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Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies

Evaluation Number 18

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1.1 Introduction

In Table 1 (Rate Constants for Bimolecular Reactions) the evaluated reactions are grouped into the classes O_x, $O(^1D)$, Singlet O_2, HO_x, NO_x, Organic Compounds, FO_x, ClO_x, BrO_x, IO_x, SO_x, and Metals. Some of the reactions in Table 1 are actually more complex than simple two-body, bimolecular, reactions. To explain the pressure and temperature dependences occasionally measured 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 $[AB]^\#$ lies between reactants and products.

$$A + B \rightarrow [AB]^\# \rightarrow C + D$$

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

The rate constants for these reactions can, in general, be reasonably well represented by the Arrhenius expression

$$k(T) = A\times\exp(-E/RT)$$

over the temperature range of atmospheric interest. Very useful correlations between the expected structure of the transition state $[AB]^\#$ and the Arrhenius 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 recommended parameters, A and E/R, are given in Table 1 as discussed below and the temperature range associated with their recommended use is given in the corresponding reaction note (e.g. “below 400 K”). Rate constants for reactions of this type are not pressure dependent.

However, even for this class of reactions, deviation in the temperature dependence from the simple Arrhenius expression mentioned above may be apparent over the full range of the experimental data considered in the evaluation, and even over the more limited temperature range used to derive the Arrhenius expression recommendation. Deviation from Arrhenius behavior is typically exhibited as curvature in the Arrhenius plot - a concave upward curvature in ln(k(T)) versus 1/T. There are several possible factors that may contribute to this curvature such as multiple reaction channels, the existence of reactant conformers, tunneling, and others. In cases where curvature was experimentally resolved, the reaction note emphasizes the temperature range over which the Arrhenius parameters given in Table 1 are applicable and also provides a recommended three-parameter expression

$$k(T) = A\times(T/298)^n\times\exp(-E/RT)$$

where n is a fit parameter, that better represents the overall temperature dependence.

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:

$$A + B \leftrightarrow [AB]^* \rightarrow C + D$$

The intermediate $[AB]^*$ is different from the transition state $[AB]^\#$, in that its lifetime substantially exceeds the characteristic time of intermolecular vibrations and, thus, it is considered a bound molecule. Of course, transition states are involved in all reactions, both forward and backward, but are not explicitly shown in the equation above. An example of a reaction of this class is ClO + NO, which normally produces Cl + NO_2. Reactions of the nonconcerted type can have more complex temperature dependences and can exhibit a pressure dependence if the lifetime of $[AB]^*$ is comparable to the rate of its collisional deactivation. This arises because the relative rate at which a complex $[AB]^*$ decomposes to products C + D or back to reactants A + B is a sensitive function of its internal 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 calculations, or, alternatively, to develop reliable theoretical bases for extrapolation of the experimental data. In several cases where sufficient data exist, reactions of this type are treated in Section 2 and included in the corresponding table for termolecular reactions.

As mentioned above, the recommended rate constant tabulation for bimolecular reactions (Table 1) is given in Arrhenius form, $k(T) = A\times\exp(-E/RT)$, and contains the following information:

1. Reaction stoichiometry and products (if known).

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

For a few reactions, the recommendations for A, E/R and k(298 K) are italicized in blue font. These represent estimates by the Panel in cases where there are either no literature data, where the existing data are judged to be of insufficient quality to base a recommendation, or where the recommendation is based on an extrapolation of very limited experimental data.

1.2 The Evaluation Procedure

The process of evaluating chemical kinetic data does not conform to a simple set of mathematical rules. There is no “one size fits all” algorithm that can be applied and each reaction must be examined on a case-by-case basis. Consideration of uncertainties in the kinetic and photochemical parameters used in atmospheric models plays a key role in determining the reliability of and uncertainty in the model results. Quite often the cause(s) of differences in experimental results from various laboratories can’t be determined with confidence and making recommendations for the uncertainties of the rate constant is often more difficult than for making recommendations of the Arrhenius parameters themselves. In many cases, investigators suggest possible qualitative reasons for disagreements among datasets. Thus, data evaluators necessarily must consider a variety of factors in assigning a recommendation, including such aspects as the chemical complexity of the system, sensitivities and shortcomings of the experimental techniques employed, similarities or trends in reactivity, and the level of agreement among studies using different techniques.

