

SECTION 1. BIMOLECULAR REACTIONS

Table of Contents

SECTION 1. BIMOLECULAR REACTIONS.....	1-1
1.1 Introduction.....	1-1
1.2 Uncertainty Estimates.....	1-2
1.3 Notes to Table 1.....	1-31
1.4 References.....	1-93

Tables

Table 1-1. Rate Constants for Second-Order Reactions.....	1-5
---	-----

Figures

Figure 1-1. Symmetric and Asymmetric Error Limits.....	1-3
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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 1-1 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 1-1) is given in Arrhenius form:

$$k(T) = A \exp((-E/R)(1/T))$$

and contains the following information:

1. Reaction stoichiometry and products (if known). The pressure dependences are included, where appropriate.
2. Arrhenius A-factor.
3. Temperature dependence and associated uncertainty (“activation temperature” $E/R \pm g$).
4. Rate constant at 298 K.
5. Uncertainty factor at 298 K.
6. Note giving basis of recommendation and any other pertinent information.

1.2 Uncertainty Estimates

For bimolecular rate constants in Table 1-1, 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 $f(298 \text{ K})$ is the uncertainty in the rate constant at $T = 298 \text{ K}$. The quantity g has been defined in this evaluation for use with $f(298 \text{ K})$ 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, $f(298 \text{ K})$ 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 1-1 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 $f(298 \text{ K})$. Explicit equations are given below for the case where g is given as $(g + a, -b)$:

For $T > 298 \text{ K}$, multiply by the factor

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

and divide by the factor

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

For $T < 298 \text{ K}$, multiply by the factor

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

and divide by the factor

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

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

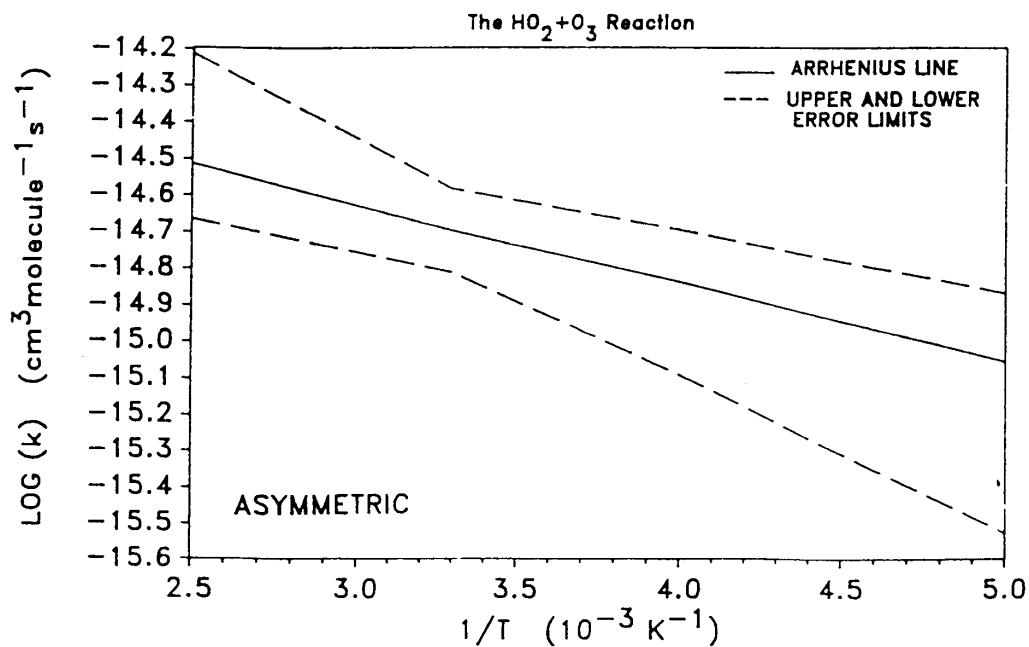
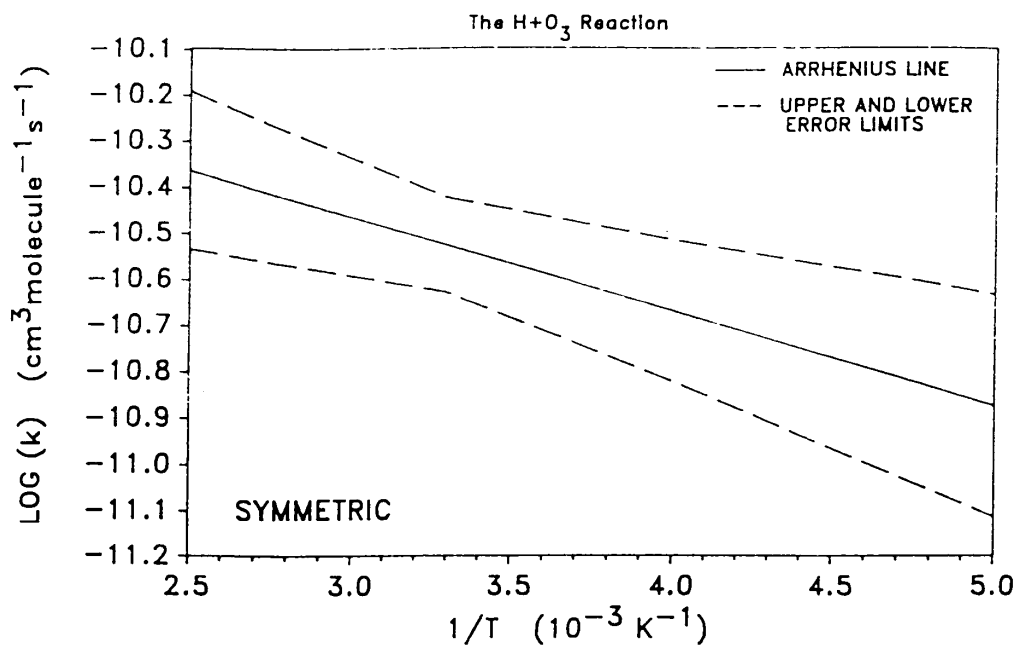


Figure 1-1. Symmetric and Asymmetric Error Limits

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 2-1)					
$O + O_3 \rightarrow O_2 + O_2$	8.0×10^{-12}	2060	8.0×10^{-15}	1.15	250	A1
O(¹D) Reactions						
$O(^1D) + O_2 \rightarrow O + O_2$	3.2×10^{-11}	-70	4.0×10^{-11}	1.2	100	A2, A3
$O(^1D) + O_3 \rightarrow O_2 + O_2$	1.2×10^{-10}	0	1.2×10^{-10}	1.3	100	A2, A4
$\quad \quad \quad \rightarrow O_2 + O + O$	1.2×10^{-10}	0	1.2×10^{-10}	1.3	100	A2, A4
$O(^1D) + H_2 \rightarrow OH + H$	1.1×10^{-10}	0	1.1×10^{-10}	1.1	100	A2, A5
$O(^1D) + H_2O \rightarrow OH + OH$	2.2×10^{-10}	0	2.2×10^{-10}	1.2	100	A2, A6
$O(^1D) + N_2 \rightarrow O + N_2$	1.8×10^{-11}	-110	2.6×10^{-11}	1.2	100	A2
$O(^1D) + N_2 \xrightarrow{M} N_2O$	(See Table 2-1)					
$O(^1D) + N_2O \rightarrow N_2 + O_2$	4.9×10^{-11}	0	4.9×10^{-11}	1.3	100	A2, A7
$\quad \quad \quad \rightarrow NO + NO$	6.7×10^{-11}	0	6.7×10^{-11}	1.3	100	A2, A7
$O(^1D) + NH_3 \rightarrow OH + NH_2$	2.5×10^{-10}	0	2.5×10^{-10}	1.3	100	A2, A8
$O(^1D) + CO_2 \rightarrow O + CO_2$	7.4×10^{-11}	-120	1.1×10^{-10}	1.2	100	A2
$O(^1D) + CH_4 \rightarrow \text{products}$	1.5×10^{-10}	0	1.5×10^{-10}	1.2	100	A2, A9
$O(^1D) + HCl \rightarrow \text{products}$	1.5×10^{-10}	0	1.5×10^{-10}	1.2	100	A10
$O(^1D) + HF \rightarrow OH + F$	1.4×10^{-10}	0	1.4×10^{-10}	2.0	100	A11
$O(^1D) + HBr \rightarrow \text{products}$	1.5×10^{-10}	0	1.5×10^{-10}	2.0	100	A12
$O(^1D) + Cl_2 \rightarrow \text{products}$	2.8×10^{-10}	0	2.8×10^{-10}	2.0	100	A13
$O(^1D) + CCl_2O \rightarrow \text{products}$	3.6×10^{-10}	0	3.6×10^{-10}	2.0	100	A2, A14
$O(^1D) + CClFO \rightarrow \text{products}$	1.9×10^{-10}	0	1.9×10^{-10}	2.0	100	A2, A14
$O(^1D) + CF_2O \rightarrow \text{products}$	7.4×10^{-11}	0	7.4×10^{-11}	2.0	100	A2, A14
$O(^1D) + CCl_4 \rightarrow \text{products}$ (CFC-10)	3.3×10^{-10}	0	3.3×10^{-10}	1.2	100	A2, A15

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
O(¹ D) + CH ₃ Br → products	1.8×10 ⁻¹⁰	0	1.8×10 ⁻¹⁰	1.3	100	A15, A16
O(¹ D) + CH ₂ Br ₂ → products	2.7×10 ⁻¹⁰	0	2.7×10 ⁻¹⁰	1.3	100	A15, A17
O(¹ D) + CHBr ₃ → products	6.6×10 ⁻¹⁰	0	6.6×10 ⁻¹⁰	1.5	100	A15, A18
O(¹ D) + CH ₃ F → products (HFC-41)	1.5×10 ⁻¹⁰	0	1.5×10 ⁻¹⁰	1.2	100	A15, A19
O(¹ D) + CH ₂ F ₂ → products (HFC-32)	5.1×10 ⁻¹¹	0	5.1×10 ⁻¹¹	1.3	100	A15, A20
O(¹ D) + CHF ₃ → products (HFC-23)	9.1×10 ⁻¹²	0	9.1×10 ⁻¹²	1.2	100	A15, A21
O(¹ D) + CHCl ₂ F → products (HCFC-21)	1.9×10 ⁻¹⁰	0	1.9×10 ⁻¹⁰	1.3	100	A15, A22
O(¹ D) + CHClF ₂ → products (HCFC-22)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	1.2	100	A15, A23
O(¹ D) + CCl ₃ F → products (CFC-11)	2.3×10 ⁻¹⁰	0	2.3×10 ⁻¹⁰	1.2	100	A2, A15
O(¹ D) + CCl ₂ F ₂ → products (CFC-12)	1.4×10 ⁻¹⁰	0	1.4×10 ⁻¹⁰	1.3	100	A2, A15
O(¹ D) + CClF ₃ → products (CFC-13)	8.7×10 ⁻¹¹	0	8.7×10 ⁻¹¹	1.3	100	A15, A24
O(¹ D) + CClBrF ₂ → products (Halon-1211)	1.5×10 ⁻¹⁰	0	1.5×10 ⁻¹⁰	1.3	100	A15, A25
O(¹ D) + CBr ₂ F ₂ → products (Halon-1202)	2.2×10 ⁻¹⁰	0	2.2×10 ⁻¹⁰	1.3	100	A15, A26
O(¹ D) + CBrF ₃ → products (Halon-1301)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	1.3	100	A15, A27
O(¹ D) + CF ₄ → CF ₄ + O (CFC-14)	–	–	2.0×10 ⁻¹⁴	1.5	–	A15, A28
O(¹ D) + CH ₃ CH ₂ F → products (HFC-161)	2.6×10 ⁻¹⁰	0	2.6×10 ⁻¹⁰	1.3	100	A15, A29
O(¹ D) + CH ₃ CHF ₂ → products (HFC-152a)	2.0×10 ⁻¹⁰	0	2.0×10 ⁻¹⁰	1.3	100	A15, A30
O(¹ D) + CH ₃ CCl ₂ F → products (HCFC-141b)	2.6×10 ⁻¹⁰	0	2.6×10 ⁻¹⁰	1.3	100	A15, A31
O(¹ D) + CH ₃ CClF ₂ → products (HCFC-142b)	2.2×10 ⁻¹⁰	0	2.2×10 ⁻¹⁰	1.3	100	A15, A32
O(¹ D) + CH ₃ CF ₃ → products (HFC-143a)	1.0×10 ⁻¹⁰	0	1.0×10 ⁻¹⁰	3.0	100	A15, A33
O(¹ D) + CH ₂ ClCClF ₂ → products (HCFC-132b)	1.6×10 ⁻¹⁰	0	1.6×10 ⁻¹⁰	2.0	100	A15, A34
O(¹ D) + CH ₂ ClCF ₃ → products (HCFC-133a)	1.2×10 ⁻¹⁰	0	1.2×10 ⁻¹⁰	1.3	100	A15, A35
O(¹ D) + CH ₂ FCF ₃ → products (HFC-134a)	4.9×10 ⁻¹¹	0	4.9×10 ⁻¹¹	1.3	100	A15, A36
O(¹ D) + CHCl ₂ CF ₃ → products (HCFC-123)	2.0×10 ⁻¹⁰	0	2.0×10 ⁻¹⁰	1.3	100	A15, A37
O(¹ D) + CHClFCF ₃ → products (HCFC-124)	8.6×10 ⁻¹¹	0	8.6×10 ⁻¹¹	1.3	100	A15, A38

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
O(¹ D) + CHF ₂ CF ₃ → products (HFC-125)	1.2×10 ⁻¹⁰	0	1.2×10 ⁻¹⁰	2.0	100	A15, A39
O(¹ D) + CCl ₃ CF ₃ → products (CFC-113a)	2×10 ⁻¹⁰	0	2×10 ⁻¹⁰	2.0	100	A15, A40
O(¹ D) + CCl ₂ FCClF ₂ → products (CFC-113)	2×10 ⁻¹⁰	0	2×10 ⁻¹⁰	2.0	100	A15, A41
O(¹ D) + CCl ₂ FCF ₃ → products (CFC-114a)	1×10 ⁻¹⁰	0	1×10 ⁻¹⁰	2.0	100	A15, A42
O(¹ D) + CClF ₂ CClF ₂ → products (CFC-114)	1.3×10 ⁻¹⁰	0	1.3×10 ⁻¹⁰	1.3	100	A15, A43
O(¹ D) + CClF ₂ CF ₃ → products (CFC-115)	5×10 ⁻¹¹	0	5×10 ⁻¹¹	1.3	100	A15, A44
O(¹ D) + CBrF ₂ CBrF ₂ → products (Halon-2402)	1.6×10 ⁻¹⁰	0	1.6×10 ⁻¹⁰	1.3	100	A15, A45
O(¹ D) + CF ₃ CF ₃ → O + CF ₃ CF ₃ (CFC-116)	–	–	1.5×10 ⁻¹³	1.5	–	A15, A46
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	A15, A47
O(¹ D) + c-C ₄ F ₈ → products	–	–	8×10 ⁻¹³	1.3	–	A15, A48
O(¹ D) + CF ₃ CHFCHFCF ₂ CF ₃ → products (HFC-43-10mee)	2.1×10 ⁻¹⁰	0	2.1×10 ⁻¹⁰	4	100	A15, A49
O(¹ D) + C ₅ F ₁₂ → products (CFC-41-12)	–	–	3.9×10 ⁻¹³	2	–	A15, A50
O(¹ D) + C ₆ F ₁₄ → products (CFC-51-14)	–	–	1×10 ⁻¹²	2	–	A15, A51
O(¹ D) + 1,2-(CF ₃) ₂ C-C ₄ F ₆ → products	–	–	2.8×10 ⁻¹³	2	–	A15, A52
O(¹ D) + SF ₆ → products	–	–	1.8×10 ⁻¹⁴	1.5	–	A53
Singlet O₂ Reactions						
O ₂ (¹ Δ) + O → products	–	–	<2×10 ⁻¹⁶	–	–	A54
O ₂ (¹ Δ) + O ₂ → products	3.6×10 ⁻¹⁸	220	1.7×10 ⁻¹⁸	1.2	100	A55
O ₂ (¹ Δ) + O ₃ → O + 2O ₂	5.2×10 ⁻¹¹	2840	3.8×10 ⁻¹⁵	1.2	500	A56
O ₂ (¹ Δ) + H ₂ O → products	–	–	4.8×10 ⁻¹⁸	1.5	–	A57
O ₂ (¹ Δ) + N → NO + O	–	–	<9×10 ⁻¹⁷	–	–	A58
O ₂ (¹ Δ) + N ₂ → products	–	–	<10 ⁻²⁰	–	–	A59
O ₂ (¹ Δ) + CO ₂ → products	–	–	<2×10 ⁻²⁰	–	–	A60
O ₂ (¹ Σ) + O → products	–	–	8×10 ⁻¹⁴	5.0	–	A61
O ₂ (¹ Σ) + O ₂ → products	–	–	3.9×10 ⁻¹⁷	1.5	–	A62

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$O_2(^1\Sigma) + O_3 \rightarrow \text{products}$	2.2×10^{-11}	0	2.2×10^{-11}	1.2	200	A63
$O_2(^1\Sigma) + H_2O \rightarrow \text{products}$	–	–	5.4×10^{-12}	1.3	–	A64
$O_2(^1\Sigma) + N \rightarrow \text{products}$	–	–	$<10^{-13}$	–	–	A65
$O_2(^1\Sigma) + N_2 \rightarrow \text{products}$	2.1×10^{-15}	0	2.1×10^{-15}	1.2	200	A66
$O_2(^1\Sigma) + CO_2 \rightarrow \text{products}$	4.2×10^{-13}	0	4.2×10^{-13}	1.2	200	A67
HO_x Reactions						
$O + OH \rightarrow O_2 + H$	2.2×10^{-11}	–120	3.3×10^{-11}	1.2	100	B 1
$O + HO_2 \rightarrow OH + O_2$	3.0×10^{-11}	–200	5.9×10^{-11}	1.1	50	B 2
$O + H_2O_2 \rightarrow OH + HO_2$	1.4×10^{-12}	2000	1.7×10^{-15}	2.0	1000	B 3
$H + O_2 \xrightarrow{M} HO_2$	(See Table 2-1)					
$H + O_3 \rightarrow OH + O_2$	1.4×10^{-10}	470	2.9×10^{-11}	1.25	200	B 4
$H + HO_2 \rightarrow \text{products}$	8.1×10^{-11}	0	8.1×10^{-11}	1.3	100	B 5
$OH + O_3 \rightarrow HO_2 + O_2$	1.7×10^{-12}	940	7.3×10^{-14}	1.2	80	B 6
$OH + H_2 \rightarrow H_2O + H$	5.5×10^{-12}	2000	6.7×10^{-15}	1.1	100	B 7
$OH + HD \rightarrow \text{products}$	5.0×10^{-12}	2130	4.0×10^{-15}	1.2	200	B 8
$OH + OH \rightarrow H_2O + O$	4.2×10^{-12}	240	1.9×10^{-12}	1.4	240	B 9
$\xrightarrow{M} H_2O_2$	(See Table 2-1)					
$OH + HO_2 \rightarrow H_2O + O_2$	4.8×10^{-11}	–250	1.1×10^{-10}	1.3	100	B10
$OH + H_2O_2 \rightarrow H_2O + HO_2$	2.9×10^{-12}	160	1.7×10^{-12}	1.15	50	B11
$HO_2 + O_3 \rightarrow OH + 2O_2$	1.0×10^{-14}	490	1.9×10^{-15}	1.15	+160 –80	B12
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	2.3×10^{-13}	–600	1.7×10^{-12}	1.3	200	B13
$\xrightarrow{M} H_2O_2 + O_2$	$1.7 \times 10^{-33}[M]$	–1000	$4.9 \times 10^{-32}[M]$	1.3	400	B13
NO_x Reactions						
$O + NO \xrightarrow{M} NO_2$	(See Table 2-1)					
$O + NO_2 \rightarrow NO + O_2$	5.6×10^{-12}	–180	1.0×10^{-11}	1.1	50	C1

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$O + NO_2 \xrightarrow{M} NO_3$	(See Table 2-1)					
$O + NO_3 \rightarrow O_2 + NO_2$	1.0×10^{-11}	0	1.0×10^{-11}	1.5	150	C 2
$O + N_2O_5 \rightarrow \text{products}$			$<3.0 \times 10^{-16}$			C 3
$O + HNO_3 \rightarrow OH + NO_3$			$<3.0 \times 10^{-17}$			C 4
$O + HO_2NO_2 \rightarrow \text{products}$	7.8×10^{-11}	3400	8.6×10^{-16}	3.0	750	C 5
$H + NO_2 \rightarrow OH + NO$	4.0×10^{-10}	340	1.3×10^{-10}	1.3	300	C 6
$OH + NO \xrightarrow{M} HONO$	(See Table 2-1)					
$OH + NO_2 \xrightarrow{M} HNO_3$	(See Table 2-1)					
$OH + NO_3 \rightarrow \text{products}$			2.2×10^{-11}	1.5		C 7
$OH + HONO \rightarrow H_2O + NO_2$	1.8×10^{-11}	390	4.5×10^{-12}	1.5	+200 -500	C 8
$OH + HNO_3 \rightarrow H_2O + NO_3$	(See Note)			1.2		C 9
$OH + HO_2NO_2 \rightarrow \text{products}$	1.3×10^{-12}	-380	4.6×10^{-12}	1.3	+270 -500	C10
$OH + NH_3 \rightarrow H_2O + NH_2$	1.7×10^{-12}	710	1.6×10^{-13}	1.2	200	C11
$HO_2 + NO \rightarrow NO_2 + OH$	3.5×10^{-12}	-250	8.1×10^{-12}	1.15	50	C12
$HO_2 + NO_2 \xrightarrow{M} HO_2NO_2$	(See Table 2-1)					
$HO_2 + NO_2 \rightarrow HONO + O_2$	(See Note)					C13
$HO_2 + NO_3 \rightarrow \text{products}$			3.5×10^{-12}	1.5		C14
$HO_2 + NH_2 \rightarrow \text{products}$			3.4×10^{-11}	2.0		C15
$N + O_2 \rightarrow NO + O$	1.5×10^{-11}	3600	8.5×10^{-17}	1.25	400	C16
$N + O_3 \rightarrow NO + O_2$			$<2.0 \times 10^{-16}$			C17
$N + NO \rightarrow N_2 + O$	2.1×10^{-11}	-100	3.0×10^{-11}	1.3	100	C18
$N + NO_2 \rightarrow N_2O + O$	5.8×10^{-12}	-220	1.2×10^{-11}	1.5	100	C19
$NO + O_3 \rightarrow NO_2 + O_2$	3.0×10^{-12}	1500	1.9×10^{-14}	1.1	200	C20
$NO + NO_3 \rightarrow 2NO_2$	1.5×10^{-11}	-170	2.6×10^{-11}	1.3	100	C21
$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2×10^{-13}	2450	3.2×10^{-17}	1.15	150	C22

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
NO ₂ + NO ₃ → NO + NO ₂ + O ₂	(See Note)					C23
NO ₂ + NO ₃ \xrightarrow{M} N ₂ O ₅	(See Table 2-1)					
NO ₃ + NO ₃ → 2NO ₂ + O ₂	8.5×10 ⁻¹³	2450	2.3×10 ⁻¹⁶	1.5	500	C24
NH ₂ + O ₂ → products			<6.0×10 ⁻²¹			C25
NH ₂ + O ₃ → products	4.3×10 ⁻¹²	930	1.9×10 ⁻¹³	3.0	500	C26
NH ₂ + NO → products	4.0×10 ⁻¹²	-450	1.8×10 ⁻¹¹	1.3	150	C27
NH ₂ + NO ₂ → products	2.1×10 ⁻¹²	-650	1.9×10 ⁻¹¹	3.0	250	C28
NH + NO → products	4.9×10 ⁻¹¹	0	4.9×10 ⁻¹¹	1.5	300	C29
NH + NO ₂ → products	3.5×10 ⁻¹³	-1140	1.6×10 ⁻¹¹	2.0	500	C30
O ₃ + HNO ₂ → O ₂ + HNO ₃			<5.0×10 ⁻¹⁹			C31
N ₂ O ₅ + H ₂ O → 2HNO ₃			<2.0×10 ⁻²¹			C32
N ₂ (A,v) + O ₂ → products			2.5×10 ⁻¹² , v=0	1.5		C33
N ₂ (A,v) + O ₃ → products			4.1×10 ⁻¹¹ , v=0	2.0		C34
Reactions of Organic Compounds						
O + CH ₃ → products	1.1×10 ⁻¹⁰	0	1.1×10 ⁻¹⁰	1.3	250	D 1
O + HCN → products	1.0×10 ⁻¹¹	4000	1.5×10 ⁻¹⁷	10	1000	D 2
O + C ₂ H ₂ → products	3.0×10 ⁻¹¹	1600	1.4×10 ⁻¹³	1.3	250	D 3
O + H ₂ CO → products	3.4×10 ⁻¹¹	1600	1.6×10 ⁻¹³	1.25	250	D 4
O + CH ₃ CHO → CH ₃ CO + OH	1.8×10 ⁻¹¹	1100	4.5×10 ⁻¹³	1.25	200	D 5
O ₃ + C ₂ H ₂ → products	1.0×10 ⁻¹⁴	4100	1.0×10 ⁻²⁰	3	500	D 6
O ₃ + C ₂ H ₄ → products	1.2×10 ⁻¹⁴	2630	1.7×10 ⁻¹⁸	1.25	100	D 7
O ₃ + C ₃ H ₆ → products	6.5×10 ⁻¹⁵	1900	1.1×10 ⁻¹⁷	1.2	200	D 8
OH + CO → Products	1.5×10 ⁻¹³ ×(1+0.6P _{atm})	0	1.5×10 ⁻¹³ ×(1+0.6P _{atm})	1.3	300	D 9
OH + CH ₄ → CH ₃ + H ₂ O	2.45×10 ⁻¹²	1775	6.3×10 ⁻¹⁵	1.1	100	D10
OH + ¹³ CH ₄ → ¹³ CH ₃ + H ₂ O	(See Note)					D11

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CH ₃ D → products	3.5×10 ⁻¹²	1950	5.0×10 ⁻¹⁵	1.15	200	D12
OH + H ₂ CO → H ₂ O + HCO	9.0×10 ⁻¹²	0	9.0×10 ⁻¹²	1.2	100	D13
OH + CH ₃ OH → products	7.3×10 ⁻¹²	620	9.1×10 ⁻¹³	1.15	250	D14
OH + CH ₃ OOH → products	3.8×10 ⁻¹²	-200	7.4×10 ⁻¹²	1.4	150	D15
OH + HC(O)OH → products	4.0×10 ⁻¹³	0	4.0×10 ⁻¹³	1.2	100	D16
OH + HCN → products	1.2×10 ⁻¹³	400	3.1×10 ⁻¹⁴	3	150	D17
OH + C ₂ H ₂ \xrightarrow{M} products	(See Table 2-1)					
OH + C ₂ H ₄ \xrightarrow{M} products	(See Table 2-1)					
OH + C ₂ H ₆ → H ₂ O + C ₂ H ₅	8.7 × 10 ⁻¹²	1070	2.4×10 ⁻¹³	1.1	100	D18
OH + C ₃ H ₈ → H ₂ O + C ₃ H ₇	1.0 × 10 ⁻¹¹	660	1.1×10 ⁻¹²	1.2	100	D19
OH + CH ₃ CHO → CH ₃ CO + H ₂ O	5.6×10 ⁻¹²	-270	1.4×10 ⁻¹¹	1.2	200	D20
OH + C ₂ H ₅ OH → products	6.9×10 ⁻¹²	230	3.2×10 ⁻¹²	1.2	100	D21
OH + CH ₃ C(O)OH → products	4.0×10 ⁻¹³	-200	8.0×10 ⁻¹³	1.25	200	D22
OH + CH ₃ C(O)CH ₃ → products	(See Note)					D23
OH + CH ₃ CN → products	7.8×10 ⁻¹³	1050	2.3×10 ⁻¹⁴	1.5	200	D24
OH+ CH ₃ ONO ₂ → products	5.0×10 ⁻¹³	810	3.3×10 ⁻¹⁴	1.5	250	D25
OH + CH ₃ C(O)O ₂ NO ₂ (PAN) → products			<4 × 10 ⁻¹⁴			D26
OH+ C ₂ H ₅ ONO ₂ → products	6.8×10 ⁻¹³	320	2.3×10 ⁻¹³	1.5	200	D27
OH + 1-C ₃ H ₇ ONO ₂ → products	7.1×10 ⁻¹³	0	7.1×10 ⁻¹³	1.5	200	D28
OH + 2-C ₃ H ₇ ONO ₂ → products	1.2×10 ⁻¹²	320	4.1×10 ⁻¹³	1.5	200	D29
HO ₂ + CH ₂ O → adduct	6.7×10 ⁻¹⁵	-600	5.0×10 ⁻¹⁴	5	600	D30
HO ₂ + CH ₃ O ₂ → CH ₃ OOH + O ₂	4.1×10 ⁻¹³	-750	5.2×10 ⁻¹²	1.3	150	D31
HO ₂ + C ₂ H ₅ O ₂ → C ₂ H ₅ OOH + O ₂	7.5×10 ⁻¹³	-700	8.0×10 ⁻¹²	1.5	250	D32
HO ₂ + CH ₃ C(O)O ₂ → products	4.3×10 ⁻¹³	-1040	1.4×10 ⁻¹¹	2	500	D33
HO ₂ + CH ₃ C(O)CH ₂ O ₂ → products	8.6×10 ⁻¹³	-700	9.0×10 ⁻¹²	2	300	D34

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
NO ₃ + CO → products			<4.0×10 ⁻¹⁹			D35
NO ₃ + CH ₂ O → products			5.8×10 ⁻¹⁶	1.3		D36
NO ₃ + CH ₃ CHO → products	1.4×10 ⁻¹²	1900	2.4×10 ⁻¹⁵	1.3	300	D37
CH ₃ + O ₂ → products			<3.0×10 ⁻¹⁶			D38
CH ₃ + O ₂ \xrightarrow{M} CH ₃ O ₂	(See Table 2-1)					
CH ₃ + O ₃ → products	5.4×10 ⁻¹²	220	2.6×10 ⁻¹²	2	150	D39
HCO + O ₂ → CO + HO ₂	5.2×10 ⁻¹²	0	5.2×10 ⁻¹²	1.4	100	D40
CH ₂ OH + O ₂ → CH ₂ O + HO ₂	9.1×10 ⁻¹²	0	9.1×10 ⁻¹²	1.3	200	D41
CH ₃ O + O ₂ → CH ₂ O + HO ₂	3.9×10 ⁻¹⁴	900	1.9×10 ⁻¹⁵	1.5	300	D42
CH ₃ O + NO → CH ₂ O + HNO	(See Note)					D43
CH ₃ O + NO \xrightarrow{M} CH ₃ ONO	(See Table 2-1)					
CH ₃ O + NO ₂ → CH ₂ O + HONO	1.1 × 10 ⁻¹¹	1200	2.0 × 10 ⁻¹³	5	600	D44
CH ₃ O + NO ₂ \xrightarrow{M} CH ₃ ONO ₂	(See Table 2-1)					
CH ₃ O ₂ + O ₃ → products	2.9×10 ⁻¹⁶	1000	1.0×10 ⁻¹⁷	3	500	D45
CH ₃ O ₂ + CH ₃ O ₂ → products	9.5×10 ⁻¹⁴	-390	3.5×10 ⁻¹³	1.2	100	D46
CH ₃ O ₂ + NO → CH ₃ O + NO ₂	2.8×10 ⁻¹²	-300	7.7×10 ⁻¹²	1.15	100	D47
CH ₃ O ₂ + NO ₂ \xrightarrow{M} CH ₃ O ₂ NO ₂	(See Table 2-1)					
CH ₃ O ₂ + CH ₃ C(O)O ₂ → products	2.0×10 ⁻¹²	-500	1.1×10 ⁻¹¹	1.5	250	D48
CH ₃ O ₂ + CH ₃ C(O)CH ₂ O ₂ → products	7.5×10 ⁻¹³	-500	4.0×10 ⁻¹²	2	300	D49
C ₂ H ₅ + O ₂ → C ₂ H ₄ + HO ₂			<2.0×10 ⁻¹⁴			D50
C ₂ H ₅ + O ₂ \xrightarrow{M} C ₂ H ₅ O ₂	(See Table 2-1)					
C ₂ H ₅ O + O ₂ → CH ₃ CHO + HO ₂	6.3 × 10 ⁻¹⁴	550	1.0×10 ⁻¹⁴	1.5	200	D51
C ₂ H ₅ O + NO \xrightarrow{M} products	(See Table 2-1)					
C ₂ H ₅ O + NO ₂ \xrightarrow{M} products	(See Table 2-1)					
C ₂ H ₅ O ₂ + C ₂ H ₅ O ₂ → products	6.8×10 ⁻¹⁴	0	6.8×10 ⁻¹⁴	2	300	D52

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$C_2H_5O_2 + NO \rightarrow \text{products}$	2.6×10^{-12}	-365	8.7×10^{-12}	1.2	150	D53
$CH_3C(O)O_2 + CH_3C(O)O_2 \rightarrow \text{products}$	2.9×10^{-12}	-500	1.5×10^{-11}	1.5	150	D54
$CH_3C(O)O_2 + NO \rightarrow \text{products}$	8.1×10^{-12}	-270	2.0×10^{-11}	1.5	100	D55
$CH_3C(O)O_2 + NO_2 \xrightarrow{M} \text{products}$	(See Table 2-1)					
$CH_3C(O)CH_2O_2 + NO \rightarrow \text{products}$	2.9×10^{-12}	-300	8.0×10^{-12}	1.5	300	D56
FO_x Reactions						
$O + FO \rightarrow F + O_2$	2.7×10^{-11}	0	2.7×10^{-11}	3.0	250	E 1
$O + FO_2 \rightarrow FO + O_2$	5.0×10^{-11}	0	5.0×10^{-11}	5.0	250	E 2
$OH + CH_3F \rightarrow CH_2F + H_2O$ (HFC-41)	2.5×10^{-12}	1430	2.1×10^{-14}	1.15	150	E 3
$OH + CH_2F_2 \rightarrow CHF_2 + H_2O$ (HFC-32)	1.7×10^{-12}	1500	1.1×10^{-14}	1.15	150	E 4
$OH + CHF_3 \rightarrow CF_3 + H_2O$ (HFC-23)	6.3×10^{-13}	2300	2.8×10^{-16}	1.2	200	E 5
$OH + CH_3CH_2F \rightarrow \text{products}$ (HFC-161)	2.5×10^{-12}	730	2.2×10^{-13}	1.15	150	E 6
$OH + CH_3CHF_2 \rightarrow \text{products}$ (HFC-152a)	9.4×10^{-13}	990	3.4×10^{-14}	1.1	100	E 7
$OH + CH_2FCH_2F \rightarrow CHFCH_2F + H_2O$ (HFC-152)	1.1×10^{-12}	730	9.7×10^{-14}	1.1	150	E 8
$OH + CH_3CF_3 \rightarrow CH_2CF_3 + H_2O$ (HFC-143a)	1.1×10^{-12}	2010	1.3×10^{-15}	1.1	100	E 9
$OH + CH_2FCHF_2 \rightarrow \text{products}$ (HFC-143)	3.9×10^{-12}	1620	1.7×10^{-14}	1.2	200	E10
$OH + CH_2FCF_3 \rightarrow CHF_2CF_3 + H_2O$ (HFC-134a)	1.05×10^{-12}	1630	4.4×10^{-15}	1.1	200	E11
$OH + CHF_2CHF_2 \rightarrow CF_2CHF_2 + H_2O$ (HFC-134)	1.6×10^{-12}	1660	6.1×10^{-15}	1.2	200	E12
$OH + CHF_2CF_3 \rightarrow CF_2CF_3 + H_2O$ (HFC-125)	6.0×10^{-13}	1700	2.0×10^{-15}	1.2	150	E13
$OH + CH_3CHFCH_3 \rightarrow \text{products}$ (HFC-281ea)	3.0×10^{-12}	490	5.8×10^{-13}	1.2	100	E14
$OH + CF_3CH_2CH_3 \rightarrow \text{products}$ (HFC-263fb)	–	–	4.2×10^{-14}	1.5	–	E15
$OH + CH_2FCF_2CHF_2 \rightarrow \text{products}$ (HFC-245ca)	2.1×10^{-12}	1620	9.2×10^{-15}	1.2	150	E16
$OH + CHF_2CHFCHF_2 \rightarrow \text{products}$ (HFC-245ea)	–	–	1.6×10^{-14}	2.0	–	E17
$OH + CF_3CHFCH_2F \rightarrow \text{products}$ (HFC-245eb)	–	–	1.5×10^{-14}	2.0	–	E18
$OH + CHF_2CH_2CF_3 \rightarrow \text{products}$ (HFC-245fa)	6.1×10^{-13}	1330	7.0×10^{-15}	1.2	150	E19

