoms. The uncertainties placed on these recommendations have been increased over those estimated by the authors to reflect the absence of any confirming investigations. (Table: 94-26, Note: 94-26) [Back to Table](#)
153. $\text{Br} + \text{CH}_3\text{SCH}_3$. It is well-established based on studies by Wine et al. [1467], Ingham et al. [639], and Nakano et al. [944] that, under atmospheric conditions, attack of Br on CH_3SCH_3 occurs predominantly by addition to the sulfur atom. Above 375K, adduct decomposition is so rapid that the addition channel is effectively negligible. Jefferson et al. [656] report high temperature experiments where the individual hydrogen transfer reactions $\text{Br} + \text{CH}_3\text{SCH}_3 \rightarrow \text{CH}_3\text{SCH}_2 + \text{HBr}$ (forward reaction) and $\text{CH}_3\text{SCH}_2 + \text{HBr} \rightarrow \text{Br} + \text{CH}_3\text{SCH}_3$ (reverse reaction) were isolated in a laser flash photolysis – resonance fluorescence system, and their kinetics were separately studied over the temperature range 386 – 604 K. These investigators determined Arrhenius expressions for the forward and reverse reactions to be $9.0 \times 10^{-11} \exp(-2386/T)$ and $8.6 \times 10^{-13} \exp(+836/T) \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, respectively. Analysis of the equilibrium data also permitted determination of the heat of formation of CH_3SCH_2 (see Appendix 1). Extrapolation of the Jefferson et al. Arrhenius expression to 298 K gives a rate constant for the non-adduct-forming part of the $\text{Br} + \text{CH}_3\text{SCH}_3$ reaction (presumably direct hydrogen abstraction) of $3.0 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. This estimated rate constant agrees quite well with the value of $(4.9 \pm 2.0) \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ obtained in a competitive kinetics study at atmospheric pressure in air by Ballesteros et al. [70], and is consistent with an upper limit of $1 \times 10^{-13} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ reported in a similar study by Maurer et al. [889]. Direct comparison of the Jefferson et al. and Ballesteros et al. kinetic data is warranted only if essentially all adduct formation is reversible in the Ballesteros et al. experiment, which is possible based on the apparent absence of an adduct + O_2 pathway [889], [944], but is not yet well-established. The recommendation for the pressure-independent bimolecular reaction is based on extrapolation of the Arrhenius expression of Jefferson et al. to the atmospheric temperature regime. The large uncertainty reflects the need for a rather long extrapolation. (Table: 06-2, Note: 06-2) [Back to Table](#)
154. $\text{Br} + \text{CH}_3\text{S(O)CH}_3$. The recommendation is based on the results of a low-pressure discharge flow – mass spectrometry study by Riffault et al. [1118]. These authors obtained an upper limit for the total rate constant of $1.5 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, and also report channel-specific rate constants in units of $10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ of 11 ± 3 for the H-abstraction channel and 1.2 ± 0.3 for the methyl elimination channel. A competitive kinetics study in 740 Torr air by Ballesteros et al. [70] reports a less sensitive upper limit rate constant of $6 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. NEW ENTRY [Back to Table](#)
155. $\text{BrO} + \text{CH}_3\text{SCH}_3$. This recommendation is an average of results obtained in the discharge flow studies of Barnes et al. [77] and Bedjanian et al. [112], and the flash photolysis studies of Ingham et al. [639] and Nakano et al. [944]. The flash photolysis studies were carried out at pressures of 60–200 Torr and give rate constants that are almost a factor of two faster than those obtained in the discharge flow studies at $P \sim 1$ Torr. The error limits in the present evaluation are adjusted to include all available data. A new study to investigate the pressure dependence of the rate constant is needed. Both Bedjanian et al. and Ingham et al. have shown that DMSO ($\text{CH}_3\text{S(O)CH}_3$) is produced with near unit yield. Ballesteros et al. [70] report that the rate constants for $\text{BrO} + \text{CH}_3\text{SCH}_3$ and $\text{BrO} + \text{CD}_3\text{SCD}_3$ are identical, a result that is consistent with reaction proceeding via formation of a short-lived adduct that rapidly decomposes to $\text{Br} + \text{DMSO}$. (Table: 06-2, Note: 06-2) [Back to Table](#)

