NBS TECHNICAL NOTE 866

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry

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Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry

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FORWARD

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The present report consists of tables of data assembled for use in modelling the chemistry of the stratosphere. It represents contributions from the Chemical Kinetics Information Center, other NSRDS data centers, and a number of individual experts. Support for the preparation of those tables has been provided by the Department of Transportation, under the Climatic Impact Assessment Program, and by the Office of Standard Reference Data.

David R. Lide, Jr.
Chief, Office of Standard
Reference Data

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<u>Appendices</u>:

Chemical Kinetic and Photochemical Data for Modelling Atmospheric Chemistry[*]

R. F. Hampson, D. Garvin, Editors

A table of data for gas phase chemical reactions and photochemistry of neutral species is presented. Specifically, it gives preferred values for reaction rate constants, photoabsorption cross sections, and quantum yields of primary photochemical processes and also cites recent experimental work. It is intended to provide the basic physical chemical data needed as input data for calculations modelling atmospheric chemistry. An auxiliary table of thermochemical data for the pertinent chemical species is given in the appendix.

Key words: Atmospheric chemistry; chemical kinetics; data evaluation; gas phase; photoabsorption cross section; photochemistry; quantum yield; rate constant.

1. Introduction

1.1. Content and History

This technical note consists of a table of data on the kinetics of chemical reactions and the photochemistry of neutral species. This is supplemented by a table of thermochemical data for the species involved. It is designed for use in modelling the chemistry of the stratosphere.

The table is an extract from the chapter "Chemistry of the Stratosphere" by H. S. Johnston, P. J. Crutzen, R. J. Cvetanovic, M. L. Corrin, D. D. Davis, E. S. Domalski, E. E. Ferguson, D. Garvin, R. F. Hampson, R. D. Hudson, L. J. Kieffer, H. I. Schiff, R. L. Taylor, D. D. Wagman, and R. T. Watson in "The Natural Stratosphere of 1974", E. Reiter, editor, Climatic Impact Assessment Program Monograph 1, U. S. Department of Transportation. The present table will also appear in the

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[*] This work was supported by the Climatic Impact Assessment Program, Office of the Secretary, Department of Transportation and by the Office of Standard Reference Data, N.B.S.

final version of the monograph to be published in the Fall of 1975.

The table includes contributions of rate evaluations by other scientists. These contributors represented in the present edition are D. L. Baulch, D. D. Drysdale and D. G. Horne, University of Leeds; J. Heicklen, Pennsylvania State University; A. C. Lloyd, University of California, Riverside; T. G. Slanger, Stanford Research Institute; J. Troe and K. Glanzer, Ecole Polytechnique Federale de Lausanne; K. H. Welge, York University; W. H. Breckenridge, University of Utah, and E. S. Domalski and D. D. Wagman of the NBS Physical Chemistry Division.

Several preliminary versions of the main table in this Note have been distributed. The history is explained below. The date of preparation of each version is given in the upper left hand corner of each page. The present version, dated November 22, 1974 supersedes all earlier tables. Addenda and errata, which may be found as Appendix 2, update the main table to March 1975.

The first version of this table of data on the chemical reactions and photochemistry of neutral species was prepared by the Chemistry Panel on the Natural Stratosphere in December, 1972 at the Fort Lauderdale, Florida meeting and received limited distribution in the first preliminary draft of CIAP Monograph No. 1. A revised and expanded version was distributed in NBSIR 73-203 in May, 1973. Another revised and expanded version was distributed in NBSIR 74-430 in January. 1974.

The present table updates these. In particular, it incorporates pertinent new data presented at the Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton, Virginia, September 1974.

The two NBS reports referred to above also contained separate tables of rate data on vibrational energy transfer processes (R. Taylor), high temperature air reactions (R. Taylor). and ion-molecule reactions (E. E. Ferguson). The high temperature air reactions have been incorporated in the present table. The other two have been published independently as indicated below.

a. Vibrational energy transfer processes - R. T. Taylor. "Energy Transfer Processes in the Stratosphere." Can. J. Chem. 52, 1436 (1974).

b. Ion-molecule reactions - E. E. Ferguson. "Rate Constants of Thermal Energy Binary Ion-Molecule Reactions of Aeronomic Interest." in Atomic Data and Nuclear Data Tables 12, 159 (1973).

The present tables (and earlier versions) include recommended values for reactions of O(^{1}D) atoms. The evaluation of these data is explained in the CIAP Monograph 1 and has been published separately as R. J. Cvetanovic, "Excited State Chemistry in the Stratosphere," Can. J. Chem. 52, 1452 (1974).

1.2. Related Data Evalutions

This table relies heavily upon other modern data evaluation work. Some pertinent sources are summarized here.

Contributors to this data survey were mentioned in section 1.1. Their evaluations are given in more detail in NBS Report 73-206 (May 1973).

Evaluations by a team of chemists at NBS have been published in J. Phys. Chem. Ref. Data 2, 267 (1973). Earlier versions of these evaluations had been distributed as NBS Report 10692 (January 1972) and NBS Report 10828 (April 1972). Additional evaluations have been published in NBSIR 73-207 (August 1973).

Evaluations by a group at the University of Leeds under the direction of D. L. Baulch have been published in "Evaluated Kinetic Data for High Temperature Reactions, volume 1, Homogeneous gas phase reactions of the H_2-O_2 system" D. L. Baulch, D. D. Drysdale, D. G. Horne and A. C. Lloyd, (Butterworths, London, 1972) and volume 2, "Homogeneous gas phase reactions of the H_2-N_2-O_2 system" D. L. Baulch D. D. Drysdale and D. G. Horne, (Butterworths, London, 1973). Earlier evaluations by the same group have appeared in five reports from the Department of Physical Chemistry, University of Leeds, entitled "High Temperature Reaction Rate Data".