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
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
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			<2×10 ⁻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

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
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
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

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{CF}_3\text{O} + \text{H}_2\text{O} \rightarrow \text{OH} + \text{CF}_3\text{OH}$	3×10^{-12}	>3600	$<2 \times 10^{-17}$	1.2	–	E64
$\text{CF}_3\text{O} + \text{NO} \rightarrow \text{CF}_2\text{O} + \text{FNO}$	3.7×10^{-11}	–110	5.4×10^{-11}		70	E65
$\text{CF}_3\text{O} + \text{NO}_2 \rightarrow \text{products}$ $\xrightarrow{\text{M}} \text{CF}_3\text{ONO}_2$	(See Note) (See Table 2-1)					E66
$\text{CF}_3\text{O} + \text{CO} \rightarrow \text{products}$ $\xrightarrow{\text{M}} \text{CF}_3\text{OCO}$	(See Table 2-1)		$<2 \times 10^{-15}$			E67
$\text{CF}_3\text{O} + \text{CH}_4 \rightarrow \text{CH}_3 + \text{CF}_3\text{OH}$	2.6×10^{-12}	1420	2.2×10^{-14}	1.1	200	E68
$\text{CF}_3\text{O} + \text{C}_2\text{H}_6 \rightarrow \text{C}_2\text{H}_5 + \text{CF}_3\text{OH}$	4.9×10^{-12}	400	1.3×10^{-12}	1.2	100	E69
$\text{CF}_3\text{O}_2 + \text{O}_3 \rightarrow \text{CF}_3\text{O} + 2\text{O}_2$			$<3 \times 10^{-15}$			E70
$\text{CF}_3\text{O}_2 + \text{CO} \rightarrow \text{CF}_3\text{O} + \text{CO}_2$			$<5 \times 10^{-16}$			E71
$\text{CF}_3\text{O}_2 + \text{NO} \rightarrow \text{CF}_3\text{O} + \text{NO}_2$	5.4×10^{-12}	–320	1.6×10^{-11}	1.1	150	E72
$\text{CF}_3\text{O}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{CF}_3\text{O}_2\text{NO}_2$	(See Table 2-1)					
ClO_x Reactions						
$\text{O} + \text{ClO} \rightarrow \text{Cl} + \text{O}_2$	3.0×10^{-11}	–70	3.8×10^{-11}	1.15	70	F 1
$\text{O} + \text{OCIO} \rightarrow \text{ClO} + \text{O}_2$	2.4×10^{-12}	960	1.0×10^{-13}	2.0	300	F 2
$\text{O} + \text{OCIO} \xrightarrow{\text{M}} \text{ClO}_3$	(See Table 2-1)					
$\text{O} + \text{Cl}_2\text{O} \rightarrow \text{ClO} + \text{ClO}$	2.7×10^{-11}	530	4.5×10^{-12}	1.3	150	F 3
$\text{O} + \text{HCl} \rightarrow \text{OH} + \text{Cl}$	1.0×10^{-11}	3300	1.5×10^{-16}	2.0	350	F 4
$\text{O} + \text{HOCl} \rightarrow \text{OH} + \text{ClO}$	1.7×10^{-13}	0	1.7×10^{-13}	3.0	300	F 5
$\text{O} + \text{ClONO}_2 \rightarrow \text{products}$	2.9×10^{-12}	800	2.0×10^{-13}	1.5	200	F 6
$\text{O}_3 + \text{OCIO} \rightarrow \text{products}$	2.1×10^{-12}	4700	3.0×10^{-19}	2.5	1000	F 7
$\text{O}_3 + \text{Cl}_2\text{O}_2 \rightarrow \text{products}$	–	–	$<1.0 \times 10^{-19}$	–	–	F 8
$\text{OH} + \text{Cl}_2 \rightarrow \text{HOCl} + \text{Cl}$	1.4×10^{-12}	900	6.7×10^{-14}	1.2	400	F 9
$\text{OH} + \text{ClO} \rightarrow \text{Cl} + \text{HO}_2$ $\rightarrow \text{HCl} + \text{O}_2$	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
$\text{OH} + \text{OCIO} \rightarrow \text{HOCl} + \text{O}_2$	4.5×10^{-13}	–800	6.8×10^{-12}	2.0	200	F11

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
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
OH + CF ₂ Cl ₂ → products (CFC-12)	~1.0×10 ⁻¹²	>3600	<6.0×10 ⁻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	1.6×10 ⁻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

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
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	-	-	<2.0×10 ⁻²¹	-	-	F47
NO + OClO → NO ₂ + ClO	2.5×10 ⁻¹²	600	3.4×10 ⁻¹³	2.0	300	F48
NO + Cl ₂ O ₂ → products	-	-	<2.0×10 ⁻¹⁴	-	-	F49
NO ₃ + OClO \xrightarrow{M} O ₂ ClONO ₂	(See Table 2-1)					
NO ₃ + HCl → HNO ₃ + Cl	-	-	<5.0×10 ⁻¹⁷	-	-	F50
HO ₂ NO ₂ + HCl → products	-	-	<1.0×10 ⁻²¹	-	-	F51
Cl + O ₂ \xrightarrow{M} ClOO	(See Table 2-1)					
Cl + O ₃ → ClO + O ₂	2.3×10 ⁻¹¹	200	1.2×10 ⁻¹¹	1.15	100	F52
Cl + H ₂ → HCl + H	3.7×10 ⁻¹¹	2300	1.6×10 ⁻¹⁴	1.25	200	F53
Cl + H ₂ O ₂ → HCl + HO ₂	1.1×10 ⁻¹¹	980	4.1×10 ⁻¹³	1.3	300	F54
Cl + NO \xrightarrow{M} NOCl	(See Table 2-1)					
Cl + NO ₂ \xrightarrow{M} ClONO (ClONO ₂)	(See Table 2-1)					
Cl + NO ₃ → ClO + NO ₂	2.4×10 ⁻¹¹	0	2.4×10 ⁻¹¹	1.5	400	F55
Cl + N ₂ O → ClO + N ₂	(See Note)					F56

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Cl + HNO ₃ → products	–	–	<2.0×10 ⁻¹⁶	–	–	F57
Cl + HO ₂ NO ₂ → products			<1×10 ⁻¹³			F58
Cl + CO \xrightarrow{M} ClCO	(See Table 2-1)					
Cl + CH ₄ → HCl + CH ₃	9.6×10 ⁻¹²	1360	1.0×10 ⁻¹³	1.05	75	F59
Cl + CH ₃ D → products	–	–	7.4×10 ⁻¹⁴	2.0	–	F60
Cl + H ₂ CO → HCl + HCO	8.1×10 ⁻¹¹	30	7.3×10 ⁻¹¹	1.15	100	F61
Cl + HC(O)OH → products			2.0×10 ⁻¹³	1.5		F62
Cl + CH ₃ O ₂ → products	–	–	1.6×10 ⁻¹⁰	1.5	–	F63
Cl + CH ₃ OH → CH ₂ OH + HCl	5.5×10 ⁻¹¹	0	5.5×10 ⁻¹¹	1.2	100	F64
Cl + CH ₃ OOH → products			5.7×10 ⁻¹¹	2.0		F65
Cl + CH ₃ ONO ₂ → products	1.3×10 ⁻¹¹	1200	2.3×10 ⁻¹³	1.5	300	F66
Cl + C ₂ H ₂ \xrightarrow{M} ClC ₂ H ₂	(See Table 2-1)					
Cl + C ₂ H ₄ \xrightarrow{M} ClC ₂ H ₄	(See Table 2-1)					
Cl + C ₂ H ₆ → HCl + C ₂ H ₅	7.7×10 ⁻¹¹	90	5.7×10 ⁻¹¹	1.1	90	F67
Cl + C ₂ H ₅ O ₂ → ClO + C ₂ H ₅ O	–	–	7.4×10 ⁻¹¹	2.0	–	F68
→ HCl + C ₂ H ₄ O ₂		–	7.7×10 ⁻¹¹	2.0	–	F68
Cl + CH ₃ CH ₂ OH → products	9.6×10 ⁻¹¹	0	9.6×10 ⁻¹¹	1.2	100	F69
Cl + CH ₃ C(O)OH → products			2.8×10 ⁻¹⁴	2.0		F70
Cl + CH ₃ CN → products	1.6×10 ⁻¹¹	2140	1.2×10 ⁻¹⁴	2.0	300	F71
Cl + C ₂ H ₅ ONO ₂ → products	1.5×10 ⁻¹¹	400	3.9×10 ⁻¹²	1.5	200	F72
Cl + CH ₃ CO ₃ NO ₂ → products	–	–	<1×10 ⁻¹⁴		–	F73
Cl + C ₃ H ₈ → HCl + C ₃ H ₇	1.2×10 ⁻¹⁰	–40	1.4×10 ⁻¹⁰	1.3	250	F74
Cl + CH ₃ C(O)CH ₃ → CH ₃ C(O)CH ₂ + HCl	7.7×10 ⁻¹¹	1000	2.7×10 ⁻¹²	1.3	500	F75
Cl + C ₂ H ₅ CO ₃ NO ₂ → products			1.1×10 ⁻¹²	2.0		F76
Cl + 1-C ₃ H ₇ ONO ₂ → products	4.5×10 ⁻¹¹	200	2.3×10 ⁻¹¹	1.5	200	F77

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Cl + 2-C ₃ H ₇ ONO ₂ → products	2.3×10 ⁻¹¹	400	6.0×10 ⁻¹²	2.0	200	F78
Cl + OCIO → ClO + ClO	3.4×10 ⁻¹¹	-160	5.8×10 ⁻¹¹	1.25	200	F79
Cl + ClOO → Cl ₂ + O ₂	2.3×10 ⁻¹⁰	0	2.3×10 ⁻¹⁰	3.0	250	F80
→ ClO + ClO	1.2×10 ⁻¹¹	0	1.2×10 ⁻¹¹	3.0	250	F80
Cl + Cl ₂ O → Cl ₂ + ClO	6.2×10 ⁻¹¹	-130	9.6×10 ⁻¹¹	1.2	130	F81
Cl + Cl ₂ O ₂ → products	-	-	1.0×10 ⁻¹⁰	2.0	-	F82
Cl + HOCl → products	2.5×10 ⁻¹²	130	1.6×10 ⁻¹²	1.5	250	F83
Cl + ClNO → NO + Cl ₂	5.8×10 ⁻¹¹	-100	8.1×10 ⁻¹¹	1.5	200	F84
Cl + ClONO ₂ → products	6.5×10 ⁻¹²	-135	1.0×10 ⁻¹¹	1.2	50	F85
Cl + CH ₃ Cl → CH ₂ Cl + HCl	3.2×10 ⁻¹¹	1250	4.8×10 ⁻¹³	1.2	200	F86
Cl + CH ₂ Cl ₂ → HCl + CHCl ₂	3.1×10 ⁻¹¹	1350	3.3×10 ⁻¹³	1.5	500	F87
Cl + CHCl ₃ → HCl + CCl ₃	8.2×10 ⁻¹²	1325	9.6×10 ⁻¹⁴	1.3	300	F88
Cl + CH ₃ F → HCl + CH ₂ F (HFC-41)	2.0×10 ⁻¹¹	1200	3.5×10 ⁻¹³	1.3	500	F89
Cl + CH ₂ F ₂ → HCl + CHF ₂ (HFC-32)	1.2×10 ⁻¹¹	1630	5.0×10 ⁻¹⁴	1.5	500	F90
Cl + CF ₃ H → HCl + CF ₃ (HFC-23)	-	-	3.0×10 ⁻¹⁸	5.0	-	F91
Cl + CH ₂ FCI → HCl + CHFCl (HCFC-31)	1.2×10 ⁻¹¹	1390	1.1×10 ⁻¹³	2.0	500	F92
Cl + CHFCl ₂ → HCl + CFCl ₂ (HCFC-21)	5.5×10 ⁻¹²	1675	2.0×10 ⁻¹⁴	1.3	200	F93
Cl + CHF ₂ Cl → HCl + CF ₂ Cl (HCFC-22)	5.9×10 ⁻¹²	2430	1.7×10 ⁻¹⁵	1.3	200	F94
Cl + CH ₃ CCl ₃ → CH ₂ CCl ₃ + HCl	2.8×10 ⁻¹²	1790	7.0×10 ⁻¹⁵	2.0	400	F95
Cl + CH ₃ CH ₂ F → HCl + CH ₃ CHF (HFC-161)	1.8×10 ⁻¹¹	290	6.8×10 ⁻¹²	3.0	500	F96
→ HCl + CH ₂ CH ₂ F	1.4×10 ⁻¹¹	880	7.3×10 ⁻¹³	3.0	500	F96
Cl + CH ₃ CHF ₂ → HCl + CH ₃ CF ₂ (HFC-152a)	6.4×10 ⁻¹²	950	2.6×10 ⁻¹³	1.3	500	F97
→ HCl + CH ₂ CHF ₂	7.2×10 ⁻¹²	2390	2.4×10 ⁻¹⁵	3.0	500	F97
Cl + CH ₂ FCH ₂ F → HCl + CHFCH ₂ F (HFC-152)	2.6×10 ⁻¹¹	1060	7.5×10 ⁻¹³	3.0	500	F98
Cl + CH ₃ CFCl ₂ → HCl + CH ₂ CFCl ₂ (HCFC-141b)	1.8×10 ⁻¹²	2000	2.2×10 ⁻¹⁵	1.2	300	F99

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Cl + CH ₃ CF ₂ Cl → HCl + CH ₂ CF ₂ Cl (HCFC-142b)	1.4×10 ⁻¹²	2420	4.2×10 ⁻¹⁶	1.2	500	F100
Cl + CH ₃ CF ₃ → HCl + CH ₂ CF ₃ (HFC-143a)	1.2×10 ⁻¹¹	3880	2.6×10 ⁻¹⁷	5.0	500	F101
Cl + CH ₂ FCHF ₂ → HCl + CH ₂ FCF ₂ (HFC-143)	5.5×10 ⁻¹²	1610	2.5×10 ⁻¹⁴	3.0	500	F102
→ HCl + CHFCHF ₂	7.7×10 ⁻¹²	1720	2.4×10 ⁻¹⁴	3.0	500	F102
Cl + CH ₂ ClCF ₃ → HCl + CHClCF ₃ (HCFC-133a)	1.8×10 ⁻¹²	1710	5.9×10 ⁻¹⁵	3.0	500	F103
Cl + CH ₂ FCF ₃ → HCl + CHF ₂ CF ₃ (HFC-134a)	–	–	1.5×10 ⁻¹⁵	1.2	–	F104
Cl + CHF ₂ CHF ₂ → HCl + CF ₂ CHF ₂ (HCF-134)	7.5×10 ⁻¹²	2430	2.2×10 ⁻¹⁵	1.5	500	F105
Cl + CHCl ₂ CF ₃ → HCl + CCl ₂ CF ₃ (HCFC-123)	4.4×10 ⁻¹²	1750	1.2×10 ⁻¹⁴	1.3	500	F106
Cl + CHFClCF ₃ → HCl + CFCICF ₃ (HCFC-124)	1.1×10 ⁻¹²	1800	2.7×10 ⁻¹⁵	1.3	500	F107
Cl + CHF ₂ CF ₃ → HCl + CF ₂ CF ₃ (HFC-125)	–	–	2.4×10 ⁻¹⁶	1.3	–	F108
Cl + C ₂ Cl ₄ \xrightarrow{M} C ₂ Cl ₅	(See Table 2-1)					
ClO + O ₃ → ClOO + O ₂	–	–	<1.4×10 ⁻¹⁷	–	–	F109
→ OCIO + O ₂	1.0×10 ⁻¹²	>4000	<1.0×10 ⁻¹⁸	–	–	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	1.0×10 ⁻¹²	1590	4.8×10 ⁻¹⁵	1.5	300	F118
→ ClOO + Cl	3.0×10 ⁻¹¹	2450	8.0×10 ⁻¹⁵	1.5	500	F118
→ OCIO + Cl	3.5×10 ⁻¹³	1370	3.5×10 ⁻¹⁵	1.5	300	F118

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{ClO} + \text{ClO} \xrightarrow{\text{M}} \text{Cl}_2\text{O}_2$	(See Table 2-1)					
$\text{ClO} + \text{OCIO} \xrightarrow{\text{M}} \text{Cl}_2\text{O}_3$	(See Table 2-1)					
$\text{HCl} + \text{ClONO}_2 \rightarrow \text{products}$	–	–	$<1.0 \times 10^{-20}$	–	–	F119
$\text{CH}_2\text{Cl} + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_2\text{ClO}_2$	(See Table 2-1)					
$\text{CHCl}_2 + \text{O}_2 \xrightarrow{\text{M}} \text{CHCl}_2\text{O}_2$	(See Table 2-1)					
$\text{CCl}_3 + \text{O}_2 \xrightarrow{\text{M}} \text{CCl}_3\text{O}_2$	(See Table 2-1)					
$\text{CFCl}_2 + \text{O}_2 \xrightarrow{\text{M}} \text{CFCl}_2\text{O}_2$	(See Table 2-1)					
$\text{CF}_2\text{Cl} + \text{O}_2 \xrightarrow{\text{M}} \text{CF}_2\text{ClO}_2$	(See Table 2-1)					
$\text{CCl}_3\text{O}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{CCl}_3\text{O}_2\text{NO}_2$	(See Table 2-1)					
$\text{CFCl}_2\text{O}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{CFCl}_2\text{O}_2\text{NO}_2$	(See Table 2-1)					
$\text{CF}_2\text{ClO}_2 + \text{NO}_2 \xrightarrow{\text{M}} \text{CF}_2\text{ClO}_2\text{NO}_2$	(See Table 2-1)					
$\text{CH}_2\text{ClO} + \text{O}_2 \rightarrow \text{CHClO} + \text{HO}_2$	–	–	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
$\text{OH} + \text{Br}_2 \rightarrow \text{HOBr} + \text{Br}$	4.2×10^{-11}	0	4.2×10^{-11}	1.3	600	G 4
$\text{OH} + \text{BrO} \rightarrow \text{products}$	–	–	7.5×10^{-11}	3.0	–	G 5
$\text{OH} + \text{HBr} \rightarrow \text{H}_2\text{O} + \text{Br}$	1.1×10^{-11}	0	1.1×10^{-11}	1.2	250	G 6
$\text{OH} + \text{CH}_3\text{Br} \rightarrow \text{CH}_2\text{Br} + \text{H}_2\text{O}$	2.35×10^{-12}	1300	3.0×10^{-14}	1.1	100	G 7

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CH ₂ Br ₂ → CHBr ₂ + H ₂ O	2.0×10 ⁻¹²	840	1.2×10 ⁻¹³	1.15	150	G 8
OH + CHBr ₃ → CBr ₃ + H ₂ O	1.35×10 ⁻¹²	600	1.8×10 ⁻¹³	1.5	100	G 9
OH + CHF ₂ Br → CF ₂ Br + H ₂ O	1.0×10 ⁻¹²	1380	1.0×10 ⁻¹⁴	1.1	100	G10
OH + CH ₂ ClBr → CHClBr + H ₂ O	2.4×10 ⁻¹²	920	1.1×10 ⁻¹³	1.1	100	G11
OH + CF ₂ ClBr → products (Halon-1211)	~1×10 ⁻¹²	>2600	<1.5×10 ⁻¹⁶	-	-	G12
OH + CF ₂ Br ₂ → products (Halon-1202)	~1×10 ⁻¹²	>2200	<5.0×10 ⁻¹⁶	-	-	G13
OH + CF ₃ Br → products (Halon-1301)	~1×10 ⁻¹²	>3600	<6.0×10 ⁻¹⁸	-	-	G14
OH + CH ₂ BrCH ₃ → products	2.9×10 ⁻¹²	640	3.4×10 ⁻¹³	1.2	150	G15
OH + CH ₂ BrCF ₃ → CHBrCF ₃ + H ₂ O	1.4×10 ⁻¹²	1340	1.6×10 ⁻¹⁴	1.2	150	G16
OH + CHFBrCF ₃ → CFBrCF ₃ + H ₂ O	7.3×10 ⁻¹³	1120	1.7×10 ⁻¹⁴	1.2	100	G17
OH + CHClBrCF ₃ → CClBrCF ₃ + H ₂ O	1.1×10 ⁻¹²	940	4.7×10 ⁻¹⁴	1.2	150	G18
OH + CHFClCF ₂ Br → CFCICF ₂ Br + H ₂ O	8.4×10 ⁻¹³	1220	1.4×10 ⁻¹⁴	1.3	200	G19
OH + CF ₂ BrCF ₂ Br → products (Halon-2402)	~1×10 ⁻¹²	>3600	<6×10 ⁻¹⁸	-	-	G20
OH + CH ₂ BrCH ₂ CH ₃ → products	3.0×10 ⁻¹²	330	1.0×10 ⁻¹²	1.1	50	G21
OH + CH ₃ CHBrCH ₃ → products	1.85×10 ⁻¹²	270	7.5×10 ⁻¹³	1.15	50	G22
HO ₂ + Br → HBr + O ₂	1.5×10 ⁻¹¹	600	2.0×10 ⁻¹²	2.0	600	G23
HO ₂ + BrO → products	3.4×10 ⁻¹²	-540	2.1×10 ⁻¹¹	1.5	200	G24
NO ₃ + HBr → HNO ₃ + Br	-	-	<1.0×10 ⁻¹⁶	-	-	G25
Cl + CH ₂ ClBr → HCl + CHClBr	1.5×10 ⁻¹¹	1070	4.1×10 ⁻¹³	1.2	300	G26
Cl + CH ₃ Br → HCl + CH ₂ Br	1.7×10 ⁻¹¹	1080	4.5×10 ⁻¹³	1.1	100	G27
Cl + CH ₂ Br ₂ → HCl + CHBr ₂	6.7×10 ⁻¹²	825	4.2×10 ⁻¹³	1.15	150	G28
Cl + CHBr ₃ → CBr ₃ + HCl	4.85×10 ⁻¹²	850	2.8×10 ⁻¹³	1.5	250	G29
Br + O ₃ → BrO + O ₂	1.7×10 ⁻¹¹	800	1.2×10 ⁻¹²	1.2	200	G30
Br + H ₂ O ₂ → HBr + HO ₂	1.0×10 ⁻¹¹	>3000	<5.0×10 ⁻¹⁶	-	-	G31
Br + NO ₂ \xrightarrow{M} BrNO ₂	(See Table 2-1)					

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Br + NO ₃ → BrO + NO ₂	–	–	1.6×10 ⁻¹¹	2.0	–	G32
Br + H ₂ CO → HBr + HCO	1.7×10 ⁻¹¹	800	1.1×10 ⁻¹²	1.3	200	G33
Br + OCIO → BrO + ClO	2.6×10 ⁻¹¹	1300	3.4×10 ⁻¹³	2.0	300	G34
Br + Cl ₂ O → BrCl + ClO	2.1×10 ⁻¹¹	470	4.3×10 ⁻¹²	1.3	150	G35
Br + Cl ₂ O ₂ → products	–	–	3.0×10 ⁻¹²	2.0	–	G36
BrO + O ₃ → products	~1.0×10 ⁻¹²	>3200	<2.0×10 ⁻¹⁷	–	–	G37
BrO + NO → NO ₂ + Br	8.8×10 ⁻¹²	–260	2.1×10 ⁻¹¹	1.15	130	G38
BrO + NO ₂ \xrightarrow{M} BrONO ₂	(See Table 2-1)					
BrO + NO ₃ → products	–	–	1.0×10 ⁻¹²	3.0	–	G39
BrO + ClO → Br + OCIO	9.5×10 ⁻¹³	–550	6.0×10 ⁻¹²	1.25	150	G40
→ Br + ClOO	2.3×10 ⁻¹²	–260	5.5×10 ⁻¹²	1.25	150	G40
→ BrCl + O ₂	4.1×10 ⁻¹³	–290	1.1×10 ⁻¹²	1.25	150	G40
BrO + BrO → products	1.5×10 ⁻¹²	–230	3.2×10 ⁻¹²	1.15	150	G41
CH ₂ BrO ₂ + NO → CH ₂ O + NO ₂ + Br	4×10 ⁻¹²	–300	1.1 × 10 ⁻¹¹	1.5	200	G42
IO_x Reactions						
O + I ₂ → IO + I	1.4×10 ⁻¹⁰	0	1.4×10 ⁻¹⁰	1.4	250	H 1
O + IO → O ₂ + I			1.2×10 ⁻¹⁰	2.0		H 2
OH + I ₂ → HOI + I			1.8×10 ⁻¹⁰	2.0		H 3
OH + HI → H ₂ O + I			3.0×10 ⁻¹¹	2.0		H 4
OH + CH ₃ I → H ₂ O + CH ₂ I	2.9×10 ⁻¹²	1100	7.2×10 ⁻¹⁴	1.5	300	H 5
OH + CF ₃ I → HOI + CF ₃	2.5×10 ⁻¹¹	2070	2.4×10 ⁻¹⁴	1.3	200	H 6
HO ₂ + I → HI + O ₂	1.5×10 ⁻¹¹	1090	3.8×10 ⁻¹³	2.0	500	H 7
HO ₂ + IO → HOI + O ₂			8.4×10 ⁻¹¹	1.5		H 8
NO ₃ + HI → HNO ₃ + I	(See Note)					H 9
Cl + CH ₃ I → CH ₂ I + HCl	2.9×10 ⁻¹¹	1000	1.0×10 ⁻¹²	1.5	250	H10

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$I + O_3 \rightarrow IO + O_2$	2.3×10^{-11}	870	1.2×10^{-12}	1.2	200	H11
$I + NO \xrightarrow{M} INO$	(See Table 2-1)					
$I + NO_2 \xrightarrow{M} INO_2$	(See Table 2-1)					
$I + BrO \rightarrow IO + Br$	–	–	1.2×10^{-11}	2.0		H12
$IO + NO \rightarrow I + NO_2$	9.1×10^{-12}	–240	2.0×10^{-11}	1.2	150	H13
$IO + NO_2 \xrightarrow{M} IONO_2$	(See Table 2-1)					
$IO + ClO \rightarrow \text{products}$	5.1×10^{-12}	–280	1.3×10^{-11}	2.0	200	H14
$IO + BrO \rightarrow \text{products}$	–	–	6.9×10^{-11}	1.5	–	H15
$IO + IO \rightarrow \text{products}$	1.5×10^{-11}	–500	8.0×10^{-11}	1.5	500	H16
$INO + INO \rightarrow I_2 + 2NO$	8.4×10^{-11}	2620	1.3×10^{-14}	2.5	600	H17
$INO_2 + INO_2 \rightarrow I_2 + 2NO_2$	2.9×10^{-11}	2600	4.7×10^{-15}	3.0	1000	H18
SO_x Reactions						
$O + SH \rightarrow SO + H$	–	–	1.6×10^{-10}	5.0	–	I 1
$O + CS \rightarrow CO + S$	2.7×10^{-10}	760	2.1×10^{-11}	1.1	250	I 2
$O + H_2S \rightarrow OH + SH$	9.2×10^{-12}	1800	2.2×10^{-14}	1.7	550	I 3
$O + OCS \rightarrow CO + SO$	2.1×10^{-11}	2200	1.3×10^{-14}	1.2	150	I 4
$O + CS_2 \rightarrow CS + SO$	3.2×10^{-11}	650	3.6×10^{-12}	1.2	150	I 5
$O + SO_2 \xrightarrow{M} SO_3$	(See Table 2-1)					
$O + CH_3SCH_3 \rightarrow CH_3SO + CH_3$	1.3×10^{-11}	–410	5.0×10^{-11}	1.1	100	I 6
$O + CH_3SSCH_3 \rightarrow CH_3SO + CH_3S$	5.5×10^{-11}	–250	1.3×10^{-10}	1.3	100	I 7
$O_3 + H_2S \rightarrow \text{products}$	–	–	$<2.0 \times 10^{-20}$	–	–	I 8
$O_3 + CH_3SCH_3 \rightarrow \text{products}$	–	–	$<1.0 \times 10^{-18}$	–	–	I 9
$O_3 + SO_2 \rightarrow SO_3 + O_2$	3.0×10^{-12}	>7000	$<2.0 \times 10^{-22}$	–	–	I 10
$OH + H_2S \rightarrow SH + H_2O$	6.0×10^{-12}	75	4.7×10^{-12}	1.2	75	I 11
$OH + OCS \rightarrow \text{products}$	1.1×10^{-13}	1200	1.9×10^{-15}	2.0	500	I 12

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
OH + CS ₂ → products	(See Note)	–	–	–	–	I13
OH + CH ₃ SH → CH ₃ S + H ₂ O	9.9×10 ⁻¹²	–360	3.3×10 ⁻¹¹	1.2	100	I14
OH + CH ₃ SCH ₃ → H ₂ O + CH ₂ SCH ₃	1.2×10 ⁻¹¹	260	5.0×10 ⁻¹²	1.15	100	I15
OH + CH ₃ SSCH ₃ → products	6.0×10 ⁻¹¹	–400	2.3×10 ⁻¹⁰	1.2	200	I16
OH + S → H + SO	–	–	6.6×10 ⁻¹¹	3.0	–	I17
OH + SO → H + SO ₂	–	–	8.6×10 ⁻¹¹	2.0	–	I18
OH + SO ₂ \xrightarrow{M} HOSO ₂	(See Table 2-1)					
HO ₂ + H ₂ S → products	–	–	<3.0×10 ⁻¹⁵	–	–	I19
HO ₂ + CH ₃ SH → products	–	–	<4.0×10 ⁻¹⁵	–	–	I19
HO ₂ + CH ₃ SCH ₃ → products	–	–	<5.0×10 ⁻¹⁵	–	–	I19
HO ₂ + SO ₂ → products	–	–	<1.0×10 ⁻¹⁸	–	–	I20
NO ₂ + SO ₂ → products	–	–	<2.0×10 ⁻²⁶	–	–	I21
NO ₃ + H ₂ S → products	–	–	<8.0×10 ⁻¹⁶	–	–	I22
NO ₃ + OCS → products	–	–	<1.0×10 ⁻¹⁶	–	–	I23
NO ₃ + CS ₂ → products	–	–	<4.0×10 ⁻¹⁶	–	–	I24
NO ₃ + CH ₃ SH → products	4.4×10 ⁻¹³	–210	8.9×10 ⁻¹³	1.25	210	I25
NO ₃ + CH ₃ SCH ₃ → CH ₃ SCH ₂ + HNO ₃	1.9×10 ⁻¹³	–500	1.0×10 ⁻¹²	1.2	200	I26
NO ₃ + CH ₃ SSCH ₃ → products	1.3×10 ⁻¹²	270	5.3×10 ⁻¹³	1.4	270	I27
NO ₃ + SO ₂ → products	–	–	<7.0×10 ⁻²¹	–	–	I28
N ₂ O ₅ + CH ₃ SCH ₃ → products	–	–	<1.0×10 ⁻¹⁷	–	–	I29
CH ₃ O ₂ + SO ₂ → products	–	–	<5.0×10 ⁻¹⁷	–	–	I30
F + CH ₃ SCH ₃ → products	–	–	2.4×10 ⁻¹⁰	2.0	–	I31
Cl + H ₂ S → HCl + SH	3.7×10 ⁻¹¹	–210	7.4×10 ⁻¹¹	1.25	100	I32
Cl + OCS → products	–	–	<1.0×10 ⁻¹⁶	–	–	I33
Cl + CS ₂ → products	–	–	<4.0×10 ⁻¹⁵	–	–	I34

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
Cl + CH ₃ SH → CH ₃ S + HCl	1.2×10 ⁻¹⁰	-150	2.0×10 ⁻¹⁰	1.25	50	I35
Cl + CH ₃ SCH ₃ → products	(See Note)	-	-	-	-	I36
ClO + OCS → products	-	-	<2.0×10 ⁻¹⁶	-	-	I37
ClO + CH ₃ SCH ₃ → products	-	-	9.5×10 ⁻¹⁵	2.0	-	I38
ClO + SO → Cl + SO ₂	2.8×10 ⁻¹¹	0	2.8×10 ⁻¹¹	1.3	50	I39
ClO + SO ₂ → Cl + SO ₃	-	-	<4.0×10 ⁻¹⁸	-	-	I37
Br + H ₂ S → HBr + SH	1.4×10 ⁻¹¹	2750	1.4×10 ⁻¹⁵	2.0	300	I40
Br + CH ₃ SH → CH ₃ S + HBr	9.2×10 ⁻¹²	390	2.5×10 ⁻¹²	2.0	100	I40
Br + CH ₃ SCH ₃ → products	(See Note)					I41
BrO + CH ₃ SCH ₃ → products	1.5×10 ⁻¹⁴	-850	2.6×10 ⁻¹³	1.3	200	I42
BrO + SO → Br + SO ₂			5.7×10 ⁻¹¹	1.4		I43
IO + CH ₃ SH → products			6.6×10 ⁻¹⁶	2.0		I44
IO + CH ₃ SCH ₃ → products			1.2×10 ⁻¹⁴	1.5		I45
S + O ₂ → SO + O	2.3×10 ⁻¹²	0	2.3×10 ⁻¹²	1.2	200	I46
S + O ₃ → SO + O ₂			1.2×10 ⁻¹¹	2.0		I47
SO + O ₂ → SO ₂ + O	2.6×10 ⁻¹³	2400	8.4×10 ⁻¹⁷	2.0	500	I48
SO + O ₃ → SO ₂ + O ₂	3.6×10 ⁻¹²	1100	9.0×10 ⁻¹⁴	1.2	200	I49
SO + NO ₂ → SO ₂ + NO	1.4×10 ⁻¹¹	0	1.4×10 ⁻¹¹	1.2	50	I50
SO + OClO → SO ₂ + ClO			1.9×10 ⁻¹²	3.0		I51
SO ₃ + H ₂ O → products	(See Note)		-	-		I52
SO ₃ + NH ₃ → products	(See Table 2-1)		-	-		
SO ₃ + NO ₂ → products			1.0×10 ⁻¹⁹	10.0		I53
SH + O ₂ → OH + SO			<4.0×10 ⁻¹⁹	-		I54
SH + O ₃ → HSO + O ₂	9.0×10 ⁻¹²	280	3.5×10 ⁻¹²	1.3	200	I55
SH + H ₂ O ₂ → products			<5.0×10 ⁻¹⁵	-		I56