A recommendation for k(298 K) is typically made by averaging the rate constants from those studies deemed to be of sufficiently high quality / reliability and free from chemical interferences that could have biased the results. In cases where a study provides reliable data over a range of temperatures of atmospheric interest, the value of k(298 K) used in the averaging process is typically obtained from a weighted non-linear least-squares fit to the data from that study, k(T) versus T, assuming equal relative uncertainties in the rate constants reported at the different temperatures. In deriving a recommended Arrhenius temperature dependence (E/R), the selected data sets are examined to ascertain the temperature range over which a standard Arrhenius fit to the data provides an adequate representation. Each data set is then scaled by a constant factor so that the Arrhenius expressions describing the individual data sets give the recommended k(298 K) and a weighted non-linear least-squares fit to all of these scaled data is then made. This typical process is helpful in avoiding biases resulting from systematic errors associated with an individual data set or from the fact that the individual data sets may have been obtained over significantly different temperature ranges. In cases where the selected data sets have been obtained over similar ranges of temperature, a fit to the combined scaled data often yields a value for E/R not very different from that obtained by averaging the E/R values from the individual studies. The recommended Arrhenius pre-exponential factor “A” is then calculated based on the recommended values for k(298 K) and E/R.

1.3 Uncertainty Estimates

The parameters f(298 K) and g given in Table 1 can be used to calculate an estimated rate constant uncertainty at any given temperature, corresponding to approximately one standard deviation, from the following expression:

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

where the exponent is an absolute value.

Note that, since f(298 K) and g have been defined to correspond to approximately one standard deviation, f(T) yields a similar uncertainty interval. The more commonly used 95% confidence limits at a given temperature can be obtained by multiplying and dividing the recommended value of the rate constant at that temperature by the factor $f^2(\mathrm{T})$. It should be emphasized that the parameter g has been defined exclusively for use with f(298 K) in the above expression and should not be interpreted as the uncertainty in the Arrhenius activation temperature (E/R). Thus, g is dependent on the value selected for f(298 K). For example, reactions for which f(298 K) is rather large may require only a small value of g to represent an adequate total rate constant uncertainty at other temperatures.

The uncertainty factor f(298 K), corresponding to approximately one standard deviation in the case of normally distributed data, was assigned such that all of the data used in deriving the average are encompassed within the band derived by multiplying and dividing k(298 K) by f^2(298 K), i.e., two standard deviations, which is considered a 95% confidence interval for the evaluation. In some cases, a slightly higher value of f(298 K) may be recommended to encompass outlying data that were not used in the averaging but could not be entirely rejected. The uncertainty factor “g” was then selected for use in the f(T) expression described below such that f^2(T) encompasses all of the data used in the evaluation over the temperature range of the recommendation. Neither f(298 K) nor g is derived from a rigorous statistical treatment of the available data, which generally are too limited to permit such analyses and, more importantly, do not follow a normal statistical distribution. Rather, the uncertainty estimation is based on knowledge of the techniques, the difficulties of the experiments, and the potential for systematic errors.

This approach is based on the fact that rate constants are typically known with greater certainty at room temperature where the experimental data are more abundant and often more reliable. The overall uncertainty normally increases at other temperatures where there are fewer data. In addition, data obtained at temperatures far distant from 298 K may be less accurate than at room temperature due to various experimental difficulties or complications.

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

Finally, there is obviously no way to quantify “unknown” errors. The spread in results among different techniques for a given reaction may provide some basis for an uncertainty estimate, but the possibility of the same, or compensating, systematic errors in all the studies can’t be disregarded. Comparisons among rate constants recommended for similar reactions or for reactions within a homologous series of compounds can also help in the assignment of uncertainty factors. For measurements subject to large systematic errors, the true rate constant may be much further from the recommended value than would be expected and allowed for with any reasonable values of f(T) based on the data available for the evaluation. For example, there have been cases in the past where the recommended rate constants have changed by factors well outside of the uncertainties that had been assigned in the absence of quantitative knowledge of systematic errors. However, as experimental techniques improve together with improved understanding of various reactive processes and with significant expansion of the kinetic and thermodynamic database for the recommendations, exceptionally large changes are becoming less likely.