Data on reactions occurring in photochemical smog have been evaluated in "The Mechanism of Photochemical Smog Formation" by K. L. Demerjian, J. A. Kerr and J. G. Calvert (Advances in Environmental Science and Technology, J. N. Pitts, Jr. and R. L. Metcalf, editors, Wiley-Interscience, volume 4, 1974).

Kinetic data for reactions of the hydroperoxyl radical have been evaluated in "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical" A. C. Lloyd, Intern. J. Chem. Kinet. 6, 169-228 (1974).

Kinetic data for reactions of chlorine atoms and chlorine oxides have been evaluated by R. T. Watson in "Chemical Kinetics Data Survey VIII. Rate Constants of ClO_x of Atmospheric Interest" NBSIR 74-516 (distributed by Chemical Kinetics Information Center, National Bureau of Standards, Washington, D. C. 20234.)

1.3. Guide to the Table

1.3.1. General

This table provides current (November 1974) information on reaction rate constants, quantum yields and absorption cross sections. For many reactions, preferred values are given. The reactions included in the table are summarized on a "reaction grid" described in section 1.3.4., Arrangement of the Table. That grid also shows processes for which data (or data evaluations) are needed.

Most of the more important stratospheric reactions are in the tables. A number of the less important ones and some related systems are included, often simply for comparison.

The following remarks summarize the content of the table. It lists 271 reactions and gives a preferred value of the rate constant for 160 reactions, 136 based on recent reviews and 24 based on recent (1972-1974) experimental work. New data entries (1972-1974) are given for 121 reactions.

Several principles have been used in the selection and presentation of data.

(a) Where a preferred value is given for a rate constant or photochemical quantity, it is so indicated by an asterisk placed ahead of the reference column.

(b) Where there is a recent published evaluation of the data and there are no newer data, the evaluation is adopted and usually, but not always, marked with an asterisk. The original data covered by the evaluation are not listed separately.

(c) Where there is an evaluation but there are new data, both are listed and a preferred value is indicated (marked by an asterisk).

(d) Where desirable, the available recent data sets are listed, and a selection is made or a preferred value is synthesized from them.

(e) The uncertainty in a preferred value given in the table is the evaluator's estimate of that value's reliability. This is a subjective judgment that, to a high degree of probability, the true value of the quantity lies within the bounds indicated.

Uncertainties are indicated in several ways:

$A < k < B$ means k lies in the range between A and B.
$k < B$ means B is an upper limit.
$k \sim B$ means that B is only a rough guide to the value of k.
$k = A \pm B$ means that a reasonably reliable estimate of the likely error can be stated. This is an estimate by the evaluator of the absolute accuracy of the preferred value. It is a subjective judgment derived from intercomparison of data sets, consideration of related reactions studied with the same technique, estimates of how well the parameters could have been controlled, and comparison with theory. It means that in the evaluators judgment, the true value will lie within the indicated limits to a high level of confidence (90 to 95 percent).

Sometimes it is more appropriate to give $\log_{10}k = C \pm D$, "k uncertain to E percent" or "k uncertain to a factor of F", all three of which are equivalent statements of multiplicative limits. The statement that k has the value k_0 and is uncertain to a factor of F means $k_0/F < k < k_0F$.

The identity of the contributor who selected a particular preferred value has been retained wherever possible. This is shown by initials after the appropriate entry in the Reaction/Reference column. The editors take responsibility for any unidentified selections and for inadvertant ommission of identification of selectors.

1.3.2. Conventions Concerning Rate Constants

a. General Convention. Almost all of the reactions in the table are elementary processes. For them the rate expression is derivable from a statement of the reaction, e.g.

$$A + 2B \rightarrow AB_2$$

$$-d[A]/dt = -(1/2)\, d[B]/dt = d[AB_2]/dt = k[A][B]^2$$

Note that the stoichiometric coefficient for B, i.e. 2, appears in the denominator before B's rate of change (which is equal to $2k[A][B]^2$) and as a power on the right hand side.

Wherever there may be any doubt an explicit rate expression is given.

b. Dissociation and Combination Reactions. Some reactions of these types are not of integral kinetic order over the stratospheric pressure and temperature range. That is, although they require an energy transfer agent, "M," they are in the "pressure fall-off region". For many such reactions we tabulate rate constants that include the effect of the energy transfer agent and give rates for various altitudes. The reactions are written to deemphasize "M," e.g.,

$$NO_2 + NO_3\ (+M) \rightarrow N_2O_5\ (+M)$$

$$HNO_3 \xrightarrow{M} HO + NO_2$$

The rate expressions to be used do not have the concentration of M in them, e.g., Rate = $k[NO_2]\,[NO_3]$ and $k[HNO_3]$ respectively. The units given for the k's. s^{-1} for first order, and cm^{+3} $molecule^{-1}s^{-1}$ for second order, are consistent with this convention.

The altitude, temperature and number density regime used in these cases is

altitude/km	temp./K	log[M]/molecule cm^{-3}
15	220	18.60
20	217	18.27
25	222	17.93
30	227	17.58
35	235	17.26
40	250	16.92
45	260	16.60

Expect for the temperature at 15 km this table follows the U. S. standard atmosphere, 1962.

c. Forward and Reverse Reactions. In some cases there are no data on a reaction of interest but there are data on the "reverse" reaction. Occasionally, for

$$A \rightarrow B\ (f)$$

$$B \rightarrow A\ (r)$$

an evaluation will use the data on the "reverse" reaction together with an equilibrium constant to obtain the other rate constant. Obviously this is an approximation but it often is a useful method of estimating non-measured physical properties.