156. BrO + CH₃SSCH₃. The recommendation is based on a competitive kinetics study in 740 Torr air by Ballesteros et al. [70]. The large uncertainty factor results from the fact that the reported rate constant is measured relative to an assumed value of $3.2 \times 10^{-13} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ for the BrO + CH₃SCH₃ rate constant, which has an uncertain pressure dependence (see above), and from the fact that there is only a single study upon which to base a recommendation. NEW ENTRY [Back to Table](#)
157. BrO + CH₃S(O)CH₃. The recommendation is based on a competitive kinetics study in 740 Torr air by Ballesteros et al. [70]. A low-pressure discharge flow – mass spectrometry study by Riffault et al. [1118], gives an upper limit that is consistent with the recommendation. The large uncertainty factor results primarily from the fact that the reported rate constant is obtained from a series of competitive kinetics experiments that are referenced to an assumed value of $3.2 \times 10^{-13} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ for the BrO + CH₃SCH₃ rate constant, which has an uncertain pressure dependence (see above). NEW ENTRY [Back to Table](#)
158. BrO + SO. This recommendation is based on the measurements of Brunning and Stief [188] performed under both excess BrO and excess SO conditions. The rate constant is supported by the lower limit assigned by Clyne and MacRobert [285] from measurements of SO₂ production. (Table 87-41, Note: 87-41) [Back to Table](#)
159. IO + CH₃SH. The value of k(298 K) comes from the study by Maguin et al. [861] using discharge flow mass spectrometry. The investigators establish a branching ratio near unity for the production of HOI. The uncertainty factor reflects the absence of any confirming investigations. (Table: 94-26, Note: 94-26) [Back to Table](#)
160. IO + CH₃SCH₃. This recommendation comes from the studies by Daykin and Wine [363] using laser photolysis – absorption spectroscopy and the studies of Maguin et al. [861], Barnes et al. [77], and Knight et al. [728] using discharge flow – mass spectrometry. These groups obtained rate constants of $\leq 3.5 \times 10^{-14}$, 1.5×10^{-14} , 8.8×10^{-15} , and $1.6 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, respectively. The studies of Maguin et al. and Barnes et al. supersede earlier, less direct measurements by the same groups, which resulted in rate constants of 1.5×10^{-11} (Martin et al. [877]) and $3.0 \times 10^{-11} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ (Barnes et al. [78]). Nakano et al. [943] have employed a laser flash photolysis – cavity ring down spectroscopy technique to investigate the temperature and pressure dependence of the rate constant. These investigators report that the 298 K rate constant increases from 1 to $25 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ as pressure increases from 5 to 100 Torr N₂, then levels off at higher pressure. Nakano et al. also investigated the temperature dependence of the rate constant at P = 100 Torr and observed a very strong negative temperature dependence, i.e., E/R = -2230 ± 460 . The pressure dependence reported by Nakano et al. appears to be in conflict with the results of Daykin and Wine, who found $k < 3.5 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ at all pressures in the range 40 – 300 Torr. The results of Nakano et al. are not used in the current recommendation pending independent verification. (Table: 06-2, Note: 06-2) [Back to Table](#)
161. S + O₂. This recommendation is based primarily on the study of Davis et al. [357]. Modest agreement at 298 K is found in the studies of Fair and Thrush [441], Fair et al. [442], Donovan and Little [412], and Clyne and Townsend [296]. The study by Clyne and Whitefield [303], which indicates a slightly negative E/R between 300 and 400 K, is encompassed by the assigned uncertainty limits. (Table: 82-57, Note: 82-57) [Back to Table](#)
162. S + O₃. This recommendation accepts the only available experimental data of Clyne and Townsend [296]. In this study the authors measure a value of the rate constant for S + O₂ in reasonable agreement with that recommended above. (Table: 82-57, Note: 82-57) [Back to Table](#)
163. SO + O₂. This recommendation is based on the low temperature measurements of Black et al. [151, 152] and Schurath and Goede [1162]. The room temperature rate constant reported by Black et al. supercedes an earlier value [151] as recommended by the authors. The recommended values for k(T) lie significantly higher than an extrapolation of the higher temperature data of Homann et al. [596], but are consistent with the more recent high temperature study of Garland [482]. A room temperature upper limit on k set by Breckenridge and Miller [175] is consistent with the recommendation. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I64. SO + O₃. The value of k(298 K) is an average of the determinations by Halstead and Thrush [543], Robertshaw and Smith [1120], Schurath and Goede [1162] and Black et al. [151, 152]. The value of E/R is an average of the values reported by Halstead and Thrush, Schurath and Goede, and Black et al. [151], with the A-factor recalculated to fit the recommendation for k(298 K). (Table: 06-2, Note: 06-2) [Back to Table](#)
- I65. SO + NO₂. The value of k(298 K) is an average of the determinations by Clyne and MacRobert [284], Black et al. [152], and Brunning and Stief [187], which agree quite well with the rate constant calculated from the relative rate measurements of Clyne et al. [280]. The Arrhenius parameters are taken from Brunning and Stief. (Table: 82-57, Note: 82-57) [Back to Table](#)
- I66. SO + OCIO. This recommendation is based on the room temperature study by Clyne and MacRobert [285]. The uncertainty reflects the absence of any confirming investigation. (Table: 82-57, Note: 82-57) [Back to Table](#)
- I67. SO₃ + 2 H₂O. Several research groups have attempted to quantify the rate of sulfuric acid formation via this reaction in the gas phase. Reiner and Arnold [1112] placed an upper limit of $2.4 \times 10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ on the rate constant, slightly lower than that determined by Wang et al. [1423]. The inability to cite the results as other than an upper limit is due to the difficulty in excluding all heterogeneous effects from the experiments. The higher rate constant reported earlier by Castleman et al. [234] may have resulted from an underestimation of the effects of such heterogeneous reactions. Subsequently, Reiner and Arnold [1113] sought to improve their rate constant determination by more detailed quantification of heterogeneous contributions. They derived a value of $1.2 \times 10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, independent of pressure (from 31–260 mbar of synthetic air). Evidence was also obtained that H₂SO₄ was, indeed, the product of the reaction.