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{SH} + \text{NO} \xrightarrow{\text{M}} \text{HSNO}$	(See Table 2-1)					
$\text{SH} + \text{NO}_2 \rightarrow \text{HSO} + \text{NO}$	2.9×10^{-11}	-240	6.5×10^{-11}	1.2	50	157
$\text{SH} + \text{Cl}_2 \rightarrow \text{ClSH} + \text{Cl}$	1.7×10^{-11}	690	1.7×10^{-12}	2.0	200	158
$\text{SH} + \text{BrCl} \rightarrow \text{products}$	2.3×10^{-11}	-350	7.4×10^{-11}	2.0	200	158
$\text{SH} + \text{Br}_2 \rightarrow \text{BrSH} + \text{Br}$	6.0×10^{-11}	-160	1.0×10^{-10}	2.0	160	158
$\text{SH} + \text{F}_2 \rightarrow \text{FSH} + \text{F}$	4.3×10^{-11}	1390	4.0×10^{-13}	2.0	200	158
$\text{HSO} + \text{O}_2 \rightarrow \text{products}$			$< 2.0 \times 10^{-17}$	-		159
$\text{HSO} + \text{O}_3 \rightarrow \text{products}$			1.0×10^{-13}	1.3		160
$\text{HSO} + \text{NO} \rightarrow \text{products}$			$< 1.0 \times 10^{-15}$	-		161
$\text{HSO} + \text{NO}_2 \rightarrow \text{HSO}_2 + \text{NO}$			9.6×10^{-12}	2.0		161
$\text{HSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_2$			3.0×10^{-13}	3.0		162
$\text{HOSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_3$	1.3×10^{-12}	330	4.4×10^{-13}	1.2	200	163
$\text{CS} + \text{O}_2 \rightarrow \text{OCS} + \text{O}$			2.9×10^{-19}	2.0		164
$\text{CS} + \text{O}_3 \rightarrow \text{OCS} + \text{O}_2$			3.0×10^{-16}	3.0		165
$\text{CS} + \text{NO}_2 \rightarrow \text{OCS} + \text{NO}$			7.6×10^{-17}	3.0		165
$\text{CH}_3\text{S} + \text{O}_2 \rightarrow \text{products}$			$< 3.0 \times 10^{-18}$	-		166
$\text{CH}_3\text{S} + \text{O}_3 \rightarrow \text{products}$	2.0×10^{-12}	-290	5.3×10^{-12}	1.15	100	167
$\text{CH}_3\text{S} + \text{NO} \rightarrow \text{products}$			$< 1.0 \times 10^{-13}$	-		168
$\text{CH}_3\text{S} + \text{NO} \xrightarrow{\text{M}} \text{products}$	(See Table 2-1)					
$\text{CH}_3\text{S} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO} + \text{NO}$	2.1×10^{-11}	-320	6.1×10^{-11}	1.15	100	169
$\text{CH}_2\text{SH} + \text{O}_2 \rightarrow \text{products}$			6.5×10^{-12}	2.0		170
$\text{CH}_2\text{SH} + \text{O}_3 \rightarrow \text{products}$			3.5×10^{-11}	2.0		171
$\text{CH}_2\text{SH} + \text{NO} \rightarrow \text{products}$			1.9×10^{-11}	2.0		172
$\text{CH}_2\text{SH} + \text{NO}_2 \rightarrow \text{products}$			5.2×10^{-11}	2.0		173
$\text{CH}_3\text{SO} + \text{O}_3 \rightarrow \text{products}$			6.0×10^{-13}	1.5		174

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{CH}_3\text{SO} + \text{NO}_2 \rightarrow \text{CH}_3\text{SO}_2 + \text{NO}$			1.2×10^{-11}	1.4		I75
$\text{CH}_3\text{SOO} + \text{O}_3 \rightarrow \text{products}$			$<8.0 \times 10^{-13}$	–		I76
$\text{CH}_3\text{SOO} + \text{NO} \rightarrow \text{products}$	1.1×10^{-11}	0	1.1×10^{-11}	2.0	100	I76
$\text{CH}_3\text{SO}_2 + \text{NO}_2 \rightarrow \text{products}$	2.2×10^{-11}	0	2.2×10^{-11}	2.0	100	I77
$\text{CH}_3\text{SCH}_2 + \text{O}_2 \xrightarrow{\text{M}} \text{CH}_3\text{SCH}_2\text{O}_2$	(See Table 2-1)					
$\text{CH}_3\text{SCH}_2 + \text{NO}_3 \rightarrow \text{products}$			3.0×10^{-10}	2.0		I78
$\text{CH}_3\text{SCH}_2\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{SCH}_2\text{O} + \text{NO}_2$			1.9×10^{-11}	2.0		I79
$\text{CH}_3\text{SS} + \text{O}_3 \rightarrow \text{products}$			4.6×10^{-13}	2.0		I80
$\text{CH}_3\text{SS} + \text{NO}_2 \rightarrow \text{products}$			1.8×10^{-11}	2.0		I81
$\text{CH}_3\text{SSO} + \text{NO}_2 \rightarrow \text{products}$			4.5×10^{-12}	2.0		I81
Metal Reactions						
$\text{Na} + \text{O}_2 \xrightarrow{\text{M}} \text{NaO}_2$	(See Table 2-1)					
$\text{Na} + \text{O}_3 \rightarrow \text{NaO} + \text{O}_2$	1.0×10^{-9}	95	7.3×10^{-10}	1.2	50	J 1
$\quad \quad \quad \rightarrow \text{NaO}_2 + \text{O}$	–	–	$<4.0 \times 10^{-11}$	–	–	J 1
$\text{Na} + \text{N}_2\text{O} \rightarrow \text{NaO} + \text{N}_2$	2.8×10^{-10}	1600	1.3×10^{-12}	1.2	400	J 2
$\text{Na} + \text{Cl}_2 \rightarrow \text{NaCl} + \text{Cl}$	7.3×10^{-10}	0	7.3×10^{-10}	1.3	200	J 3
$\text{NaO} + \text{O} \rightarrow \text{Na} + \text{O}_2$	3.7×10^{-10}	0	3.7×10^{-10}	3.0	400	J 4
$\text{NaO} + \text{O}_2 \xrightarrow{\text{M}} \text{NaO}_3$	(See Table 2-1)					
$\text{NaO} + \text{O}_3 \rightarrow \text{NaO}_2 + \text{O}_2$	1.1×10^{-9}	570	1.6×10^{-10}	1.5	300	J 5
$\quad \quad \quad \rightarrow \text{Na} + 2\text{O}_2$	6.0×10^{-11}	0	6.0×10^{-11}	3.0	800	J 5
$\text{NaO} + \text{H}_2 \rightarrow \text{NaOH} + \text{H}$	2.6×10^{-11}	0	2.6×10^{-11}	2.0	600	J 6
$\text{NaO} + \text{H}_2\text{O} \rightarrow \text{NaOH} + \text{OH}$	2.2×10^{-10}	0	2.2×10^{-10}	2.0	400	J 7
$\text{NaO} + \text{NO} \rightarrow \text{Na} + \text{NO}_2$	1.5×10^{-10}	0	1.5×10^{-10}	4.0	400	J 8
$\text{NaO} + \text{CO}_2 \xrightarrow{\text{M}} \text{NaCO}_3$	(See Table 2-1)					
$\text{NaO} + \text{HCl} \rightarrow \text{products}$	2.8×10^{-10}	0	2.8×10^{-10}	3.0	400	J 9

Reaction	A-Factor ^a	E/R	k(298 K) ^a	f(298 K) ^b	g	Notes
$\text{NaO}_2 + \text{O} \rightarrow \text{NaO} + \text{O}_2$	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
$\text{NaOH} + \text{CO}_2 \xrightarrow{\text{M}} \text{NaHCO}_3$	(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 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

- A1. $O + O_3$. The recommended rate expression is from Wine et al. [1316] and is a linear least squares fit of all data (unweighted) from Davis et al. [319], McCrumb and Kaufman [795], West et al. [1294], Arnold and Comes [29], and Wine et al. [1316].
- A2. $O(^1D)$ Reactions. The rate constants are for the disappearance of $O(^1D)$, which includes physical quenching or deactivation. Where information is available, product yields are given. The rate constant recommendations are based on averages of the absolute rate constant measurements reported by Streit et al. [1123], Davidson et al. [312] and Davidson et al. [311] 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. [18], Amimoto et al. [17], and Force and Wiesenfeld [405,406] 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 [1317–1319] for N_2O , H_2O , N_2 , H_2 , O_3 , CO_2 , and CF_2O ; by Brock and Watson (private communication, 1980) for N_2 , O_2 and CO_2 ; by Lee and Slanger [701,702] for H_2O and O_2 ; by Gericke and Comes [427] for H_2O ; and by Shi and Barker [1057] for N_2 and CO_2 , and Talukdar and Ravishankara [1157] for H_2 . The weight of the evidence from these studies indicates that the results of Heidner and Husain [494], Heidner et al. [493] and Fletcher and Husain [399,400] contain a systematic error. For the critical atmospheric reactants, such as N_2O , H_2O , and CH_4 , the recommended absolute rate constants are in good agreement with the previous relative measurements when compared with N_2 as the reference reactant. A similar comparison with O_2 as the reference reactant gives somewhat poorer agreement.
- A3. $O(^1D) + O_2$. The deactivation of $O(^1D)$ by O_2 leads to the production of $O_2(^1\Delta)$ with an efficiency of $80 \pm 20\%$: Noxon [901], Biedenkapp and Bair [119], Snelling [1096], and Lee and Slanger [701]. The $O_2(^1\Delta)$ is produced in the $v=0, 1$, and 2 vibrational levels in the amounts 60%, 40%, and $<3\%$, Gauthier and Snelling [424] and Lee and Slanger [701].
- A4. $O(^1D) + O_3$. The branching result for reaction of $O(^1D)$ with O_3 to give $O_2 + O_2$ or $O_2 + O + O$ is from Davenport et al. [306]. This is supported by measurements of Amimoto et al. [18] who reported that on average one ground state O is produced per $O(^1D)$ reaction with O_3 . It seems unlikely that this could result from 100% quenching of the $O(^1D)$ by O_3 .
- A5. $O(^1D) + H_2$. Wine and Ravishankara [1318] have determined the yield of $O(^3P)$ is $<4.9\%$. The major products are $H + OH$. Koppe et al. [649] report a 2.7 times larger rate coefficient at a kinetic energy of 0.12eV. This does not agree with the observations of Davidson et al. [312], who reported that k is independent of temperature (200–350 K) and Matsumi et al. [791] who report no change in k when hot $O(^1D)$ is moderated with Ar.
- A6. $O(^1D) + H_2O$. Measurements of the $O_2 + H_2$ product yield were made by Zellner et al. [1361] ($1 + 0.5$ or -1%) and by Glinski and Birks [445] ($0.6 + 0.7$ or -0.6%). The yield of $O(^3P)$ from $O(^1D) + H_2O$ is reported to be $<(4.9 \pm 3.2)\%$ by Wine and Ravishankara [1318] and $(2 \pm 1)\%$ by Takahashi et al. [1146].

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.

- A7. $O(^1D) + N_2O$. 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. [309]; Volltrauer et al. [1236]; Marx et al. [790] and Lam et al. [675], with a spread in $R = k(NO + NO)/k(Total) = 0.52 - 0.62$. Cantrell et al. [198] reported a measurement of $R = 0.57$ and an analysis of all measurements from 1957–1994 leads 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 [189]). The $O(^1D)$ translational energy and temperature dependence effects are not clearly resolved. Wine and Ravishankara [1318] have determined that the yield of $O(^3P)$ from $O(^1D) + N_2O$ is $<4.0\%$. The uncertainty for this reaction includes factors for both the overall rate coefficient and the branching ratio. A direct measurement by Greenblatt and Ravishankara [455] of the NO yield from the $O(^1D) + N_2O$ reaction in synthetic air 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. These authors suggest that their results support the recommendations and reduce the uncertainty in the collected rate parameters by over a factor of two.

To calculate the rates of NO 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 N_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.

- A8. $O(^1D) + NH_3$. Sanders et al. [1024] have detected the products $NH(a1\Delta)$ and OH formed in the reaction. They report that the yield of $NH(a1\Delta)$ is in the range 3–15% of the amount of OH detected.
- A9. $O(^1D) + CH_4$. The reaction products are (a) $CH_3 + OH$, (b) CH_3O or $CH_2OH + H$ and (c) $CH_2O + H_2$. Lin and DeMore [739] 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. [202] used a molecular beam experiment to observe H and CH_3O (or CH_2OH) products. They reported that the yield of H_2 was <25% of the yield of H from (b). Satyapal et al. [1029] observed the production of H atoms in a pulsed laser experiment and reported a yield of H of (25±8)%. Matsumi et al. [791] measured the yields of H and $O(^3P)$ in low pressure gas mixtures and reported the yield of H was (15±3)% and the yield of $O(^3P)$ was <5%. Wine and Ravishankara [1318] reported that the yield of $O(^3P)$ was <4.3%. Takahashi et al. [1146] reported that the $O(^3P)$ yield is <1%. We recommend the following branching ratios: (a) (75±15)%, (b) (20±7)%, (c) (5±5)%.
- A10. $O(^1D) + HCl$. The recommendation is the average of measurements by Davidson et al. [312] and Wine et al. [1325]. Product studies by the latter indicate: $O(^3P) + HCl$ (9±5)%; $H + ClO$ (24±5)%; and $OH + Cl$ (67±10)%. Takahashi et al. [1146] report the $O(^3P)$ yield is (15±4)%.
- A11. $O(^1D) + HF$. Rate coefficient and product yield measured by Wine et al. (1984, private communication). The $O(^3P)$ yield is less than 4%.
- A12. $O(^1D) + HBr$. Rate coefficient and products measured by Wine et al. [1325]. Product yields: $HBr + O(^3P)$ (20±7)%, $H + BrO$ <4.5%, and $OH + Br$ (80±12)%.
- A13. $O(^1D) + Cl_2$. Rate coefficient and $O(^3P)$ product were measured by Wine et al. [1314], who reported $Cl_2 + O(^3P)$ (25±10)%. Takahashi et al. [1146] reported that the ClO yield is (74±15)%, in excellent agreement. An indirect study by Freudenstein and Biedenkapp [409] is in reasonable agreement on the yield of ClO .
- A14. $O(^1D) + COCl_2$, $COClF$ and COF_2 . For the reactions of $O(^1D)$ with $COCl_2$ and $COClF$ the recommended rate constants are derived from data of Fletcher and Husain [401]. For consistency, the recommended values for these rate constants were derived using a scaling factor (0.5) which corrects for the difference between rate constants from the Husain laboratory and the recommendations for other $O(^1D)$ rate constants in this table. The recommendation for COF_2 is from the data of Wine and Ravishankara [1319]. Their result is preferred over the value of Fletcher and Husain [401] 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 $O(^1D)$ reactions, it is assumed that E/R equals zero, and therefore the value shown for the A -factor has been set equal to $k(298\text{ K})$.
- A15. $O(^1D) + \text{halocarbons}$. The halocarbon rate constants are for the total disappearance of $O(^1D)$ and probably include physical quenching. Products of the reactive channels may include $CX_3O + X$, $CX_2O + X_2$ (or $2X$), and $CX_3 + XO$, where $X = H, F, Cl, \text{ or } Br$ 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 $O(^1D)$ proceeding through physical quenching and reactive channels. For CCl_4 : quenching = (14±6)% and reaction = (86±6)% (Force and Wiesenfeld [405]), ClO yield = (90±19)% (Takahashi et al. [1146]; for $CFCl_3$: quenching = (25±10)%, ClO formation = (60±15)% (Donovan, private communication, 1980), ClO yield = (88±18)% (Takahashi et al.); for CF_2Cl_2 : quenching = (14±7)% and reaction = (86±14)% (Force and Wiesenfeld [405]), quenching = (20±10)%, ClO formation = (55±15)% (Donovan), quenching = (19±5)% and ClO formation = (87±18%) (Takahashi et al.).
- A16. $O(^1D) + CH_3Br$. The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is 0±7%.
- A17. $O(^1D) + CH_2Br_2$. The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is (5±7)%.
- A18. $O(^1D) + CHBr_3$. The recommendation is based on data from Thompson and Ravishankara [1165]. The rate coefficient is somewhat large compared to analogous compounds. They report that the yield of $O(^3P)$ from physical quenching is (32±8)%.
- A19. $O(^1D) + CH_3F$ (HFC-41). The recommendation is the average of measurements of Force and Wiesenfeld [405] and Schmoltnner et al. [1039]. The $O(^3P)$ product yield was reported to be (25±3)% by Force and Wiesenfeld, (11±5)% by Schmoltnner et al., and (19±5)% by Takahashi et al. [1146]. Burks and Lin [175] reported observing vibrationally excited HF as a product. Park and Wiesenfeld [929] observed OH .

- A20. $O(^1D) + CH_2F_2$ (HFC-32). The recommendation is based upon the measurement of Schmoltnner et al. [1039], who reported that the yield of $O(^3P)$ is $(70 \pm 11)\%$. Green and Wayne [453] 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 [175] reported observing vibrationally excited HF as a product.
- A21. $O(^1D) + CHF_3$ (HFC-23). The recommendation is the average of measurements of Force and Wiesenfeld [405] and Schmoltnner et al. [1039]. 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 [175] and Aker et al. [15], which indicate the formation of HF + CF_2O products.
- A22. $O(^1D) + CHCl_2F$ (HCFC-21). The recommendation is based upon the measurement by Davidson et al. [311] of the total rate coefficient (physical quenching and reaction). Takahashi et al. [1146] report the yield of ClO is $(74 \pm 15)\%$.
- A23. $O(^1D) + CHClF_2$ (HCFC-22). The recommendation is based upon the measurements by Davidson et al. [311] and Warren et al. [1277] 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 [453] 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. [41] 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. [1277] also report a yield of $O(^3P)$ of $(28 \pm 6)\%$, which they interpret as the product of physical quenching.
- A24. $O(^1D) + CClF_3$ (CFC-13). The recommendation is based on the measurement by Ravishankara et al. [985] who report $(31 \pm 10)\%$ physical quenching. Takahashi et al. [1146] report the yields of $O(^3P)$ $(16 \pm 5)\%$ and ClO $(85 \pm 18)\%$.
- A25. $O(^1D) + CClBrF_2$ (Halon 1211). The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is $(36 \pm 4)\%$.
- A26. $O(^1D) + CBr_2F_2$ (Halon 1202). The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is $(54 \pm 6)\%$.
- A27. $O(^1D) + CBrF_3$ (Halon 1301). The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is $(59 \pm 8)\%$. Lorenzen-Schmidt et al. [753] 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.
- A28. $O(^1D) + CF_4$ (CFC-14). The recommendation is based upon the measurement by Ravishankara et al. [985], who report $(92 \pm 8)\%$ physical quenching. Force and Wiesenfeld [405] measured a quenching rate coefficient about 10 times larger. Shi and Barker [1057] 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.
- A29. $O(^1D) + CH_3CH_2F$ (HFC 161). The recommendation is based on data from Schmoltnner et al. [1039]. They report that the yield of $O(^3P)$ from physical quenching is $(18 \pm 5)\%$.
- A30. $O(^1D) + CH_3CHF_2$ (HFC-152a). The recommendation is based on the measurements of Warren et al. [1277], who report $(54 \pm 7)\%$ physical quenching.
- A31. $O(^1D) + CH_3CCl_2F$ (HCFC-141b). The recommendation is based upon the measurement of Warren et al. [1277], who report $(31 \pm 5)\%$ physical quenching.
- A32. $O(^1D) + CH_3CClF_2$ (HCFC-142b). The recommendation is based upon the measurement of Warren et al. [1277], who report $(26 \pm 5)\%$ physical quenching. This agrees very well with Green and Wayne [453], who measured the loss of CH_3CF_2Cl relative to the loss of N_2O , when the recommendation for N_2O is used.
- A33. $O(^1D) + CH_3CF_3$ (HFC-143a). The recommendation is based upon the relative rate measurement of Green and Wayne [453], 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.
- A34. $O(^1D) + CH_2ClCClF_2$ (HCFC-132b). The recommendation is based upon the relative rate measurement of Green and Wayne [453], 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.

- A35. $O(^1D) + CH_2ClCF_3$ (HCFC-133a). The recommendation is based upon the measurement of Warren et al. [1277], who report (20±5)% physical quenching. This agrees with Green and Wayne [453] who measured the loss of CH_2ClCF_3 relative to the loss of N_2O , when the recommendation for N_2O is used.
- A36. $O(^1D) + CH_2FCF_3$ (HFC-134a). The recommendation is based on the measurement of Warren et al. [1277] 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 $O(^1D)$.
- A37. $O(^1D) + CHCl_2CF_3$ (HCFC-123). The recommendation is based upon measurements by Warren et al. [1277]. The relative rate measurement of Green and Wayne [453], 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.
- A38. $O(^1D) + CHClFCF_3$ (HCFC-124). The recommendation is based upon the measurement of Warren et al. [1277], who report (31 ± 10)% physical quenching.
- A39. $O(^1D) + CHF_2CF_3$ (HFC-125). The recommendation is based upon the measurement of Warren et al. [1277], who report (85+15/-22)% physical quenching. Green and Wayne [453] 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 .
- A40. $O(^1D) + CCl_3CF_3$ (CFC-113a). The recommendation is an estimate based on analogy to similar compounds.
- A41. $O(^1D) + CCl_2FCClF_2$ (CFC-113). The recommendation is an estimate based on analogy to similar compounds.
- A42. $O(^1D) + CCl_2FCF_3$ (CFC-114a). The recommendation is an estimate based on analogy to similar compounds.
- A43. $O(^1D) + CClF_2CClF_2$ (CFC-114). The recommendation is based on the measurement by Ravishankara et al. [985], who report (25 ± 9)% physical quenching.
- A44. $O(^1D) + CClF_2CF_3$ (CFC-115). The recommendation is based on the measurement by Ravishankara et al. [985], who report (70 ± 7)% physical quenching.
- A45. $O(^1D) + CBrF_2CBrF_2$ (Halon 2402). The recommendation is based on data from Thompson and Ravishankara [1165]. They report that the yield of $O(^3P)$ from physical quenching is (25±7)%. Lorenzen-Schmidt et al. [753] measured the Halon removal rate relative to the N_2O removal rate and report that the rate coefficient for the Halon destruction path is $(8.8 ± 1.2) × 10^{-11}$, in fair agreement with the result of Thompson and Ravishankara.
- A46. $O(^1D) + C_2F_6$ (CFC-116). The recommendation is based on a measurement by Ravishankara et al. [985], who report (85 ± 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.
- A47. $O(^1D) + CHF_2CF_2CF_2CHF_2$ (HFC 338 pcc). The recommendation is based on data from Schmoltnner et al. [1039]. They report that the yield of $O(^3P)$ from physical quenching is (97 ± 9)%.
- A48. $O(^1D) + c-C_4F_8$. The recommendation for perfluorocyclobutane is based upon the measurement by Ravishankara et al. [985], 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.
- A49. $O(^1D) + CF_3CHFCHFCF_2CF_3$ (HFC 43-10 mee). The recommendation is based on data from Schmoltnner et al. [1039]. The rate coefficients for this compound and CHF_2CF_3 do not follow the reactivity trend of other HFCs. Schmoltnner et al. report that the yield of $O(^3P)$ from physical quenching is (91±4)%.
- A50. $O(^1D) + C_5F_{12}$ (CFC 41-12). The recommendation is based on data from Ravishankara et al. [985]. They report that the yield of $O(^3P)$ from physical quenching is (79±12)%.
- A51. $O(^1D) + C_6F_{14}$ (CFC 51-14). The recommendation is based on data from Ravishankara et al. [985]. They report that the yield of $O(^3P)$ from physical quenching is (75±9)%.
- A52. $O(^1D) + 1,2-(CF_3)_2c-C_4F_6$. The recommendation is based on data from Ravishankara et al. [985]. They report that the yield of $O(^3P)$ from physical quenching is (84±16)%.
- A53. $O(^1D) + SF_6$. The recommendation is based upon measurements by Ravishankara et al. [985] who report (32±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.
- A54. $O_2(^1Δ) + O$. The recommendation is based on the upper limit reported by Clark and Wayne [232].

- A55. $O_2(^1\Delta) + O_2$. The recommendation is the average of eight room temperature measurements: Steer et al. [1108], Findlay and Snelling [392], Borrell et al. [140], Leiss et al. [706], Tachibana and Phelps [1140], Billington and Borrell [127], Raja et al. [977], and Wildt et al. [1306]. 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 [231], Findlay et al. [391], and McLaren et al. [797]. Wildt et al. [1307] report observations of weak emissions in the near IR due to collision-induced radiation. Wildt et al. [1308] give rate coefficients for this process.
- A56. $O_2(^1\Delta) + O_3$. The recommendation is the average of the room temperature measurements of Clark et al. [230], Findlay and Snelling [393], Becker et al. [95], and Collins et al. [266]. Several less direct measurements agree well with the recommendation (McNeal and Cook [798], Wayne and Pitts [1290], and Arnold and Comes [30]). 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 O_3 destruction near the peak of the Hartley band. For example, measurements of the number of O_3 molecules destroyed per photon absorbed: Von Ellenrieder et al. [1237], Ravishankara et al. [991], Lissi and Hecklen [746], and references cited therein and measurements of O_3 loss and O atom temporal profiles in pulsed experiments Klais et al. [633] and Arnold and Comes [30]. Anderson et al. [26] report that the rate coefficient for atom exchange between $O_2(^1\Delta)$ and O_3 is $< 5 \times 10^{-16}$ at 300 K.
- A57. $O_2(^1\Delta) + H_2O$. The recommendation is the average of the measurements reported by Becker et al. [94] and Findlay and Snelling [392]. An earlier study by Clark and Wayne [231] reported a value about three times larger.
- A58. $O_2(^1\Delta) + N$. The recommendation is an upper limit based upon the measurement reported by Westenberg et al. [1301], who used ESR to detect $O_2(X^3\Sigma$ and $a^1\Delta)$, $O(^3P)$ and $N(^4S)$ with a discharge flow reactor. They used an excess of $O_2(^1\Delta)$ and measured the decay of N and the appearance of O at 195 and 300 K. They observed that the reaction of N with $O_2(^1\Delta)$ is somewhat slower than its reaction with $O_2(^3\Sigma)$. The recommended rate constant value for the latter provides the basis for the recommendation. Clark and Wayne [232,233] and Schmidt and Schiff [1036] reported observations of an $O_2(^1\Delta)$ reaction with N that is about 30 times faster than the recommended limit. Schmidt and Schiff attribute the observed loss of $O_2(^1\Delta)$ in excess N to a rapid energy exchange with some constituent in discharged nitrogen, other than N.
- A59. $O_2(^1\Delta) + N_2$. The recommendation is based upon the measurements by Findlay et al. [391] and Becker et al. [94]. Other studies obtained higher values for an upper limit: Clark and Wayne [231] and Steer et al. [1108].
- A60. $O_2(^1\Delta) + CO_2$. The recommendation is based on the measurements reported by Findlay and Snelling [392] and Leiss et al. [706]. Upper limit rate coefficients reported by Becker et al. [94], McLaren et al. [797], and Singh et al. [1074] are consistent with the recommendation.
- A61. $O_2(^1\Delta) + O$. The recommendation is based on the measurement reported by Slinger and Black [1088].
- A62. $O_2(^1\Delta) + O_2$. The recommendation is the average of values reported by Martin et al. [788], Lawton et al. [686], and Lawton and Phelps [687], who are in excellent agreement. Measurements by Thomas and Thrush [1164], Chatha et al. [214], and Knickelbein et al. [639] are in reasonable agreement with the recommendation. Knickelbein et al. report an approximate unit yield of $O_2(^1\Delta)$ product.
- A63. $O_2(^1\Delta) + O_3$. The recommendation is based upon the room temperature measurements of Gilpin et al. [439], Slinger and Black [1088], Choo and Leu [229], and Shi and Barker [1057]. Measurements by Snelling [1096], Amimoto and Wiesenfeld [19], Ogren et al. [903], and Turnipseed et al. [1208] are in very good agreement with the recommendation. The temperature dependence is derived from the results of Choo and Leu. The yield of $O + 2O_2$ products is reported to be $(70 \pm 20)\%$ by Slinger and Black and Amimoto and Wiesenfeld.
- A64. $O_2(^1\Delta) + H_2O$. The recommendation is the average of room temperature measurements reported by Stuhl and Niki [1127], Filseth et al. [390], Wildt et al. [1306], and Shi and Barker [1057]. These data cover a range of about a factor of two. Measurements reported by O'Brien and Myers [902], Derwent and Thrush [342], and Thomas and Thrush [1164] are in good agreement with the recommendation. Wildt et al. [1306] report that the yield of $O_2(^1\Delta) \geq 90\%$.
- A65. $O_2(^1\Delta) + N$. The recommendation is based on the limit reported by Slinger and Black [1088].

- A66. $O_2(^1\Delta) + N_2$. The recommendation is the average of measurements reported by Izod and Wayne [566], Stuhl and Welge [1130], Filseth et al. [390], Martin et al. [788], Kohse-Höinghaus and Stuhl [646], Choo and Leu [229], Wildt et al. [1306], and Shi and Barker [1057]. Less direct measurements reported by Noxon [901], Myers and O'Brien [843], and Chatha et al. [214] are consistent with the recommendation. Kohse-Höinghaus and Stuhl observed no significant temperature dependence over the range 203–349 K.
- A67. $O_2(^1\Delta) + CO_2$. The recommendation is the average of measurements reported by Filseth et al. [390], Davidson et al. [310], Avilés et al. [51], Muller and Houston [840], Choo and Leu [229], Wildt et al. [1306], and Shi and Barker [1057] at room temperature. The temperature dependence is from the work of Choo and Leu. Muller and Houston and Singh and Setser [1075] give evidence that $O_2(^1\Delta)$ is a product. Wildt et al. report that the yield of $O_2(^1\Delta) \geq 90\%$.
- B1. $O + OH$. The rate constant for $O + OH$ is a fit to three temperature dependence studies: Westenberg et al. [1300], Lewis and Watson [727], and Howard and Smith [532]. This recommendation is consistent with earlier work near room temperature as reviewed by Lewis and Watson [727] and with the measurements of Brune et al. [160]. The ratio $k(O + HO_2)/k(O + OH)$ measured by Keyser [621] agrees with the rate constants recommended here.
- B2. $O + HO_2$. The recommended values are based on the results of studies over a range of temperatures by Keyser [620] and Nicovich and Wine [871] and the room temperature studies of Sridharan et al. [1099], Ravishankara et al. [991], and Brune et al. [160]. Earlier studies by Hack et al. [467] and Burrows et al. [176,179] are not considered, because the $OH + H_2O_2$ reaction was important in these studies and the value used for its rate constant in their analyses has been shown to be in error. Data from Ravishankara et al. [991] at 298 K show no dependence on pressure between 10 and 500 torr N_2 . The ratio $k(O + HO_2)/k(O + OH)$ measured by Keyser [621] agrees with the rate constants recommended here. Sridharan et al. [1097] showed that the reaction products correspond to abstraction of an oxygen atom from HO_2 by the O reactant. Keyser et al. [625] reported $<1\%$ $O_2(^1\Delta)$ yield.
- B3. $O + H_2O_2$. There are two direct studies of the $O + H_2O_2$ reaction: Davis et al. [320] and Wine et al. [1316]. The recommended value is a fit to the combined data. Wine et al. suggest that the earlier measurements may be too high because of secondary chemistry. The A-factor for both data sets is quite low compared to similar atom-molecule reactions. An indirect measurement of the E/R by Roscoe [1006] is consistent with the recommendation.
- B4. $H + O_3$. The recommendation is an average of the results of Lee et al. [693] and Keyser [616], which are in excellent agreement over the 200–400 K range. An earlier study by Clyne and Monkhouse [251] 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. Results by Finlayson-Pitts and Kleindienst [397] agree well with the present recommendations. Reports of a channel forming $HO_2 + O$ (Finlayson-Pitts and Kleindienst [397]: ~25%, and Force and Wiesenfeld [406]: ~40%) have been contradicted by other studies (Howard and Finlayson-Pitts [531]: <3%; Washida et al. [1280]: <6%; Finlayson-Pitts et al. [398]: <2%; and Dodonov et al. [357]: <0.3%). Secondary chemistry is believed to be responsible for the observed O-atoms in this system. Washida et al. [1281] measured a low limit (<0.1%) for the production of singlet molecular oxygen in the reaction $H + O_3$.
- B5. $H + HO_2$. There are five studies of this reaction: Hack et al. [471], Hack et al. [469], Thrush and Wilkinson [1171], Sridharan et al. [1099] and Keyser [623]. 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 HO_2 reactant. The recommendation is based on the data of Sridharan et al. and Keyser because their measurements were the most direct and required the fewest corrections. The other measurements, $(5.0 \pm 1.3) \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by Thrush and Wilkinson [1171] and $(4.65 \pm 1) \times 10^{-11}$ by Hack et al. [469] are in reasonable agreement with the recommended value. Three of the studies reported the product channels: (a) 2OH, (b) $H_2O + O$, and (c) $H_2 + O_2$. Hack et al. [471] $k_a/k = 0.69$, $k_b/k = 0.02$, and $k_c/k = 0.29$; Sridharan et al. [1099] $k_a/k = 0.87 \pm 0.04$, $k_b/k = 0.02 \pm 0.02$, $k_c/k = 0.09 \pm 0.045$; and Keyser [623] $k_a/k = 0.90 \pm 0.04$, $k_b/k = 0.02 \pm 0.02$, and $k_c/k = 0.08 \pm 0.04$. Hislop and Wayne [511], Keyser et al. [625], and Michelangeli et al. [825] reported on the yield of $O_2(^1\Sigma)$ formed in channel (c) as $(2.8 \pm 1.3) \times 10^{-4}$, $<8 \times 10^{-3}$, and $<2.1 \times 10^{-2}$ respectively of the total reactions. Keyser found the rate coefficient and product yields to be independent of temperature for $245 < T < 300 \text{ K}$.
- B6. $OH + O_3$. Recommended values are based on the results of studies over a range of temperatures by Anderson and Kaufman [23], Ravishankara et al. [990], Smith et al. [1091] and Nizkorodov et al. [895] and the room

temperature measurements of Kurylo [660], Zahniser and Howard [1353], and Kulcke et al. [655]. 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 obtained in the above-mentioned studies. The values reported by Kulcke et al. [655] and Nizkorodov et al. [899] have been corrected for a minor contribution from $k(\text{HO}_2 + \text{O}_3)$.

- B7. $\text{OH} + \text{H}_2$. The $\text{OH} + \text{H}_2$ reaction has been the subject of numerous studies (see Ravishankara et al. [983] for a review of experimental and theoretical work). The recommendation is fixed to the average of nine studies at 298 K: Greiner [457], Stuhl and Niki [1129], Westenberg and de Haas [1298], Smith and Zellner [1093], Atkinson et al. [43], Overend et al. [923], Tully and Ravishankara [1198], Zellner and Steinert [1360], and Ravishankara et al. [983]. Results reported by Talukdar et al. [1153] are in excellent agreement.
- B8. $\text{OH} + \text{HD}$. The recommendation is based on direct measurements made by Talukdar et al. [1153] using pulsed photolysis-laser induced fluorescence over the temperature range 248–418 K. The recommendation is in excellent agreement with the ratio $k(\text{OH} + \text{H}_2)/k(\text{OH} + \text{HD}) = 1.65 \pm 0.05$ at 298 K reported by Ehhalt et al. [375] when combined with the recommended $k(\text{OH} + \text{H}_2)$.
- B9. $\text{OH} + \text{OH}$. The recommendation for the $\text{OH} + \text{OH}$ reaction is the average of six measurements near 298 K: Westenberg and de Haas [1297], McKenzie et al. [796], Clyne and Down [240], Trainor and von Rosenberg [1185], Farquharson and Smith [384], and Wagner and Zellner [1239]. The rate constants for these studies all fall between $(1.4 \text{ and } 2.3) \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. The temperature dependence is from Wagner and Zellner, who reported rate constants for the range $T = 250\text{--}580\text{ K}$.
- B10. $\text{OH} + \text{HO}_2$. A study by Keyser [624] 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 [619], Thrush and Wilkinson [1170], Sridharan et al. [1098,1100], Temps and Wagner [1160], and Rozenshtein et al. [1010], and atmospheric pressure studies that gave rate coefficients near 11×10^{-11} : Lii et al. [735], Hochanadel et al. [517], DeMore [329], Cox et al. [278], Burrows et al. [178], and Kurylo et al. [666]. Laboratory measurements using a discharge flow experiment and a chemical model analysis of the results by Keyser [624] demonstrate that the previous discharge flow measurements were probably subject to interference from small amounts of O and H. In the presence of excess HO_2 these atoms generate OH and result in a rate coefficient measurement that falls below the true value.