The table contains notations to warn the reader when this procedure has been used, such as "based on reverse reaction," or when both reactions f and r are listed together "$k_f = k_r K_{eq}$" or $k_r = k_f/K_{eq}$. These expressions, which are those used in the analyses, are based on equating the two rates at equilibrium.

$$R_f = R_r$$

$$k_f[A] = k_r[B]$$

$$K_{eq} = [B]/[A] = k_f/k_r.$$

1.3.3. Convention Concerning Optical Absorption Coefficients

These are reported in the table as "absorption cross sections per molecule, base e". They are defined by the equations

$$I/I_o = \exp(-\sigma[N]\ell)$$

$$\sigma = (1/([N]\ell))\ln\,(I_o/I)$$

where I_o and I are the intensities of incident and transmitted light, σ is the absorption cross section, cm^2 $molecule^{-1}$, [N] is the concentration of absorbers, molecules cm^{-3}, and ℓ is the path length, cm. Other definitions and units are frequently used. The terms "absorption coefficient" and "extinction coefficient" are common. It is always necessary to know what concentration units path length units and type of logarithim (base e or base 10) are used in the definition. To convert "cross-sections" to absorption coefficients in (atm at 273 K)$^{-1}$ cm^{-1}, base e, multiply by 2.69×10^{19}.

1.3.4. Arrangement of the Tables

a. Reaction Grid. The contents of the data table and the location of a reaction in it are shown on the "reaction grid," that follows this discussion.

This grid shows the molecules of interest for stratospheric chemistry along the top and left edges. The symbol "K" in the intersection for two reactants means that data for the reaction are in the table. Combination reactions, $A + B + M \rightarrow AB + M$ are above the main diagonal. Bimolecular reactions, typically $A + B \rightarrow C + D$, are below the diagonal.

The first four columns in the reaction grid indicate whether the table contains the following data for a particular species listed along the left edge of the grid: 1. (ABS. σ), ultraviolet or visible photoabsorption cross section; 2. (Q.Y.), quantum yields for primary photochemical processes; 3. (E.TR.), rate coefficients for processes involving energy transfer from excited species; and 4. (DISS.) rate data for its thermal dissociation.

b. <u>Sequence of Reactions</u>. The order in which reactions are listed follows the grid. All reactions of O atoms, the first species, shown in its <u>row and column</u> are listed first, then those of the second species, $O(^1D)$, with all species other than O atoms, and so on. Thus a particular reaction is placed with the reactant highest (or to the left) on the grid. Bimolecular and combination reactions with the same reactants appear together in the table.

The algorithm used to assign reaction locations is to construct an ordered ascending sequence of number pairs (or triplets), one for each reaction according to the following rules:

(1) Assign numbers to each reactant in an equation. Use the numbers at the left side of the grid.

(2) Arrange this set of numbers in ascending order, e.g. 1, 3 not 3, 1; 4, 10, 11 not 10, 11, 4.

(3) Order the sets in ascending order, giving priority to the lower number in the corresponding position of two sets being compared, e.g. 1,4; 1,7; 4,10,10; 4,10,11; 18, 24 etc. This completes the assignment of reaction sequence.

If a reaction is not filed according to this scheme, a cross reference appears at the proper spot. Exceptions are made principally to put forward and reverse reactions together.

c. <u>Status of the Data</u>. The reaction grid also shows what data are available and what are needed. A "dash" (-) means that the reaction may be ignored for stratospheric chemistry. An "0" means that data are needed or existing data should be evaluated. Often this means the reaction is important, but at times it means that data are required so that the importance of the reaction can be assessed. A blank intersection merely means that no decision can be made at present. Finally, data are included in the table for some reactions that are unimportant. They are presented for comparison.

2. Chemical Reaction Matrix

K = Data in table, O = Data selection or new data needed,
- = Unimportant for stratospheric chemistry, E = Data elsewhere in the chapter, (Blank) = Role of process not assessed