Kolb et al. [735] attempted to measure the gas phase rate constant using a turbulent flow reactor designed to minimize wall effects. Their results, when analyzed as representing a bimolecular reaction, support a rate constant in the range $(1 - 7) \times 10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. However, a more detailed analysis of the data indicated that the gas phase reaction was second order in water vapor. The reaction rate was also observed to increase as the temperature was lowered from 333 K to 243 K. These observations, together with calculations by Morokuma and Mugurama [933], led the latter authors to suggest that SO₃ consumption likely involved its reaction with the water dimer or the reaction SO₃-H₂O + H₂O, leading to the formation of sulfuric acid.

A laminar flow reactor study by Lovejoy et al. [847] over the temperature range 250 to 360 K also revealed SO₃ loss to be second order in water concentration and independent of pressure (from 20 to 80 Torr of N₂ at 300 K). These latter authors measured a strong negative temperature dependence for the rate constant and a significant kinetic isotope effect ($k_{\text{H}_2\text{O}} \approx 2k_{\text{D}_2\text{O}}$), leading them to describe the reaction as proceeding via the rapid association between SO₃ and H₂O followed by a slower reaction between the adduct and water to form sulfuric acid. Lovejoy et al.'s measurement of a -13 kcal mol⁻¹ "activation" energy was viewed as energetically inconsistent with a SO₃ + water dimer reaction mechanism since it would require a large negative activation energy for the SO₃ + (H₂O)₂ step. Jayne et al. [655] have carried out a turbulent flow reactor study over the temperature range 283 to 370 K and the pressure range 100 to 760 Torr N₂. Their results provide further support for a mechanism involving formation of an SO₃-H₂O adduct that reacts with a second H₂O to form H₂SO₄, and the rate constants they report agree quite well with those reported by Lovejoy et al. The recommended expression for first order loss of SO₃,

$$k^1 = 8.5 \times 10^{-41} \exp(+6540/T) [\text{H}_2\text{O}]^2 \text{ s}^{-1} \quad ([\text{H}_2\text{O}] \text{ in molec cm}^{-3})$$

is the best fit of the combined data of Lovejoy et al. and Jayne et al. to an Arrhenius form. NEW ENTRY [Back to Table](#)

- I68. SO₃ + NO₂. This recommendation is based on the study of Penzhorn and Canosa [1045] using second derivative UV spectroscopy. These authors observe the production of a white aerosol, which they interpret to be the adduct NSO₅. This claim is supported by ESCA spectra. (Table: 85-37, Note: 85-37) [Back to Table](#)
- I69. SH + O₂. This upper limit for k(298 K) is based on the study by Stachnik and Molina [1229] utilizing experiments sensitive to the production of OH. Somewhat higher upper limits of 1.0×10^{-7}

¹⁷ and 1.5×10^{-17} were assigned by Friedl et al. [472] and Wang et al. [1421] respectively from the detection sensitivities for OH detection and SH decay respectively. An even higher upper limit by Black [148], based on the lack of SH decay, may have been complicated by SH regeneration. Much less sensitive upper limits have been calculated by Tsee et al. [1308], Nielsen [974], and Cupitt and Glass [336]. Stachnik and Molina [1229] also report a somewhat higher upper limit ($< 1.0 \times 10^{-18}$) for the rate constant for the sum of the two SH + O₂ reaction channels (producing OH + SO and H + SO₂). (Table: 85-37, Note: 85-37) [Back to Table](#)