1.8 NO_x Reactions

1.8.1 Table 1C: NO_x Reactions

Reaction	Temperature Range of Exp. Data (K) [a]	A-Factor	E/R	k(298 K)[b]	f(298 K)[c]	g	Note
$O + NO \xrightarrow{M} NO_2$		(See Table 2-1)					
$O + NO_2 \rightarrow NO + O_2$	199–2300	5.1×10^{-12}	-210	1.04×10^{-11}	1.1	20	C 1
$O + NO_2 \xrightarrow{M} NO_3$		(See Table 2-1)					
$O + NO_3 \rightarrow O_2 + NO_2$	298–329	1.0×10^{-11}	0	1.0×10^{-11}	1.5	150	C 2
$O + N_2O_5 \rightarrow$ products	223–300			$<3.0\times10^{-16}$			C 3
$O + HNO_3 \rightarrow OH + NO_3$	298			$<3.0\times10^{-17}$			C 4
$O + HO_2NO_2 \rightarrow$ products	228–297	7.8×10^{-11}	3400	8.6×10^{-16}	3.0	750	C 5
$H + NO_2 \rightarrow OH + NO$	195–2000	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)					
$OH + NO_3 \rightarrow$ products	298			2.2×10^{-11}	1.5		C 7
$OH + HONO \rightarrow H_2O + NO_2$	278–1400	1.8×10^{-11}	390	4.5×10^{-12}	1.5	+200 –500	C 8
$OH + HNO_3 \rightarrow H_2O + NO_3$	218–1100	(See Note)			1.2		C 9
$OH + HO_2NO_2 \rightarrow$ products	218–335	1.3×10^{-12}	–380	4.6×10^{-12}	1.3	+270 –500	C10
$OH + NH_3 \rightarrow H_2O + NH_2$	228–2360	1.7×10^{-12}	710	1.6×10^{-13}	1.2	200	C11
$HO_2 + NO \rightarrow NO_2 + OH$	183–1270	3.3×10^{-12}	–270	8.0×10^{-12}	1.15	20	C12
$NO_2^* + H_2O \rightarrow OH + HONO$		(See Note)					C13
$HO_2 + NO_2 \xrightarrow{M} HO_2NO_2$		(See Table 2-1)					
$HO_2 + NO_2 \rightarrow HONO + O_2$	220–358	(See Note)					C14
$HO_2 + NO_3 \rightarrow$ products	263–338			3.5×10^{-12}	1.5		C15
$HO_2 + NH_2 \rightarrow$ products	298			3.4×10^{-11}	2.0		C16
$N + O_2 \rightarrow NO + O$	280–1220	1.5×10^{-11}	3600	8.5×10^{-17}	1.25	400	C17
$N + O_3 \rightarrow NO + O_2$	298			$<2.0\times10^{-16}$			C18