Combination Reactions: A + B + M → AB + M

		ABS.σ	Q.Y.	E.TR.	DISS.	O	O(1D)	O(1S)	O2	O2(1Δ)	O2(1Σ)	O3	N	NO	NO2	NO3	N2	N2O	N2O5	NH	NH2	NH3	H	HO	HO2	H2	H2O	H2O2	HNO	HNO2	HNO3	SO	SO2	SO3	S2O	HS	H2S	HSO3	H2SO4	Cl	ClO	ClO2	ClO3	HCl	HOCl	HOClO	NOCl	NO2Cl	Cl2	CO	CO2	CHO	CH2O	CH3	CH3O	CH3O2	CH3OH	CH3OOH	CH3NO2	CH3NO3	CH4	C2H4	C2H6	C3H6	C3H8	C4H10
1	O	-	-	-	-	K			K			-	K	K	K	-	K	-	-			-	K	K	-		-	-			-		K	-					-													-	-	-	-	-										
2	O(1D)	-	-	K	-	-	-					-				-	K	-	-						-		-	-						-																																
3	O(1S)	-	-	K	-	K	-					-	-				-	-	-						-		-	-						-	-																						-										
4	O2	K	O	E	-		K	K	-	-	-	-		K	-	-	-	-	-			-	K	-	-		-	-		-	-		-	-	-				-	K										-			-	K	-	-										
5	O2(1Δ)			K	-		-		K	-		-		-	-	-	-	-	-			-		-	-		-	-			-			-					-											-			-		-	-										
6	O2(1Σ)			K	-		-		K	-	-	-		-	-	-	-	-	-			-		-	-		-	-			-			-					-											-			-		-	-										
7	O3	K	K	E	K	K	K	K	-	K	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-				-											-		-	-	-	-	-										
8	N	-	-	-	-	-	-	-	K		-	K	K	-	-	-	-	-	-	-	-	-			-		-	-	-	-	-	-	-	-	-				-											-		-	-	-	-	-										
9	NO	K	O		K	K	K	K	K	K		K	K	K	-	-	-	-	-	-	-	-	K	K	K		-	-	-	-	-	-	-	-	-				-	K										-			-	K	K	K										
10	NO2	K	K	O	K	K	K	K	K			K	K	K	K	K	-	-	-	-	-	-		K	O		-	-	-	-	-	-	-	-	-				-	K										-			-	K	K	K										
11	NO3	K	K	O	K				K			-		K	K	K	-	-	-	-	-	-	-	O	-		-	-	-	-	-	-	-	-	-				-											-			-													
12	N2	-	-	E	K	K	K	K	K	K	K	-	-	-	-	-	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-				-											-		-	-	-	-	-										
13	N2O	E	O	-	K	K	K	K	-	-	-	-		-	-	-	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-				-											-		-	-	-	-	-										
14	N2O5	K	K	O	K	K			-	-	-				-	-	-	-	-	-	-	-	-	-	-		-	-	-	-	-	-	-	-	-				-											-				-												
15	NH				-		-		O								-	-		-		-					-	-	-	-	-								-											-		-	-	-	-	-										
16	NH2				-	K	-		O			O		K			-	-				-	K					-	-	-	-								-											-																
17	NH3			-	K	K	K	K	-			O		-	K		-	-			-	-	-	-				-	-	-	-																			-		-	-	-	-	-										
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21	H2	-	-	-	K	K	K	-	K	-	-	-		K	-	-	-	-	-	-	K	-	-	K	K	-																																								
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23	H2O2	K	O	-	K	K	K		K	-	-	-		K	-		-	-				-	K	K	-	-	K	-	-	-	-								-											-	-	-	-	-	-	-										
24	HNO	O	O		K				K					-			-	-				-	K	K		-	-		K										-											-		-	-	-	-	-										
25	HNO2	E	K	O	-	K			-			-			-		-	-					K	K	-	-			-	O									-											-		-	-	-	-	-										
26	HNO3	K	K	O	K	K			-	-	-	-			-	-	-	-	-	-	-	O	K	K	-	-	-	-	-	-	-								-													-	-	-	-	-										
27	SO	O	O		-				K	K		K	-				-															K		-	-				-											-			-													
28	SO2	O	O	O	-				-	K	-	K	-	K		K	-	-	K					K	K	-							-																	-			-	K												
29	SO3	O	O	-	-	K			-	-	-	-	-				-							O		-	K					K	-																	-			-													
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37	ClO2	K			K	K							K	K			-						K		O															K																										
38	ClO3																-								O																																									
39	HCl	K			-	K	K										-						O	K																-																										
*40	HOCl					K											-																							K																										
41	HOClO																-																																																	
42	NOCl																-																							K																										
43	NO2Cl																-																							K								-																		
44	Cl2	K	O		-	K				-							-																																-																	
45	CO			E	-		K		-	K		K	-	-	-	-	-	K	-	-	-	-		K	K	-	-	-	-	-	-	-	-	-	-				-		K									-		-	-		-	-										
46	CO2	-	-	E	-	-	K	K	-	-	-	-		-	-	-	-	-	-	-	-	-	-		-		-	-	-	-	-		-	-	-				-											-	-															
47	CHO				-	K	-		K				-				-	-				-	-			-	-			-	-								-											-	-															
48	CH2O	K	K		-	K			-	-	-	-		-			-	-				-	K	K	K	-	-	-	-	-	-																			-	-		-													
49	CH3				-	K	-		K				-		K		-	-				-				-	-				-																			-	-															
50	CH3O				-		-		K				-	K	K		-	-					-			-	-				-								-											K	-					-										
51	CH3O2				-				O				-	K	K	-	-	-				-	-		K	-	-			-	-	-	-	-	-				-											-	-					K										
52	CH3OH																																																																	
53	CH3OOH	O	O		-					-	-						-	-				-	-				-	-	-	-	-		-	-	-				-											-		-	-	-	-	-										
54	CH3NO2	O	K	O	-					-	-						-	-				-	-				-	-	-	-	-		-																	-		-	-	-	-	-										
55	CH3NO3	O	O	O	-					-	-	-					-	-				-	-				-	-	-	-	-		-																	-		-	-	-	-	-										
56	CH4	-	-	-	-	K	K	K	-	-	-	K		-	-	-	-	-	-	-	-	-	-	K	-		-	-	-	-	-		-	-	-				-	K	K									-		-	-	-	-	-										
57	C2H4				-	K						K												K	K																K																									
58	C2H6				-	K	K																	K	K																																									
† 59	C3H6				-	K						K												K																	K																									
∇ 60	C3H8				-																			K	K																																									
‡ 61	CF2Cl2	K			-		K																																																											

November 22, 1974

Bimolecular Reactions: A + B → C + D + ...