The temperature dependence is from Keyser [624], who covered the range 254 to 382 K. A flow tube study by Schwab et al. [1043] reported $k = (8.0 +3/-4) \times 10^{-11}$. These workers measured the concentrations of HO_2 , 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 [365] employing an isotope labelled ^{18}OH 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 ^{16}OH gave $k = 6 \times 10^{-11}$. It should be noted that their control experiments were subject to the errors described by Keyser [624] due to the presence of small amounts of H and O, whereas their ^{18}OH measurements were not. Kurylo et al. [666] found no evidence of significant scrambling in isotope studies of the OH and HO_2 reaction. An additional careful study of the reaction temperature dependence would be useful. Hippler and Troe [509] 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.

- B11. $\text{OH} + \text{H}_2\text{O}_2$. The recommendation is a fit to the temperature dependence studies of Keyser [618], Sridharan et al. [1101], Wine et al. [1320], Kurylo et al. [670], and Vaghjiani et al. [1224]. The data from these studies have been revised to account for the H_2O_2 UV absorption cross section recommendations in this evaluation. The first two references contain a discussion of some possible reasons for the discrepancies with earlier work and an assessment of the impact of the new value on other kinetic studies. All of these measurements agree quite well and overlap one another. Measurements by Lamb et al. [676] agree at room temperature but indicate a quite different temperature dependence with k increasing slightly with decreasing temperature. Their data were not incorporated in the fit. Measurements at room temperature by Marinelli and Johnston [781] and Turnipseed et al. [1208] agree well with the recommendation. Hippler and Troe [509] have analysed data for this reaction at temperatures up to 1250 K.
- B12. $\text{HO}_2 + \text{O}_3$. The recommended values are based on results of studies over a range of temperatures by DeMore [327] at 231 to 334 K, Zahniser and Howard [1353] at 245 to 365 K, Manzanares et al. [772] at 298 K, Sinha et al. [1084] at 243 to 413 K, Wang et al. [1275] at 233 to 400 K and Herndon et al. [501] at 200 to 298 K. The data of Simonaitis and Heicklen [1069] and DeMore and Tschuikow-Roux [338] 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 ^{18}O labelled HO_2 by Sinha et al. [1084], who reported that the reaction occurs $75 \pm 10\%$ via H atom transfer at 297 K and by Nelson and Zahniser [851], 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 $94 \pm 5\%$ at $226 \pm 11\text{ K}$ to $88 \pm 5\%$ at $355 \pm 8\text{ K}$.

- B13. $\text{HO}_2 + \text{HO}_2$. Two separate expressions are given for the rate constant for the $\text{HO}_2 + \text{HO}_2$ 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 have negative temperature coefficients. The bimolecular expression is obtained from data of Cox and Burrows [277], Thrush and Tyndall [1167,1168], Kircher and Sander [627], Takacs and Howard [1144,1145], Sander [1016] and Kurylo et al. [672]. Data of Rozenshtein et al. [1010] 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 [1169] and Dobis and Benson [355] are inconsistent with the recommendation. The termolecular expression is obtained from data of Sander et al. [1021], Simonaitis and Hecklen [1071], and Kurylo et al. [672] at room temperature and Kircher and Sander [627] for the temperature dependence. This equation applies to $M = \text{air}$. On this reaction system there is general agreement among investigators on the following aspects of the reaction at high pressure ($P \sim 1\text{ atm}$): (a) the HO_2 UV absorption cross section: Paukert and Johnston [934], Cox and Burrows [277], Hochanadel et al. [517], Sander et al. [1021], Kurylo et al. [673], and Crowley et al. [295]; (b) the rate constant at 300K: Paukert and Johnston [934], Hamilton and Lii [476], Cox and Burrows [277], Lii et al. [734], Tsuchiya and Nakamura [1190], Sander et al. [1021], Simonaitis and Hecklen [1071], Kurylo et al. [672], Andersson et al. [27], and Crowley et al. [295] (all values fall in the range $(2.5\text{ to }4.7) \times 10^{-12}\text{ cm}^3\text{ molecule}^{-1}\text{ s}^{-1}$); (c) the rate constant temperature dependence: Cox and Burrows [277], Lii et al. [734], and Kircher and Sander [627]; (d) the rate constant water vapor dependence: Hamilton [475], Hochanadel et al. [516], Hamilton and Lii [476], Cox and Burrows [277], DeMore [327], Lii et al. [736], Sander et al. [1021], and Andersson et al. [27]; (e) the H/D isotope effect: Hamilton and Lii [476] and Sander et al. [1021]; and (f) the formation $\text{H}_2\text{O}_2 + \text{O}_2$ as the major products at 300 K: Su et al. [1133], Niki et al. [887], Sander et al. [1021], and Simonaitis and Hecklen [1071]. Sahetchian et al. [1014,1015] give evidence for the formation of a small amount of H_2 ($\sim 10\%$) at temperatures near 500 K, but Baldwin et al. [58] and Ingold [560] give evidence that the yield must be much less. Glinski and Birks [445] 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. [1112]). For systems containing water vapor, the multiplicative factor given by Lii et al. [736] and Kircher and Sander [627] can be used: $1 + 1.4 \times 10^{-21} [\text{H}_2\text{O}] \exp(2200/T)$. Lightfoot et al. [732] 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 elevated temperature. A high temperature study by Hippler et al. [510] confirms the strong curvature.
- C1. $\text{O} + \text{NO}_2$. The recommended values are based on the results of studies over a range of temperatures by Gierczak et al. [428], Ongstad and Birks [909], Slinger et al. [1089] and Geers-Muller and Stuhl [425] and the room temperature study of Paulson et al. [935]. In the most recent study of Gierczak et al. [428], 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. [315] and Bemand et al. [110] 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.
- C2. $\text{O} + \text{NO}_3$. Based on the study of Graham and Johnston [451] 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.
- C3. $\text{O} + \text{N}_2\text{O}_5$. Based on Kaiser and Japar [600].
- C4. $\text{O} + \text{HNO}_3$. The upper limit reported by Chapman and Wayne [212] is accepted.
- C5. $\text{O} + \text{HO}_2\text{NO}_2$. The recommended value is based on the study of Chang et al. [211]. 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.

- C6. H + NO₂. The recommended value of k_{298} is derived from the studies of Wagner et al. [1241], Bemand and Clyne [108], Clyne and Monkhouse [251], Michael et al. [820] and Ko and Fontijn [644]. The temperature dependence is from the studies of Wagner et al. and Ko and Fontijn. The data from Wategaonkar and Setser [1284] and Agrawalla et al. [14] were not considered.
- C7. OH + NO₃. The recommendation is derived from an average of the results of Boodaghians et al. [137], Mellouki et al. [806], Becker et al. [91] and Mellouki et al. [809]. There are no temperature dependence data. The reaction products are probably HO₂ + NO₂.
- C8. OH + HONO. The recommended rate expression is derived from the work of Jenkin and Cox [577], which supersedes the earlier room temperature study of Cox et al. [284]. Recent results from the Ravishankara group [173] suggest that the reaction may have a small negative temperature dependence.
- C9. OH + HNO₃. The recent study of Brown et al. [159] furnishes the most comprehensive set of rate measurements for N₂ 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. [1091], involving the formation of a bound, relatively long-lived HO·HNO₃ complex, as well as the direct reaction channel. Studies of the effects of isotopic substitution on the reactions OD+DNO₃, OH+DNO₃, OD+HNO₃ and ¹⁸OH+HNO₃, by Brown et al. [158] 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:

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

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 $k([M],T)$ and the values of the Arrhenius parameters for k_0 , k_2 , and k_3 derived by Brown et al. [159] for N₂ 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. [159], Stachnik et al. [1103], Devolder et al. [343] and Margitan and Watson [776].

The reaction yield of NO₃ (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. [158] and the theoretical calculations of Xia and Lin [1338].

- C10. OH + HO₂NO₂. The recommendation for both k at 298 K and the Arrhenius expression is based upon the data of Trevor et al. [1186], Barnes et al. [64], C. A. Smith et al. [1091] and Barnes et al. [66]. 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±193) 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±30) K. The early Barnes et al. study [64] 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 N₂ and temperature range 268–295 K with no rate constant variation being observed. In addition, k_{298} derived in Barnes et al. [64] 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 [747] 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.
- C11. OH + NH₃. The recommended value at 298 K is the average of the values reported by Stuhl [1125], Smith and Zellner [1094], Perry et al. [943], Silver and Kolb [1061], Stephens [1111] and Diau et al. [346]. The values reported by Pagsberg et al. [925] and Cox et al. [283] 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 [660] and Hack et al. [465] 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 [1094] and Diau et al. [346], and the A-factor has been selected to fit the recommended room temperature value.

- 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 [530], Leu [713], Howard [527], Glaschick-Schimpf et al. [440], Hack et al. [468], Thrush and Wilkinson [1170] and Jemi-Alade Thrush [574], and Seeley et al. [1047]. All of these are in quite good agreement. The results of Imamura and Washida [559] were not considered due to the relatively large uncertainty limits reported in this study. An earlier study, Burrows et al. [176] has been disregarded because of an error in the reference rate constant, k(OH + H₂O₂). The room temperature study of Rozenshtein et al. [1010] 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 K) is obtained from the Arrhenius line.
- C13. HO₂ + NO₂. Tyndall et al. [1212] 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.
- C14. HO₂ + NO₃. The recommendation for k₂₉₈ is based on a weighted average of the data of Hall et al. [473], Mellouki et al. [806], Becker et al. [91] and Mellouki et al. [809]. 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. [809], which obtained a value of 1.0 +0.0/-0.3 at 298 K.
- 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 [659] and the relative studies of Cheskis and Sarkisov [225] and Pagsberg et al. [925]. 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.
- C16. N + O₂. The recommended expression is derived from a least squares fit to the data of Kistiakowsky and Volpi [629], Wilson [1310], Becker et al. [93], Westenberg et al. [1301], Clark and Wayne [233], Winkler et al. [1328] and Barnett et al. [74]. k(298 K) is derived from the Arrhenius expression and is in excellent agreement with the average of all of the room temperature determinations.
- C17. N + O₃. The recommendation is based on the results of Barnett et al. [74]. 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. [1121] and Garvin and Broida [423] cast doubt on the much faster rates reported by Phillips and Schiff [948], and Chen and Taylor [221].
- C18. N + NO. The recommended temperature dependence is based on the discharge flow-resonance fluorescence studies of Wennberg and Anderson [1293], and the discharge flow-resonance fluorescence and flash photolysis-resonance fluorescence studies of Lee et al. [695]. There is relatively poor agreement between these studies and the results of Clyne and McDermid [248], Kistiakowsky and Volpi [630], Herron [502], Phillips and Schiff [948], Lin et al. [741], Ishikawa et al. [563], Sugawara et al. [1134], Cheah and Clyne [215], Husain and Slater [549], Clyne and Ono [255], Brunning and Clyne [161] and Jeoung et al. [587].
- C19. N + NO₂. The recommendation for k₂₉₈ is from the discharge flow-resonance fluorescence study of Wennberg and Anderson [1293]. The latter study had significantly better sensitivity for N(⁴S) than the discharge flow-resonance fluorescence study of Clyne and Ono [255], which obtained a value about four times smaller. The results of Husain and Slater [549] and Clyne and McDermid [248] 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. [564] suggested an upper limit of $3.3 \times 10^{-13} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for the corresponding reaction involving N(²D) and N(²P) atoms (sum of all reaction channels).
- C20. NO + O₃. The recommended values are based on the results of studies over a range of temperatures by Birks et al. [129], Lippmann et al. [743], Ray and Watson [997], Michael et al. [814], Borders and Birks [139] and Moonen et al. [833] and the room temperature studies of Stedman and Niki [1105] and Bemand et al. [110]. 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 [236], Birks et al., Schurath et al. [1042], and Michael et al. have reported individual Arrhenius parameters for the two primary reaction channels producing ground and excited molecular oxygen.

- C21. $\text{NO} + \text{NO}_3$. The recommendation is based on the studies of Hammer et al. [477], Sander and Kircher [1020] and Tyndall et al. [1213], which are in excellent agreement.
- C22. $\text{NO}_2 + \text{O}_3$. The recommended expression is derived from a least squares fit to the data of Davis et al. [318], Graham and Johnston [450], Huie and Herron [543], and Cox and Coker [279]. The data of Verhees and Adema [1228] and Stedman and Niki [1105] were not considered because of systematic discrepancies with the other studies.
- 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 [304]; Johnston and Tao [591]; Cantrell et al. [196]) and NO (Hjorth et al. [512], and Cantrell et al. [199]) 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.
- C24. $\text{NO}_3 + \text{NO}_3$. The recommendation for $k(298 \text{ K})$ is from the studies of Graham and Johnston [451] and Biggs et al. [123]. The temperature dependence is from Graham and Johnston.
- 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. [464] and Jayanty et al. [572] 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 [708]), 8×10^{-15} (Pagsberg et al. [925]), 1.5×10^{-17} (Cheskis and Sarkisov [225]), 3×10^{-18} (Lozovsky et al. [760]), 1×10^{-17} (Patrick and Golden [933]) and 7.7×10^{-18} (Michael et al. [816]) and 6×10^{-21} (Tyndall et al. [1215]). 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.
- C26. $\text{NH}_2 + \text{O}_3$. There is poor agreement among the recent studies of Cheskis et al. [224], $k(298) = 1.5 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Patrick and Golden [933], $k(298 \text{ K}) = 3.25 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Hack et al. [463], $1.84 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, Bulatov et al. [166], $1.2 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$, and Kurasawa and Lesclaux [658], $0.63 \times 10^{-13} \text{ cm}^3 \text{ s}^{-1}$. 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).
- 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. [710], Hancock et al. [478], Sarkisov et al. [1028], Stief et al. [1119], Andresen et al. [28] Whyte and Phillips [1302], Dreier and Wolfrum [367], Atakan et al. [33], Wolf et al. [1329], Diau et al. [344] and Imamura and Washida [559]. The results of Gordon et al. [447], Gehring et al. [426], Hack et al. [470] and Silver and Kolb [1062] 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 [1244] 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 [359], Silver and Kolb [1065], Atakan et al., Stephens et al. [1110], Park and Lin [930]) agree on a value around 0.1 at 300 K, with $\text{N}_2 + \text{H}_2\text{O}$ making up the balance.
- C28. $\text{NH}_2 + \text{NO}_2$. There have been four studies of this reaction (Hack et al. [470]; Kurasawa and Lesclaux [657]; Whyte and Phillips [1302]; and Xiang et al. [1339]). 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 $N_2O + H_2O$. Just as for the $NH_2 + NO$ 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.

- C29. $NH + NO$. The recommendation is derived from the room temperature results of Hansen et al. [481], Cox et al. [274] and Harrison et al. [483]. The temperature dependence is from Harrison et al.
- C30. $NH + NO_2$. The recommendation is derived from the temperature-dependence study of Harrison et al. [483].
- C31. $O_3 + HNO_2$. Based on Kaiser and Japar [599] and Streit et al. [1124].
- C32. $N_2O_5 + H_2O$. The recommended value at 298 K is based on the studies of Tuazon et al. [1193], Atkinson et al. [49] and Hjorth et al. [513]. Sverdrup et al. [1136] 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 Table 59 for heterogeneous rate data for this reaction.
- C33. $N_2(A, v) + O_2$. Rate constants for the overall reaction for the $v=0, 1$ and 2 vibrational levels of $N_2(A)$ have been made by Dreyer et al. [368], Zipf [1374], Piper et al. [951], Iannuzzi and Kaufman [557], Thomas and Kaufman [1163] and De Sousa et al. [324]. 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 $k(T, v) = k(v, 298K)(T/300)^{0.55}$ for $v=0, 1, 2$. The observation of high N_2O production initially reported by Zipf [1374] has not been reproduced by other groups, and the branching ratio for this channel is probably less than 0.02 (Iannuzzi et al. [556], Black et al. [132], De Sousa et al. [324], Fraser and Piper [407]). The branching ratios for the other channels are poorly established, although there is strong evidence for the formation of both $O(^3P)$ and $O_2(B^3\Sigma_u^-)$.
- C34. $N_2(A, v) + O_3$. The only study is that of Bohmer and Hack [136], 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 $N_2(A)$, respectively. This study determined that the NO channel accounts for about 20% of the reaction products.
- D1. $O + CH_3$. The recommended $k(298 \text{ K})$ is the weighted average of three measurements by Washida and Bayes [1282], Washida [1279], and Plumb and Ryan [956]. The E/R value is based on the results of Washida and Bayes [1282], who found k to be independent of temperature between 259 and 341 K.
- D2. $O + HCN$. Because it is a very slow reaction, there are no studies of this reaction below 450 K. Davies and Thrush [313] studied this reaction between 469 and 574 K while Perry and Melius [945] 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 Roth et al. [1007], Szekely et al. [1137], and Louge and Hanson [754] have not been considered. This reaction has two reaction pathways: $O + HCN \rightarrow H + NCO$, $\Delta H = -2 \text{ kcal/mol}$ (k_a); and $O + HCN \rightarrow CO + NH$ (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.
- D3. $O + C_2H_2$. The value at 298 K is an average of ten measurements (Arrington et al. [31], Sullivan and Warneck [1135], Brown and Thrush [156], Hoyermann et al. [533, 534], Westenberg and deHaas [1295], James and Glass [569], Stuhl and Niki [1128], Westenberg and deHaas [1299], and Aleksandrov et al. [16]). There is reasonably good agreement among these studies. Arrington et al. [31] did not observe a temperature dependence, an observation that was later shown to be erroneous by Westenberg and deHaas [1295]. Westenberg and deHaas [1295], Hoyermann et al. [534] and Aleksandrov et al. [16] 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., $C_2HO + H$ or $CH_2 + CO$. 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 $C_2HO + H$ channel contributes no more than 7% to the net reaction at 298 K, while a similar study by Vinckier et al. [1234] suggests that both CH_2 and C_2HO are formed.

- D4. $O + H_2CO$. The recommended values for A, E/R and $k(298\text{ K})$ are the averages of those determined by Klemm [635] (250 to 498 K) using flash photolysis-resonance fluorescence, by Klemm et al. [636] (298 to 748 K) using discharge flow-resonance fluorescence, and Chang and Barker [208] (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. [884], Herron and Penzhorn [504], and Mack and Thrush [762]. 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.
- D5. $O + CH_3CHO$. The recommended $k(298\text{ K})$ is the average of three measurements by Cadle and Powers [185], Mack and Thrush [763], and Singleton et al. [1078], 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 [763], Avery and Cvetanovic [50], and Singleton et al. [1078]).
- D6. $O_3 + C_2H_2$. The database for this reaction is not well established. Room temperature measurements (Cadle and Schadt [186]; DeMore [325]; DeMore [326]; Stedman and Niki [1106]; Pate et al. [932]; and Atkinson and Aschmann [34]) 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 [34], 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 [325,326]). 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 [326], and DeMore and Lin [336]). The anhydride intermediates in several alkyne ozonations have been isolated in low temperature solvent experiments (DeMore and Lin [336]).
- D7. $O_3 + C_2H_4$. The rate constant of this reaction is well established over a large temperature range, 178 to 360 K. Our recommendation is based on the data of DeMore [325], Stedman et al. [1107], Herron and Huie [503], Japar et al. [570,571], Toby et al. [1176], Su et al. [1132], Adeniji et al. [10], Kan et al. [606], Atkinson et al. [38], and Bahta et al. [55].
- D8. $O_3 + C_3H_6$. 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 [503], 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 [325], and is consistent with, but 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 [290], Stedman et al. [1107], Japar et al. [570,571], and Atkinson et al. [38] are in good agreement (10% or better) with the recommendation.
- D9. $OH + CO$. 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. [89]) and the values reported by Dreier and Wolfrum [366], Husain et al. [547], Ravishankara and Thompson [986], Paraskevopoulos and Irwin [927], Hofzumahaus and Stuhl [518]. The results of Jonah et al. [593] 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 [922], Perry et al. [944], Chan et al. [207], Biermann et al. [121], Cox et al. [284], Butler et al. [184], Paraskevopoulos and Irwin [926,927], DeMore [330], Hofzumahaus and Stuhl [518], Hynes et al. [554]). In addition, Niki et al. [892] have measured k relative to $OH + C_2H_4$ 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 [927], DeMore [330], Hofzumahaus and Stuhl [518], and Hynes et al. [554]) as well as those in air (Niki et al. [894], Hynes et al. [554]), 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. [121]) has been resolved and is attributed to secondary reactions (DeMore [330], Hofzumahaus and Stuhl [518]). The results of Butler et al. [184] have to be re-evaluated in the light of refinements in the rate coefficient for the $OH + H_2O_2$ reaction. The corrected rate coefficient is in approximate agreement with the recommended value. Currently,

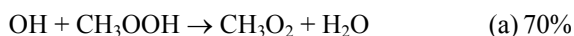
there are no indications to suggest that the presence of O₂ has any effect on the rate coefficient other than as a third body. The E/R value in the pressure range 50–760 torr has been shown to be essentially zero between 220 and 298 K by Hynes et al. [554]. Further substantiation of the temperature independence of k at 1 atm. may be worthwhile. Beno et al. [111] observe an enhancement of k with water vapor, which is in conflict with the flash photolysis studies; e.g., Ravishankara and Thompson [986], Paraskevopoulos and Irwin [927], and Hynes et al. [554]. The uncertainty factor is for 1 atm. of air.

The bimolecular channel yields H + CO₂ while the addition leads to HOCO. In the presence of O₂, the HOCO intermediate is converted to HO₂ + CO₂ (DeMore [330], Miyoshi et al. [827]). Miyoshi et al. report a rate constant for the reaction of HOCO with O₂ 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 HO₂ and CO₂.

- D10. OH + CH₄. This reaction has been extensively studied. The most recent data are from Vaghjani and Ravishankara [1223], Saunders et al. [1030], Finlayson-Pitts et al. [396], Dunlop and Tully [370], Mellouki et al. [812], and Gierczak et al. [434], who measured the absolute rate coefficients for this reaction using discharge flow and pulsed photolysis techniques. Sharkey and Smith [1056] have reported a high value ($7.7 \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) for k(298 K), and this value has not been considered here. The current recommendation for k(298 K) was derived from the results of Vaghjani 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 Vaghjani 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.
- D11. OH + ¹³CH₄. This reaction has been studied relative to the OH + CH₄ reaction, since the ratio of the rate coefficients is the quantity needed for quantifying methane sources. Rust and Stevens [1011], Davidson et al. [308], and Cantrell et al. [200] have measured k₁₂/k₁₃ 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 k₁₂/k₁₃ to be independent of temperature between 273 and 353 K.
- D12. OH + CH₃D. 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. [433]. 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 [334] 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 [448] 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 [370], Gierczak et al. [1153], Gordon and Mulac [448]).
- D13. OH + H₂CO. The value for k(298 K) is the average of those determined by Niki et al. [893], Atkinson and Pitts [46], Stief et al. [1120], Yetter et al. [1345], and Temps and Wagner [1161]. The value reported by Morris and Niki [836] agrees within the stated uncertainty. There are two relative values that are not in agreement with the recommendations. The value of Niki et al. [886] relative to OH + C₂H₄ is higher, while the value of Smith [1095] relative to OH + OH is lower. The latter data are also at variance with the negligible temperature dependence observed in the two flash photolysis studies. The later report of Niki et al. [893] is assumed to supersede the earlier rate constant. The rate coefficient reported by Zabarnick et al. [1348] at and above 298 K are consistently higher than the average value recommended here, but overlap within the combined uncertainty. The combined data set suggests E/R = 0, although a slight negative temperature dependence cannot be ruled out. The abstraction reaction shown in the table is the major channel (Temps and Wagner [1161], Niki et al. [892]); other channels may contribute to a small extent (Horowitz et al. [525]).
- D14. OH + CH₃OH. The recommended value for k(298 K) is the average of seven direct studies (Overend and Paraskevopoulos [921], Ravishankara and Davis [979], Hagele et al. [472], Meier et al. [800], Greenhill and O'Grady [456], Wallington and Kurylo [1264], and Hess and Tully [506]). When these measurements were not at exactly 298 K, their values have been recalculated for 298 K by using the E/R recommended here.

Indirect measurements by Campbell et al. [190], Barnes et al. [65], Tuazon et al. [1194] and Klopffer et al. [638] 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, and Hess and Tully. The recommended value of E/R was calculated using the results obtained in the temperature range of 240 to 400 K by Greenhill and O'Grady [456], Wallington and Kurylo [1264], Hess and Tully, Meier et al., and Haegle et al. 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 $\text{CH}_2\text{OH} + \text{H}_2\text{O}$ or from the OH group to give $\text{CH}_3\text{O} + \text{H}_2\text{O}$. The results of Hagele et al., Meier et al., and Hess and Tully suggest that H abstraction from the methyl group to give $\text{CH}_2\text{OH} + \text{H}_2\text{O}$ is the dominant channel below room temperature. At 298 K, for example, the branching ratio for the formation of CH_2OH is about 0.85 and increases as the temperature decreases. In the Earth's atmosphere, the eventual products of $\text{OH} + \text{CH}_3\text{OH}$ reaction are the same: CH_2O and HO_2 .

- D15. $\text{OH} + \text{CH}_3\text{OOH}$. The recommended value for $k(298 \text{ K})$ is the average of the rate coefficients measured by Niki et al. [891] and Vaghjiani and Ravishankara [1222], which differ by nearly a factor of two. Niki et al. measured the rate coefficient relative to that for OH with C_2H_4 ($= 8.0 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) by monitoring CH_3OOH disappearance using an FTIR system. Vaghjiani and Ravishankara monitored the disappearance of OH , OD , and ^{18}OH in excess CH_3OOH in a pulsed photolysis-LIF system. They measured k between 203 and 423 K and report a negative activation energy with $E/R = -190 \text{ K}$; the recommended E/R is based on their results. The reaction of OH with CH_3OOH occurs via abstraction of H from the oxygen end to produce the CH_3OO radical and from the CH_3 group to produce the CH_2OOH radical, as originally proposed by Niki et al. and confirmed by Vaghjiani and Ravishankara. CH_2OOH is unstable and falls apart to CH_2O and OH within a few microseconds. The possible reaction of CH_2OOH with O_2 is unimportant under atmospheric conditions (Vaghjiani and Ravishankara). The recommended branching ratios are,



(from Vaghjiani and Ravishankara) and are nearly independent of temperature.

- D16. $\text{OH} + \text{HC(O)OH}$. The recommended value of $k(298 \text{ K})$ is the average of those measured by Zetzsch and Stuhl [1363], Wine et al. [1311], Jolly et al. [592], Dagaut et al. [303], and Singleton et al. [1083]. 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 $\text{OH} + \text{HC(O)OH}$ reaction to be the same as that for $\text{OH} + \text{DC(O)OH}$ 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 CO_2 and H. End product studies are also consistent with the formation of CO_2 and H_2O in this reaction (Singleton et al. [1083]). The products of this reaction would be mostly HC(O)O and H_2O . The fate of HC(O)O in the atmosphere will be to give HO_2 either directly via reaction with O_2 or via thermal decomposition to H atom, which adds to O_2 .

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.

- D17. $\text{OH} + \text{HCN}$. This reaction is pressure dependent. The recommended value is the high pressure limit measured by Fritz et al. [414] using a laser photolysis-resonance fluorescence apparatus. Phillips [947] 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.
- D18. $\text{OH} + \text{C}_2\text{H}_6$. There are nineteen studies of this reaction at 298 K (Greiner [458], Howard and Evenson [529], Overend et al. [923], Lee and Tang [697], Leu [713], Tully et al. [1199], Jeong et al. [584], Tully et al. [1197], Nielsen et al. [879], Zabarnick et al. [1348], Wallington et al. [1266], Smith et al. [1091], Baulch et al. [88], Bourmada et al. [144], Abbatt et al. [2], Schiffman et al. [1033], Talukdar et al. [1155], Sharkey and Smith [1056] and Anderson and Stephens [24]). 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 C_2H_6 and C_3H_8 has been measured by Finlayson-Pitts [396]. Our recommendations are in reasonable agreement with this ratio. Crowley et al. [294] have measured k at 247, 294, and 303 K, and the results are in agreement with the recommendations.

- D19. OH + C_3H_8 . There are many measurements of the rate coefficients at 298 K. In this evaluation we have considered only the direct measurements (Greiner [458], Tully et al. [1199], Droege and Tully [369], Schmidt et al. [1037], Baulch et al. [88], Bradley et al. [147], Abbatt et al. [2], Schiffman et al. [1033], Talukdar et al. [1155], Anderson and Stephens [24] and Mellouki et al. [812]). The 298 K value is the average of these ten studies. Greiner, Tully et al. [1196], Droege and Tully, Talukdar et al. and Mellouki et al. have measured the temperature dependence of this reaction. The recommended E/R was obtained from a linear least squares analysis of the data of Droege and Tully below 400 K and the data of Talukdar et al., Anderson and Stephens, and Mellouki et al. The A-factor was adjusted to reproduce $k(298\text{ K})$. This reaction has two possible channels, i.e., abstraction of the primary and the secondary H-atom. Therefore, non-Arrhenius behavior is exhibited over a wide temperature range, as shown by Tully et al. and Droege and Tully. 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 C_2H_6 and C_3H_8 has been measured by Finlayson-Pitts et al. [396]. Our recommendations are in reasonable agreement with this ratio.

- D20. OH + CH_3CHO . There are six measurements of this rate coefficient at 298 K (Morris et al. [838], Niki et al. [886], Atkinson and Pitts [46], Kerr and Sheppard [613], Semmes et al. [1054], and Michael et al. [815]). The recommended value of $k(298\text{ K})$ is the average of these measurements. Atkinson and Pitts, Semmes et al., and Michael et al. measured the temperature dependence of this rate coefficient and found it to exhibit a negative temperature dependence. The recommended E/R is the average value of these studies. The A-factor has been adjusted to yield the recommended value of $k(298\text{ K})$.
- D21. OH + C_2H_5OH . The recommended value for $k(298\text{ K})$ is the average of those reported by Campbell et al. [190], Overend and Paraskevopoulos [921], Ravishankara and Davis [979], Cox and Goldstone [288], Kerr and Stocker [614], Wallington and Kurylo [1264], and Hess and Tully [505]. The value reported by Meier et al. is nearly a factor of two lower than that recommended here. The recommended value of E/R was obtained by using the data of Wallington and Kurylo, Hess and Tully, and Meier et al. The temperature dependent rate coefficient values of Meier et al. were assumed to have the same systematic error that, hence, would not be reflected in the derivation of the E/R value. The A-factor has been adjusted to yield the recommended value of $k(298\text{ K})$. This reaction has three possible product channels: (a) $CH_3CH_2O + H_2O$, (b) $CH_3CHOH + H_2O$, and (c) $CH_2CH_2OH + H_2O$. At atmospheric temperatures, channel (b) is the major pathway (Meier et al. [801], Hess and Tully [505]), accounting for more than 75% of the reaction. The branching ration for channel (b) is expected to increase with decreasing temperature, based on the work of Hess and Tully [505]. The CH_3CHOH radical that is produced in channel (b) and CH_3CH_2O radical formed in channel (a) will both rapidly react with O_2 leading to CH_3CHO and HO_2 . However, the CH_2CH_2OH radical produced in channel (c) will lead to a different set of products in the atmosphere. The exact values for these reaction pathways under atmospheric temperatures have not been quantified. Extrapolations of the higher temperature data to atmospheric temperatures may not be valid.
- D22. OH + $CH_3C(O)OH$. The recommended $k(298\text{ K})$ is the average of the values obtained by Dagaut et al. [303] and Singleton et al. [1082]. The earlier results of Zetzsch and Stuhl [1363] are lower than these values, but within the uncertainty of the recommended value. The temperature dependence has been studied by Dagaut et al., who observe a very slight increase in k with temperature between 298 and 440 K and by Singleton et al., who observe a significant decrease with increase in temperature between 298 and 446 K. Further, Singleton et al. observe that the Arrhenius plot is curved. While Dagaut et al. observed that the acetic acid dimer reacts twice as fast as the monomer, Singleton et al. found the dimer to be essentially unreactive toward OH! The latter observations are consistent with the mechanism for the OH + $HC(O)OH$ reaction, which is discussed in the note for that reaction. It is also consistent with the decrease in reactivity upon D substitution on the carboxylic site and no change upon substitution on the methyl group (Singleton et al. [1082]). Thus, there is some uncertainty as to the T dependence and the reaction mechanism. Here we recommend a slightly

negative T dependence, based on an average of both temperature dependence studies but with an uncertainty that encompasses both the studies. The A factor and E/R suggest that this reaction may not be a simple metathesis reaction. Based on the analogy with OH + HC(O)OH reaction and the evidence of Singleton et al., the products are expected to be mostly CH₃C(O)O + H₂O. In the atmosphere, CH₃C(O)O is expected to give CH₃ + CO₂.

- D23. OH + CH₃C(O)CH₃. The rate coefficient for this reaction has been measured at temperatures close to 298 K by Cox et al. [286], Zetzsch [1362], Chiorboli et al. [227], Kerr and Stocker [614], Wallington and Kurylo [1265], LeCalve et al. [690], Wollenhaupt et al. [1330], and Gierczak et al. [429]. 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. and Gierczak 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. 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 CH₃ + CH₃C(O)OH, CH₃OH + CH₃C(O), CH₄ + CH₃CO₂, H₂O + CH₃C(O)CH₂. The branching ratios for the formation of different sets of products will, most likely, vary with temperature. Wollenhaupt and Crowley (2000) have deduced that CH₃ 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. [1227]. The results of Gierczak et al. on OH + CD₃C(O)CD₃ 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. Because of this conflicting evidence, we have not recommended the products of this reaction.

- D24. OH + CH₃CN. This rate coefficient has been measured as a function of temperature by Harris et al. [482] between 298 and 424 K, Kurylo and Knable [667] between 250 and 363 K, Rhasa [1002] between 295 and 520 K, and Hynes and Wine [552] between 256 and 388 K. In addition, the 298 K value has been measured by Poulet et al. [961]. 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 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, O₂ 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 O₂. The recommended k(298 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.
- D25. OH + CH₃ONO₂. The rate coefficient for this reaction at 298 K has been measured by Kerr and Stocker [614], Nielsen et al. [881], Gaffney et al. [417], Talukdar et al. [417], Kakesu et al. [604] and Shallcross et al. [1055]. 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 [36], 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, ¹⁸OH, and OD) and methyl

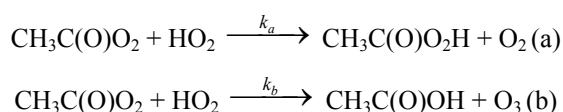
nitrate (CH_3ONO_2 and CD_3ONO_2) are all consistent with this reaction proceeding via an H-atom abstraction pathway. Accordingly, the recommended value of $k(298\text{ K})$ is based on an average of the values given by Gaffney et al, Talukdar et al., Kakesu et al. and Shallcross et al. Further verification 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.