- I70. SH + O₃. The value for k(298 K) is an average of the determinations by Friedl et al. [472] (laser-induced fluorescence detection of SH), Schonle et al. [1161] (mass spectrometric detection of reactant SH and product HSO) as revised by Schindler and Benter [1153], and Wang and Howard [1420] (laser magnetic resonance detection of SH). The temperature dependence is from Wang and Howard with the A-factor calculated to agree with the recommended value for k(298 K). The recommendation for g reflects the fact that the temperature dependence comes from measurements above room temperature and, thus, extrapolation to lower temperatures may be subject to additional uncertainties. Wang and Howard report observing a minor reaction channel that produces H + SO + O₂. A theoretical study by Resende and Ornellas [1115] concludes that if reaction occurs on the ground state potential energy surface, the rate constant should be several orders of magnitude slower than the experimental value. (Table: 06-2, Note: 06-2) [Back to Table](#)
- I71. SH + H₂O₂. This recommended upper limit for k(298 K) is based on the study of Friedl et al. [472]. Their value is calculated from the lack of SH decay (measured by laser-induced fluorescence) and the lack of OH production (measured by resonance fluorescence). The three possible product channels are H₂S + HO₂, HSOH + OH, and HSO + H₂O. (Table: 85-37, Note: 85-37) [Back to Table](#)
- I72. SH + NO₂. This recommendation is based on the measurements of Wang et al. [1421]. These authors suggest that the lower values of k(298 K) reported by Black [148], Friedl et al. [472], and Bulatov et al. [194] are due to SH regeneration from the H₂S source compound. In the study by Stachnik and Molina [1229], attempts were made at minimizing such regeneration, and the reported value of k(298 K) was significantly higher than that from the earlier studies, but still 30% lower than that measured by Wang et al., who used two independent SH source reactions. A slightly higher rate constant measured by Schonle et al. [1161], as revised by Schindler and Benter [1153], has not been recommended due to the somewhat more limited database for their determination. The reaction as written represents the most exothermic channel. In fact, HSO has been detected as a product by Leu and Smith [808], Bulatov et al. [194], Schonle et al. [1161], and Wang et al. [1421]. The absence of a primary deuterium isotope effect, as observed by Wang et al. [1421], coupled with the large magnitude of the rate constant suggests that the (four-center intermediate) channels producing SO + HNO and OH + SNO are of minor importance. No evidence for a three-body combination reaction was found by either Black [148] or Friedl et al. [472]. Based on a pressure independence of the rate constant between 30 and 300 torr, Black set an upper limit of 7.0×10^{-31} for the termolecular rate constant. Similarly, Stachnik and Molina [1229] observed no change in decay rate between 100 and 730 torr with O₂ (although these O₂ experiments were designed primarily to limit SH regeneration). The recommendation given here is supported by the discharge flow laser-induced fluorescence study of the SD + NO₂ reaction by Fenter and Anderson [450]. These investigators report a rate constant at 298 K of 6.8×10^{-11} cm³ molec⁻¹ s⁻¹, which compares favorably with the value of 7.1×10^{-11} cm³ molecule⁻¹ s⁻¹ determined in the Wang et al. study of the same reaction. Fenter and Anderson also obtained an E/R value of -210 K, very similar to the -237 K value derived by Wang et al. for the SH reaction. (Table: 97-4, Note: 97-4) [Back to Table](#)
- I73. SH + N₂O. The recommendation is the upper limit rate constant reported by Herndon et al. [572]. As discussed by Herndon et al., the much faster (four orders of magnitude) rate constant reported by Ravichandran et al. [1089] appears to result from mis-interpretation of the source of electronically excited HSO, chemiluminescence from which was employed by Ravichandran et al. to follow the reaction kinetics. NEW ENTRY [Back to Table](#)
- I74. SH + Cl₂. The recommended 298 K rate constant is based on the work of Nesbitt and Leone [957], who studied the kinetics of the Cl + H₂S → SH + HCl, SH + Cl₂ → ClSH + Cl chain reaction. Fenter and Anderson [449] employed a discharge flow – laser induced fluorescence technique to study the SD + Cl₂ reaction over the temperature range 273–373 K. The 298 K rate constant

reported by Fenter and Anderson is about 20% faster than the one reported by Nesbitt and Leone, which is consistent with the expected secondary kinetic isotope effect. The recommended value of E/R is taken from the work of Fenter and Anderson; the recommended value for the parameter g reflects the absence of any confirming studies and uncertainty in the isotope effect on E/R. (Table: 06-2, Note: 06-2) [Back to Table](#)

- I75. SH + BrCl; SH + Br₂; SH + F₂. The recommendations for these reactions are derived from the data of Fenter and Anderson [449] for the SD radical. The uncertainties have been increased over those estimated by the investigators to reflect the absence of any confirming investigations and the influence of the secondary isotope effect. For the BrCl reaction, the channel producing ClSD + Br was found to be described by the rate expression $k = 2.3 \times 10^{-11} \exp(100/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. (Table: 92-20, Note: 06-2) [Back to Table](#)
- I76. HSO + O₂. This recommendation is based on the study by Lovejoy et al. [851], who employed laser magnetic resonance monitoring of HSO in a discharge flow system. The upper limit thus derived for k(298 K) is nearly two orders of magnitude lower than measured by Bulatov et al. [196]. (Table 87-41, Note: (Table: 92-20, Note: 92-20)) [Back to Table](#)
- I77. HSO + O₃. This recommendation is based on the determinations by Friedl et al. [472] and Wang and Howard [1420]. In the first study, performed at higher O₃ concentrations, greater quantities of HSO were produced in the flow tube and SH approached a steady state due to its generation via HSO + O₃. The rate constant for this reaction was thus determined relative to SH + O₃ from measurements of the steady state SH concentration as a function of the initial SH concentration. In the second study, the rate constant and its branching ratio were measured at two temperatures. At room temperature, the overall rate constant is in excellent agreement with that of Friedl et al. More recently, Lee et al. [795] determined a room temperature rate constant of $4.7 \times 10^{-14} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$ for the sum of all reaction channels not producing HS. This value is approximately 30% greater than that measured by Wang and Howard for the same channels. Lee et al. derive an Arrhenius activation energy of 1120 K for these channels from data between 273 and 423 K, in agreement with the more limited temperature-dependent data of Wang and Howard.