* and Cl2O
† and higher olefins, alkynes and aromatics
∇ and higher alkanes
‡ and other chlorofluorocarbons

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^6 molecule^{-2} s^{-1}$	Notes and Reliability of log k
1,1M	$O + O + M \rightarrow O_2 + M$			
	*Johnston (1968) review	1000< T <8000	$3.80 \times 10^{-30}\ T^{-1} \exp(-170/T)$ M = O_2	±0.3
	Campbell, Gray (1973)	298	4.8×10^{-33} M = N_2	±0.03
		196	11.1×10^{-33}	±0.02
	Taylor (1974) review	2000–10000	$1.7 \times 10^{-32}\ T^{-1/2}$ M = N_2	
			$2.2 \times 10^{-28}\ T^{-3/2}$ M = O_2	
			$6.2 \times 10^{-28}\ T^{-3/2}$ M = O	
			$8.3 \times 10^{-33}\ T^{-1/2}$ M = N, NO	
1,3	$O + O(^1S) \rightarrow$		see $O(^1S) + O \rightarrow$	
1,4M	$O(^3P) + O_2 + M \rightarrow O_3 + M$ (f)			
7,M	$O_3 + M \rightarrow O + O_2 + M$ (r)			
	*This Survey (D.D.D. and D.G.)	200–346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$ M = Ar	±.07
			Rel. M eff.: Ar(1.0), N_2(1.6), O_2(1.7), H_2O(15)	
	Johnston (1968) eval.	200–1000	$k_f = 4.6 \times 10^{-35} \exp(1050/T)$ M = O_3	±0.1
			$k_r = 1.65 \times 10^{-9} \exp(-11400/T) cm^3 molecule^{-1} s^{-1}$	±0.1
			Rel. M eff.: O_3(1.0), Ar(0.25), O_2(0.44), N_2(0.39)	
	Huie, Herron, Davis (1972)	200–346	$k_f = 6.6 \times 10^{-35} \exp(510/T)$ M = Ar	
			Rel. M efficiencies: Ar(1.0), He(0.9), N_2(1.7)	
	Mulcahy, Williams (1968)	213–386	$k_f = 4.7 \times 10^{-35} \exp(840/T)$ M = Ar	
			Rel. M eff.: Ar(1.0), He(0.8), CO_2(3.4), O_2(1.1)	
	Meaburn, et al (1968)	300	$k_f = 1.0 \times 10^{-33}$ M = CO_2	
			Rel. M eff.: CO_2(1.0), CO(0.44), N_2O(0.88)	