- D26. $\text{OH} + \text{CH}_3\text{C}(\text{O})\text{O}_2\text{NO}_2$ (PAN). This reaction has been studied by four groups, Winer et al. [1326], Wallington et al. [1248], Tsalkani et al. [1187], and Talukdar et al. [1152]. 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. [1152] 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 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.
- D27. $\text{OH} + \text{C}_2\text{H}_5\text{ONO}_2$. The rate constant for this reaction at 298 K has been measured by Kerr and Stocker [614], Nielsen et al. [881], Talukdar et al. [1154], Kakesu et al. [604], and Shallcross et al. [1055]. 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, with a large uncertainty. 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 $\leq 298\text{ K}$. The large uncertainty encompasses the results of Kerr and Stocker and Nielsen et al.
- D28. $\text{OH} + 1\text{-C}_3\text{H}_7\text{ONO}_2$. The reaction has been studied by Kerr and Stocker [614] and Atkinson and Aschmann [36] at room temperature and by Nielsen et al. [881] 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.
- D29. $\text{OH} + 2\text{-C}_3\text{H}_7\text{ONO}_2$. The reaction has been studied by Atkinson and Aschman [36], Atkinson et al [37] and Becker and Wirtz [98] at room temperature and by Talukdar et al. [1117] 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.
- D30. $\text{HO}_2 + \text{CH}_2\text{O}$. There is sufficient evidence to suggest that HO_2 adds to CH_2O (Su et al. [1131,1133], Veyret et al. [1231], Zabel et al. [1349], Barnes et al. [70], and Veyret et al. [1230]). The recommended $k(298\text{ K})$ is the average of values obtained by Su et al. [1131], Veyret et al. [1231], and Veyret et al. [1230]. The temperature dependence observed by Veyret et al. [1230] 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 is a great deal of discrepancy between measured values of the equilibrium constants for this reaction.
- D31. $\text{HO}_2 + \text{CH}_3\text{O}_2$. This recommendation is from Tyndall et al. [1210]. 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 CH_3OOH and O_2 . They used this product yield information with their evaluated UV absorption cross sections for HO_2 and CH_3O_2 to reanalyze the UV absorption profiles measured in kinetics experiments by Dagaut et al. [301] and by Lightfoot et al. [733], 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 CH_3O_2 and HO_2 are independent of temperature at the wavelengths used for the kinetics studies.

D32. $\text{HO}_2 + \text{C}_2\text{H}_5\text{O}_2$. The recommended value is the weighted average of those measured by Cattell et al. [205], Dagaut et al. [302], Fenter et al. [389], and Maricq and Szente [778]. 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 $\text{C}_2\text{H}_5\text{O}_2$ and HO_2 . The absorption cross section of $\text{C}_2\text{H}_5\text{O}_2$ is not well-defined. The value reported by Dagaut et al. would be ~30% higher if the cross sections used by Maricq and Szente were used. The recommended E/R is that measured by Dagaut et al., Fenter et al., and Maricq and Szente. Wallington and Japar [1263] have shown that $\text{C}_2\text{H}_5\text{O}_2\text{H}$ and O_2 are the only products of this reaction.

D33. $\text{HO}_2 + \text{CH}_3\text{C}(\text{O})\text{O}_2$. This recommendation is from Tyndall et al. [1210]. 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. [293], Moortgat et al. [834], and Horie and Moortgat [522], 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. [834] and Tomas et al. [1180].

D34. $\text{HO}_2 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{O}_2$. This recommendation is from Tyndall et al. [1210]. This reaction has been studied by only Bridier et al. [152] and Tyndall et al. based their recommendation on this one study.

D35. $\text{NO}_3 + \text{CO}$. The upper limit is based on the results of Hjorth et al. [514], who monitored isotopically labeled CO loss in the presence of NO_3 by FTIR. Burrows et al. [180] 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 $\text{NO}_2 + \text{CO}_2$, if the reaction occurs.

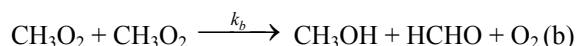
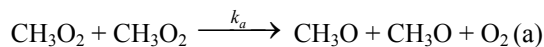
D36. $\text{NO}_3 + \text{CH}_2\text{O}$. There are three measurements of this rate coefficient at 298 K: Atkinson et al. [48], Cantrell et al. [201], and Hjorth et al. [515]. The value reported by Atkinson et al. [48], $k = (3.23 \pm 0.26) \times 10^{-16} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, 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 $\text{NO}_3 + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$ 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. [1195]). 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 HNO_3 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.

D37. $\text{NO}_3 + \text{CH}_3\text{CHO}$. There are four measurements of this rate constant: Morris and Niki [837], Atkinson et al. [48], Cantrell et al. [195], and Dlugokencky and Howard [349]. The value reported by Atkinson et al. [48], $k = (1.34 \pm 0.28) \times 10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, 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. [1195]. 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.

- D38. $\text{CH}_3 + \text{O}_2$. This bimolecular reaction is not expected to be important, based on the results of Baldwin and Golden [57], 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. [632] 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. [116] 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 [1053] and Plumb and Ryan [956] confirm the low value for this rate coefficient. Previous studies of Washida and Bayes [1282] 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 [1359] suggests that this reaction is important at combustion temperature but is unimportant for the atmosphere.
- D39. $\text{CH}_3 + \text{O}_3$. The recommended A-factor and E/R are those obtained from the results of Ogryzlo et al. [904]. The results of Simonaitis and Heicklen [1070], based on an analysis of a complex system, are not used. Washida et al. [1281] 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 (Schmoltnr et al. [1038], Kleinermanns and Luntz [634], Hunziker et al. [544], and Inoue and Akimoto [561]) have shown this reaction to be a poor source of CH_3 . Therefore, the results of Washida et al. are also not used.
- D40. $\text{HCO} + \text{O}_2$. The value of $k(298 \text{ K})$ is the average of the determinations by Washida et al. [1283], Shibuya et al. [1059], Veyret and Lesclaux [1229], Langford and Moore [680], Nesbitt et al. [859], Temps et al. [1161] and Ninomiya et al. [896]. There are three measurements of k where HCO was monitored via the intracavity dye laser absorption technique (Reilly et al. [998], Nadochenko et al. [844], and Gill et al. [435]). 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. [1175] 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. [535] suggest that this reaction proceeds via addition at low temperature and abstraction at higher temperatures.
- D41. $\text{CH}_2\text{OH} + \text{O}_2$. The rate coefficient was first measured directly by Radford [973] 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 [52] was in error. Wang et al. [1273] 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. [352], Grotheer et al. [460], Payne et al. [937], Grotheer et al. [461] and Nesbitt et al. [862] 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. [461] and Nesbitt et al. [862], 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.
- D42. $\text{CH}_3\text{O} + \text{O}_2$. The recommended value for $k(298 \text{ K})$ is the average of those reported by Lorenz et al. [752] and Wantuck et al. [1276]. The recommended E/R was obtained using the results of Gutman et al. [462] (413 to 608 K), Lorenz et al. [752] (298 to 450 K), and Wantuck et al. [1276] (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. [61] and Batt and Robinson [85]) are in reasonable agreement with the derived expression. This value is consistent with the 298 K results of Cox et al. [285], obtained from an end product analysis study, and with the upper limit measured by Sanders et al. [1025]. 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. [889].
- D43. $\text{CH}_3\text{O} + \text{NO}$. The reaction of CH_3O with NO proceeds mainly via addition to form CH_3ONO (Batt et al. [84], Wiebe and Heicklen [1305], Frost and Smith [415], and Ohmori et al. [905]). However, a fraction of the

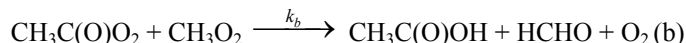
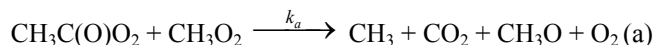
energized CH₃ONO adducts decompose to CH₂O + HNO, and appear to be a bimolecular channel. This reaction has been investigated recently by direct detection of CH₃O via laser-induced fluorescence (Zellner [1357]; Frost and Smith [415]; Ohmori et al. [905]). The previous end-product studies (Batt et al. [84], Wiebe and Heicklen [1305]) are generally consistent with this conclusion. Since the fraction of the CH₃ONO adduct that falls apart to CH₂O + 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 [415] and Ohmori et al. [905] for lower atmospheric conditions.

- D44. CH₃O + NO₂. The reaction of CH₃O with NO₂ proceeds mainly via the formation of CH₃ONO₂. However, a fraction of the energized adducts fall apart to yield CH₂O + HNO₂. The bimolecular rate coefficient reported here is for the fraction of the reaction that yields CH₂O and HNO₂. It is not meant to represent a bimolecular metathesis reaction. The recommended value was derived from the study of McCaulley et al. [794] and is discussed in the section on association reactions.
- D45. CH₃O₂ + O₃. This recommendation is from Tyndall et al. [1210]. Their recommendation is based mostly on the recent study by Tyndall et al. [1220]. The temperature dependence is based on the assumption that the only possible reaction which can occur is the O atom transfer from the CH₃O₂ radical and that the activation energy of ~2 kcal mol⁻¹ for this O-atom transfer is similar to that in the HO₂ + O₃ reaction.
- D46. CH₃O₂ + CH₃O₂. This recommendation is from Tyndall et al. [1210]. There are two confirmed sets of products for this reaction.



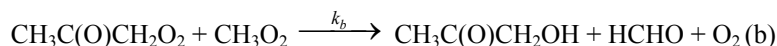
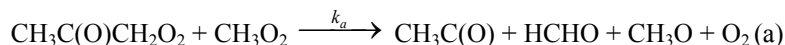
The relative product yield, k_a/k_b , was evaluated by Tyndall et al. to be $(26.2 \pm 6.6) \times \exp((-1130 \pm 240)/T)$. They concluded that there was no evidence for the formation of the CH₃OOCH₃. The kinetics of this reaction has been studied by using UV absorption following pulsed photolytic production 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 HO₂ 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 CH₃O that leads to the unavoidable occurrence of the CH₃O₂ + HO₂ side reaction; this side reaction consumes another CH₃O₂ radical.

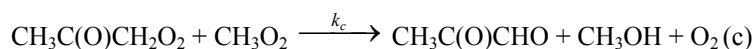
- D47. CH₃O₂ + NO. This recommendation is from Tyndall et al. [1210]. They evaluated the available information to deduce that the main set of products under atmospheric conditions is CH₃O + NO₂. They noted, however, that a very small yield, <0.5%, of CH₃ONO₂ is also possible. The rate coefficient for the reaction at 298 K and its temperature dependence is based on numerous direct studies of this reaction that have been reported.
- D48. CH₃O₂ + CH₃C(O)O₂. This recommendation is from Tyndall et al. [1210]. 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. [1005] and Villenave et al. [1232]. Their recommended temperature dependence for the overall rate coefficient is based on analogy with other RO₂ reactions.

- D49. CH₃O₂ + CH₃C(O)CH₂O₂. This recommendation is from Tyndall et al. [1210]. 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. [152] and Jenkin et al. [578]. 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 RO₂ reactions.

- D50. C₂H₅ + O₂. This is a complex reaction that involves the formation of an C₂H₅O₂ adduct, which can either be stabilized by collisions or fall apart to HO₂ and C₂H₄ (Wagner et al. [1238], Bozzelli and Dean [146], and Kaiser et al. [601]). The fraction of the energized adducts that fall apart to give HO₂ and C₂H₄ will decrease with increasing pressure and decreasing temperature, i.e., as the C₂H₅O₂ formation increases. The C₂H₄-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.
- D51. C₂H₅O + O₂. The recommendation is based on the pulsed laser photolysis studies of Gutman et al. [462] and Hartmann et al. [484]. In both these studies, removal of C₂H₅O in an excess of O₂ 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 Heicklen [1347] is in reasonable agreement with the recommended value.
- D52. C₂H₅O₂ + C₂H₅O₂. k(298 K) has been studied by Adachi et al. [7], Anastasi et al. [22], Munk et al. [841], Cattell et al. [205], Anastasi et al. [21], Wallington et al. [1254], Bauer et al. [87], and Fenter et al. [389]. All the above determinations used only UV absorption to monitor C₂H₅O₂ and hence measured k/σ, where σ is the absorption cross section of C₂H₅O₂ 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 HO₂. HO₂ is formed by the reaction of CH₃CH₂O with O₂ and it reacts with C₂H₅O₂ to enhance the observed rate coefficient (see Wallington et al. [1256] or Lightfoot et al. [731] 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., Anastasi et al., Cattell et al., Bauer et al. and Fenter et al. The observed products (Niki et al. [890]), suggest that at 298 K the channel to yield 2 C₂H₅O + O₂ accounts for about 60% of the reaction; the channel to yield CH₃CHO + C₂H₅OH + O₂ accounts for about 40% of the reaction; and the channel to yield C₂H₅O₂C₂H₅ + O₂ 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.
- D53. C₂H₅O₂ + NO. The recommended k(298 K) is obtained from the results of Plumb et al. [958], Sehested et al. [1051], Daele et al. [300], Eberhard and Howard [371], and Maricq and Szente [779]. 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 CH₃O₂ + 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 Szente, which are in good agreement.
- D54. CH₃C(O)O₂ + CH₃C(O)O₂. This reaction has been studied by Addison et al. [8], Basco and Parmar [83], Moortgat et al. [834] Maricq and Szente [779], and Roehl et al. [1005], using UV absorption techniques. The recommended value is obtained from the data of Moortgat et al., Maricq and Szente, 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 peroxyradical. 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 CH₃O₂ and other stable products in their data analysis (Moortgat et al., Maricq and Szente). The recommended temperature dependence was calculated from the data of Moortgat et al. and Maricq and Szente. Addison et al. reported the formation of O₃, which was attributed to the reaction channel which produces CH₃C(O)OCH₃C(O) + O₃. Moortgat et al. place an upper limit of 2% for this channel. The main products of this reaction appear to be CH₃C(O)O + O₂. The CH₃C(O)O radicals rapidly decompose to give CH₃ and CO₂.
- D55. CH₃C(O)O₂ + NO. This recommendation is from Tyndall et al. [1210]. These authors have argued that the only set of products of importance in the atmosphere is the production of CH₃ + CO₂ + NO₂. This is because

the alkoxy radical produced upon O abstraction from the peroxy radical by NO will be unstable towards decomposition to give CH₃ and CO₂. 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 CH₃C(O)O₂ with NO₂. The temperature dependence of this rate coefficient were derived from a set of direct measurement and kept consistent with the observed temperature dependence of the rate coefficient for the CH₃C(O)O₂ + NO₂ reaction.

- D56. CH₃C(O)CH₂O₂ + NO. This recommendation is from Tyndall et al. [1210]. They deduced, based on the results of Sehested et al. [1048], Jenkin et al. [578] and Orlando et al. [918], that the products of this reaction are CH₃C(O)CH₂O + NO₂. The CH₃C(O)CH₂O radical decomposes rapidly to give CH₃C(O) + CH₂O. 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 NO₂, the monitored species, via the reaction of peroxy radicals (such as CH₃C(O)O₂ and CH₃O₂) with NO. The temperature dependence of the reaction is derived based on analogy with other peroxy radical reactions.
- E1. O + FO. The recommended value is based on results of the room temperature study of Bedzhanyan et al. [106] The temperature dependence of the rate constant is expected to be small, as it is for the analogous ClO reaction.
- E2. O + FO₂. 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.
- E3. OH + CH₃F (HFC-41). The recommended values for k(298 K) and E/R are averages of these parameters derived from fits to the data of Schmoltner et al. [1039], Nip et al [898], Hsu and DeMore [538], and DeMore [335] (with the relative rate constants from the last two studies recalculated based on the current recommendations for the rate constants for the OH + CH₃CHF₂ and OH + CH₃Cl reference reactions respectively.) The A factor was then calculated. The renormalization procedure for relative rate measurements referenced to the OH + CH₃CHF₂ reaction is discussed in the note for that reaction. The results of Howard and Evenson [528], Jeong and Kaufman [586], and Wallington and Hurley [1260] 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.
- E4. OH + CH₂F₂ (HFC-32). The recommended value of k(298 K) is an average from the studies of Nip et al. [898], Jeong and Kaufman [586], Talukdar et al. [1150], Hsu and DeMore [538] (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 Szilagyi et al. [1138]. 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 [528], Clyne and Holt [244], and Bera and Hanrahan [113] were not used in deriving the recommended parameters.
- E5. OH + CHF₃ (HFC-23). The recommended values for k(298 K) and E/R are averages of the values Schmoltner et al. [1039], and Hsu and DeMore [538] (recalculated based on the current recommendation for the rate constant for the OH + CHF₂CF₃ reference reaction). The results of Jeong and Kaufman [586], and Medhurst et al. [799], being predominantly above room temperature, were not used in deriving the recommended parameters. The results from Clyne and Holt [244] and Bera and Hanrahan [113] were also not used due to their inconsistency with the other studies. The room temperature values of Howard and Evenson [528] and Nip et al [898] are encompassed within the 2σ confidence limits.
- E6. OH + CH₃CH₂F (HFC-161). The recommended value for k(298 K) is an average of the values from Nip et al. [898], Schmoltner et al. [1039], and Kozlov et al. [651]. 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 [538] reports a temperature dependence that is markedly different from those of Schmoltner et al. [1039] and Kozlov et al. [651], 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 OH + CH₃CHF₂ (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. [651], which was conducted over an extended temperature range above and below room temperature. Singleton et al. [1080] determined that 85 ± 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.

- E7. OH + CH₃CHF₂ (HFC-152a). The recommended value for k(298 K) is an average of the values from Howard and Evenson [529], Handwerk and Zellner [480], Nip et al. [898], Gierczak et al. [431] (two different absolute determinations), Hsu and DeMore [538] (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 [651]. 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. [431]) has been more clearly demonstrated by the study of Kozlov et al. [651] 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 [244], Brown et al. [154], Nielsen [875], and Liu et al. [749] (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. [431] and Kozlov et al. [651] 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 [538]

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

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.

- E8. OH + CH₂FCH₂F (HFC-152). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [787], Kozlov et al. [651], and DeMore et al. [341] (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. [651] 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 [651] are in excellent agreement with the three relative rate data sets of DeMore et al. [341]. 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.
- E9. OH + CH₃CF₃ (HFC-143a). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [787], Orkin et al. [910], Talukdar et al. [1150] (two different determinations), and Hsu and DeMore [538] (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 [244] were not used due to their inconsistency with the other studies.
- E10. OH + CH₂FCHF₂ (HFC-143). The recommended temperature dependence is based on results of the relative rate study of Barry et al. [79] 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 [787] and Barry et al. The significantly higher values reported by Clyne and Holt [244] were not used in the derivation of the recommended parameters.

- E11. OH + CH₂FCF₃ (HFC-134a). The recommended value for k(298 K) is an average of the values from Martin and Paraskevopoulos [787], Bednarek et al. [101], Orkin and Khamaganov [912], Leu and Lee [711], Gierczak et al. [431] (two different determinations), Liu et al. [749], and DeMore [333] (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. [1365] is in excellent agreement with the recommendation. The data of Jeong et al. [584], Brown et al. [154], and Clyne and Holt [244] were not used in deriving the recommended parameters.
- E12. OH + CHF₂CHF₂ (HFC-134). The preferred rate expression is based on results of the three relative rate measurements by DeMore [333] (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 [244] agrees within the 2σ confidence limits.
- E13. OH + CHF₂CF₃ (HFC-125). The recommended rate expression is derived from a combined fit to the temperature dependence data of Talukdar et al. [1150] and DeMore [333] and the room temperature data of Martin and Paraskevopoulos [787]. The data of Brown et al. [154] and Clyne and Holt [244] were not used in deriving the recommended parameters.
- E14. OH + CH₃CHFCH₃ (HFC-281ea). The recommended parameters were derived from a fit to the data of DeMore and Wilson [340] 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.
- E15. OH + CH₃CH₂CF₃ (HFC-263fb). Based on room temperature measurement of Nelson et al. [853].
- E16. OH + CH₂FCF₂CHF₂ (HFC-245ca). The absolute rate constant results of Zhang et al. [1368] differ from the relative rate data (Hsu and DeMore [538]) 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 [538] recalculated using the current recommendation for the rate constant of the OH + CH₄ reference reaction).
- E17. OH + CHF₂CHFCH₂ (HFC-245ea). Based on room temperature measurement of Nelson et al. [853].
- E18. OH + CH₂FCHFCF₃ (HFC-245eb). Based on room temperature measurement of Nelson et al. [853].
- E19. OH + CHF₂CH₂CF₃ (HFC-245fa). The recommended room temperature value is the mean of the values reported by Orkin et al. [910] and Nelson et al. [853], 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.
- 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. [420], 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.
- E21. OH + CHF₂CHF₂CF₃ (HFC-236ea). The recommended value for k(298 K) averages the values reported by Hsu and DeMore [538] 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. [853] by an absolute technique. The temperature dependence is from Hsu and DeMore [538], with the A-factor adjusted to fit the recommended room temperature value. The higher and somewhat more scattered values of Garland et al. [420] and Zhang et al. [1368] were not used in deriving the recommended expression.
- 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 [538] (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. [432]. The higher results of Nelson et al. [853] and of Garland and Nelson [421], which superseded the earlier results of Garland et al. [421], were not used. A relative rate determination at room temperature by Barry et al. [77] yields a rate constant in excellent agreement with the recommended value. However, the

extremely small rate constant ratio measured (relative to $\text{OH} + \text{CH}_3\text{CF}_2\text{CH}_2\text{CF}_3$) resulted in fairly large uncertainties. Hence this determination was not directly used in the evaluation.

- E23. $\text{OH} + \text{CF}_3\text{CHF}\text{CF}_3$ (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. [849], Zellner et al. [1358], and Zhang et al. [1368] and the relative rate studies of Hsu and DeMore [538] (two determinations which have been recalculated based on the current recommendations for the rate constants for the reference reactions $\text{OH} + \text{CH}_4$ and $\text{OH} + \text{CHF}_2\text{CF}_3$).
- E24. $\text{OH} + \text{CH}_3\text{CF}_2\text{CH}_2\text{CF}_3$ (HFC-365mfc). The recommended value of $k(298 \text{ K})$ is an average of the values obtained from the individual rate expressions by Mellouki et al. [813] and Barry et al. [77] (renormalized to the current recommendation for the rate constant for the reference reaction $\text{OH} + \text{CH}_3\text{CCl}_3$). The value for E/R is an average of the values for this parameter from the same two studies.
- E25. $\text{OH} + \text{CF}_3\text{CH}_2\text{CH}_2\text{CF}_3$ (HFC-356mff). The recommended value of $k(298 \text{ K})$ is an average of the values from Nelson et al. [853] and Zhang et al. [1368]. 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.
- E26. $\text{OH} + \text{CH}_2\text{FCH}_2\text{CF}_2\text{CF}_3$ (HFC-356mcf). The recommended parameters are based on a fit to the data of Nelson et al. [853].
- E27. $\text{OH} + \text{CHF}_2\text{CF}_2\text{CF}_2\text{CHF}_2$ (HFC-338pcc). The recommended values for both $k(298 \text{ K})$ and E/R are averages of these values taken from the individual fits to the data of Schmoltner et al. [1039] and Zhang et al. [1370].
- 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. [853].
- E29. $\text{OH} + \text{CF}_3\text{CHFCH}\text{F}\text{CF}_2\text{CF}_3$. (HFC-43-10mee). The recommended rate expression is derived from a combined fit to the data from Schmoltner et al. [1039] and Zhang et al. [1370].
- 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. [853]. 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 $k(298 \text{ K})$.
- E31. $\text{OH} + \text{CH}_2=\text{CHF}$. The recommended parameters were derived from a fit to the data of Perry et al. [941].
- E32. $\text{OH} + \text{CH}_2=\text{CF}_2$. The recommended value for $k(298 \text{ K})$ is from Howard [526]. 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.
- 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. [911], and Orkin et al. [916]. The value for E/R is from a fit to the data of Orkin et al. [916], with the value for A calculated to yield the recommended value for $k(298 \text{ K})$.
- 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. [832] and Schneider and Wallington [1040]) and laboratory measurements (Huey et al. [542]) 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.
- 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. [1255], Inoue et al. [562], and Tokuhashi et al. [1177] (two independent studies). The recommended value for E/R is derived from the data of and Tokuhashi et al. [1177]. The A factor was calculated to agree with the recommended value for $k(298 \text{ K})$.
- 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. [1177] (two independent absolute measurement studies) and the relative rate study of Chen et al. [220] (recalculated based on the current recommendation for the rate constant for the $\text{OH} + \text{CH}_2\text{Cl}_2$ reference reaction).

- E37. OH + CF₃CH(OH)CF₃. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1177] (two independent absolute measurement studies).
- E38. OH + CH₃OCHF₂ (HFOC-152a). The recommended rate expression is derived from a fit to the data of Orkin et al. [914] below 400 K.
- E39. OH + CH₃OCF₃ (HFOC-143a). The preferred rate expression is derived from a combined fit to the data of Orkin et al. [914] and Hsu and DeMore [539] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₃CHF₂ and OH + CH₂F₂ reference reactions). The renormalization procedure for relative rate measurements referenced to the OH + CH₃CHF₂ reaction is discussed in the note for that reaction. The room temperature result of Zhang et al. [1371] 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.
- 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 [539] (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. [917], and Wilson et al. [1309]. The more scattered measurements of Garland et al. [420] were not used in derivation of the preferred value.
- E41. OH + CHF₂OCF₃ (HFOC-125). The recommended rate expression is based on results of the relative rate study of Hsu and DeMore [539] (recalculated using the rate constant for the CHF₃ reference reaction given in this evaluation). Additional measurements by Hsu and DeMore [539] 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. [1371] lies significantly higher than the recommended value, possibly due to the presence of reactive impurities in the sample.
- E42. OH + CHF₂OCH₂CF₃ (HFOC-245fa). The recommended rate expression is derived from a fit to the data of Orkin et al. [914] below 400 K.
- E43. OH + CH₃OCF₂CHF₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1179] (two independent absolute measurement studies). A room temperature measurement by Heathfield et al. [490] is nearly an order of magnitude higher than recommended and may be affected by reactive impurities.
- E44. OH + CH₃OCF₂CF₃. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1178] (two independent absolute measurement studies). The expression, as expected, is similar to those for the OH + CH₃OCF₃ and OH + CH₃OCF₂CF₂CF₃ reactions.
- E45. OH + CH₃OCF₂CF₂CF₃. The recommended value for k(298 K) is an average of the values reported by Tokuhashi et al. [1178] (two independent absolute measurement studies) and Nonomiya et al. [896] (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.
- E46. OH + CH₃OCF(CF₃)₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1178] (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.
- E47. OH + CHF₂OCH₂CF₂CHF₂. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1179] (two independent absolute measurement studies).
- E48. OH + CHF₂OCH₂CF₂CF₃. The recommended parameters were derived from a fit to the data (below 400 K) of Tokuhashi et al. [1179] (two independent absolute measurement studies).
- E49. F + O₃. The recommended value is based on results of the room temperature study of Bedzhanyan et al. [103] and the temperature-dependent study of Wagner et al. [1242]. The value appears to be quite reasonable in view of the well-known reactivity of atomic chlorine with O₃.
- E50. F + H₂. The value of k at 298 K seems to be well established with the results reported by Zhitneva and Pshezhetskii [1373], Heidner et al. [491,492], Wurzburg and Houston [1337], Dodonov et al. [356], Clyne et al. [249], Bozzelli [145], Igoshin et al. [558], Clyne and Hodgson [242] and Stevens et al. [1115] 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.

- E51. $F + H_2O$. The recommended temperature-independent value is based on results reported in the study by Stevens et al. [1115] 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. [416] and Walther and Wagner [1268]. 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.
- E52. $F + HNO_3$. The recommendation is based on results of the temperature-dependent study of Wine et al. [1324] and the room temperature results of Mellouki et al. [805], Rahman et al. [975] and Becker et al. [90]. The values at room temperature are in good agreement. The study of Wine et al. [1324] 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.
- E53. $F + CH_4$. The recommended room temperature value is the mean of the results of Wagner et al. [1240], Clyne et al. [249], Kompa and Wanner [648], Foon and Reid [404], Fasano and Nogar [386], and Persky et al. [946]. The temperature dependence is that reported by Persky et al. in a competitive study using the reaction $F + D_2$ 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.
- E54. $FO + O_3$. Recommended upper limit is based on the results of Li et al. [729] in a study using a discharge flow-mass spectrometric technique. FO was produced in the reaction of F atoms with excess O_3 . No appreciable decay of FO, and only a small increase in FO_2 , was detected, allowing an upper limit to the rate constant of $10^{-14} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to be derived. A two orders of magnitude higher upper limit was derived by Sehested et al. [1052]. A lower value of the upper limit was derived by Colussi and Grela [268] from a re-analysis of data on the quantum yields for ozone destruction in F_2/O_3 mixtures reported by Starrico et al. [1104]. The results of the recent, more direct, study of Li et al. [729] are preferred over the earlier results of Starrico et al. There are two possible pathways which are exothermic, resulting in the production of $F + 2O_2$ or $FO_2 + O_2$.
- E55. $FO + NO$. The recommended value is based on results of the temperature-dependent study of Bedzhanyan et al. [105] and the value reported by Ray and Watson [996] for k at 298 K using the discharge flow-mass spectrometric technique.
- E56. $FO + FO$. The recommended value is based on the results of Bedzhanyan et al. [104] and Clyne and Watson [260]. Wagner et al. [1242], in a less direct study, report a higher value. The results of Bedzhanyan et al. indicate the predominant reaction channel is that to produce $2F + O_2$.
- E57. $FO_2 + O_3$. Recommended value is based on results of Sehested et al. [1052]. A higher upper limit has been reported by Li et al. [729].
- E58. $FO_2 + NO$. Recommended values are based on results of Li et al. [729], 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. [1052].
- E59. $FO_2 + NO_2$. Recommended values are based on results of Li et al. [729], 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. [1052]. This discrepancy might be attributable to a small NO impurity in the NO_2 sample used in the Sehested et al. study.
- E60. $FO_2 + CO$. Recommended value is based on results of Sehested et al. [1052], the only published study of this reaction.
- E61. $FO_2 + CH_4$. Recommended value is based on results of Li et al. [729]. 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. [1052].
- E62. $CF_3O + O_2$. The recommendation is based upon the results of Turnipseed et al. [1202] 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 K) limits. By comparison to other reactions involving abstraction by O_2 the A-factor is likely to be much smaller.

- 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. [1202], Wallington and Ball [1251], and Bourbon et al. [141]. 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 Sente [777], Nielsen and Sehested [880], and Wallington et al. [1261] are consistent with the $k(298\text{ K})$ recommendation. Measurements reported by Fockenberg et al. [402] and Meller and Moortgat [802] 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.
- 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. [1200]. 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. [1262] are consistent with the recommendation.
- E65. $\text{CF}_3\text{O} + \text{NO}$. The recommendation is based upon the room temperature rate coefficients reported by Sehested and Nielsen [1050], Turnipseed et al. [1202], and Jensen et al. [581] which are in very good agreement. An earlier low value given by Bevilacqua et al. [115] 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. [142] and Bhatnagar and Carr [117] and a temperature dependence study by Dibble et al. [347] are in good agreement with the recommendation. The reaction products have been reported by Chen et al. [218] Bevilacqua et al. [115], Bhatnagar and Carr and Dibble et al.
- 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. [217] 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.
- E67. $\text{CF}_3\text{O} + \text{CO}$. The kinetics of this reaction were studied by Turnipseed et al. [1200], 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 [1252] report a yield of $96 \pm 8\%$ CO_2 at one atmosphere and $296 \pm 2\text{ K}$.
- E68. $\text{CF}_3\text{O} + \text{CH}_4$. The absolute rate coefficients reported by Saathoff and Zellner [1013], Barone et al. [75], Jensen et al. [581], Bourbon et al. [143], and Bednarek et al. [102] at room temperature are in excellent agreement. Kelly et al. [611] 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 $298 \pm 2\text{ K}$. This does not agree with the ratio of our recommended values, which is 0.017. A relative rate measurement reported by Chen et al. [219] using FTIR methods also gives a low result for the rate coefficient. A relative rate measurement reported by Wallington and Ball [1252], $R = 0.0152 \pm 0.0023$ 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. [115].
- 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 [1013], Barone et al. [75], and Bourbon et al. [143]. These workers are in excellent agreement. Chen et al. [219] 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. [611] 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 $298 \pm 2\text{ K}$. This does not agree with the ratio of our recommended values, which is 0.017. A relative rate measurement reported by Wallington and Ball [1252], $R = 0.0152 \pm 0.0023$ 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 CF₃O with organic compounds.

- E70. CF₃O₂ + O₃. The recommended upper limit is given by the measurements reported by Ravishankara et al. [987] who used chemical ionization detection of CF₃O₂ with a flow tube reactor. No measurable reaction was observed in their study. The less direct studies of Nielsen and Sehested [880], Maricq and Szente [777] and Turnipseed et al. [1202] all report somewhat larger upper limits to the rate coefficient. An observable reaction was reported in an indirect measurement by Meller and Moortgat [802]. Their result for the CF₃O + O₃ reaction is not consistent with the value recommended above. Their study may have interference from unknown reactions. The products are assumed to be CF₃O + 2O₂.
- E71. CF₃O₂ + CO. The recommended upper limit is reported by Turnipseed et al. [1200] who used chemical ionization mass spectrometric detection of CF₃OO with a flow tube reactor at 296 K. This result is at odds with an earlier study by Czarnowski and Schumacher [298], who deduced a "fast reaction" when they observed the thermal decomposition of CF₃OOOCF₃ to accelerate in the presence of CO at 315–343K. It is possible that the reaction of CF₃O with CO could account for their observations.
- E72. CF₃O₂ + NO. The recommendation is an average of the room temperature rate coefficients reported by Plumb and Ryan [957], Dognon et al. [358], Peeters et al. [939], Bevilacqua et al. [115], Sehested and Nielsen [1050], Turnipseed et al. [1202], Bourbon et al. [142], and Bhatnagar and Carr [117], 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.
- F1. O + ClO. There have been five studies of this rate constant over an extended temperature range using a variety of techniques: Leu [716]; Margitan [775]; Schwab et al. [1044]; Ongstad and Birks [909]; and Nicovich et al. [873]. 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 [1354] and Ongstad and Birks [908]. Values reported in the early studies of Bemand et al. [109] and Clyne and Nip [254] are significantly higher and were not used in deriving the recommended value. Leu and Yung [725] were unable to detect O₂(¹Δ) or O₂(¹Σ) and set upper limits to the branching ratios for their production of 4.4 × 10⁻⁴ and 2.5 × 10⁻² respectively.
- F2. O + OCIO. The recommended value is based on results of the DF-RF study of Gleason et al. [443]. 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 [267], 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. [269] 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. [109], 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 → ClO₃ + 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 [267] and Colussi et al. [269].
- F3. O + Cl₂O. Recommended value is based on the results of Stevens and Anderson [1114] and Miziolek and Molina [828], which are in good agreement. The significantly lower values of Wecker et al. [1291] are not included, nor are earlier results by Basco and Dogra [82] and Freeman and Phillips [408] due to data analysis difficulties in both studies.
- F4. O + HCl. Fair agreement exists between the results of Brown and Smith [157], Wong and Belles [1331], Ravishankara et al. [984], Hack et al. [466] and Singleton and Cvetanovic [1077] 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. [56]. 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.