Reaction	Temperature Range of Exp. Data (K) [a]	A-Factor	E/R	k(298 K)[b]	f(298 K)[c]	g	Note
$N + NO \rightarrow N_2 + O$	196–3660	2.1×10^{-11}	–100	3.0×10^{-11}	1.3	100	C19
$N + NO_2 \rightarrow N_2O + O$	223–700	5.8×10^{-12}	–220	1.2×10^{-11}	1.5	100	C20
$NO + O_3 \rightarrow NO_2 + O_2$	195–443	3.0×10^{-12}	1500	1.9×10^{-14}	1.1	200	C21
$NO + NO_3 \rightarrow 2NO_2$	209–703	1.5×10^{-11}	–170	2.6×10^{-11}	1.3	100	C22
$NO_2 + O_3 \rightarrow NO_3 + O_2$	259–362	1.2×10^{-13}	2450	3.2×10^{-17}	1.15	150	C23
$NO_2 + NO_3 \rightarrow NO + NO_2 + O_2$	236–538	(See Note)					C24
$NO_2 + NO_3 \xrightarrow{M} N_2O_5$		(See Table 2-1)					
$NO_3 + NO_3 \rightarrow 2NO_2 + O_2$	298–1100	8.5×10^{-13}	2450	2.3×10^{-16}	1.5	500	C25
$NH_2 + O_2 \rightarrow$ products	295–2300			$<6.0\times10^{-21}$			C26
$NH_2 + O_3 \rightarrow$ products	248–380	4.3×10^{-12}	930	1.9×10^{-13}	3.0	500	C27
$NH_2 + NO \rightarrow$ products	200–2500	4.0×10^{-12}	–450	1.8×10^{-11}	1.3	150	C28
$NH_2 + NO_2 \rightarrow$ products	250–910	2.1×10^{-12}	–650	1.9×10^{-11}	3.0	250	C29
$NH + NO \rightarrow$ products	269–3350	4.9×10^{-11}	0	4.9×10^{-11}	1.5	300	C30
$NH + NO_2 \rightarrow$ products	300	3.5×10^{-13}	–1140	1.6×10^{-11}	2.0	500	C31
$O_3 + HNO_2 \rightarrow O_2 + HNO_3$	226–300			$<5.0\times10^{-19}$			C32
$N_2O_5 + H_2O \rightarrow 2HNO_3$	290–298			$<2.0\times10^{-21}$			C33
$N_2(A,v) + O_2 \rightarrow$ products	80–560			2.5×10^{-12}, v=0	1.5		C34
$N_2(A,v) + O_3 \rightarrow$ products	298			4.1×10^{-11}, v=0	2.0		C35

Shaded areas indicate changes or additions since JPL10-6.

[a] Temperature range of available experimental data. This is not necessarily the range of temperature over which the recommended Arrhenius parameters are applicable. See the corresponding note for each reaction for such information.

[b] Units are cm^3 $molecule^{-1}$ s^{-1}.

[c] f(298 K) is the uncertainty factor at 298 K. To calculate the uncertainty at other temperatures, use the expression:

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

Note that the exponent is an absolute value.