Reactions of O with O and O_2

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Stuhl, Niki (1971)	300	$k_f = 5.4 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = N_2	
			Rel. M efficiencies:	
			$N_2(1.0)$ $O_2(1.18)$, CO(1.24)	
	Donovan, Husain, Kirsch (1970)	300	$k_f = 5.0 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = Ar	
			Rel. M efficiencies:	
			Ar(1.0), Kr(0.98), He(0.92)	
	Hippler, Troe (1971)	300	$k_f = 8 \times 10^{-34}$ M = N_2	
	Slanger, Black (1970)	300	$k_f = 4.4 \times 10^{-34}$ M = Ar, Rel. eff. Ar(1.0), $N_2(1.6)$	
	Francis (1969)	300	$k_f = 1.24 \times 10^{-34}$ M = O_2	
	Sauer (1967)	300	$k_f = 2.28 \times 10^{-34}$ M = Ar	
	Ball and Larkin (1973)	295	$k_f = 5.4 \pm 1.2 \times 10^{-34}$ M = N_2	
			Rel. efficiencies: $N_2(1.0)$, $O_2(1.09)$, Ar(0.78)	
	Hippler, Schippert, Troe (1974)	300	$k_f \sim 8 \times 10^{-34}$ cm^{6}molecule^{-2}s^{-1} M = N_2	(a)
			$k_{f(\infty)} = 2.8 \times 10^{-12}$ cm^{3}molecule^{-1}s^{-1}	(a,b)
			(a) Reevaluation of work in Hippler, Troe (1971)	
			(b) 2d order high pressure limit	
1.4M	$O + O_2 + M \rightarrow O_3^* + M$			
	Bevan, Johnson (1973)	300	5.4×10^{-34}cm^{6}molecule^{-2}s^{-1} M = O_2	(a)
			Rel. efficiencies: $O_2(1.0)$, Ar(0.50), $N_2O(2.4)$,	
			$CO_2(2.5)$, $SF_6(5.7)$	
	von Rosenberg, Trainor (1974)	300	3×10^{-34} cm^{6}molecule^{-2}s^{-1}	(b)
			(a) Vibrationally excited O_3 followed as fn. of time using absn. 250< λ <330nm.	
			(b) Vibrationally excited O_3 followed as fn. of time using i.r. emission at 9.6 and 14.3 μm	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1.7	$O(^3P) + O_3 \to O_2 + O_2$			
	*This Survey (D.D.D., H.I.S, and H.J.)	220-1000	$1.9 \times 10^{-11} \exp(-2300/T)$	±0.1 (a)
	Hampson (1973) eval.	220-1000	$1.9 \times 10^{-11} \exp(-2300/T)$	
	McCrumb, Kaufman (1972)	269-409	$1.1 \times 10^{-11} \exp(-2155/T)$	
	Lundell, Ketcheson, Schiff (1969)	300	1.5×10^{-14}	
	Husain, Kirsch, Donovan (1972)	300	1.3×10^{-14}	
	Davis, Wong, Lephardt (1973)	220-353	$2.0 \times 10^{-11} \exp(-2280/T)$	
	(a) The preferred value of this survey is based on the high temperature data included in Hampson (1973) and the low temperature data of McCrumb and Kaufman and of Davis, et al.			
1.8M	$O + N + M \to NO + M$			
	*Baulch, et al (1973) review	200-400	$1.8 \times 10^{-31}(T)^{-0.5} cm^6 molecule^{-2} s^{-1}$, $M = N_2$	±0.2
	Taylor (1974)	2000-10000	$2.8 \times 10^{-28} T^{-3/2}$ $M = N_2, O_2, N, O$ $5.5 \times 10^{-27} T^{-3/2}$ $M = NO$	
1.9	$O + NO \to N + O_2$ (f)			
4.8	$O_2 + N \to NO + O$ (r)			
	*Baulch, et al (1973) review	1000-3000	$k_f = 2.5 \times 10^{-15} T \exp(-19500/T)$	±0.12 at 1000K (a)
		300-3000	$k_r = 1.1 \times 10^{-14} T \exp(-3150/T)$	±0.12 300<T<1500K
			(a) $k_f = k_r K_{eq}$. Error in log k increases to ±0.3 at 3000K	
	Taylor (1974)	2000-10000	$k_r = 2.2 \times 10^{-14}(T) \exp(-3560/T)$	
1.9	$O + NO \to NO_2 + h\nu$			
	Becker, et al (1973)	300	4.2×10^{-18}	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
1,9M	O + NO + M -> NO_2 + M (f)			
10,M	NO_2 + M -> NO + O + M (r)			
	*Baulch, et al (1973) review	200-500	$k_f = 3.0 \times 10^{-33} \exp(940/T)$ cm^{6}molecule^{-2}s^{-1}, M = O_2	±0.08
			Rel. M efficiencies: $O_2(1.0)$, Ar(1.0), $N_2(1.4)$	
		1400-2400	$k_r = 1.8 \times 10^{-8} \exp(-33000/T)$cm^{3}molecule^{-1}s^{-1}	±0.1
			M = Ar	
	Hampson, et al (1973a) review	200-500	accepts above recommendation	
	Slanger, Wood, Black (1973)	296	$k_f = 6.0 \times 10^{-32}$ M = Ar	(a)
		241	$k_f = 13.0 \times 10^{-32}$ M = Ar	(a)
	Hippler, Schippert, Troe (1974)	300	$k_f = 7.4 \times 10^{-32}$ cm^{6}molecule^{-2}s^{-1} M = N_2	
			$k_{f(\infty)} = 3.0 \times 10^{-11}$ cm^{3}molecule^{-1}s^{-1}	(b)
	Atkinson, Pitts (1974)	300-392	$k_f = 2.6 \times 10^{-32} \exp(450 \pm 100/T)$ M = N_2O	
			(a) slightly higher but supports recommendation.	
			(b) 2d order high pressure limit	
1,9M	O + NO + M -> NO_2 + M + hv			
	Becker, et al (1973)	300	7×10^{-32} cm^{6}molecule^{-2}s^{-1}	
1,10	O(3p) + NO_2 -> NO + O_2 (f)			
4,9	O_2 + NO -> NO_2 + O (r)			
	*This survey (D.D.D.)	230-550	$k_f = 9.1 \times 10^{-12}$	±0.06
	Baulch, et al (1973)	300-550	$k_f = 1.7 \times 10^{-11} \exp(-300/T)$	
			$k_r = k_f/K_{eq} = 2.8 \times 10^{-12} \exp(-23400/T)$	±0.1
	Davis, Herron and Huie (1973)	230-339	$k_f = 9.1 \times 10^{-12}$	
	Clyne, Cruse (1971)	300	$k_f = 8.3 \times 10^{-12}$	
	Harker, Johnston (1972)	300	$k_f = 9.2 \times 10^{-12}$	(a)
	Clyne, Cruse (1972)	298	$k_f = 6.1 \times 10^{-12}$	
			(continued)	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Slanger, et al (1973)	300	$k_f = 9.3 \times 10^{-12}$	(b)
		240	$k_f = 10.5 \times 10^{-12}$	
	Hampson, et al (1973a) review	220-500	$k_f = 9.1 \times 10^{-12}$	±0.08
	Stuhl, Niki (1970)	300	$k_f = 4.4 \times 10^{-12}$	(b)
	Bemand, Clyne, Watson (1973)	230-1055	$k_f = 1.75 \times 10^{-10} \times (T)^{-0.52}$	(c)
		298	$k_f = 9.5 \pm 1.1 \times 10^{-12}$	
		(a) $k/k(O + NO + M)$ measured, where $k(ref) = 6.9 \times 10^{-32}$		
		(b) Similar techniques were used by Slanger and by Stuhl and Niki: Flash photolysis - chemiluminescence.		
		(c) Based on this work (198 <T/K< 1055) and other recent work.		
1,10M	$O + NO_2 + M \rightarrow NO_3 + M$ (f)			
11,M	$NO_3 + M \rightarrow NO_2 + O + M$ (r)			
	*Hampson, et al (1973a) review	298	$k_f = 1.0 \times 10^{-31}$ cm^6 molecule^{-2}s^{-1} $M = N_2$	±0.2
	Baulch, et al (1973) review	295	$k_f = 6.3 \times 10^{-32}$ $M = N_2$	±0.4
			$k_r \sim 8 \times 10^{-42}$ cm^{3}molecule^{-1}s^{-1}, $M = N_2$	(a)
	Hippler, Schippert, Troe (1974)	300	$k_f = 8.0 \times 10^{-32}$ cm^{6}molecule^{-2}s^{-1} $M = N_2$	
			$k_{f(\infty)} = 2.0 \times 10^{-11}$ cm^{3}molecule^{-1}s^{-1}	(b)
			(a) No reliable data. Value based on k_f	
			(b) 2d order high pressure limit	
1,12	$O + N_2 \rightarrow N + NO$		See reverse reaction	
1,12M	$O + N_2 + M \rightarrow N_2O + M$ (f)			
13,M	$N_2O + M \rightarrow N_2 + O + M$ (r)			
	Baulch, et al (1973) review	1300-2500	$k_f = 3.9 \times 10^{-35} \exp(-10400/T)$ cm^{6}molecule^{-2}s^{-1} $M = Ar$	±0.2 (a)