The lack of an isotope effect when SD was employed in the Friedl et al. study suggests that the products of the HSO + O₃ reaction are SH + 2O₂ (analogous to those for HO₂ + O₃). However, Wang and Howard found that only 70% of the reaction leads to HS formation. In addition, their observations of HO₂ production in the presence of O₂ suggests the existence of a reaction channel producing HSO₂ + O₂ followed by HSO₂ + O₂ → HO₂ + SO₂. At the present time, no recommendation is given for the product channels. Further mechanistic work is suggested, since it is important to understand whether this reaction in the atmosphere leads to HS regeneration or to oxidation of the sulfur. (Table: 92-20, Note: 94-26) [Back to Table](#)

- I78. HSO + NO; HSO + NO₂. The recommendations for these reactions are based on the study by Lovejoy et al. [851] in which laser magnetic resonance was used to monitor HSO in a discharge flow system. Their upper limit for the NO reaction is a factor of 25 lower than the rate constant measured by Bulatov et al. [195] using intracavity laser absorption at pressures between 10 and 100 torr. Since it is unlikely that this reaction rate undergoes a factor of 25 increase between 1 torr (the pressure of the Lovejoy et al. work) and 10 torr, the higher rate constant may be due to secondary chemistry associated with the HSO production methods employed.

The recommendation for the NO₂ reaction is a factor of 2 higher than the rate constant reported by Bulatov et al. [194]. Lovejoy et al. have attributed this difference to HSO regeneration under the experimental conditions used by Bulatov et al. [194]. The product assignment for this reaction is discussed in the note for the HSO₂ + O₂ reaction. (Table 87-41, Note: 87-41) [Back to Table](#)

- I79. HSO₂ + O₂. This recommendation is based on the rate of HO₂ formation measured by Lovejoy et al. [851] upon addition of O₂ to the HSO + NO₂ reaction system. While HSO₂ was not observed directly, a consideration of the mechanistic possibilities for HSO + NO₂, coupled with measurements of the HO₂ production rate at various O₂ pressures, led these authors to suggest that HSO₂ is both a major product of the HSO + NO₂ reaction and a precursor for HO₂ via reaction with O₂. (Table 87-41, Note: 87-41) [Back to Table](#)

180. $\text{HOSO}_2 + \text{O}_2$. This recommendation is based on the studies of Gleason et al. [511] and Gleason and Howard [509] in which the HOSO_2 reactant was monitored using a chemical ionization mass spectrometric technique. Gleason and Howard conducted their measurements over the 297–423 K temperature range in the only temperature dependence investigation. Thus, the parameter g has been increased from their quoted limits to account for the potential uncertainties in extrapolating their data to sub-ambient temperatures. The value of $k(298 \text{ K})$ derives further support from the studies of Margitan [867] and Martin et al. [879], both of whom used modeling fits of OH radical decays in the $\text{OH} + \text{SO}_2 + \text{M}$ reaction system in the presence of O_2 and NO . In this latter analysis, the HOSO_2 reacts with O_2 yielding HO_2 , which subsequently regenerates OH through its reaction with NO . The infrared spectrum of HOSO_2 has been recorded in low temperature matrix isolation experiments by Hashimoto et al. [557] and Nagase et al. [942]. Mass spectrometric detection of HOSO_2 in the gas phase has also been reported by Egsgaard et al. [432]. (Table: 06-2, Note: 06-2) [Back to Table](#)
181. $\text{CS} + \text{O}_2$. The recommendation given for $k(298 \text{ K})$ is based on the work of Black et al. [150] using laser-induced fluorescence to monitor CS. This value agrees with the somewhat less precise determination by Richardson [1117] using OCS formation rates. The latter author presents evidence that this reaction channel dominates over the one producing $\text{SO} + \text{CO}$ by more than a factor of 10. Measurements by Richardson at 293 K and 495 K yield an E/R of 1860 K. However, use of this activation energy with the recommended value of $k(298 \text{ K})$ results in an unusually low Arrhenius A-factor of $1.5 \times 10^{-16} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. In view of this, no recommendation is given for the temperature dependence. (Table: 85-37, Note: 85-37) [Back to Table](#)
182. $\text{CS} + \text{O}_3$; $\text{CS} + \text{NO}_2$. The $k(298 \text{ K})$ recommendations for both reactions accept the results of Black et al. [150], who used laser-induced fluorescence to monitor the CS reactant in a room temperature experiment. The uncertainty factors reflect the absence of any confirming measurements. (Table: 85-37, Note: 85-37) [Back to Table](#)
183. $\text{CH}_3\text{S} + \text{O}_2$. This upper limit is based on the study by Tyndall and Ravishankara [1354]. Somewhat higher upper limits were derived in the earlier studies of Balla et al. [69] and Black and Jusinski [149]. (Table: 90-1, Note: 90-1) [Back to Table](#)
184. $\text{CH}_3\text{S} + \text{O}_3$. The recommendation for $k(298 \text{ K})$ is the average of room temperature rate constants reported by Tyndall and Ravishankara [1355], Domine et al. [408], Turnipseed et al. [1335], and Martinez et al. [882]. The recommendation for E/R is the average of values obtained from least squares fits of the temperature-dependent data of Turnipseed et al. and Martinez et al. using only rate constants at temperatures below 345 K. A failure to observe significant reaction in the study by Black and Jusinski [149] is interpreted as due to rapid regeneration of CH_3S in their system. Tyndall and Ravishankara [1355] corrected their measured 298 K rate constant downward by ~20% to account for CH_3S regeneration via the $\text{CH}_3\text{SO} + \text{O}_3$ reaction, but the magnitude of the correction is now highly uncertain in light of the results of Domine et al. and Turnipseed et al. Domine et al. measured the yield of CH_3SO to be 15%. (Table: 06-2, Note: 06-2) [Back to Table](#)
185. $\text{CH}_3\text{S} + \text{NO}$. The upper limit for the bimolecular reaction between CH_3S and NO is based on estimates by Balla et al. [69], who conducted a temperature dependence study of the termolecular reaction. (Table: 92-20, Note: 92-20) [Back to Table](#)
186. $\text{CH}_3\text{S} + \text{NO}_2$. The recommendation for $k(298 \text{ K})$ is the average of room temperature rate constants reported by Tyndall and Ravishankara [1354], Domine et al. [406], Turnipseed et al. [1335], Martinez et al. [882], and Chang et al. [244]. The recommendation for E/R is the average of values reported by Turnipseed et al., Martinez et al., and Chang et al. An earlier study by Balla et al. [69] appears to have been affected by secondary reactions resulting from high radical concentrations. Tyndall and Ravishankara determined the NO yield to be $(80 \pm 20)\%$. Together with the unity yield of CH_3SO obtained by Domine et al., this implies that the primary reaction channel is as written. (Table: 06-2, Note: 06-2) [Back to Table](#)
187. $\text{CH}_2\text{SH} + \text{O}_2$. This recommendation is the average of the rate constant obtained by Rahman et al. [1086] in a fast flow mass spectrometer system and that from Anastasi et al. [23] using a pulse radiolysis – kinetic absorption apparatus. The value of Anastasi et al. is nearly twice that of Rahman et al. It is difficult at present to indicate a preference for the results of one study over the other, and the value of $f(298 \text{ K})$ has been chosen to reflect this uncertainty. Since this is a fast bimolecular