1.12 BrO_x Reactions

1.12.1 Table 1G: BrO_x Reactions

Reaction	Temperature Range of Exp. Data (K) [a]	A-Factor	E/R	k(298 K)[b]	f(298 K)[c]	g	Note
$O + BrO \rightarrow Br + O_2$	231–328	1.9×10^{-11}	–230	4.1×10^{-11}	1.5	150	G 1
$O + HBr \rightarrow OH + Br$	221–554	5.8×10^{-12}	1500	3.8×10^{-14}	1.3	200	G 2
$O + HOBr \rightarrow OH + BrO$	233–423	1.2×10^{-10}	430	2.8×10^{-11}	3.0	300	G 3
$O + BrONO_2 \rightarrow NO_3 + BrO$	227–339	1.9×10^{-11}	–215	3.9×10^{-11}	1.25	40	G 4
$OH + Br_2 \rightarrow HOBr + Br$	230–360	2.1×10^{-11}	–240	4.6×10^{-11}	1.1	50	G 5
$OH + BrO \rightarrow$ products	230–355	1.7×10^{-11}	–250	3.9×10^{-11}	1.4	100	G 6
$OH + HBr \rightarrow H_2O + Br$	230–360	5.5×10^{-12}	–200	1.1×10^{-11}	1.1	100	G 7
$OH + CH_3Br \rightarrow CH_2Br + H_2O$	233–400	1.42×10^{-12}	1150	3.0×10^{-14}	1.07	100	G 8
$OH + CH_2Br_2 \rightarrow CHBr_2 + H_2O$	244–375	2.0×10^{-12}	840	1.2×10^{-13}	1.1	100	G 9
$OH + CHBr_3 \rightarrow CBr_3 + H_2O$	230–370	9.0×10^{-13}	360	2.7×10^{-13}	1.05	20	G10
$OH + CH_2ClBr \rightarrow CHClBr + H_2O$	230–376	2.1×10^{-12}	880	1.1×10^{-13}	1.07	100	G11
$OH + CHClBr_2 \rightarrow CClBr_2 + H_2O$	230–330	9.0×10^{-13}	420	2.2×10^{-13}	1.07	20	G12
$OH + CHCl_2Br \rightarrow CCl_2Br + H_2O$	230–330	9.4×10^{-13}	510	1.7×10^{-13}	1.07	20	G13
$OH + CHF_2Br \rightarrow CF_2Br + H_2O$ (Halon-1201)	233–460	7.85×10^{-13}	1300	1.0×10^{-14}	1.07	100	G14
$OH + CF_2Br_2 \rightarrow$ products (Halon-1202)	298	1×10^{-12}	>2200	$<5\times10^{-16}$			G15
$OH + CF_3Br \rightarrow$ products (Halon-1301)	460	1×10^{-12}	>3600	$<6\times10^{-18}$			G16
$OH + CF_2ClBr \rightarrow$ products (Halon-1211)	373	1×10^{-12}	>3500	$<8\times10^{-18}$			G17
$OH + CH_3CH_2Br \rightarrow$ products	233–422	2.9×10^{-12}	640	3.4×10^{-13}	1.2	150	G18
$OH + CH_2BrCH_2Br \rightarrow$ products	292–366	1.75×10^{-11}	1290	2.3×10^{-13}	1.15	200	G19
$OH + CH_2BrCF_3 \rightarrow CHBrCF_3 + H_2O$ (Halon-2301)	280–460	9.5×10^{-13}	1200	1.7×10^{-14}	1.2	150	G20
$OH + CHFBrCF_3 \rightarrow CFBrCF_3 + H_2O$ (Halon-2401)	279–460	7.3×10^{-13}	1120	1.7×10^{-14}	1.2	100	G21
$OH + CHClBrCF_3 \rightarrow CClBrCF_3 + H_2O$ (Halothane, Halon-2311)	298–460	1.1×10^{-12}	940	4.7×10^{-14}	1.2	150	G22
$OH + CHFClCF_2Br \rightarrow CFClCF_2Br + H_2O$	315–372	8.4×10^{-13}	1220	1.4×10^{-14}	1.3	200	G23
$OH + CF_2BrCF_2Br \rightarrow$ products (Halon-2402)	460	1×10^{-12}	>3600	$<6\times10^{-18}$			G24