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k
			$k_r = 8.3 \times 10^{-10} \exp(-29000/T)\ cm^3 molecule^{-1}s^{-1}$	
			$M = Ar$	±0.2
		900-2100	$k_f = 5.5 \times 10^{-15} \exp(-11330/T)\ cm^3 molecule^{-1}s^{-1}$	±0.2 (a,b)
			$k_r = 1.3 \times 10^{+11} \exp(-30000/T) s^{-1}$	±0.2 (c)
			(a) $k_f = k_r K_{eq}$	
			(b) 2d order high pressure limit	
			(c) 1st order high pressure limit	
1,13	$O + N_2O \rightarrow N_2 + O_2$ (1)			
1,13	$O + N_2O \rightarrow NO + NO$ (2)			
9,9	$NO + NO \rightarrow N_2O + O$ (2r)			
	Baulch, et al (1973) review	1200-2000	$k_1 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	±0.4 (a)
			$k_2 = 1.7 \times 10^{-10} \exp(-14.1 \times 10^3/T)$	±0.3
		1200-2000	$k_{2r} = 2.2 \times 10^{-12} \exp(-32100/T)$	±0.3 (b)
			(a) Based on $k_1/k_2 = 1$	
			(b) $d[NO]/dt = -2k_{2r}[NO]^2$	
	Taylor (1974) review	2000-10000	$k_{2r} = 0.4 T^{-5/2} \exp(-43000/T)$	
1,14	$O + N_2O_5 \rightarrow$ products			
	Davis (1974)	300	$< 2 \times 10^{-13}$	preliminary
1,16	$O + NH_2 \rightarrow HNO + H$ (a)			
	$\rightarrow HO + NH$ (b)			
	Gehring, et al (1973)	300	3.5×10^{-12} $(k_a + k_b)$	
1,17	$O + NH_3 \rightarrow HO + NH_2$ (f)			
16,19	$HO + NH_2 \rightarrow O + NH_3$ (r)			
	*Kurylo, et al (1969) (D.G.)	361-677	$k_f = 6.6 \times 10^{-12} \exp(-3300/T)$	±0.3

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
	Baulch, et al (1973) review	300-1000	$k_f = 2.5 \times 10^{-12} \exp(-3020/T)$	±0.2
		300-1000	$k_r = k_f/K_{eq} = 1 \times 10^{-13}$	±0.2 (a)
	Albers, et al (1969)	300-1000	$k_f = 2 \times 10^{-12} \exp(-3000/T)$	
	Kondratiev (1970) review	350-1000	$k_f = 1.8 \times 10^{-12} \exp(-2500/T)$	
			Data of Albers, et al provide an upper limit	
			when extrapolated to 220K	
			(a) $HO + NH_2 \rightarrow NH + H_2O$ may be preferred channel.	
1,18M	$O + H + M \rightarrow HO + M$			
	Schofield (1973) review	1000-3000	~2 x 10^{-32} $cm^6molecule^{-2}s^{-1}$ M = Ar	±1 estimate
	Baulch, et al (1972) review		No recommendation	
1,19	$O + HO \rightarrow H + O_2$ (f)			
4,18	$O_2 + H \rightarrow O + HO$ (r)			
	*Wilson (1972) review	300-2000	$k_f = 4.2 \pm 1.7 \times 10^{-11}$	±0.3
	*Baulch, et al (1972) review	700-2500	$k_r = 3.7 \times 10^{-10} \exp(-8450/T)$	±0.1
	Baulch, et al (1972) review	300	$k_f = 3.8 \pm 1.7 \times 10^{-11}$	±0.17
1,19M	$O + HO + M \rightarrow HO_2 + M$			
	Baulch, et al (1972) review		no recommendation	
1,20	$O + HO_2 \rightarrow HO + O_2$			
	Lloyd (1974) review	~300	$8 \times 10^{-11} \exp(-500/T)$	estimate
1,21	$O + H_2 \rightarrow HO + H$ (f)			
18,19	$H + HO \rightarrow O + H_2$ (r)			
	Baulch, et al (1972) review	400-2000	$k_f = 3.0 \times 10^{-14}(T)\exp(-4480/T)$	±0.1
			$k_r = k_f/K_{eq} = 1.4 \times 10^{-14}(T)\exp(-3500/T)$	±0.15