reaction, one would expect the products to be $\text{HO}_2 + \text{CH}_2\text{S}$, by analogy with the reaction between CH_2OH and O_2 . (Table: 94-26, Note: 94-26) [Back to Table](#)

- I88. $\text{CH}_2\text{SH} + \text{O}_3$. The value of $k(298 \text{ K})$ comes from the study by Rahman et al. [1086] using fast flow – mass spectrometry. The uncertainty factor reflects the absence of any confirming investigations. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I89. $\text{CH}_2\text{SH} + \text{NO}$. The value of $k(298 \text{ K})$ comes from the study by Anastasi et al. [23] using a pulse radiolysis – kinetic absorption apparatus. The uncertainty factor reflects the absence of any confirming investigations. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I90. $\text{CH}_2\text{SH} + \text{NO}_2$. This recommendation averages the rate constant obtained by Rahman et al. [1086] in a fast flow – mass spectrometry system with that from Anastasi et al. [23], using a pulse radiolysis kinetic absorption apparatus. The value of Rahman et al. is nearly twice that of Anastasi et al. It is difficult at present to indicate a preference for the results of one study over the other, and the value of $f(298 \text{ K})$ has been chosen to reflect this uncertainty. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I91. $\text{CH}_3\text{SO} + \text{O}_3$. This recommendation is the average of values reported by Domine et al. [408] and Borissenko et al. [161]. It is supported by the study of Tyndall and Ravishankara [1355], in which the rate constant was derived from a complex analysis of the $\text{CH}_3\text{S} + \text{O}_3$ reaction system. Borissenko et al. measured the rate constant relative to the rate constant for the $\text{CH}_3\text{SO} + \text{NO}_2$ reaction; they report that $\text{CH}_3\text{SO} + \text{NO}_2$ is faster by a factor of 47. Domine et al. place the direct yield of CH_2SO at approximately 10% and that of CH_3S at 13% at low pressure. Borissenko et al. report that the SO_2 yield is near unity in 100–600 Torr N_2 . (Table: 06-2, Note: 06-2) [Back to Table](#)
- I92. $\text{CH}_3\text{SO} + \text{NO}_2$. This recommendation is based on the direct measurements of Domine et al. [406]. The results are supported by somewhat less direct measurements of Tyndall and Ravishankara [1354], Mellouki et al. [901], and Kukui et al. [740]. The results of Kukui et al. suggest a small negative activation energy, but their data set is not extensive enough to warrant a recommendation for E/R without independent confirmation. Borissenko et al. [161] report that the SO_2 yield drops from ~0.4 in 100 Torr N_2 to ~0.25 in 660 Torr N_2 . (Table: 06-2, Note: 06-2) [Back to Table](#)
- I93. $\text{CH}_3\text{SOO} + \text{O}_3$, $\text{CH}_3\text{SOO} + \text{NO}$, $\text{CH}_3\text{SOO} + \text{NO}_2$. These recommendations are based on the experiments of Turnipseed et al. [1335] in which CH_3S was monitored by LIF in equilibrium with CH_3SOO . The upper limit for the O_3 reaction was determined from experiments at 227 K. The results for the NO and NO_2 reactions were independent of temperature over the ranges 227–256 K and 227–246 K, respectively. The uncertainties placed on these recommendations have been increased over those estimated by the authors to reflect the absence of any confirming investigations. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I94. $\text{CH}_3\text{SO}_2 + \text{NO}_2$. This recommendation is based on the study by Ray et al. [1106] using a discharge flow reactor equipped with laser-induced fluorescence and mass spectrometric detection. The CH_3SO_2 was produced by the sequential oxidation of CH_3S and CH_3SO by NO_2 and is to be differentiated from the weakly bound adduct, CH_3SOO , formed by the reaction of CH_3S with O_2 at low temperature (Turnipseed et al. [1335]). The uncertainty limit on the rate constant has been increased over that given by the authors to reflect the absence of any confirming investigation. However, some additional support for this recommendation does come from the study of the $\text{CH}_3\text{S} + \text{NO}_2$ reaction by Tyndall and Ravishankara [1354]. These authors observed fluorescence from a product species tentatively identified as CH_3SO_2 , produced by the reaction of CH_3SO with NO_2 . Computer simulation of the rise and fall of the fluorescence signal yielded an approximate rate constant value for the reaction $\text{CH}_3\text{SO}_2 + \text{NO}_2$ of $7.0 \times 10^{-12} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. However, an unambiguous differentiation between the production and disappearance rate constants was not possible. (Table: 97-4, Note: 97-4) [Back to Table](#)
- I95. $\text{CH}_3\text{SCH}_2 + \text{NO}_3$. This recommendation is based on the experiments of Butkovskaya and Le Bras [209]. The uncertainty factor reflects the absence of any confirming investigation. (Table: 94-26, Note: 94-26) [Back to Table](#)
- I96. $\text{CH}_3\text{SCH}_2\text{O}_2 + \text{NO}$. The recommended 298 K rate constant is based on the experiments of Urbanski et al. [1360], which are less impacted by secondary chemistry complications than the experiments of Wallington et al. [1402] or Turnipseed et al. [1337]; the error limits are chosen to encompass the rate