- F5. O + HOCl. Recommended value is based on results of Schindler et al. [1035]. 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.
- F6. O + ClONO₂. The results reported by Molina et al. [830] and Kurylo [661] are in good agreement, and these data have been used to derive the preferred Arrhenius expression. The value reported by Ravishankara et al. [980] 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.
- F7. O₃ + OClO. The recommended value is based on results over the temperature range 262–296 K reported by Wongdontri-Stuper et al. [1332]. Within the indicated uncertainty limits it also encompasses the somewhat lower room temperature result of Birks et al. [128].
- F8. O₃ + Cl₂O₂. The recommended upper limit is that determined by DeMore and Tschuikow-Roux [339]. It refers to a temperature of 195 K, and while the reaction possibly could be faster at higher temperatures, the value of the rate at the higher temperatures would be of no significance because of the thermal decomposition of the dimer.
- F9. OH + Cl₂. The recommended room temperature value is the average of the results reported by Boodaghians et al. [138], Loewenstein and Anderson [750], Ravishankara et al. [981], and Leu and Lin [721]. The temperature dependence is from Boodaghians et al. Loewenstein and Anderson determined that the exclusive products are Cl + HOCl.
- F10. OH + ClO. The reaction has two known product channels under atmospheric conditions: OH + ClO → Cl + HO₂ and OH + ClO → HCl + O₂. Most studies measure the rate coefficients for the overall reaction (OH + ClO → products) that is presumably the sum of the two channels. The recommendation for the Cl + HO₂ channel is obtained from the difference between a critical assessment of the measurements of the overall reaction and the recommendation for the HCl + O₂ channel as discussed below. The assessment of the overall reaction (OH + ClO → products) is based on a fit to the 219–373 K data of Hills and Howard [508], the 208–298 K data of Lipson et al. [745], the 234–356 K data of Kegley-Owen et al. [610] and the 298 K data of Poulet et al. [965]. Data reported in the studies of Burrows et al. [181], Ravishankara et al. [981], and Leu and Lin [721] 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) [1269], Bedjanian et al. (230–360 K) [100] and Tyndall et al. (298 K) [1211] 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 [721] (>0.65); Burrows et al. [181] (0.85±0.2) and Hills and Howard [508] (0.86±0.14). Poulet et al. [965] 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 [744] and diode laser spectroscopy [1270] 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 [1270] 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. [1211] and Bedjanian et al. [100] are noted but are not considered in this evaluation.

- F11. OH + OClO. The recommended value is that reported by Poulet et al. [969], 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 + O₂ was determined to be close to unity, but experimental uncertainty would allow it to be as low as 0.80.
- 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. [831], Keyser [622], Ravishankara et al. [993] and Battin-

Leclerc et al. [86]. 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 [1143], Zahniser et al. [1355], Smith and Zellner [1093], Ravishankara et al. [984], Hack et al. [466], Husain et al. [547], Cannon et al. [191], Husain et al. [548], and Smith and Williams [1092] had reported somewhat lower room temperature values. The data of Sharkey and Smith [1056] over the temperature range 138–216 K and Battin-Leclerc et al. [86] 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.

- F13. OH + HOCl. In the only reported study of this system Ennis and Birks [379] 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.
- F14. OH + ClNO₂. The recommended value is based on results of the direct study of Ganske et al. [418,419] 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.
- F15. OH + ClONO₂. The results reported by Zahniser et al. [1352] and Ravishankara et al. [980] 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.
- F16. OH + CH₃Cl. The recommended rate expression is derived from a combined fit (for T ≤ 400 K) of the data from the relative rate study by Hsu and DeMore [537] (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. [914] and Herndon et al. [500]. Data from the earlier studies of Howard and Evenson [528], Perry et al. [942], Davis et al. [317], Paraskevopoulos et al. [928], Taylor et al. [1158], and Jeong and Kaufman [586] are reasonably well encompassed within the 2σ limits. The room temperature value from Taylor et al. [1158] 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. [281] and Brown et al. [155].
- 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. [1233] and Herndon et al. [500] and the relative rate study of Hsu and DeMore [537] (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 renormalized using a rate constant of the reference reaction calculated from the data of Schmoltner et al. [1039] and Kozlov et al. [650] above room temperature. The results of Cox et al. [281] and Davis et al. [317] support this recommendation. The results from Taylor et al. [1159], Jeong and Kaufman [586], Perry et al. [942] and Howard and Evenson [528] lie considerably higher and were not used in deriving the recommended parameters.
- 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 [537] (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. [1159] (which superseded Taylor et al. [1158]), Jeong and Kaufman [586], Davis et al. [317], and Howard and Evenson [528]. The recommended value of E/R is an average of values for this parameter derived in the first four of the above studies.
- 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. [281]. 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 [528] and Clyne and Holt [243]. 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.
- F20. OH + CH₂FCI (HCFC-31). The recommended value for k(298 K) is an average of the values from the relative rate study of DeMore [335] (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 [528], Paraskevopoulos et al. [928], Watson et al. [1286], Handwerk and Zellner [480] and Jeong and Kaufman

[586]. 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.

- F21. OH + CHFCl₂ (HCFC-21). The recommended rate expression is derived from a combined fit to the data of Howard and Evenson [528], Perry et al. [942], Watson et al. [1286], Chang and Kaufman [209], Paraskevopoulos et al. [928], Jeong and Kaufman [586], and Fang et al. [382]. The rate constants reported by Clyne and Holt [244] are significantly higher than those from the other seven studies and were not used in deriving the recommended parameters.
- 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 [538] (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 [912], Fang et al. [382], Atkinson et al. [43], Watson et al. [1286], Chang and Kaufman [209], Paraskevopoulos et al. [928] and Jeong and Kaufman [586]. The more scattered results of Handwerk and Zellner [480] are in general agreement. The results from the studies of Howard and Evenson [528] and Clyne and Holt [244] are significantly different from those of the other studies and were not used in the derivation.
- 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 [210] at about 480 K. This expression is compatible with the upper limits reported by Atkinson et al. [43], Howard and Evenson [528], Cox et al. [281] and Clyne and Holt [243]. None of the investigators reported any evidence for reaction.
- 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 [210] at about 480 K. This expression is compatible with the upper limits reported by Atkinson et al. [43], Howard and Evenson [528], Cox et al. [281] and Clyne and Holt [243]. None of the investigators reported any evidence for reaction.
- F25. OH + CH₂ClCH₃. The recommended value for k(298 K) is an average of the values reported by Howard and Evenson [529], Paraskevopoulos et al. [928], Kasner et al. [608], and Herndon et al. [500]. 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 [782] were not used to derive the recommended parameters, as they are somewhat more scattered.
- 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. [1156] and Finlayson-Pitts et al. [395], and a relative rate study of DeMore [332] (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. [1156]. These studies indicate both a lower k(298 K) and E/R than was reported in earlier studies: Nelson et al. [856], Jeong and Kaufman [585], and Kurylo et al. [664]. More recent measurements by Jiang et al. [588] and Lancar et al. [678] yield rate constants that are slightly higher at 298 K than this recommendation.
- 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 [541] (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. [678], Zhang et al. [1365] (together with the data at 330 K and above from Liu et al. [749], Talukdar et al. [1150] above 253 K (two studies), and Mors et al. [839]). The temperature-dependence data of Brown et al. [154] were not considered because the relatively large rate constants and Arrhenius curvature are suggestive of sample impurities.
- F28. OH + CH₃CF₂Cl (HCFC-142b). The recommended value for k(298 K) is an average of the values from Howard and Evenson [529], Cox et al. [281], Paraskevopoulos et al. [928], Mors et al. [839], Watson et al. [1286], Handwerk and Zellner [480], Liu et al. [749], Gierczak et al. [431], and Fang et al. [383]. 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. [154] and Clyne and Holt [244] were not used to derive the recommended parameters. The 270 K data of Zhang et al. [1365] are in reasonable agreement with the recommendation.
- F29. OH + CH₂ClCF₂Cl (HCFC-132b). The recommended rate expression was derived from the data of Watson et al. [1288], which were corrected by these authors for the presence of alkene impurities. The data of Jeong et al. [584], indicating faster rate constants, may have been affected by such impurities; hence they were not included in deriving the recommendation.
- F30. OH + CH₂ClCF₃ (HCFC-133a). The recommended value of k₂₉₈ is the average of the values of Howard and Evenson [529] and Handwerk and Zellner [480] adjusted to 298 K. The recommended temperature

dependence was derived from the data of Handwerk and Zellner [480]. The data of Clyne and Holt [244] were not used in deriving the recommended parameters but (below 400 K) are encompassed within the 2σ limits.

- F31. OH + CHCl₂CF₂Cl (HCFC-122). The recommended rate expression is derived from a combined fit to the data of Orkin and Khamaganov [912] (below 400 K) and DeMore [335] (two determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₂Cl₂ and OH + CHCl₂CF₃ reference reactions).
- F32. OH + CHFClCFCl₂ (HCFC-122a). The recommended rate expression was derived from the relative rate data of Hsu and DeMore [538] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CHF₂ reference reaction, as discussed in the note for that reaction).
- F33. OH + CHCl₂CF₃ (HCFC-123). The recommended value of k_{298} is the average of the values from the absolute studies of Gierczak et al. [431] (two determinations) Liu et al. [749], and Yamada et al. [1342], and from the relative rate study by Hsu and DeMore [538] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CHF₂ 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 [875], Watson et al. [1288], Clyne and Holt [244], and Brown et al. [154] and the room temperature data of Howard and Evenson [529] were not used in the derivations.
- F34. OH + CHFClCF₂Cl (HCFC-123a). The recommended rate expression is based on the data of Orkin and Khamaganov [912].
- F35. OH + CHFClCF₃ (HCFC-124). The recommended value for $k(298\text{ K})$ is an average of the values from the studies of Watson et al. [1288], Gierczak et al. [431] (2 studies), Yamada et al. [1342], and Hsu and DeMore [538] (two relative rate determinations which have been recalculated based on the current recommendations for the rate constants of the OH + CH₄ and OH + CHF₂CHF₂ reference reactions). The room temperature rate constant of Howard and Evenson [529] 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. [431] and Yamada et al. [1342]).
- F36. OH + CH₃CF₂CFCl₂ (HCFC-243cc). The recommended rate expression is derived from the temperature-dependence data of Nelson et al. [852]. 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 OH + CH₃CF₂Cl.
- F37. OH + CHCl₂CF₃CF₂ (HCFC-225ca). The recommended value for $k(298\text{ K})$ is an average of the values from Nelson et al. [852] and Zhang et al. [1366]. The recommendation for E/R is taken from Nelson et al. [852]. The temperature-dependence data of Brown et al. [153] 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. [1366] are in reasonable agreement with those of Nelson et al. [852] over the temperature range of measurement overlap. However, the complete Zhang et al. [1366] data set yields a value for E/R much larger than currently recommended for the OH + CHCl₂CF₃ (HFC-123) reaction, for which the activation energy should be similar.
- F38. OH + CF₂CICF₂CHFCl (HCFC-225cb). The recommended rate expression is derived from a combined fit to the temperature-dependence data of Nelson et al. [852] and Zhang et al. [1366], which are in excellent agreement.
- F39. OH + CH₂=CHCl. The recommended value for $k(298\text{ K})$ is an average of the values reported by Howard [526], Perry et al. [941], Liu et al. [748] and [1343]. 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.
- F40. OH + CH₂=CCl₂. The recommended value for $k(298\text{ K})$ is an average of the values reported by Edney et al. [373], Tuazon et al. [1191], Abbatt and Anderson [1], Zhang et al. [1367], Canosa-Mas et al. [193] and [1341]. 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. [628] 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.

- 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 [526], Chang and Kaufman [209], Kirchner et al. [628], Klopffer et al. [638], Edney et al. [373] and Tichenor et al. [1172]. The recommended value of E/R is an average of values for this parameter derived by Chang and Kaufman [209], Kirchner et al. [628] and Tichenor et al. [1172]. The value for $k(298\text{ K})$ derived from a relative rate study by Winer et al. [1327] 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. [589] 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. [1172].
- 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 [526], Chang and Kaufman [209], and Kirchner et al. [628]. The room temperature value reported by Winer et al. [1327] 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 [209] and Kirchner et al. [628]. A study by Tichenor et al. [1173] 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.
- F43. $\text{OH} + \text{CH}_3\text{OCl}$. The recommended rate expression is derived from a fit to the data of Crowley et al. [294], the only reported study of this reaction.
- 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. [78] (using three independent techniques), Dobe et al. [350], Nelson et al. [856], Ballestra-Garcia et al. [59], and Scollard et al. [1045]. The temperature dependence is derived from a fit to the data of Dobe et al. [350]. The A factor was then calculated to agree with the recommended value for $k(298\text{ K})$.
- F45. $\text{HO}_2 + \text{Cl}$. The recommendations for the two reaction channels are based upon the results by Lee and Howard [703] 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 [717], Poulet et al. [967], Burrows et al. [176]) or to $\text{Cl} + \text{H}_2$ (Cox [275]). The contribution of the reaction channel producing $\text{OH} + \text{ClO}$ (21% at room temperature) is much higher than the upper limit reported by Burrows et al. (1% of total reaction). Cattell and Cox [206], 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 [355] reports a total rate constant in good agreement with this recommendation but a much lower contribution ($5 \pm 3\%$) of the channel producing $\text{OH} + \text{ClO}$. The rate constant for the channel producing $\text{ClO} + \text{OH}$ can be combined with that for the reaction $\text{ClO} + \text{OH} > \text{Cl} + \text{HO}_2$ 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.
- F46. $\text{HO}_2 + \text{ClO}$. Three new studies by Nickolaisen et al [865], Knight et al. [640], and Laszlo et al. [682] have been added to the previous five studies of this rate constant (Reimann and Kaufman, [999]; Stimpfle et al. [1122]; Leck et al. [691]; Burrows and Cox [177]; Cattell and Cox [206]). 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 [715], 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. [394], 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-HO₂ 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.

- F47. H₂O + ClONO₂. This recommendation is based on the upper limits to the homogeneous bimolecular rate constant reported by Atkinson et al. [49], and by Hatakeyama and Leu [487,488]. Atkinson et al. observed by FTIR analysis the decay of ClONO₂ in the presence of H₂O 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. [1008] 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.
- F48. NO + OCIO. The Arrhenius expression was estimated based on 298 K data reported by Bemand, Clyne and Watson [109].
- F49. NO + Cl₂O₂. The recommended upper limit is that determined by Friedl (private communication) in a study using a DF-MS technique.
- F50. NO₃ + HCl. The recommended upper limit is that reported by Mellouki et al. [807] 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. [197] and Canosa-Mas et al. [194]; the latter study also reports Arrhenius parameters at higher temperatures (333–473 K).
- F51. HO₂NO₂ + HCl. This upper limit is based on results of static photolysis-FTIR experiments reported by Leu et al. [720].
- F52. Cl + O₃. The results reported for $k(298\text{ K})$ by Watson et al. [1287], Zahniser et al. [1356], Kurylo and Braun [665], Clyne and Nip [253], Nicovich et al. [868] and Seeley et al. [1046] are in good agreement, and have been used to determine the preferred value at this temperature. The values reported by Leu and DeMore [717] (due to the wide error limits) and Clyne and Watson [259] (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. The two most 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 [331] directly determined the ratio $k(\text{Cl} + \text{O}_3)/k(\text{Cl} + \text{CH}_4)$ at 197–217 K to be within 15% of that calculated from the absolute rate constant values recommended here. Vanderzanden and Birks [1226] 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 [328], in connection with the Cl₂ photosensitized decomposition of ozone. However Choo and Leu [228] 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. [172], 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.
- F53. Cl + H₂. This Arrhenius expression is based on the data below 300 K reported by Watson et al. [1285], Lee et al. [694], Miller and Gordon [826], and Kita and Stedman [631]. The results of these studies are in excellent agreement below 300 K; the data at higher temperatures are in somewhat poorer agreement. The results of Watson et al., Miller and Gordon, and Kita and Stedman agree well (after extrapolation) with the results of Benson et al. [112] and Steiner and Rideal [1109] at higher temperatures. For a discussion of the large body

of rate data at high temperatures, see the review by Baulch et al. [89][86]. The room temperature value of Kumaran et al. [656], in a study primarily at high temperatures, is in excellent agreement with this recommendation. Miller and Gordon and Kita and Stedman also measured the rate of the reverse reaction, and found the ratio to be in good agreement with equilibrium constant data.

- F54. Cl + H₂O₂. The absolute rate coefficients determined at ~298 K by Watson et al. [1287], Leu and DeMore [717], Michael et al. [824], Poulet et al. [967] and Keyser [617] range in value from (3.6–6.2) × 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 H₂O₂ 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 [498], using mass spectrometry, confirmed that this reaction proceeds only by the abstraction mechanism giving HCl and HO₂ as products.
- F55. Cl + NO₃. The recommended value at room temperature is based on the discharge flow-EPR study of Mellouki et al. [805] and the discharge flow-mass spectrometric study of Becker et al. [92]. The results of these direct absolute rate studies are preferred over results of the earlier relative rate studies of Cox et al. [276], Burrows et al. [180], and Cox et al. [287], in all of which NO₃ was monitored in the photolysis of Cl₂-ClONO₂-N₂ 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. [287] in which the complications must have been temperature independent.
- F56. Cl + N₂O. 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. [609]. The largest value reported was 10⁻¹⁷ cm³ molecule⁻¹ 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.
- F57. Cl + HNO₃. The recommended upper limit at room temperature is that reported in the study of Wine et al. [1324], in which long-path laser absorption spectroscopy was used to look for the appearance of NO₃ following the pulsed laser photolysis of Cl₂-HNO₃ mixtures with no evidence for NO₃ 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. [1350]. Higher values obtained in earlier studies (Leu and DeMore [717], Kurylo et al. [671], and Clark et al. [234]) as well as the higher temperature results of Poulet et al. [967] are not used.
- F58. Cl + HO₂NO₂. The only study of this reaction is by Simonaitis and Leu [1072] using the low pressure discharge flow technique coupled with resonance fluorescence detection of Cl and mass spectrometric detection of HO₂NO₂ ion fragments. Consistent results were obtained monitoring either Cl or HO₂NO₂ decays and retrieved rate constants were less than 1 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ for all conditions. Impurities in the HO₂NO₂ sample (especially H₂O₂) complicated the measurements. A limited temperature study over the 298–399 K range suggests that E/R is in the range of 500 – 1500. Given the experimental difficulties, only an upper limit is recommended for the reaction rate.
- F59. Cl + CH₄. The values of k at 298 K reported from thirteen absolute rate constant studies (Manning and Kurylo [770], Whytock et al. [1303], Michael and Lee [817], Lin et al. [740], Zahniser et al. [1351], Keyser [615], Ravishankara and Wine [988], Heneghan et al. [499], Dobis and Benson [353], Sawerysyn et al. [1031], Beichert et al. [107], Seeley et al. [1046], and Pilgrim et al. [950]) fall in the range (0.92 – 1.13) × 10⁻¹³, with a mean value of 0.99 × 10⁻¹³. An earlier absolute study by Watson et al. [1287] gives rate constant values slightly higher than those of the aforementioned studies, which 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.

The values derived for k at 298 K from the competitive chlorination studies of Pritchard et al. [970], Pritchard et al. [971], Knox [641], Knox and Nelson [643], Lee and Rowland [692], and Lin et al. [740] range from (0.8–1.6) × 10⁻¹³ when the original data are referenced to the presently recommended rate constant values for the reactions of Cl with H₂ and C₂H₆. Of these relative rate studies, that of Lin et al. [740], yields a room temperature rate constant (1.07 × 10⁻¹³) that is most consistent with the absolute measured values. Thus, the recommended value for k at 298 K (1.0 × 10⁻¹³) is derived from an unweighted average of the rate constants from the thirteen preferred absolute studies and the relative rate study of Lin et al. [740].

There have been nine absolute studies of the temperature dependence of k in which the measurements extend below 300 K (Watson et al. [1287], Manning and Kurylo [770], Whytock et al. [1303], Lin et al. [740],

Zahniser et al. [1351], Keyser [615], Ravishankara and Wine [988], Heneghan et al. [499], and Seeley et al. [1046]). 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. [1303], Zahniser et al. [1351] and Keyser [615]), and in each case a strong non-linear Arrhenius behavior was observed. Ravishankara and Wine [988] 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. [1287], Manning and Kurylo [770], and Seeley et al. [1046]) and those who only studied it above 300 K (Clyne and Walker [258], Poulet et al. [966], and Lin et al. [740]). The agreement between all studies below 300 K is reasonably good, with values of E/R ranging from (1063–1320) K, and $k(230\text{ K})$ in the range $(2.6\text{--}3.2) \times 10^{-14}$. There have not been any absolute studies at stratospheric temperatures other than those which utilized the resonance fluorescence technique. Ravishankara and Wine [988] have suggested that the results obtained using the discharge flow and competitive chlorination techniques may be in error at the lower temperatures (<240 K) due to a non-equilibration of the $^2P_{1/2}$ and $^2P_{3/2}$ states of atomic chlorine. Ravishankara and Wine 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. [1287], which appear to be systematically high due to reactive impurities) yields $E/R = 1253\text{ K}$ and $k(298\text{ K}) = 1.0 \times 10^{-13}$.

The competitive chlorination results differ from those obtained in the absolute studies in that linear Arrhenius behavior is observed. The values of E/R are consistently larger than those obtained from the absolute studies, with an average value of approximately 1500 K. Until the hypothesis of Ravishankara and Wine [988] is re-examined, the preferred Arrhenius expression attempts to best fit the results obtained between 200 and 300 K from all sources. Thus, using the relative rate results of Lin et al. [740] (referenced to the current recommendation for the $\text{Cl} + \text{C}_2\text{H}_6$ reaction) as representative of the relative rate studies below 300 K, together with the composite fit to the absolute studies given above, we obtain a recommended E/R value of 1360 K. Taken with the recommended value for $k(298\text{ K}) = 1.0 \times 10^{-13}$, we compute an Arrhenius A factor of 9.6×10^{-12} . However, the A-factor thus derived seems somewhat low (on a per hydrogen atom basis) when compared with the A-factors for some similar reactions.

- F60. $\text{Cl} + \text{CH}_3\text{D}$. Recommended value is based on results of Wallington and Hurley [1259].
- F61. $\text{Cl} + \text{H}_2\text{CO}$. The results from five of the six published studies (Michael et al. [821], Anderson and Kurylo [25], Niki et al. [885], Fasano and Nogar [385] and Poulet et al. [962]) are in good agreement at $\sim 298\text{ K}$, but are $\sim 50\%$ greater than the value reported by Foon et al. [403]. 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.
- F62. $\text{Cl} + \text{HC(O)OH}$. The room temperature kinetics of this reaction have been studied by Wallington et al. [1245] and Li et al. [728]. 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. [1221] 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.
- F63. $\text{Cl} + \text{CH}_3\text{O}_2$. Recommended value is based on results of Maricq et al. [780], Jungkamp et al. [598], and Daele and Poulet [299]. 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. [780] 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.

- F64. Cl + CH₃OH. This recommendation at 298 K) is based on results of the absolute rate studies of Michael et al. [822], Payne et al. [937], Dobe et al. [351], Pagsberg et al. [924] and Tyndall et al. [1214], and results obtained in the competitive chlorination studies of Wallington et al. [1267], Lightfoot et al. [733], Nelson et al. [855] 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: CH₂OH + HCl, channel (a) and CH₃O + HCl, channel (b). Product analysis and isotopic substitution have established that the reaction proceeds via channel (a) rather than via channel (b). See Radford [973], Radford et al. [974], Meier et al. [800], and Payne et al. [937]. This reaction has been used in the laboratory as a source of CH₂OH and as a source of HO₂ by the reaction of CH₂OH with O₂.
- F65. Cl + CH₃OOH. The only study of this reaction was by Wallington et al [1245], who measured the rate relative to Cl + C₂H₆ at 295 K and atmospheric pressure.
- F66. Cl + CH₃ONO₂. This reaction has been studied at 298 K by Nielsen et al [881] 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 (Cl + C₂H₆). 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.
- F67. Cl + C₂H₆. The absolute rate coefficients reported in all four studies (Davis et al. [314], Manning and Kurylo [770], Lewis et al. [726], and Ray et al. [995]) are in good agreement at 298 K. The value reported by Davis et al. was probably overestimated by ~10% (the authors assumed that I_f was proportional to [Cl]^{0.9}, whereas a linear relationship between I_f and [Cl] probably held under their experimental conditions). The preferred value at 298 K was taken to be a simple mean of the four values (the value reported by Davis et al. was reduced by 10%), i.e., 5.7 × 10⁻¹¹. The two values reported for E/R are in good agreement; E/R = 61 K (Manning and Kurylo) and E/R = 130 K (Lewis et al.). A simple least squares fit to all the data would unfairly weight the data of Lewis et al. due to the larger temperature range covered. Therefore, the preferred value of 7.7 × 10⁻¹¹ exp(-90/T) is an expression which best fits the data of Lewis et al. and Manning and Kurylo between 220 and 350 K. The recent temperature-dependent results of Dobis and Benson [354] and room temperature results of Kaiser et al. [602], Hooshiyar and Niki [521] and Beichert et al. [107] are in good agreement with the recommendation.
- F68. Cl + C₂H₅O₂. Recommended value is based on results of Maricq et al. [780].
- F69. Cl + CH₃CH₂OH. The rate coefficient for this reaction has been studied at 298 K by four groups using a relative rate technique: Nelson et al. [855] (relative to Cl + cyclohexane), Wallington et al. [1267] (relative to Cl + C₂H₆), Edelbuttel-Einhaus et al. [372] (relative to Cl + C₂H₆), and Taatjes et al. [1139]. Nelson et al measured this rate constant relative to the Cl + cyclohexane while the others used the Cl + C₂H₆ 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: CH₂CH₂OH + HCl, channel (a); CH₃CHOH, channel (b); and CH₃CH₂O 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.
- F70. Cl + CH₃C(O)OH. Koch and Moortgat [645] 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 CO₂ 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 CH₂C(O)OH radical followed by reaction with O₂ to form a peroxy radical. Thermal decomposition of the peroxy radical produces HCHO, CO₂, and atomic H. In the laboratory system, the HCHO reacts with atomic chlorine to yield CO.
- F71. Cl + CH₃CN. The recommendation is based on results of the study of Tyndall et al. [1216]. 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 [667], Poulet et al. [961], and Olbregts et al. [906]. Product studies reported by Tyndall et al. show that reaction proceeds predominantly by hydrogen atom abstraction.

- F72. $\text{Cl} + \text{C}_2\text{H}_5\text{ONO}_2$. Wallington et al. [1258] and Nielsen et al [881] 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.
- F73. $\text{Cl} + \text{CH}_3\text{CO}_2\text{NO}_2$ (PAN). The recommended value is based on results of the relative rate study of Wallington et al. [1245]. 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. [1187] 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.
- F74. $\text{Cl} + \text{C}_3\text{H}_8$. The recommended room temperature value is the mean of results of the competitive chlorination studies of Pritchard et al. [971], Knox and Nelson [643], Atkinson and Aschmann [35], Wallington et al. [1267], and Hooshiyar and Niki [521], and the absolute rate studies of Lewis et al. [726] and Beichert et al. [107]. The temperature dependence is from Lewis et al. The A-factor from that study has been adjusted slightly to fit the recommended room temperature value.
- F75. $\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{CH}_3$. The rate coefficient for this reaction has only been reported at 298 K. Wallington et al. [1267] and Olsson et al. [907] 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. [900] 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. [1267], 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 $k(298 \text{ K})$. 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 $\text{Cl} + \text{CH}_3\text{C}(\text{O})\text{CH}_3$, we recommend an E/R value of 1000 K with a γ value of 500 K. Such a temperature dependence is consistent with this reaction proceeding via H atom abstraction. This E/R and $k(298 \text{ K})$ 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 $\text{CH}_3\text{C}(\text{O})\text{CH}_2$ and HCl.
- F76. $\text{Cl} + \text{C}_2\text{H}_5\text{CO}_2\text{NO}_2$. Wallington et al. [1245] have measured this rate constant relative to $\text{Cl} + \text{CH}_3\text{Cl}$. The recommended value is adjusted from that given by Wallington et al. using the currently recommended value for the reference reaction rate constant.
- F77. $\text{Cl} + 1\text{-C}_3\text{H}_7\text{ONO}_2$. Wallington et al. [1258] and Nielsen et al [881] 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 $\text{OH} + \text{CH}_3\text{ONO}_2$. This is consistent with observed OH/Cl A-factor ratios for primary H-abstraction from alkanes.
- F78. $\text{Cl} + 2\text{-C}_3\text{H}_7\text{ONO}_2$. This reaction has been measured by Wallington et al [1258] 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.
- F79. $\text{Cl} + \text{OCIO}$. The data of Toohey [1181] are in good agreement with the results of Bemand et al. [109] 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 [1181] is accepted but with error limits that encompass the temperature independence reported in the earlier study.
- F80. $\text{Cl} + \text{ClOO}$. The recommended value is based on the results of studies by Mauldin et al. [792] and Baer et al. [54], 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. [590], Cox et al. [282], and Ashford et al. [32]. 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 [863], 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.

- F81. Cl + Cl₂O. The preferred value was determined from results of the temperature-dependent study of Stevens and Anderson [1114] and the results of two independent absolute rate coefficient studies reported by Ray et al. [995], which used the discharge flow-resonance fluorescence and discharge flow-mass spectrometric techniques. This value has been confirmed by Burrows and Cox [177], 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 [80] has been rejected.
- F82. Cl + Cl₂O₂. 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 [289] in a study using a static photolysis technique with photodiode array UV spectroscopy.
- F83. Cl + HOCl. This recommendation is based on results over the temperature range 243–365 K reported by Cook et al. [270] and the room temperature result of Vogt and Schindler [1235]. There is a significant discrepancy in the reported values of the product branching ratios. Ennis and Birks [378] reported that the major reaction channel is that to give the products Cl₂ + OH with a yield of 91±6%, whereas Vogt and Schindler report this yield to be 24±11%, with the major reaction channel giving HCl + ClO as products.
- F84. Cl + 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. [213] provides rate data for each Cl atom spin state, and they attribute the low value reported by Nelson and Johnston [854] in a laser flash photolysis-resonance fluorescence study to reaction of the Cl ²P_{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 [459]. The results of Clyne and Cruse [239] 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. [213], Nesbitt et al. [861], and Kita and Stedman [631]. The recommended temperature dependence is from the study of Abbatt et al. [4].
- F85. Cl + ClONO₂. Recommended value is based on the results of Yokelson et al. [1346] and those of Margitan [773]. These results are in excellent agreement; the slightly higher values of Kurylo et al. [668] 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 Cl₂ + NO₃ as products.
- F86. Cl + CH₃Cl. The recommended room temperature value is the mean of results of the absolute rate studies of Manning and Kurylo [770] and Beichert et al. [107] and the relative rate study of Wallington et al. [1245]. The temperature dependence is from Manning and Kurylo. The A-factor from that study has been adjusted slightly to fit the recommended room temperature value. The results reported by Clyne and Walker [258] and Manning and Kurylo [770] are in good agreement at 298 K. However, the value of the activation energy measured by Manning and Kurylo is significantly lower than that measured by Clyne and Walker. Both groups of workers measured the rate constant for the Cl + CH₄ and, similarly, the activation energy measured by Manning and Kurylo was significantly lower than that measured by Clyne and Walker. It is suggested that the discharge flow-mass spectrometric technique used by Clyne and Walker was in this case subject to a systematic error, and that the flash photolysis results of Manning and Kurylo provide the basis for the recommended rate constant.
- F87. Cl + CH₂Cl₂. The recommended value is based on results of the relative rate study of Tschuikow-Roux et al. [1188] normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation. The room temperature value is in good agreement with results of the relative rate study of Niki et al. [888] and the absolute rate study of Beichert et al. [107]. The higher results of Clyne and Walker [258] were not used.
- F88. Cl + CHCl₃. There have been three recent studies of this reaction. In the studies of Beichert et al. [107] by an absolute technique and Brahan et al. [148] by a relative technique, room temperature values about 50% greater than the previous recommendation, which was based on the relative study of Knox [642], were reported. Talhaoui et al. [1148] in a temperature-dependent absolute rate study by the discharge flow-mass spectrometric technique reported a room temperature value in excellent agreement with the previous recommendation. The recommended room temperature value is the mean of the values reported in the studies of Knox, Beichert et al., Brahan et al., and Talhaoui et al. The temperature dependence is from Talhaoui et al. and Knox. The A-factor has been fitted to the recommended room temperature value.
- F89. Cl + CH₃F (HFC-41). The recommended value is based on results of the temperature-dependent relative rate study of Tschuikow-Roux et al. [1188] and the relative rate studies of Tuazon et al. [1192] and Wallington et

al. [1253] at room temperature. The results of the absolute rate study of Manning and Kurylo [770] are in good agreement at room temperature but show a weaker temperature dependence, which is encompassed within the error limits.

- F90. Cl + CH₂F₂ (HFC-32). The recommended room temperature value is the mean of results of the relative rate studies of Tschuikow-Roux et al. [1189] and of Nielsen et al. [876], both normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation. The temperature dependence is from Tschuikow-Roux et al. The A-factor from that study has been adjusted to fit the recommended room temperature value.
- F91. Cl + CF₃H (HFC-23). Recommended value is based on results of Coomber and Whittle [271].
- F92. Cl + CH₂FCI (HCFC-31). The recommended value is based on the room temperature results of Tuazon et al. [1192] and the temperature dependence reported by Tschuikow-Roux et al. [1188], normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation.
- F93. Cl + CHFCl₂ (HCFC-21). The recommended room temperature value is the mean of results of the relative rate study of Tuazon et al. [1192] and the absolute rate study of Talhaoui et al. [1148]. The temperature dependence is from Talhaoui et al. The A-factor from that study has been adjusted to fit the recommended room temperature value. These results are preferred over the earlier results of Glavas and Heicklen [441].
- F94. Cl + CHF₂Cl (HCFC-22). The recommended room temperature value is the mean of results of the relative rate studies of Tuazon et al. [1192] and the absolute rate studies of Sawerysyn et al. [1032] and Talhaoui et al. [1148]. The temperature dependence is from Talhaoui et al. The A-factor from that study has been adjusted to fit the recommended room temperature value.
- F95. Cl + CH₃CCl₃. Recommended value is based on results of the absolute rate study of Talhaoui et al. [1149]. It is consistent with the previous recommendation, which was a much higher upper limit reported by Wine et al. [1321] in a study in which it was concluded that a reactive impurity accounted for a significant fraction of the Cl atom removal. The value reported by Platz et al. [955] is in agreement with the recommendation.
- F96. Cl + CH₃CH₂F (HFC-161). The recommended values for the two reaction channels are based on results of the relative rate study of Tschuikow-Roux et al. [1189], normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation.
- F97. Cl + CH₃CHF₂ (HFC-152a). The recommended values for the two reaction channels are based on results of the relative rate study of Yano and Tschuikow-Roux [1344], normalized to the value of the rate constant for the reference reaction (Cl + C₂H₆) recommended in this evaluation. The overall rate constant value is in good agreement with results of the room temperature relative rate studies of Wallington and Hurley [1259], and Tuazon et al. [1192].
- F98. Cl + CH₂FCH₂F (HFC-152). The recommended value is based on results of the relative rate study of Yano and Tschuikow-Roux [1344], normalized to the value of the rate constant for the reference reaction (Cl + C₂H₆) recommended in this evaluation.
- F99. Cl + CH₃CFCl₂ (HCFC-141b). The recommended value is based on results of absolute rate studies of Talhaoui et al. [1149] by the discharge flow - mass spectrometric technique and Warren and Ravishankara [1278] by the pulsed photolysis-resonance fluorescence technique and the relative rate studies of Wallington and Hurley [1259] and Tuazon et al. [1192].
- F100. Cl + CH₃CF₂Cl (HCFC-142b). The recommended room temperature value is based on results of the relative rate studies of Wallington and Hurley [1259], and Tuazon et al. [1192], and the absolute rate study of Talhaoui et al. [1149]. The temperature dependence is from Talhaoui et al. The A-factor from that study has been adjusted to fit the recommended room temperature value.
- F101. Cl + CH₃CF₃ (HFC-143a). The recommended value is based on results of the relative rate study of Tschuikow-Roux et al. [1189], normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation.
- F102. Cl + CH₂FCHF₂ (HFC-143). The recommended values for the two reaction channels are based on results of the relative rate study of Tschuikow-Roux et al. [1189] normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation.
- F103. Cl + CH₂ClCF₃ (HCFC-133a). The recommended value is based on results of the direct study of Jourdain et al. [595] using the discharge flow-mass spectrometric technique to monitor the decay of the HCFC in the presence of a large excess of Cl atoms. The A-factor is lower than expected.