Reaction	Temperature Range of Exp. Data (K) [a]	*A*-Factor	*E*/R	*k*(298 K)[b]	*f*(298 K)[c]	*g*	Note
$OH + CH_2BrCH_2CH_3 \rightarrow$ products	210–480	3.0×10^{-12}	330	1.0×10^{-12}	1.05	50	G25
$OH + CH_3CHBrCH_3 \rightarrow$ products	210–480	1.85×10^{-12}	270	7.5×10^{-13}	1.05	50	G26
$OH + CHBr{=}CF_2 \rightarrow$ products	250–370	1.3×10^{-12}	–370	4.5×10^{-12}	1.1	20	G27
$OH + CFBr{=}CF_2 \rightarrow$ products	250–370	2.0×10^{-12}	–400	7.6×10^{-12}	1.1	20	G28
$OH + CH_2{=}CBrCF_3 \rightarrow$ products	220–370	1.06×10^{-12}	–380	3.8×10^{-12}	1.05	20	G29
$OH + CH_2{=}CBrCF_2CF_3 \rightarrow$ products	250–370	9.5×10^{-12}	–370	3.3×10^{-12}	1.05	20	G30
$OH + CH_2{=}CHCF_2CF_2Br \rightarrow$ products	250–370	8.7×10^{-12}	–200	1.7×10^{-12}	1.1	20	G31
$HO_2 + Br \rightarrow HBr + O_2$	230–355	4.8×10^{-12}	310	1.7×10^{-12}	1.3	150	G32
$HO_2 + BrO \rightarrow$ products	210–360	4.5×10^{-12}	–460	2.1×10^{-11}	1.15	100	G33
$NO_3 + HBr \rightarrow HNO_3 + Br$	298			$<1.0\times10^{-16}$			G34
$Cl + CH_3Br \rightarrow HCl + CH_2Br$	210–700	1.46×10^{-11}	1040	4.45×10^{-13}	1.03	50	G35
$Cl + CH_2Br_2 \rightarrow HCl + CHBr_2$	222–395	6.3×10^{-12}	800	4.3×10^{-13}	1.1	50	G36
$Cl + CHBr_3 \rightarrow CBr_3 + HCl$	273–363	4.85×10^{-12}	850	2.8×10^{-13}	1.3	200	G37
$Cl + CH_2ClBr \rightarrow HCl + CHClBr$	298	*6.8×10^{-12}*	*870*	3.7×10^{-13}	1.2	100	G38
$Br + O_3 \rightarrow BrO + O_2$	195–422	1.6×10^{-11}	780	1.2×10^{-12}	1.15	100	G39
$Br + H_2O_2 \rightarrow HBr + HO_2$	298–378	*1×10^{-11}*	*>3000*	$<5\times10^{-16}$			G40
$Br + NO_2 \xrightarrow{M} BrNO_2$		(See Table 2-1)					
$Br + NO_3 \rightarrow BrO + NO_2$	298			1.6×10^{-11}	2.0		G41
$Br + H_2CO \rightarrow HBr + HCO$	223–480	1.7×10^{-11}	800	1.1×10^{-12}	1.2	125	G42
$Br + CH_2{=}C(CH_3)CHO \rightarrow$ products	301			2.3×10^{-11} (1 atm air)	1.5		G43
$Br + CH_3C(O)CH{=}CH_2 \rightarrow$ products	301			1.9×10^{-11} (1 atm air)	1.5		G44
$Br + CH_2{=}C(CH_3)CH{=}CH_2 \overset{M}{\leftrightarrow} X \xrightarrow{O_2}$ products	210–298	(See Note)					G45
$Br + CH_2{=}C(CH_3)CH{=}CH_2 \rightarrow CH_2{=}C(\cdot CH_2)CH{=}CH_2 + HBr$	526–673	1.2×10^{-11}	2100	1.0×10^{-14}	2.0	200	G46
$Br{-}CH_2{=}C(CH_3)CH{=}CH_2 + O_2 \rightarrow$ products	297			3.2×10^{-13}	1.5		G47
$Br + OClO \rightarrow BrO + ClO$	267–423	2.6×10^{-11}	1300	3.4×10^{-13}	2.0	300	G48

Reaction	Temperature Range of Exp. Data (K) [a]	*A*-Factor	*E*/R	*k*(298 K)[b]	*f*(298 K)[c]	*g*	Note
$Br + Cl_2O \rightarrow BrCl + ClO$	220–402	2.1×10^{-11}	470	4.3×10^{-12}	1.3	150	G49
$Br + Cl_2O_2 \rightarrow$ products	223–298	5.9×10^{-12}	170	3.3×10^{-12}	1.3	200	G50
$BrO + O_3 \rightarrow$ products	298	*1×10^{-12}*	*>3200*	$<2\times10^{-17}$			G51
$BrO + NO \rightarrow NO_2 + Br$	224–425	8.8×10^{-12}	–260	2.1×10^{-11}	1.15	130	G52
$BrO + NO_2 \xrightarrow{M} BrONO_2$		(See Table 2-1)					
$BrO + NO_3 \rightarrow$ products	298			1.0×10^{-12}	3.0		G53
$BrO + ClO \rightarrow Br + OClO$	200–400	9.5×10^{-13}	–550	6.0×10^{-12}	1.2	100	G54
$\rightarrow Br + ClOO$		2.3×10^{-12}	–260	5.5×10^{-12}	1.2	100	
$\rightarrow BrCl + O_2$		4.1×10^{-13}	–290	1.1×10^{-12}	1.2	100	
$BrO + BrO \rightarrow$ products	220–348	1.5×10^{-12}	–230	3.2×10^{-12}	1.15	150	G55
$OBrO + O_3 \rightarrow$ products	298			$<1.5\times10^{-15}$			G56
$OBrO + NO \rightarrow$ products	240–350	2.4×10^{-13}	–610	1.8×10^{-12}	3	200	G57
$CH_2BrO_2 + NO \rightarrow CH_2O + NO_2 + Br$	298	*4×10^{-12}*	*–300*	1.1×10^{-11}	1.5	200	G58

Shaded areas indicate changes or additions since JPL10-6. Italicized blue text denote estimates.