constants reported in all three studies. The E/R value is taken from Urbanski et al., who report the only available temperature dependence data. The recommended value for the parameter g is larger than reported by Urbanski et al. pending independent confirmation of their result. (Table: 06-2, Note: 06-2) [Back to Table](#)

197. $\text{CH}_3\text{SCH}_2\text{O}_2 + \text{CH}_3\text{SCH}_2\text{O}_2$. The recommended 298 K rate constant is the average of values reported by Wallington et al. [1402] using a pulse radiolysis – UV absorption technique and Urbanski et al. [1360] using a laser flash photolysis – tunable diode laser absorption technique. Urbanski et al. observed that the reaction produces formaldehyde with unit yield, suggesting that the dominant reaction pathway is $2 \text{CH}_3\text{SCH}_2\text{O}_2 \rightarrow 2 \text{CH}_3\text{SCH}_2\text{O} + \text{O}_2$ ($\text{CH}_3\text{SCH}_2\text{O}$ rapidly decomposes to $\text{CH}_3\text{S} + \text{H}_2\text{CO}$). NEW ENTRY [Back to Table](#)
198. $\text{CH}_3\text{SS} + \text{O}_3$. This recommendation is based on the discharge flow-photoionization mass spectroscopy study by Domine et al. [408]. The uncertainty factor reflects the absence of any confirming investigations. The rate constant ratio for the reactions of CH_3SS with O_3 and NO_2 is consistent with the rate constant ratio for the corresponding CH_3S reactions. (Table: 92-20, Note: 92-20) [Back to Table](#)
199. $\text{CH}_3\text{SS} + \text{NO}_2$; $\text{CH}_3\text{SSO} + \text{NO}_2$. These recommendations are based on the discharge flow – photoionization mass spectrometry study by Domine et al. [406]. The rate constant ratio for these two reactions agrees with that observed for other RS/RSO radicals with NO_2 . The assigned uncertainties reflect this agreement but acknowledge the absence of any confirming investigation. In the Domine et al. study, CH_3SSO was produced by reacting away all CH_3SS with high NO_2 concentrations. Thus, as expected, O atom transfer may be the primary channel in the CH_3SS reaction. (Table: 92-20, Note: 92-20) [Back to Table](#)
- J1. $\text{Na} + \text{O}_3$. The recommendation is based on the measurements of Ager et al. [15], Worsnop et al. [1484] as corrected in Worsnop et al. [1485], and Plane et al. [1061]. The data of Worsnop et al. supersede earlier work from that laboratory (Silver and Kolb [1187]). Measurements made by Husain et al. [623] at 500 K are somewhat lower, probably because they did not recognize that secondary chemistry, $\text{NaO} + \text{O}_3 \rightarrow \text{Na} + 2\text{O}_2$, interferes with the rate coefficient measurement. The temperature dependence is from results of Worsnop et al. [1485] (214–294 K) and Plane et al. [1061] (208–377K). Ager et al. [15] estimate that the $\text{NaO}_2 + \text{O}$ product channel is $\leq 5\%$. Evidence that the NaO product is in the $^2\Sigma^+$ excited electronic state was reported by Shi et al. [1181] and Wright et al. [1486]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- J2. $\text{Na} + \text{N}_2\text{O}$. The recommendation incorporates the data of Husain and Marshall [622], Ager et al. [15], Plane and Rajasekhar [1062], and Worsnop et al. [1485]. Silver and Kolb [1187] measured a rate coefficient at 295 K that is lower and is superseded by Worsnop et al. [1485]. Helmer and Plane [568] report a measurement at 300 K in excellent agreement with the recommendation. Earlier, less direct studies are discussed by Ager et al. [15]. The NaO product does not react significantly with N_2O at room temperature [k (for $\text{Na} + \text{N}_2 + \text{O}_2$ products) $\leq 10^{-16}$ and k (for $\text{NaO}_2 + \text{N}_2$ products) $\leq 2 \times 10^{-15}$ (Ager et al.). Wright et al. [Wright, 1993 #1863] used UV photoelectron spectroscopy to determine the product NaO is formed predominantly in the excited $^2\Sigma^+$ state. (Table: 92-20, Note: 94-26) [Back to Table](#)
- J3. $\text{Na} + \text{Cl}_2$. Two measurements of the rate coefficient for this reaction are in excellent agreement: Silver [1183] and Talcott et al. [1277]. The recommended value is the average of these room temperature results. (Table 87-41, Note: 87-41) [Back to Table](#)
- J4. $\text{NaO} + \text{O}$. The recommendation is based on measurements by Plane and Husain [1060] and Griffin et al. [527]. The $\text{Na} + \text{O}_3$ reaction produces NaO predominately in the low lying $A \ ^2\Sigma^+$ state which can radiatively and collisionally decay slowly to the $X \ ^2\Pi$ ground state. The Plane and Husain [1060] experiment was configured so the the predominant reactant was $\text{NaO} \ X \ ^2\Pi$ while the Griffin et al. [527] experiment was designed to maximize $\text{NaO} \ A \ ^2\Sigma^+$ concentrations. While the two states may not have identical reaction rate constants, their energy difference is small compared to reaction exothermicity and both states show reaction rate constants near the collisional limit. Since this reaction in the atmosphere will probably proceed through a mixture of the two lowest NaO electronic states and data are available at only one temperature for each state, the recommended rate