- F104. $\text{Cl} + \text{CH}_2\text{FCF}_3$ (HFC-134a). The recommended value is based on results of the relative rate studies of Wallington and Hurley [1259], and Tuazon et al. [1192], and the absolute rate study of Sawerysyn et al. [1032].
- F105. $\text{Cl} + \text{CHF}_2\text{CHF}_2$ (HFC-134). The recommended value is based on results of the relative rate study of Nielsen et al. [877] and that of Yano and Tschuikow-Roux [1344], normalized to the value of the rate constant for the reference reaction ($\text{Cl} + \text{C}_2\text{H}_6$) recommended in this evaluation.
- F106. $\text{Cl} + \text{CHCl}_2\text{CF}_3$ (HCFC-123). The recommended value is based on results of the temperature-dependent study of Warren and Ravishankara [1278] using the pulsed photolysis-resonance fluorescence technique, and the relative rate studies of Wallington and Hurley [1259] and Tuazon et al. [1192] at room temperature.
- F107. $\text{Cl} + \text{CHFClCF}_3$ (HCFC-124). The recommended value is based on results of the temperature-dependent study of Warren and Ravishankara [1278] using the pulsed photolysis-resonance fluorescence technique and the relative rate study of Tuazon et al. [1192] at room temperature. The A-factor is lower than expected.
- F108. $\text{Cl} + \text{CHF}_2\text{CF}_3$ (HFC-125). Recommended value is based on results of the relative rate studies of Tuazon et al. [1192] and Sehested et al. [1049].
- 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 [1113]. 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. [337] and Wongdontri-Stuper et al. [1332]; the Arrhenius parameters for k_2 were estimated.
- 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 [259]).
- F111. $\text{ClO} + \text{NO}$. The absolute rate coefficients determined in the four discharge flow-mass spectrometric studies (Clyne and Watson [259], Leu and DeMore [719], Ray and Watson [996] and Clyne and MacRobert [245]) and the discharge flow laser magnetic resonance study of Lee et al. [704] are in excellent agreement at 298 K, and are averaged to yield the preferred value. The value reported by Zahniser and Kaufman [1354] 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 [719] and Lee et al. are in excellent agreement. Although the E/R value reported by Zahniser and Kaufman [1354] 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.
- F112. $\text{ClO} + \text{NO}_3$. The recommended value is based on results reported by Cox et al. [276], Cox et al. [287] Biggs et al. [124], and Kukui et al. [652]. Biggs et al. report the rate constant to be independent of temperature, consistent with the results of Cox et al. [287]. This recent study of Kukui et al. supersedes the earlier study of Becker et al. [92] from the same laboratory, which had indicated the major products to be $\text{OCIO} + \text{NO}_2$. There is now agreement among all studies that the major reaction channel forms $\text{ClOO} + \text{NO}_2$ (see Biggs et al. [124] Cox et al. [287], and Kukui et al. From a study of the OCIO/NO_3 system Friedl et al. [413] conclude that at 220 K the formation of $\text{ClOO} + \text{NO}_2$ is favored.
- F113. $\text{ClO} + \text{N}_2\text{O}$. The Arrhenius expression was estimated based on the $\sim 600 \text{ K}$ data of Walker (reported in Clyne and Watson [259]).
- F114. $\text{ClO} + \text{CO}$. The Arrhenius expression was estimated based on the $\sim 600 \text{ K}$ data of Walker (reported in Clyne and Watson [259]).
- F115. $\text{ClO} + \text{CH}_4$. The Arrhenius expression was estimated based on the $\sim 600 \text{ K}$ data of Walker (reported in Clyne and Watson [259]).
- F116. $\text{ClO} + \text{H}_2\text{CO}$. Poulet et al. [968] have reported an upper limit of $10^{-15} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ for k at 298 K using the discharge flow-EPR technique.
- F117. $\text{ClO} + \text{CH}_3\text{O}_2$. The recommended expressions for the overall rate constant is based on the results of Helleis et al. [495]. It is consistent with the room temperature measurements of Simon et al. [1067] and Kenner et al. [612]. The results of Kukui et al. [654] 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 $\text{ClOO} + \text{CH}_3\text{O}$ (a) and $\text{CH}_3\text{OCl} + \text{O}_2$ (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. [495], Simon et al. [1067], Kukui et al. and Helleis et al. [496] but it is reported to be the minor channel by Biggs et al. [122] and Daele and Poulet [299]. Because of this large discrepancy, no branching ratios are recommended. The branching ratio studies that go down to low temperatures (Helleis et al. [495], Kukui et al. , and Helleis et al. [496]) report that reaction channels (a) and (b) are both significant down to lower polar stratospheric temperatures.

- F118. $\text{ClO} + \text{ClO}$. There are three bimolecular channels for this reaction: $\text{ClO} + \text{ClO} \rightarrow \text{Cl}_2 + \text{O}_2$ (k_1); $\text{ClO} + \text{ClO} \rightarrow \text{ClOO} + \text{Cl}$ (k_2); and $\text{ClO} + \text{ClO} \rightarrow \text{OClO} + \text{Cl}$ (k_3). The recommended values for the individual reaction channels are from the study of Nickolaisen et al. [864]. 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 [237], Clyne and White [263], and Clyne et al. [250], and those of other studies reported by Hayman et al. [489], Cox and Derwent [280], Simon et al. [1068], Horowitz et al. [523], and Horowitz et al. [524]. The room temperature branching ratio are $k_1:k_2:k_3 = 0.29:0.50:0.21$. 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 Cl_2O_2 dimer is given in Table 3.
- F119. $\text{HCl} + \text{ClONO}_2$. 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: $10^{-19} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ by a static wall-less long-path UV absorption technique and a steady-state flow FTIR technique (Molina et al. [829]); 5×10^{-18} using a flow reactor with FTIR analysis (Friedl et al. [411]); and 8.4×10^{-21} using a static photolysis system with FTIR analysis (Hatakeyama and Leu [487] and Leu et al. [720]), and 1.5×10^{-19} by FTIR analysis of the decay of ClONO_2 in the presence of HCl in large-volume (2500 and 5800 liters) Teflon or Teflon-coated chambers (Atkinson et al. [40]). Earlier, Birks et al. [128] 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.
- F120. $\text{CH}_2\text{ClO} + \text{O}_2$. The CH_2ClO radical is reported to be resistant to unimolecular dissociation into $\text{Cl} + \text{CH}_2\text{O}$ products, according to chain reaction/product analysis studies by Sanhueza and Hecklen [1026] and Niki et al. [888] and kinetics studies by Catoire et al. [204]. The recommendation is based on the work of Kaiser and Wallington [603] who studied the competition between reaction with O_2 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 [42]. The fate of CH_2ClO in the atmosphere is this reaction with O_2 .
- F121. $\text{CH}_2\text{ClO}_2 + \text{HO}_2$. The recommendation is based on the measurement reported by Catoire et al. [204], who used pulsed photolysis with UV absorption detection at 1 atm pressure and 251–588 K.
- F122. $\text{CH}_2\text{ClO}_2 + \text{NO}$. The recommendation is based on the value reported by Sehested et al. [1051], who used pulsed radiolysis and UV absorption detection of NO_2 to measure the rate coefficient. The temperature dependence is estimated by analogy to similar $\text{RO}_2 + \text{NO}$ reactions.
- F123. $\text{CCl}_3\text{O}_2 + \text{NO}$. The recommendation is based upon the measurements of Ryan and Plumb [1012] and Dognon et al. [358], 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 CCl_3O primary product of the reaction of CCl_3O_2 with NO decomposes rapidly to eliminate Cl, according to Lesclaux et al. [709].
- F124. $\text{CCl}_2\text{FO}_2 + \text{NO}$. The recommendation is based on the measurements made by Dognon et al. [358] 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 [707]. The CCl_2FO radical primary product of the $\text{CCl}_2\text{FO}_2 + \text{NO}$ reaction is reported by Lesclaux et al. [709] and Wu and Carr [1336] to rapidly decompose to eliminate Cl and to give the products indicated.
- F125. $\text{CClF}_2\text{O}_2 + \text{NO}$. The recommendation is based on the measurements made by Dognon et al. [358], who used pulsed photolysis with mass spectrometry detection at 1–10 torr and 228–413 K, and Sehested et al. [1051], who used pulsed radiolysis with UV absorption detection of the NO_2 product at one atm and 298 K. Wu and Carr [1336] observed the CClF_2O radical primary product to rapidly dissociate to CF_2O and Cl.
- G1. $\text{O} + \text{BrO}$. The preferred value is based on the value reported by Thorn et al. [1166] using a dual laser flash photolysis/long path absorption/resonance fluorescence technique. Clyne et al. [252] reported a value approximately 40% lower.
- G2. $\text{O} + \text{HBr}$. Results of the flash photolysis-resonance fluorescence study of Nava et al. [846] for 221–455 K and the laser flash photolysis-resonance fluorescence study of Nicovich and Wine [872] for 250–402 K provide

the only data at stratospheric temperatures. Results reported include those of Singleton and Cvetanovic [1076] for 298–554 K by a phase-shift technique, and discharge flow results of Brown and Smith [157] for 267–430 K and Takacs and Glass [1142] 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.

- G3. O + HOBr. Recommended room temperature value is the mean of results of Monks et al. [1166] and Kukui et al. [653]. The temperature dependence is from Nesbitt et al. [860]. 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.
- G4. OH + Br₂. The recommended room temperature value is the average of the values reported by Boodaghians et al. [138], Loewenstein and Anderson [750], and Poulet et al. [963]. The temperature independence is from Boodaghians et al. Loewenstein and Anderson determined that the exclusive products are Br + HOBr.
- G5. OH + BrO. Recommended room temperature value is that reported by Bogan et al. [135]. This study, using discharge flow reactor techniques and beam sampling mass spectrometry, is the only experimental measurement of this rate constant. Because of the difficulty of analyzing the data, we assign a large uncertainty factor. The authors suggest that the reaction proceeds by recombination to form vibrationally excited HOObR that dissociates to Br + HO₂.
- G6. OH + HBr. The preferred value at room temperature is the average of the values reported by Ravishankara et al. [989] using FP-RF, by Jourdain et al. [597] using DF-DPR, by Cannon et al. [191] using FP-LIF, and by Ravishankara et al. [992] using LFP-RF and LFP-LIF techniques. In this latest study the HBr concentration was directly measured in-situ in the slow flow system by UV absorption. The rate constant determined in this re-investigation is identical to the value recommended here. The data of Ravishankara et al. [989] show no dependence on temperature over the range 249–416 K. Values reported by Takacs and Glass [1141] and by Husain et al. [547] are a factor of 2 lower and were not included in the derivation of the preferred value. Data by Sims et al. [1073] are in good agreement with the recommendation at 298 K but show a negative temperature dependence at lower temperatures.
- G7. OH + CH₃Br. The recommended rate expression is derived from a combined fit to the data from the relative rate study of Hsu and DeMore [537] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CHF₂ reference reaction, as discussed in the note for that reaction) and the absolute determinations by Chichinin et al. [226], Mellouki et al. [811] and Zhang et al. [1369]. 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. [317] and Howard and Evenson [528].
- G8. OH + CH₂Br₂. The recommended value for k(298 K) is an average of the values from the absolute studies of Mellouki et al. [811] and Zhang et al. [1364] and from the relative rate measurements of DeMore [335] (recalculated based on the current recommendation for the rate constant for the OH + CH₂Cl₂ reference reaction) and Orlando et al. [920] (recalculated based on the current recommendation for the rate constant for the OH + CH₃(CO)CH₃ reference reaction). The recommended value of E/R is from the study of Mellouki et al. [811].
- G9. OH + CHBr₃. The recommended rate expression is derived from a fit to the data from the relative rate study of DeMore [335] (recalculated based on the current recommendation for the rate constant for the OH + CH₂Cl₂ reference reaction). The results of Orkin et al. [914] are higher by a factor of 2 but have the same temperature dependence. They are encompassed within the 2σ confidence limits.
- G10. OH + CHF₂Br. The recommended values for k(298 K) and E/R are derived from a fit to the data of Talukdar et al. [1151] (two studies), Orkin and Khamaganov [913], and Hsu and DeMore [538] (a relative rate measurement recalculated using the current recommendation for the rate constant for the OH + CH₄ reference reaction). These data are preferred over the consistently higher results reported by Brown et al. [153].
- G11. OH + CH₂ClBr. The recommended value for k(298 K) is an average of the values from two relative rate studies by DeMore [335] (recalculated based on the current recommendation for the rate constant for the OH + CH₂Cl₂ reference reaction) and Bilde et al. [126] (recalculated using the current recommendation for the rate constant for the OH + CH₂Br₂ reference reaction) and two absolute determinations by Orkin et al. [915], 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.

- G12. 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. [174] in a study using pulsed photolysis-LIF and DF-LMR techniques. A less sensitive upper limit was reported by Clyne and Holt [243].
- G13. 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. [174] in a study using pulsed photolysis-LIF and DF-LMR techniques.
- G14. 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 [913]. 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. [174] 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 [688].
- G15. 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. [500]. 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. [972] (which include earlier data reported by the same research group in Xing et al. [1340]) 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. [363] seems too low for this reaction when compared with the recommendation for presumably slower (and better studied) OH reaction with CH₃CH₂F.
- G16. OH + CH₂BrCF₃. The recommended values for k(298 K) and E/R are from a combined fit to the data of Nelson et al. [849] and Orkin and Khamaganov [913].
- G17. OH + CHFBrCF₃. The recommended rate expression is derived from a combined fit to the data (below 400 K) of Orkin and Khamaganov [913] and Brown et al. [153].
- G18. OH + CHClBrCF₃. The recommended rate expression is derived from a fit to the data of Orkin and Khamaganov [913] (for T ≤ 400 K). The room temperature value measured by Brown et al. [154] lies somewhat higher than this recommendation but is encompassed within the 2σ confidence limits.
- G19. OH + CHFClCF₂Br. The recommended rate expression is derived from a fit to the data from the relative rate study of DeMore [335] (recalculated based on the current recommendation for the rate constant for the OH + CH₃CCl₃ reference reaction).
- G20. 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 [913]. 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. [174] in a study using pulsed photolysis-LIF and DF-LMR techniques at room temperature is understandably higher.
- G21. 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. [363], Teton et al. [1162], Nelson et al. [850], Herndon et al. [500], Gilles et al. [436], and Kozlov et al. [650]. 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.
- G22. OH + CH₃CHBrCH₃. The recommended values for k(298 K) and E/R are averages of the parameters derived from a fit to the data (T ≤ 300 K) of Herndon et al. [500] and Kozlov et al. [650] which are in excellent agreement. The A factor was then calculated. The room temperature relative rate determination by Donaghy et al. [363] and the absolute temperature dependent data of Teton et al. [1162] 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.
- G23. HO₂ + Br. This recommendation is based on results obtained over the 260–390 K temperature range in the study by Toohey et al. [1183], using a discharge flow system with LMR detection of HO₂ decay in excess Br. The room temperature value reported in this study is a factor of 3 higher than that reported by Poulet et al. [964] using LIF and MS techniques and is an order of magnitude larger than the value of Posey et al. [959]. The uncertainty in E/R is set to encompass the value E/R = 0, as it is for other radical-radical reactions. The value determined by Laverdet et al. [685] using DF-EPR techniques is in good agreement with this

recommendation. The reactions of Br atoms with H₂O₂, HCHO, and HO₂ are all slower than the corresponding reactions of Cl atoms by one to two orders of magnitude.

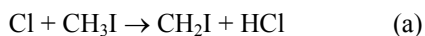
- G24. HO₂ + BrO. The recommendation is based on results of the temperature-dependent studies of Larichev et al. [681], Elrod et al. [377], and Li et al. [730]. The studies of Larichev et al. and Elrod et al. were done under pseudo-first-order conditions with excess HO₂; the study of Li et al. was done under pseudo-first-order conditions with either HO₂ or BrO in excess. The recommended room temperature value is the mean of the values reported in these studies, with the values of Li et al. under both conditions included. These studies all report a similar negative temperature dependence. The room temperature value of Bridier et al. [151], which was not obtained under pseudo-first-order decay conditions, was not included in derivation of the recommendation. Larichev et al. have determined an upper limit of 1.5% for production of HBr and O₃. From a study of the reverse reaction above room temperature, Mellouki et al. [810] determined by extrapolation that the yield of HBr + O₃ is an insignificant fraction (<0.01%) of the total reaction down to 200 K.
- G25. NO₃ + HBr. The recommended upper limit is the upper limit reported by Mellouki et al. [807] 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. [194] reported a value that is consistent, within experimental error, with the upper limit of Mellouki et al.
- G26. Cl + CH₂ClBr. Recommended value is based on results of Tschuikow-Roux et al. [1188] (normalized to the value of the rate constant for the reference reaction (Cl + CH₄) recommended in this evaluation) and Bilde et al. [126] (normalized to most recent values for the rate coefficients for the reference reactions, i.e., the rate coefficients for the Cl + CH₄ reaction given in JPL 00-3 [1019] and for Cl + CH₂Br₂ given in the current recommendation, respectively.) The products of this reaction are expected to be CHClBr and HCl.
- G27. Cl + CH₃Br. Recommended value is based on results of the absolute rate studies of Gierczak et al. [430], Orlando et al. [920], Kambanis et al. [605] and Piety et al. [949]. Results of these studies are in excellent agreement. Results of the relative rate study Tschuikow-Roux et al. [1188] were not used in derivation of the recommended value. The product of this reaction is expected to be mostly CH₂Br and HCl. The possible production of CH₃Cl + Br is very small in the atmosphere [446].
- G28. Cl + CH₂Br₂. Recommended value is based on results of the absolute rate studies of Gierczak et al. [430], Orlando et al. [920], and Kambanis et al. [605]. Results of these studies are in excellent agreement. Results of the relative rate study of Tschuikow-Roux et al. [1188] were not used in derivation of the recommended value. The products of this reaction are expected to be CHBr₂ and HCl.
- G29. Cl + CHBr₃. The recommendation is based on the only reported study of this reaction by Kambanis et al. [605], who employed a very low pressure reactor and monitored reactants and products using mass spectrometry. The products of this reaction are CBr₃ and HCl.
- G30. Br + O₃. The results reported for k(298 K) by Clyne and Watson [261], Leu and DeMore [718], Michael et al. [818], Michael and Payne [823], and Toohey et al. [1184] 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. [868] are in excellent agreement with this recommendation.
- G31. 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. [1183] 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 [714] and Posey et al. [959] using the discharge flow-mass spectrometric technique. The much higher value reported by Heneghan and Benson [498] 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. [810] have measured the rate of the reverse reaction.
- G32. Br + NO₃. The recommended value is that reported by Mellouki et al. [807] in a study using DF-DPR techniques.
- G33. Br + H₂CO. There have been two studies of this rate constant as a function of temperature: Nava et al. [848], using the flash photolysis-resonance fluorescence technique, and Poulet et al. [962], 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. [689], using the discharge flow-EPR technique, has been shown to be in error due to secondary chemistry (Poulet et al.).

- G34. Br + OCIO. The recommended value at room temperature is the mean of the values reported by Clyne and Watson [262] and Toohey [1181]. In the study of Clyne and Watson, correction for the effect of the rapid reverse reaction was required. The temperature dependence reported by Toohey [1181] is accepted but with increased error limits.
- G35. Br + Cl₂O. The recommended value is based on results reported by Stevens and Anderson [1114] and by Sander and Friedl [1018], which are in good agreement.
- G36. Br + Cl₂O₂. The recommended value is that determined by Friedl (private communication) in a study using a DF-MS technique.
- G37. BrO + O₃. There have been two recent studies of this reaction. Rattigan et al. [978] report an overall rate constant of $\sim 10^{-17}$ cm³ molecule⁻¹s⁻¹ over the temperature range 318–343 K. Rowley et al. [1009] 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. [793]. The pre-exponential factor was estimated, and E/R was calculated.
- G38. BrO + NO. The results of the three low pressure mass spectrometric studies (Clyne and Watson [261]; Ray and Watson [996]; Leu [712]) and the high pressure UV absorption study (Watson et al. [1289]), 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 [238]). 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.
- G39. BrO + NO₃. The recommended value is the geometric mean of the lower and upper limits reported by Mellouki et al. [807] in a study using DF-DPR techniques. These reported limits are encompassed within the indicated uncertainty limits.
- G40. BrO + ClO. Friedl and Sander [412], 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 [1018]) 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 [1182], 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. [960], 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 [262] and the very low value derived in the flash photolysis study of Basco and Dogra [81] 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 [412] and Turnipseed et al. [1205]. 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. [507] and Basco and Dogra [81].
- G41. 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. [438] 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 [1023], Mauldin et al. [793], Bridier et al. [151], Rowley et al. [1009], Laszlo et al. [683], and Gilles et al.) come into very good agreement among themselves and also with results of the mass spectrometric studies of Clyne and Watson [261] and Lancar et al. [677]. This provides the basis for the recommended room temperature value.

The temperature dependence is based on results of Sander and Watson, Turnipseed et al. [1204] and Gilles et al.

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 [1023], Turnipseed et al. [1204] and Lancar et al. [677], by Jaffe and Mainquist [568] from 258 to 333 K, by Cox et al. [292] from 278 to 348 K and by Mauldin et al. [793] 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 $k_2 = 2.8 \times 10^{-14} \exp(860/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$.

- G42. $\text{CH}_2\text{BrO}_2 + \text{NO}$. The recommendation is based on the 298 K measurement of Sehested et al. [1051], 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. [216] and Orlando et al. [919]. 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. [878].
- H1. $\text{O} + \text{I}_2$. Based on the room temperature data of Ray and Watson [996] and Laszlo et al. [684]. The molecular beam study of Parrish and Herschbach [931] suggests a zero activation energy, consistent with the near gas kinetic value of k at 298 K.
- H2. $\text{O} + \text{IO}$. Based on results of Laszlo et al. [684], 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 .
- H3. $\text{OH} + \text{I}_2$. Based on the data of Loewenstein and Anderson [751] and Jenkin et al. [575].
- H4. $\text{OH} + \text{HI}$. Based on the data of Lancar et al. [679] and MacLeod et al. [765].
- H5. $\text{OH} + \text{CH}_3\text{I}$. The recommended rate expression is derived from a fit to the data of Brown et al. [155], the only reported study of this reaction.
- H6. $\text{OH} + \text{CF}_3\text{I}$. The recommended rate expression is derived from a fit to the data of Gilles et al. [437]. The results from the studies by Garraway and Donovan [422] and Berry et al. [114] 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. [155] agrees within the 2σ limits.
- H7. $\text{HO}_2 + \text{I}$. Based on the data of Jenkin et al. [580], the only reported study of this reaction.
- H8. $\text{HO}_2 + \text{IO}$. The recommended value is the average of the values reported by Jenkin et al. [579] and Maguin et al. [768].
- 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. [679]).
- 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. [53] 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. [605] between 273 and 363 K, Bilde and Wallington [125] at 298 K, and Cotter et al. [273] 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 [125]. 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 CH_3ICl via reaction with O_2 cannot be ignored. Further, the possible atmospheric photolysis of CH_3ICl 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 $\text{CH}_3\text{Cl} + \text{I}$ (Goliff and Rowland [446]). Based on the results of Bilde and Wallington and Goliff and Rowland, we recommend that the rate coefficient for the $\text{Cl} + \text{CH}_3\text{I} \rightarrow \text{CH}_3\text{Cl} + \text{I}$ 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 $\sim 14 \text{ kcal mol}^{-1}$ at 298 K, the branching ratio for the production of CH_3Cl and I in the atmosphere will be likely less than that at 298 K.

- H11. $\text{I} + \text{O}_3$. Based on the room temperature data of Jenkin and Cox [576] and Sander [1017], and the temperature dependent data of Buben et al. [164] and Turnipseed et al. [1207].
- H12. $\text{I} + \text{BrO}$. Based on results of Laszlo et al. [683], the only reported study of this rate constant. This value was derived from modeling the simultaneous decay of BrO and IO in a $\text{Br}_2/\text{I}_2/\text{N}_2\text{O}$ system.
- H13. $\text{IO} + \text{NO}$. Based on the data of Ray and Watson [996], Daykin and Wine [322], Buben et al. [165], and Turnipseed et al. [1207].
- H14. $\text{IO} + \text{ClO}$. Based on results of Turnipseed et al. [1206], 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 .
- H15. $\text{IO} + \text{BrO}$. Based primarily on results of Laszlo et al. [683]. Gilles et al. [438] reported the following Arrhenius expression for non-iodine atom producing channels: $2.5 \times 10^{-11} \exp(260/T) \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$. 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: $6 \times 10^{-11} < k < 10 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$, the range of which is consistent with the results of Laszlo et al.
- H16. $\text{IO} + \text{IO}$. Changed from the previous recommendation, which was based on the results of Sander [1017]. 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. [485], 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. [684]. 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 I_2O_2 is the dominant reaction channel in the IO self-reaction.
- H17. $\text{INO} + \text{INO}$. Based on the data of Van den Bergh and Troe [1225].
- H18. $\text{INO}_2 + \text{INO}_2$. Based on the data of Van den Bergh and Troe [1225].
- I1. $\text{O} + \text{SH}$. This recommendation accepts the results of Cupitt and Glass [296]. The large uncertainty reflects the absence of any confirming investigation.
- I2. $\text{O} + \text{CS}$. The room temperature recommendation is an average of the rate constants determined by Slagle et al. [1087], Bida et al. [118], Lilenfeld and Richardson [737], and Hancock and Smith [479]. The temperature dependence is that of Lilenfeld and Richardson, with the A-factor adjusted to yield the recommended value of $k(298 \text{ K})$.
- I3. $\text{O} + \text{H}_2\text{S}$. This recommendation is derived from an unweighted least squares fit of the data of Singleton et al. [1079] and Whytock et al. [1304]. The results of Slagle et al. [1085] 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. [1085] and Hollinden et al. [519]. 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, $\Delta E/R$ 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. [1085], Singleton et al. [1079], and Singleton et al. [1081]. In the latter two studies, an upper limit of 20% was placed on the displacement channel. Direct observations of product HSO was made in the reactive scattering experiments of Clemo et al. [235] and Davidson et al. [307]. 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 [1090]. 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 stratospheric chemistry.

- I4. O + OCS. The value of $k(298\text{ K})$ is the average of the determinations by Westenberg and de Haas [1296], Klemm and Stief [637], Wei and Timmons [1292], Manning et al. [771], and Breckenridge and Miller [150]. The recommended value of E/R is the average value taken from the first three listed studies. Hsu et al. [536] 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. [222] and Nickolaissen et al. [866] respectively.
- I5. O + CS₂. The value of $k(298\text{ K})$ is an average of the rate constants determined by Wei and Timmons [1292], Westenberg and de Haas [1296], Slagle et al. [1086], Callear and Smith [188], Callear and Hedges [187], Homann et al. [520], and Graham and Gutman [449]. 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 data of Westenberg and de Haas. The principal reaction products are thought to be CS + SO. However, Hsu et al. [536] 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 [449] 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 [272] determined the branching ratios for the CO and OCS producing channels to be (3.0±1.0)% and (8.5±1.0)% respectively.
- I6. O + CH₃SCH₃. This recommendation is based on a fit of the data from Nip et al. [897], Lee et al. [700], and Lee et al. [699]. Product studies by Cvetanovic et al. [297] indicate that the reaction proceeds almost entirely by addition followed by rapid fragmentation to the products as written. Pavanaja et al. [936] 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.
- I7. O + CH₃SSCH₃. This recommendation averages the 298 K rate constants of Nip et al. [897] and Lee et al. [696], which differ by nearly a factor of 2. The temperature dependence is that of Nip et al.; Lee et al. having reported no temperature dependence over the limited range of 270–329 K. The A -factor has been adjusted to yield the recommended (averaged) value of $k(298\text{ K})$. Product studies by Cvetanovic et al. [297] indicate that the reaction proceeds mainly by addition followed by rapid fragmentation to the products as written. Pavanaja et al. [936] 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.
- I8. O₃ + H₂S. This upper limit was determined by Becker et al. [96] from measurements of the rates of SO₂ production and O₃ consumption. The heterogeneous reaction between H₂S and O₃ is far more efficient in most laboratory systems.
- I9. O₃ + CH₃SCH₃. This rate constant upper limit is based on the measurements of Martinez and Herron [789], which represent the only reported study of this reaction.
- I10. SO₂ + O₃. This recommendation is based on the limited data of Davis et al. [318] at 300 K and 360 K in a stopped flow investigation using mass spectrometric and UV spectroscopic detection.
- I11. OH + H₂S. The values of $k(298\text{ K})$ and E/R are derived from a composite unweighted least squares fit to the individual data points of Perry et al. [943], Cox and Sheppard [291], Wine et al. [1313], Leu and Smith [723], Michael et al. [819], Lin [738], Lin et al. [742], Barnes et al. [63], and Lafage et al. [674]. The studies of Leu and Smith [723], Lin et al. [742], Lin [738], and Lafage et al. [674] 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 $E/R = 400\text{ K}$ for the abstraction channel, in good agreement with the E/R value determined above room temperature by Westenberg and de Haas [1297]. The results of these latter workers lie systematically higher (by about 70%), presumably due to secondary reactions. The room temperature value measured by Stuhl [1126] lies just outside the 2σ error limit set for $k(298\text{ K})$.
- I12. OH + OCS. The value of $k(298\text{ K})$ is an average of the determinations by Wahner and Ravishankara [1243] and Cheng and Lee [223]. The room temperature rate constants from these studies are a factor of 3 higher

than the earlier determination by Leu and Smith [722]. 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 H₂S 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 [1243] supersedes the study of Ravishankara et al. [982], which minimized complications due to secondary and/or excited state reactions that presumably were interfering with the experiments of Atkinson et al. [45] and of Kurylo [663]. The upper limit for

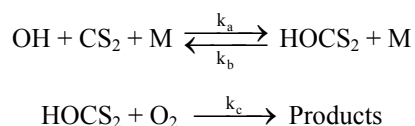
k(298 K) reported by Cox and Sheppard [291] is too insensitive to permit comparison with the more recent studies. The room temperature measurements of Wahner and Ravishankara demonstrate the lack of an effect of total pressure (or O₂ partial pressure) on the rate constant and are supported by the more limited pressure and O₂ 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 [669] that the predominant reaction pathway is to produce SH + CO₂ 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 [454] 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.

113. OH + CS₂. There is a consensus of experimental evidence that this reaction proceeds very slowly as a direct bimolecular process. Wine et al. [1322] set an upper limit on k(298 K) of 1.5 × 10⁻¹⁵ cm³ molecule⁻¹ s⁻¹. A consistent upper limit is also reported by Iyer and Rowland [565] for the rate of direct product 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 [724] and of Biermann et al. [120], which set somewhat higher upper limits on k(298 K). The more rapid reaction rates measured by Atkinson et al. [45], Kurylo [663], and Cox and Sheppard [291] 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. [1312].

An accelerating effect of O₂ on the OH + CS₂ reaction rate has been observed by Jones et al. [594], Barnes et al. [69], and Hynes et al. [553], 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 [663] and Kurylo and Laufer [669] followed by its reaction with O₂:



Hynes et al. [553], Murrells et al. [842], Becker et al. [97], and Bulatov et al. [167] directly observed the approach to equilibrium in this reversible adduct formation. In the Hynes et al. study, the equilibrium constant was measured as a function of temperature, and the heat of formation of HOCS₂ was calculated (-27.4 kcal/mole). A rearrangement of this adduct followed by dissociation into OCS and SH corresponds to the bimolecular (low k) channel referred to earlier. Hynes et al. [553] measured the rate constant for this process in the absence of O₂ (at approximately one atmosphere of N₂) to be < 8 × 10⁻¹⁶ cm³ molecule⁻¹ s⁻¹. Hynes et al. [553], Murrells et al. [842], and Diau and Lee [345] agree quite well on the value of k_c, with an average value of 2.9 × 10⁻¹⁴ being reported independent of temperature and pressure. Diau and Lee also report the rate constants for the reactions of the adduct (CS₂OH) with NO and NO₂ to be 7.3 × 10⁻¹³ and 4.2 × 10⁻¹¹ respectively.

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

$$1/k_{\text{eff}} = (k_b/k_a k_c)(1/P_{\text{O}_2}) + (1/k_a)(1/P_{\text{M}})$$

where P_{O_2} is the partial pressure of O_2 and P_M equals $P_{O_2} + P_{N_2}$. The validity of this expression requires that k_a and k_b are invariant with the P_{O_2}/P_{N_2} ratio. A $1/k$ vs $1/P_{O_2}$ plot of the data of Jones et al. [594] taken at atmospheric pressure exhibits marked curvature, suggesting a more complex mechanistic involvement of O_2 , whereas the data of Barnes et al. [69] and Hynes et al. [553] 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 O_2 and N_2 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_{O_2} , and the other at fixed P_{O_2} and varying P_M (i.e., varying added N_2). Within each data set, rate constants calculated from both fits agree reasonably well for mole fractions of O_2 near 0.2 (equivalent to air) but disagree by more than a factor of 2 for measurements in a pure O_2 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 O_2 (at 700 torr total pressure) to -2900 K for experiments in a 50 torr O_2 plus 650 torr N_2 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., $P_{O_2}/P_{N_2} = 0.25$) at atmospheric pressure. Since most CS_2 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. [553], 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.

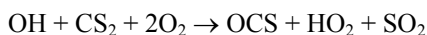
$$k(298\text{ K}) = 1.2 \times 10^{-12} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$$

The uncertainty factor, $f(298\text{ K}) = 1.5$, encompasses the results of Barnes et al. [69] within 2σ . To compute values of k below 298 K, we have accepted the analysis of Hynes et al.

$$k(T) = \{1.25 \times 10^{-16} \exp(4550/T)\} / \{T + 1.81 \times 10^{-3} \exp(3400/T)\}$$

This recommendation is only valid for one atmosphere pressure of air. It is interesting to note that measurements by Hynes et al. [553] at approximately 250 K and 700 torr total pressure result in k_{eff} values that are independent of the amount of O_2 for partial pressures between 145–680 torr. This suggests that the adduct is quite stable with respect to dissociation into the reactants ($OH + CS_2$) at this low temperature and the that effective rate constant for reactant removal approaches the elementary rate constant for adduct formation.

From a mechanistic viewpoint, the primary products of reaction c determine the products of CS_2 oxidation in air. Lovejoy et al. [757] have shown that the yields of both HO_2 and SO_2 are equal and near unity. Together with the earlier mentioned unity yield of OCS , these observations suggest that the oxidation equation



describes this atmospheric system. Further insight is provided by the mechanistic study of Stickel et al. [1116], 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 $CS_2OH + O_2$ reaction or as products of a secondary reaction between a primary product and O_2 . These same authors report an SO_2 yield of (1.15 ± 0.10) , with the results suggesting that only about 75% of the SO_2 formed as a prompt product, with the remainder generated via a slow reaction of SO (generated as a prompt product of the $CS_2OH + O_2$ reaction) with O_2 . Insight into the specific reaction pathways can be gleaned from the study of Lovejoy et al. [756] in which k_c for the reaction of $DOCS_2 + O_2$ was found to be the same as that for $HOCS_2$, indicating that simple H atom abstraction is not the likely process. Rather, HO_2 production most likely involves complex formation followed by HO_2 elimination. Lovejoy et al. [758] found that the ^{18}O atom in the ^{18}OH reactant is transferred predominantly ($90 \pm 20\%$) to the SO_2 product. These findings are consistent with an S–O–bonded CS_2 –OH adduct and preservation of the S–O bond in the steps leading to SO_2 formation. Additional work involving direct intermediate observations would be helpful in elucidating this reaction mechanism.