[a] Temperature range of available experimental data. This is not necessarily the range of temperature over which the recommended Arrhenius parameters are applicable. See the corresponding note for each reaction for such information.

[b] Units are cm^3 $molecule^{-1}$ s^{-1}.

[c] *f*(298 K) is the uncertainty factor at 298 K. To calculate the uncertainty at other temperatures, use the expression:

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

Note that the exponent is an absolute value.

1.7 HO_x Reactions

1.7.1 Table 1B: HO_x Reactions

Reaction	Temperature Range of Exp. Data (K)[a]	*A*-Factor	*E*/R	*k*(298 K)[b]	*f*(298 K)[c]	*g*	Note
$O + OH \rightarrow O_2 + H$	136–515	1.8×10^{-11}	–180	3.3×10^{-11}	1.15	50	B1
$O + HO_2 \rightarrow OH + O_2$	229–391	3.0×10^{-11}	–200	5.9×10^{-11}	1.05	50	B2
$O + H_2O_2 \rightarrow OH + HO_2$	283–386	1.4×10^{-12}	2000	1.7×10^{-15}	1.2	100	B3
$H + O_2 \xrightarrow{M} HO_2$		(See Table 2-1)					
$H + O_3 \rightarrow OH + O_2$	196–424	1.4×10^{-10}	470	2.9×10^{-11}	1.1	40	B4
$H + HO_2 \rightarrow 2\ OH$	245–300	7.2×10^{-11}	0	7.2×10^{-11}	1.2	100	B5
$\rightarrow O + H_2O$		1.6×10^{-12}	0	1.6×10^{-12}	1.5	100	
$\rightarrow H_2 + O_2$		6.9×10^{-12}	0	6.9×10^{-12}	1.4	100	
$OH + O_3 \rightarrow HO_2 + O_2$	190–357	1.7×10^{-12}	940	7.3×10^{-14}	1.15	50	B6
$OH + H_2 \rightarrow H_2O + H$	200–1050	2.8×10^{-12}	1800	6.7×10^{-15}	1.05	100	B7
$OH + HD \rightarrow$ products	248–418	5.0×10^{-12}	2130	4.0×10^{-15}	1.15	50	B8
$OH + OH \rightarrow H_2O + O$	233–580	1.8×10^{-12}	0	1.8×10^{-12}	1.25	50	B9
$\xrightarrow{M} H_2O_2$		(See Table 2-1)					
$OH + HO_2 \rightarrow H_2O + O_2$	252–420	4.8×10^{-11}	–250	1.1×10^{-10}	1.15	50	B10
$OH + H_2O_2 \rightarrow H_2O + HO_2$		(See Note)					B11
$HO_2 + O_3 \rightarrow OH + 2O_2$	197–413	1.0×10^{-14}	490	1.9×10^{-15}	1.15	80	B12
$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	222–1120	3.0×10^{-13}	–460	1.4×10^{-12}	1.15	100	B13
$\xrightarrow{M} H_2O_2 + O_2$		2.1×10^{-33} [M]	–920	4.6×10^{-32} [M]	1.2	200	
$HO_2 + HO_2{\cdot}H_2O \rightarrow$ products	298–350	5.4×10^{-11}	410	1.4×10^{-11}	2	100	B14

Shaded areas indicate changes or additions since JPL10-6.

[a] Temperature range of available experimental data. This is not necessarily the range of temperature over which the recommended Arrhenius parameters are applicable. See the corresponding note for each reaction for such information.

[b] Units are cm^3 $molecule^{-1}$ s^{-1}.

[c] *f*(298 K) is the uncertainty factor at 298 K. To calculate the uncertainty at other temperatures, use the expression:

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

Note that the exponent is an absolute value.