constant is an average of the two measurements. Plane and Husain [1060] reported that ~0.01 of the Na product is in the 3^2P excited state, while Griffin et al. [527] report a Na 3^2P product branching ratio of 0.14 ± 0.04 . This difference is consistent with the orbital correlation predictions of products for reaction of each NaO state as presented by Herschbach et al. [578]. (Table: 06-2, Note: 06-2) [Back to Table](#)

- J5. NaO + O₃. This reaction was studied by Silver and Kolb [1187], Ager et al. [15], and Plane et al. [1061], who agree on the rate coefficient and branching ratio. This agreement may be fortuitous because Silver and Kolb used an indirect method and an analysis based on their rate coefficient for the Na + O₃ reaction, which is about 1/2 of the recommended value. Ager et al. employed a somewhat more direct measurement, but the study is complicated by a chain reaction mechanism in the Na/O₃ system. Plane et al. reported rate coefficient measurements for the NaO₂ + O₂ product channel over the temperature range 207–377 K using pulsed photolysis LIF methods. The recommendation for that channel is based on all three studies, and the recommendation for the Na + 2O₂ channel is based upon the results of Silver and Kolb and Ager et al. The latter reaction channel may also have a significant temperature dependence. (Table: 94-26, Note: 94-26) [Back to Table](#)
- J6. NaO + H₂. The recommendation is based on a measurement by Ager and Howard [14]. They also reported a significant Na + H₂O product channel and that a small fraction of the Na from this channel is in the 3^2P excited state. (Table 87-41, Note: 87-41) [Back to Table](#)
- J7. NaO + H₂O. The recommendation is based on a room temperature measurement by Ager and Howard [14] and a temperature dependent measurement by Cox and Plane [331] with the more extensive temperature dependent data favored. (Table: 06-2, Note: 06-2) [Back to Table](#)
- J8. NaO + NO. The recommendation is based on an indirect measurement reported by Ager et al. [15]. (Table 87-41, Note: 87-41) [Back to Table](#)
- J9. NaO + HCl. There is only one indirect measurement of the rate coefficient for this reaction, that from the study by Silver et al. [1189]. They indicate that the products are NaCl and OH, although some NaOH and Cl production is not ruled out. (Table: 85-37, Note: 85-37) [Back to Table](#)
- J10. NaO₂ + O. The recommendation is based on a flow tube study at 300 K by Helmer and Plane [568]. (Table: 94-26, Note: 94-26) [Back to Table](#)
- J11. NaO₂ + NO. This reaction is endothermic. The upper limit recommended is from an experimental study by Ager et al. [15]. (Table 87-41, Note: 87-41) [Back to Table](#)
- J12. NaO₂ + HCl. The recommendation is based on a measurement reported by Silver and Kolb [1186]. They indicated that the products are NaCl + HO₂, but NaOOH + Cl may be possible products. (Table 87-41, Note: 87-41) [Back to Table](#)
- J13. NaOH + HCl. The recommendation is based on the study by Silver et al. [1189], which is the only published study of this reaction. (Table: 85-37, Note: 85-37) [Back to Table](#)
- J14. NaHCO₃ + H. The recommendation is based on measurements at 307 and 227 K by Cox et al. [332]. It is consistent with an upper limit reported by Ager and Howard [13]. NEW ENTRY [Back to Table](#)

1.4 References

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