114. $OH + CH_3SH$. This recommendation is based on a composite fit to the data of Atkinson et al. [44], Wine et al. [1313], Wine et al. [1323], and Hynes and Wine [551], which are in excellent agreement. The results from the relative rate study of Barnes et al. [63] are in agreement with this recommendation and indicate that the higher value of Cox and Sheppard [291] is due to complications resulting from the presence of O_2 and NO in their reaction system. MacLeod et al. [766,767] and Lee and Tang [698] 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. [1323] 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 [1218] 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. Hynes and Wine [551] failed to observe any effect of O₂ on the rate constant.

- I15. OH + CH₃SCH₃. This recommendation is based on the results of Hynes et al. [555], Wine et al. [1313], Hsu et al. [540], Abbatt et al. [3], and Barone et al. [76]. The earlier higher rate constant values of Atkinson et al. [45] and Kurylo [662] are presumably due to reactive impurities, while those of MacLeod et al. [767] were most likely overestimated because of heterogeneous reactions. Absolute determinations lower than those recommended were obtained by Martin et al. [785], Wallington et al. [1247], and Nielsen et al. [883]. While the reasons for these differences are not readily apparent, these results are encompassed within the 2σ error limits of the 298 K recommendation. Hynes et al. have demonstrated the importance of a second reaction channel involving addition of OH to dimethyl sulfide (approximately 30% in 1 atmosphere of air at 298 K). More recently, Hynes et al. and Barone et al. have examined the reaction mechanism in more detail using fully deuterated DMS. Both groups report similar rate constants for the bimolecular (non-adduct-forming) rate constant and adduct bond strengths (13.0 and 10.1 kcal/mole—Hynes et al.; 10.2 and 10.7 kcal/mole—Barone et al.) from second and third law calculations, respectively. Values of the rate constant for the reaction of the adduct with O₂ were also nearly identical (8 × 10⁻¹³ cm³ molecule⁻¹ s⁻¹ from Hynes et al., and 10⁻¹² cm³ molecule⁻¹ s⁻¹ from Barone et al. for both DMS and d⁶-DMS) independent of pressure and temperature.

The recommendation given here is for the abstraction reaction only. Confirmation of the products as written is obtained from the study of Stickel et al. [1118] who determined an HDO product yield of (0.84±0.15) for the OD + CH₃SCH₃. Further mechanistic insight comes from the studies of Barnes et al. [72,73] and Turnipseed et al. [1203] who find that the abstraction product, CH₃SCH₂, leads predominantly to CH₃S under atmospheric conditions. Barnes et al. measure a 0.7% yield of OCS under low NO_x conditions, which they attribute to further oxidation of CH₃S. Both Barnes et al. and Turnipseed et al. find a significant (20–30%) yield of dimethyl sulfoxide, apparently produced via the reaction of the DMS–OH adduct with O₂. Zhao et al. [1372] determined an upper yield of 0.07 for CH₃ elimination in the OD + CH₃SCH₃ reaction system.

Due to the rapid decomposition of a DMS–OH adduct, only the direct abstraction channel is measured in the absence of O₂. The reaction of the adduct with O₂, as quantified most recently by Hynes et al. and Barone et al., is responsible for the majority of the products formed in the atmospheric oxidation of DMS. An increase in the observed rate constant (k_{obs}) with increasing O₂ concentration has clearly been observed by Hynes et al. [555], Wallington et al. [1247], Barnes et al. [62], Nielsen et al. [883], Barone et al. [76], and Hynes et al. [550]. This O₂ effect has been suggested as an explanation for the higher rate constants obtained in many of the earlier relative rate studies. Hynes et al. give the following expression for the observed rate constant in one atmosphere of air:

$$k_{\text{obs}} = \frac{T \exp(-234/T) + 8.46 \times 10^{-10} \exp(7230/T) + 2.68 \times 10^{-10} \exp(7810/T)}{1.04 \times 10^{11} T + 88.1 \exp(7460/T)}$$

This expression was derived empirically from the analysis of a complex data set, which also yielded a value of the rate constant for reaction of the adduct with O₂ that was a factor of 4 larger than the values derived by Hynes et al. [550] and Barone et al. [76] and appeared to be both pressure and temperature dependent. The effect of these revisions in the adduct + O₂ rate constant on the k_{obs} expression is not easily ascertained.

- I16. OH + CH₃SSCH₃. This recommendation is based on the temperature-dependent studies of Wine et al. [1313] and Abbatt et al. [3] and the room temperature relative rate study of Cox and Sheppard [291]. Domine and Ravishankara [361] have observed both CH₃S (via laser-induced fluorescence) and CH₃SOH (via photoionization mass spectrometry) as products of this reaction. At 298 K, the yield of CH₃S alone was quantified at approximately 30%. An FTIR product study of the photooxidation of dimethyl disulfide by Barnes et al. [71] presents evidence that oxidation of the CH₃SOH product is the principal source of the methane sulfonic acid observed.
- I17. OH + S. This recommendation is based on the study by Jourdain et al. [596]. Their measured value for k(298 K) compares favorably with the recommended value of k(O + OH) when one considers the slightly greater exothermicity of the present reaction.
- I18. OH + SO. The value recommended for k(298 K) is an average of the determinations by Fair and Thrush [380] and Jourdain et al. [596]. Both sets of data have been corrected using the present recommendation for the O + OH reaction.

- I19. $\text{HO}_2 + \text{H}_2\text{S}$, $\text{HO}_2 + \text{CH}_3\text{SH}$, $\text{HO}_2 + \text{CH}_3\text{SCH}_3$. These upper limits are taken from the discharge flow laser magnetic resonance study of Mellouki and Ravishankara [808]. The H_2S value disagrees with the rate constant reported by Bulatov et al. [171] 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. [63] and Niki (reported as a private communication in the Mellouki and Ravishankara paper).
- I20. $\text{HO}_2 + \text{SO}_2$. This upper limit is based on the atmospheric pressure study of Graham et al. [452]. A low pressure laser magnetic resonance study by Burrows et al. [176] places a somewhat higher upper limit on $k(298 \text{ K})$ of 4×10^{-17} (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. [938].
- I21. $\text{NO}_2 + \text{SO}_2$. This recommendation is based on the study of Penzhorn and Canosa [940] 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 [567], much of which may have been due to heterogeneous processes. Penzhorn and Canosa suggest that the products of this reaction are $\text{NO} + \text{SO}_3$.
- I22. $\text{NO}_3 + \text{H}_2\text{S}$. This recommendation accepts the upper limit set by Dlugokencky and Howard [348] 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. [1249] and Cantrell et al. [197].
- I23. $\text{NO}_3 + \text{OCS}$. This upper limit is based on the relative rate data of MacLeod et al. [764].
- I24. $\text{NO}_3 + \text{CS}_2$. This upper limit is based on the study of Burrows et al. [180]. A somewhat higher upper limit was derived in the relative rate data of MacLeod et al. [764].
- I25. $\text{NO}_3 + \text{CH}_3\text{SH}$. The recommended values are derived from a composite fit to the data of Wallington et al. [1249], Rahman et al. [975], and Dlugokencky and Howard [348]. The room temperature rate constant derived in the relative rate experiments of MacLeod et al. [764] 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. [583] 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.
- I26. $\text{NO}_3 + \text{CH}_3\text{SCH}_3$. The recommended values are derived from a composite fit to the data of Wallington et al. [1249], Tyndall et al. [1209], and Dlugokencky and Howard [348]. The relative rate study of Atkinson et al. [47] 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 [323] and Wallington et al. [1250] are also in agreement with the recommended value. Jensen et al. [582] propose a mechanism that involves hydrogen abstraction as the first step to explain their observed product distribution. In a later study, Jensen et al. [583] measured a kinetic isotope effect for the rate constant for CH_3SCH_3 vs. that for CD_3SCD_3 of $k_{\text{H}}/k_{\text{D}} = (3.8 \pm 0.6)$, providing further confirmation of such abstraction. Butkovskaya and Le Bras [182] utilized chemical titration of the primary radical produced from $\text{NO}_3 + \text{CH}_3\text{SCH}_3$ in a discharge flow mass spectrometer 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 $\text{CH}_3 + \text{CH}_3\text{SONO}_2$.
- I27. $\text{NO}_3 + \text{CH}_3\text{SSCH}_3$. The recommended values were derived from a composite fit to the data of Wallington et al. [1249] and Dlugokencky and Howard [348]. The investigation by Atkinson et al. [39] 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. [764] can be considered to be erroneous. Based on their observations of intermediate and end products, Jensen et al. [583] proposed a reaction mechanism in which the initial addition of NO_3 to one of the sulfur atoms results in formation of $\text{CH}_3\text{S} + \text{CH}_3\text{SO} + \text{NO}_2$.
- I28. $\text{NO}_3 + \text{SO}_2$. This recommended upper limit for $k(298 \text{ K})$ is based on the study by Daubendiek and Calvert [305]. Considerably higher upper limits have been derived by Burrows et al. [180], Wallington et al. [1249], Canosa–Mas et al. [192], and Dlugokencky and Howard [348].
- I29. $\text{N}_2\text{O}_5 + \text{CH}_3\text{SCH}_3$. This recommendation is based on the value estimated by Tyndall and Ravishankara [1219] from the study by Atkinson et al. [47].

130. $\text{CH}_3\text{O}_2 + \text{SO}_2$. This recommendation accepts the results from the study of Sander and Watson [1022], which is believed to be the most appropriate for stratospheric modeling purposes. These authors conducted experiments using much lower CH_3O_2 concentrations than employed in the earlier investigations of Sanhueza et al. [1027] and Kan et al. [607], both of which resulted in $k(298\text{ K})$ values approximately 100 times greater. A later report by Kan et al. [606] 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 stratospheric conditions to compete with the adduct decomposition. This interpretation, unfortunately, does not explain the high rate constant derived by Cocks et al. [265] under conditions of low $[\text{CH}_3\text{O}_2]$.
131. $\text{F} + \text{CH}_3\text{SCH}_3$. This recommendation is based on the discharge flow mass spectrometric study by Butkovskaya et al. [183]. 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.
132. $\text{Cl} + \text{H}_2\text{S}$. This recommendation is based on the study by Nicovich et al. [870], 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 [857], who refined the data of Braithwaite and Leone [149], but is significantly greater than the values reported by Clyne and Ono [256], Clyne et al. [247], and Nava et al. [847]. 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 . 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. [761] also measured a temperature-independent rate constant but report a value at 298 K, about 40% greater than that of Nicovich et al. However, the presence of 4000 torr of CF_3Cl bath gas in the Lu et al. may suggest a slight pressure dependence of the reaction, although Nicovich et al. observed no pressure dependence for pressures ranging up to 600 torr with N_2 .
133. $\text{Cl} + \text{OCS}$. This upper limit is based on the minimum detectable decrease in atomic chlorine measured by Eibling and Kaufman [376]. Based on the observation of product SCl , these authors set a lower limit on $k(298\text{ K})$ of 10^{-18} for this reaction channel. Considerably higher upper limits on $k(298\text{ K})$ were determined in the studies of Clyne et al. [247] and Nava et al. [847].
134. $\text{Cl} + \text{CS}_2$. This upper limit for the overall reaction is based on determinations by Nicovich et al. [869] and Wallington et al. [1246]. The first authors confirm that the reaction proceeds via reversible adduct formation as suggested by Martin et al. [783]. The much larger rate constant values determined by Martin et al. may possibly be attributed to reactive impurities in the CS_2 sample. Nicovich et al. set an upper limit on the rate constant for the adduct (CS_2Cl) reacting with O_2 of 2.5×10^{-16} at room temperature.
135. $\text{Cl} + \text{CH}_3\text{SH}$. This recommendation is based on the results of Nicovich et al. [870], who used laser photolysis with resonance fluorescence detection to study the reactions of Cl with H_2S , D_2S , CH_3SH , and CD_3SD . The room temperature determination by Nesbitt and Leone [857] is in good agreement with the value recommended. The $k(298\text{ K})$ value from the study by Mellouki et al. [804] 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 [858] report that less than 2% of the reaction occurs via abstraction of an H atom from the CH_3 group.
136. $\text{Cl} + \text{CH}_3\text{SCH}_3$. Stickel et al. [1117] have used laser photolysis resonance fluorescence to measure that rate constant between 240–421 K, over the pressure range of 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} 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 $(\text{CH}_3)_2\text{SCl}$ adduct becomes competitive with hydrogen atom abstraction with increasing pressure. These investigators also observed a negative temperature dependence for the reaction. Butkovskaya et al. [183] conducted a discharge flow mass spectrometric study at 298 K, in which they determined that the reaction proceeds to form $\text{HCl} + \text{CH}_3\text{SCH}_2$ almost exclusively at 1 torr total pressure. The sum of all other possible channels was estimated at less than 3%. Zhao et al. [1372] used laser photolysis coupled with CH_3 detection by time-resolved tunable diode laser

absorption spectroscopy to determine an upper limit for CH₃ elimination at 298 K and pressures between 10–30 torr. Room temperature measurements by Nielsen et al. [882] at 740 torr and Kinnison et al. [626] at 760 torr agree quite well with the results of Stickel et al. Kinnison et al. also observed the rate constant to increase from 3.6×10^{-10} to 4.2×10^{-10} cm³ molec⁻¹ s⁻¹ when the bath gas was changed from pure N₂ to synthetic air, suggesting that the (CH₃)₂S₂ adduct reacts with O₂.

- I37. ClO + OCS; ClO + SO₂. These recommendations are based on the discharge flow mass spectrometric data of Eibling and Kaufman [376]. The upper limit on k(298 K) for ClO + OCS was set from the minimum detectable decrease in ClO. No products were observed. The upper limit on k(298 K) for ClO + SO₂ is based on the authors' estimate of their SO₃ 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 Cl + O₃ source reaction.
- I38. ClO + CH₃SCH₃. This recommendation is based on the study by Barnes et al. [67] using discharge flow mass spectrometry. The authors prefer the present value of the rate constant to one a factor of 4 higher, which they determined in an earlier version of their apparatus. The uncertainty factor reflects the absence of any confirming investigations.
- I39. ClO + SO. The value of k(298 K) is an average of the determinations by Clyne and MacRobert [246] and Brunning and Stief [162]. The temperature independence is taken from the latter study with the A-factor recalculated to fit the k(298 K) recommendation.
- I40. Br + H₂S, Br + CH₃SH. These recommendations are based on the study by Nicovich et al. [867] 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.
- I41. Br + CH₃SCH₃. Wine et al. [1315] used laser photolysis resonance fluorescence to study reversible adduct formation in the Br + CH₃SCH₃ reaction system over the temperature range 260 – 310 K from which they derive a (CH₃)₂S–Br bond strength of 14.5 ± 1.2 kcal mole⁻¹. Above 375 K, adduct decomposition is so rapid that the addition channel is effectively negligible. Extrapolation of these data to conditions typical of the springtime Arctic boundary layer (760 torr, 230 – 270 K) leads these authors to suggest that under such conditions, the addition of Br to CH₃SCH₃ proceeds with a rate constant of approximately 1.3×10^{-10} cm³ molecule⁻¹ s⁻¹. Researchers from the same laboratory (Jefferson et al. [573]) studied the abstraction reaction over the temperature range 386 – 604 K. These authors observed the reactants to be in equilibrium with the products HBr + CH₃SCH₂ and determined Arrhenius expressions for the forward and reverse reactions respectively of $9.0 \times 10^{-11} \exp(-2386/T)$ cm³ molecule⁻¹ s⁻¹ and $8.6 \times 10^{-13} \exp(836/T)$ cm³ molecule⁻¹ s⁻¹. Analysis of the equilibrium data also permitted determination of the heat of formation of CH₃SCH₂ (see Appendix 1).
- I42. BrO + CH₃SCH₃. This recommendation is based on the discharge flow mass spectrometric study by Bedjanian et al. [99], performed at 1 torr over the temperature range 233–320 K. The rate constant at 298 K is nearly identical to that derived by Barnes et al. [67], using a similar experimental system. Bedjanian et al. also determined a near unity yield for the production of dimethylsulfoxide and suggest that the reaction proceeds via production of an adduct that decomposes into the sulfoxide and bromine atoms.
- I43. BrO + SO. This recommendation is based on the measurements of Brunning and Stief [163] performed under both excess BrO and excess SO conditions. The rate constant is supported by the lower limit assigned by Clyne and MacRobert [246] from measurements of SO₂ production.
- I44. IO + CH₃SH. The value of k(298 K) comes from the study by Maguin et al. [769] 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.
- I45. IO + CH₃SCH₃. This recommendation comes from the studies by Daykin and Wine [321] using laser photolysis absorption spectroscopy and by Maguin et al. [769] and Barnes et al. [67] using discharge flow mass spectrometry. These groups obtained rate constants of $\leq 3.5 \times 10^{-14}$, 1.5×10^{-14} , and 8.8×10^{-15} respectively. The last two studies supersede earlier, less direct measurements by the same groups, which resulted in rate constants of 1.5×10^{-11} (Martin et al. [784]) and 3.0×10^{-11} (Barnes et al. [68]).
- I46. S + O₂. This recommendation is based primarily on the study of Davis et al. [316]. Modest agreement at 298 K is found in the studies of Fair and Thrush [380], Fair et al. [381], Donovan and Little [364], and Clyne and Townsend [257]. The study by Clyne and Whitefield [264], which indicates a slightly negative E/R between 300 and 400 K, is encompassed by the assigned uncertainty limits.

147. S + O₃. This recommendation accepts the only available experimental data of Clyne and Townsend [257]. In this study the authors measure a value of the rate constant for S + O₂ in reasonable agreement with that recommended above.
148. SO + O₂. This recommendation is based on the low temperature measurements of Black et al. [133,134]. The room temperature value accepts the results of the more recent paper as recommended by the authors. The uncertainties cited reflect the need for further confirmation and the fact that these results lie significantly higher than an extrapolation of the higher temperature data of Homann et al. [520]. A room temperature upper limit on k set by Breckenridge and Miller [150] is consistent with the Black et al. data.
149. SO + O₃. The value of k(298 K) is an average of the determinations by Halstead and Thrush [474], Robertshaw and Smith [1004], and Black et al. [133,134] using widely different techniques. The value of E/R is an average of the values reported by Halstead and Thrush and Black et al. [134], with the A-factor recalculated to fit the recommendation for k(298 K).
150. SO + NO₂. The value of k(298 K) is an average of the determinations by Clyne and MacRobert [245], Black et al. [133], and Brunning and Stief [162], which agree quite well with the rate constant calculated from the relative rate measurements of Clyne et al. [241]. The Arrhenius parameters are taken from Brunning and Stief.
151. SO + OCIO. This recommendation is based on the room temperature study by Clyne and MacRobert [246]. The uncertainty reflects the absence of any confirming investigation.
152. SO₃ + H₂O. Several research groups have attempted to quantify the rate of sulfuric acid formation via this reaction in the gas phase. Reiner and Arnold [1000] 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. [1274]. 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. [203] may have resulted from an underestimation of the effects of such heterogeneous reactions. Subsequently, Reiner and Arnold [1001] 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. [647] attempted to measure the gas phase reaction using a turbulent flow reactor designed to minimize wall effects. Their results, when analyzed as representing a bimolecular reaction, support a rate constant between $(1 - 7) \times 10^{-15} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$. However, a more considered 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 [835], led the latter authors to suggest that SO₃ consumption likely involved its reaction with the water dimer or the reaction of SO₃H₂O + H₂O, leading to the formation of sulfuric acid.
- A laminar flow reactor study by Lovejoy et al. [755] over the temperature range 256–360 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 the SO₃ + water dimer reaction mechanism since it would require a large negative activation energy for the SO₃ + (H₂O)₂ step. The first order expression for SO₃ loss derived by these authors is $2.26 \times 10^{-43} T \exp(6544/T) [\text{H}_2\text{O}]^2$ and is recommended here.
153. SO₃ + NO₂. This recommendation is based on the study of Penzhorn and Canosa [940] 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.
154. SH + O₂. This upper limit for k(298 K) is based on the study by Stachnik and Molina [1102] utilizing experiments sensitive to the production of OH. Somewhat higher upper limits of 1.0×10^{-17} and 1.5×10^{-17} were assigned by Friedl et al. [410] and Wang et al. [1272] respectively from the detection sensitivities for OH detection and SH decay respectively. An even higher upper limit by Black [130], based on the lack of SH decay, may have been complicated by SH regeneration. Much less sensitive upper limits have been calculated by Tiee et al. [1174], Nielsen [874], and Cupitt and Glass [296]. Stachnik and Molina [1102] 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).
155. SH + O₃. The value for k(298 K) is an average of the determinations by Friedl et al. [410] (laser-induced fluorescence detection of SH), Schonle et al. [1041] (mass spectrometric detection of reactant SH and product

HSO) as revised by Schindler and Benter [1034], and Wang and Howard [1271] (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 $k(298\text{ K})$. $\Delta E/R$ 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 $\text{H} + \text{SO} + \text{O}_2$.

156. $\text{SH} + \text{H}_2\text{O}_2$. This recommended upper limit for $k(298\text{ K})$ is based on the study of Friedl et al. [410]. 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 yield: $\text{H}_2\text{S} + \text{HO}_2$, $\text{HSOH} + \text{OH}$, and $\text{HSO} + \text{H}_2\text{O}$.
157. $\text{SH} + \text{NO}_2$. This recommendation is based on the measurements of Wang et al. [1272]. These authors suggest that the lower values of $k(298\text{ K})$ reported by Black [130], Friedl et al. [410], and Bulatov et al. [168] are due to SH regeneration from the H_2S source compound. In the study by Stachnik and Molina [1102], attempts were made at minimizing such regeneration, and the reported value of $k(298\text{ K})$ 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. [1041], as revised by Schindler and Benter [1034], 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 [723], Bulatov et al. [168], Schonle et al. [1041], and Wang et al. [1272]. The absence of a primary deuterium isotope effect, as observed by Wang et al. [1272], coupled with the large magnitude of the rate constant suggests that the (four-center intermediate) channels producing $\text{SO} + \text{HNO}$ and $\text{OH} + \text{SNO}$ are of minor importance. No evidence for a three-body combination reaction was found by either Black [130] or Friedl et al. [410]. Based on a pressure independence of the rate constant between 30–300 torr, Black set an upper limit of 7.0×10^{-31} for the termolecular rate constant. Similarly, Stachnik and Molina [1102] saw no change in decay rate between 100 and 730 torr with O_2 (although these O_2 experiments were designed primarily to limit SH regeneration). The recommendation given here is supported by the recent discharge flow laser-induced fluorescence study of the $\text{SD} + \text{NO}_2$ reaction by Fenter and Anderson [388]. These investigators report a rate constant at 298 K of $6.8 \times 10^{-11} \text{ cm}^3 \text{ molec}^{-1} \text{ s}^{-1}$, which compares favorably with the value of $7.1 \times 10^{-11} \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ determined in the Wang et al. 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.
158. $\text{SH} + \text{Cl}_2$; $\text{SH} + \text{BrCl}$; $\text{SH} + \text{Br}_2$; $\text{SH} + \text{F}_2$. The recommendations for these reactions are derived from the data of Fenter and Anderson [387] 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 $\text{ClSD} + \text{Br}$ was found to be described by the rate expression $k = 2.3 \times 10^{-11} \exp(100/T)$.
159. $\text{HSO} + \text{O}_2$. This recommendation is based on the study by Lovejoy et al. [759], who employed laser magnetic resonance monitoring of HSO in a discharge flow system. The upper limit thus derived for $k(298\text{ K})$ is nearly two orders of magnitude lower than measured by Bulatov et al. [170].
160. $\text{HSO} + \text{O}_3$. This recommendation is based on the determinations by Friedl et al. [410] and Wang and Howard [1271]. In the first study, performed at higher O_3 concentrations, greater quantities of HSO were produced in the flow tube and SH approached a steady state due to its generation via $\text{HSO} + \text{O}_3$. The rate constant for this reaction was thus determined relative to $\text{SH} + \text{O}_3$ 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. [705] determined a room temperature rate constant of 4.7×10^{-14} 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 273–423 K, in agreement with the more limited temperature 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 $\text{HSO} + \text{O}_3$ reaction are $\text{SH} + 2\text{O}_2$ (analogous to those for $\text{HO}_2 + \text{O}_3$). However, Wang and Howard found that only 70% of the reaction leads to HS formation. In addition, their observations of HO_2 production in the presence of O_2 suggests the existence of a reaction channel producing $\text{HSO}_2 + \text{O}_2$ followed by $\text{HSO}_2 + \text{O}_2 \rightarrow \text{HO}_2 + \text{SO}_2$. 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.

- I61. $\text{HSO} + \text{NO}$; $\text{HSO} + \text{NO}_2$. The recommendations for these reactions are based on the study by Lovejoy et al. [759] 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. [169] 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 NO_2 reaction is a factor of 2 higher than the rate constant reported by Bulatov et al. [168]. Lovejoy et al. have attributed this difference to HSO regeneration under the experimental conditions used by Bulatov et al. [168]. The product assignment for this reaction is discussed in the note for the $\text{HSO}_2 + \text{O}_2$ reaction.
- I62. $\text{HSO}_2 + \text{O}_2$. This recommendation is based on the rate of HO_2 formation measured by Lovejoy et al. [759] upon addition of O_2 to the $\text{HSO} + \text{NO}_2$ reaction system. While HSO_2 was not observed directly, a consideration of the mechanistic possibilities for $\text{HSO} + \text{NO}_2$, coupled with measurements of the HO_2 production rate at various O_2 pressures, led these authors to suggest that HSO_2 is both a major product of the $\text{HSO} + \text{NO}_2$ reaction and a precursor for HO_2 via reaction with O_2 .
- I63. $\text{HOSO}_2 + \text{O}_2$. This recommendation is based on the studies of Gleason et al. [444] and Gleason and Howard [442] 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, $\Delta E/R$ 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 [774] and Martin et al. [786], 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. [486] and Nagase et al. [845]. Mass spectrometric detection of HOSO_2 in the gas phase has also been reported by Egsgaard et al. [374].
- I64. $\text{CS} + \text{O}_2$. The recommendation given for $k(298 \text{ K})$ is based on the work of Black et al. [132] using laser-induced fluorescence to monitor CS. This value agrees with the somewhat less precise determination by Richardson [1003] 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 1.5×10^{-10} . In view of this, no recommendation is given for the temperature dependence.
- I65. $\text{CS} + \text{O}_3$; $\text{CS} + \text{NO}_2$. The $k(298 \text{ K})$ recommendations for both reactions accept the results of Black et al. [132], 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.
- I66. $\text{CH}_3\text{S} + \text{O}_2$. This upper limit is based on the study by Tyndall and Ravishankara [1217]. Somewhat higher upper limits were derived in the earlier studies of Balla et al. [60] and Black and Jusinski [131].
- I67. $\text{CH}_3\text{S} + \text{O}_3$. This recommendation is based on the temperature-dependent study of Turnipseed et al. [1201] and the room temperature determinations of Tyndall and Ravishankara [1218] and Domine et al. [362]. Domine et al. measured the yield of CH_3SO to be 15% at low pressure and used this value to revise the corrections applied in the Tyndall and Ravishankara investigation to account for CH_3S regeneration by $\text{CH}_3\text{SO} + \text{O}_3$. A failure to observe significant reaction in the study by Black and Jusinski [131] is interpreted as due to rapid regeneration of CH_3S in their system. The value of g has been set larger than that derived by Turnipseed et al. to reflect the existence of only one temperature dependence investigation.
- I68. $\text{CH}_3\text{S} + \text{NO}$. The upper limit for the bimolecular reaction between CH_3S and NO is based on estimates by Balla et al. [60], who conducted a temperature dependence study of the termolecular reaction.
- I69. $\text{CH}_3\text{S} + \text{NO}_2$. This recommendation is based on the temperature dependent data of Turnipseed et al. [1201] and the room temperature results of Tyndall and Ravishankara [1217]. The room temperature value of Domine et al. [360] is encompassed by the recommended uncertainty factor. The value of $\Delta E/R$ has been set larger than that derived by Turnipseed et al. to reflect the existence of only one temperature dependence investigation. An earlier study by Balla et al. [60] yielded a room temperature rate constant nearly a factor of two higher than the present recommendation, which may be attributed to secondary reactions at higher radical concentrations. Tyndall and Ravishankara determined the NO yield to be $(80 \pm 20)\%$. Together with

the unity yield of CH₃SO obtained by Domine et al., this implies that the primary reaction channel is as written.

170. CH₂SH + O₂. This recommendation is the average of the rate constant obtained by Rahman et al. [976] in a fast flow mass spectrometer system and that from Anastasi et al. [20] 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 $k(298\text{ K})$ has been chosen to reflect this uncertainty. Since this is a fast bimolecular reaction, one would expect the products to be HO₂ + CH₂S, by analogy with the reaction between CH₂OH and O₂.
171. CH₂SH + O₃. The value of $k(298\text{ K})$ comes from the study by Rahman et al. [976] using fast flow mass spectrometry. The uncertainty factor reflects the absence of any confirming investigations.
172. CH₂SH + NO. The value of $k(298\text{ K})$ comes from the study by Anastasi et al. [20] using a pulse radiolysis kinetic absorption apparatus. The uncertainty factor reflects the absence of any confirming investigations.
173. CH₂SH + NO₂. This recommendation averages the rate constant obtained by Rahman et al. [976] in a fast flow mass spectrometer system with that from Anastasi et al. [20], 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 $k(298\text{ K})$ has been chosen to reflect this uncertainty.
174. CH₃SO + O₃. This recommendation is based on the study by Domine et al. [362]. It is supported by the study of Tyndall and Ravishankara [1218], in which the rate constant was derived from a complex analysis of the CH₃S + O₃ reaction system. Domine et al. place the direct yield of CH₂SO at approximately 10% and that of CH₃S at 13% at low pressure.
175. CH₃SO + NO₂. This recommendation is based on the direct measurements of Domine et al. [360]. The results are supported by somewhat less direct measurements of Tyndall and Ravishankara [1217] and Mellouki et al. [803].
176. CH₃SOO + O₃, CH₃SOO + NO, CH₃SOO + NO₂. These recommendations are based on the experiments of Turnipseed et al. [1201] in which CH₃S was monitored by LIF in equilibrium with CH₃SOO. The upper limit for the O₃ reaction was determined from experiments at 227 K. The results for the NO and NO₂ 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.
177. CH₃SO₂ + NO₂. This recommendation is based on the study by Ray et al. [994] using a discharge flow reactor equipped with laser-induced fluorescence and mass spectrometric detection. The CH₃SO₂ was produced by the sequential oxidation of CH₃S and CH₃SO by NO₂ and is to be differentiated from the weakly bound adduct, CH₃SOO, formed by the reaction of CH₃S with O₂ at low temperature (Turnipseed et al. [1201]). 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 CH₃S + NO₂ reaction by Tyndall and Ravishankara [1217]. These authors observed fluorescence from a product species tentatively identified as CH₃SO₂, produced by the reaction of CH₃SO with NO₂. Computer simulation of the rise and fall of the fluorescence signal yielded an approximate rate constant value for the reaction CH₃SO₂ + NO₂ 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.
178. CH₃SCH₂ + NO₃. This recommendation is based on the experiments of Butkovskaya and Le Bras [182]. The uncertainty factor reflects the absence of any confirming investigation.
179. CH₃SCH₂O₂ + NO. This recommendation is based on the experiments of Wallington et al. [1257]. The uncertainty factor reflects the absence of any confirming investigation.
180. CH₃SS + O₃. This recommendation is based on the discharge flow photoionization mass spectroscopy study by Domine et al. [362]. The uncertainty factor reflects the absence of any confirming investigations. The rate constant ratio for the reactions of CH₃SS with O₃ and NO₂ is consistent with the rate constant ratio for the corresponding CH₃S reactions.
181. CH₃SS + NO₂; CH₃SSO + NO₂. These recommendations are based on the discharge flow photoionization mass spectroscopy study by Domine et al. [360]. The rate constant ratio for these two reactions agrees with that observed for other RS/RSO radicals with NO₂. The assigned uncertainties reflect this agreement but acknowledge the absence of any confirming investigation. In the Domine et al. study, CH₃SSO was produced by reacting away all CH₃SS with high NO₂ concentrations. Thus, as expected, O atom transfer may be the primary channel in the CH₃SS reaction.

- J1. Na + O₃. The recommendation is based on the measurements of Ager et al. [13], Worsnop et al. [1333] as corrected in Worsnop et al. [1334], and Plane et al. [953]. The data of Worsnop et al. supersede earlier work from that laboratory (Silver and Kolb [1063]). Measurements made by Husain et al. [546] at 500 K are somewhat lower, probably because they did not recognize that secondary chemistry, NaO + O₃ → Na + 2O₂, interferes with the rate coefficient measurement. The temperature dependence is from results of Worsnop et al. [1334] (214–294 K) and Plane et al. [953] (208–377K). Ager et al. [13] estimate that the NaO₂ + O product channel is ≤ 5%. Evidence that the NaO product is in the ²Σ⁺ excited electronic state was reported by Shi et al. [1058] and Wright et al. [1335].
- J2. Na + N₂O. The recommendation incorporates the data of Husain and Marshall [545], Ager et al. [13], Plane and Rajasekhar [954], and Worsnop et al. [1334]. Silver and Kolb [1063] measured a rate coefficient at 295 K that is lower and is superseded by Worsnop et al. [1334]. Helmer and Plane [497] report a measurement at 300 K in excellent agreement with the recommendation. Earlier, less direct studies are discussed by Ager et al. [13]. The NaO product does not react significantly with N₂O at room temperature [k (for Na + N₂ + O₂ products) ≤ 10⁻¹⁶ and k (for NaO₂ + N₂ products) ≤ 2 × 10⁻¹⁵ (Ager et al.)]. Wright et al. [1335] used UV photoelectron spectroscopy to determine the product NaO is formed predominantly in the excited ²Σ⁺ state.
- J3. Na + Cl₂. Two measurements of the rate coefficient for this reaction are in excellent agreement: Silver [1060] and Talcott et al. [1147]. The recommended value is the average of these room temperature results.
- J4. NaO + O. The recommendation is based on a measurement at 573 K by Plane and Husain [952]. They reported that ≤ 1% of the Na product is in the 3²P excited state.
- J5. NaO + O₃. This reaction was studied by Silver and Kolb [1063], Ager et al. [13], and Plane et al. [953], 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.
- J6. NaO + H₂. The recommendation is based on a measurement by Ager and Howard [12]. They also reported a significant Na + H₂O product channel and that a small fraction of the Na from this channel is in the 3²P excited state.
- J7. NaO + H₂O. The recommendation is based on a measurement by Ager and Howard [12].
- J8. NaO + NO. The recommendation is based on an indirect measurement reported by Ager et al. [13].
- J9. NaO + HCl. There is only one indirect measurement of the rate coefficient for this reaction, that from the study by Silver et al. [1066]. They indicate that the products are NaCl and OH, although some NaOH and Cl production is not ruled out.
- J10. NaO₂ + O. The recommendation is based on a flow tube study at 300 K by Helmer and Plane [497].
- J11. NaO₂ + NO. This reaction is endothermic. The upper limit recommended is from an experimental study by Ager et al. [13].
- J12. NaO₂ + HCl. The recommendation is based on a measurement reported by Silver and Kolb [1064]. They indicated that the products are NaCl + HO₂, but NaOOH + Cl may be possible products.
- J13. NaOH + HCl. The recommendation is based on the study by Silver et al. [1066], which is the only published study of this reaction.

1.4 References

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