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
1,22	$0 + H_20$ -> HO + HO		See reverse reaction	
1,22	$0 + H_20$ -> H + HO_2			
	Baulch, et al (1972) review		no recommendation	
1,23	$0(^3P) + H_20_2 = HO_2 + OH$ (a) $= H_20 + 0_2$ (b)			
	*This Survey (D.D.D.)	283-373	k(a+b) = 2.75 x 10^{-12}exp(-2125/T)cm^{3}molecule^{-1}s^{-1}	±0.07 (a)
	Foner, Hudson (1962)	300	$\lesssim$ 4 x 10^{-15}	
	Davis, Wong, Schiff (1974)	283-373	k(a+b) = 2.75 x 10^{-12} exp(-2125/T)	±0.06
	Albers, et al. (1971)	370-800	k(a + b) = 4.6 x 10^{-11} exp(-3220/T)	
		(a) There is presently no basis for assigning relative k values to the two possible channels for this reaction.		
1,25	$0 + HNO_2$ -> HO + NO_2			
	This survey (D.G.)		No data. Probably faster than 0 + HNO_3, since it is 94 kJ/mol more exothermic.	
	Baulch, et al (1973) review		No recommendation	
1,26	$0 + HNO_3$ -> HO + NO_3			
	*Hampson, et al (1973) review	300	< 1.5 x 10^{-14}	
	Morley, Smith (1972)	300	<1.3 x 10^{-14}	
	Chapman, Wayne (1974)	300	< 3 x 10^{-17}	
	Baulch, et al (1973) review	300	<10^{-14}	approximate upper limit
1,28M	$0 + SO_2 + M$ -> $SO_3 + M$			
	*Davis (1974) (D.D.D.,D.G.)	220-353	3.4 x 10^{-32} exp (-1130/T) cm^{6}molecule^{-2}s^{-1} M = N_2 N_2(1.0), He(.45), Ar(.87), SO_2(56)	
	Schofield (1973) review	250-1000	1 x 10^{-33} exp(+500/T) cm^6 molecule^{-2}s^{-1}, M = 0_2, N_2, Ar, He	±0.3 at 300K ±0.6 at other Temp

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Reactions of 0 with H_20 to SO_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1,29	$O + SO_3 \rightarrow SO_2 + O_2$			
	Schofield (1973) review	1480-1550	$5 \times 10^{-10} \exp(-6000/T)$	Uncertain
	Jacob, Winkler (1972)	300-500	$3 \times 10^{-16} \exp(-500/T)$	
1,31	$O + HS \rightarrow H + SO$			
	Cupitt, Glass (1974)	295	$1.6 \pm 0.5 \times 10^{-10}$	
1,32	$O + H_2S \rightarrow HO + HS$			
	Hollinden, Kurylo, Timmons (1970)	205-300	$2.9 \times 10^{-13} \exp(-750/T)$	(a)
			(a) Assumes stoichiometry of 3.5	
1,36	$O + ClO \rightarrow Cl + O_2$			
	Watson (1974) review	300	$5.3 \pm 0.8 \times 10^{-11}$	±0.1
1,37	$O + OClO \rightarrow ClO + O_2$			
	Watson (1974) review	300	5×10^{-13}	±0.2
1,39	$O + HCl \rightarrow HO + Cl$			
	Balakhnin, et al (1971)	295-371	$1.74 \pm 0.6 \times 10^{-12} \exp(-2260/T)$	
	Brown, Smith (1974)	293-440	$2.5 \times 10^{-12} \exp(-2970 \pm 150/T)$	
	Wong, Belles (1972)	356-628	$1.9 \pm 0.3 \times 10^{-11} \exp(-3580/T)$	
1,39	$O + HCl(v = 1) \rightarrow HO + Cl$ (a) $\rightarrow O + HCl(v = 0)$ (b)			
	Arnoldi, Wolfrum (1974)	300	$3.6 \pm 1.2 \times 10^{-12}$	(a)
	Brown, Glass, Smith (1974)	196-397	$8.2 \times 10^{-12} \exp(-650/T)$	(a)
			(a) Total rate constant for sum of two reaction paths.	
1,40	$O + Cl_2O \rightarrow 2ClO$			
	*Watson (1974) review	300	$1.4 \pm 0.2 \times 10^{-11}$	
1,44	$O + Cl_2 \rightarrow ClO + Cl$			
	*Watson (1974) review	300	6.3×10^{-14}	± 0.1

Reactions of O with SO_3 to Cl_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1,47	$O + CHO \rightarrow CO_2 + H$ (a)			
	$\rightarrow CO + HO$ (b)			
	*Washida, et al (1973)	297	$2.1 \pm 0.4 \times 10^{-10}$ $(k_a + k_b)$	
1,48	$O + CH_2O \rightarrow CHO + OH$			
	*Demerjian, et al (1974) review	300	1.6×10^{-13}	
	Mack, Thrush (1973)	300	1.5×10^{-13}	± 0.05
1,49	$O + CH_3 \rightarrow CH_2O + H$ (a)			
	$\rightarrow CHO + H_2$ (b)			
	Washida, Bayes (1973)	300	$k_a = 1.23 \times 10^{-10}$	± 0.1
	Washida, et al (1973)	300	k_b negligible $k_b/k_a < 0.05$	
	Morris, Niki (1972)	300	$k_a = 9 \times 10^{-11}$	
	Peeters, Mahnen (1973)	1100-1900	$k_a = 2.2 \times 10^{-10} \exp(-1000/T)$	
	Slagle, Pruss, Gutman (1974)	300	$1.85 \pm 0.28 \times 10^{-10}$	
1,56	$O + CH_4 \rightarrow$ products			
	*Herron, Huie (1973) review	350-1000	$3.5 \times 10^{-11} \exp(-4550/T)$	± 0.11
1,57	$O + C_2H_4 \rightarrow CH_3 + HCO$ (a)			
	$\rightarrow CH_2CO + H_2$ (b)			
	*Herron, Huie (1973) evaluation	200-500	$5.5 \times 10^{-12} \exp(-565/T)$ $(k_a + k_b)$	± 0.08
	Pruss, Slagle, Gutman (1974)	300	$k_b = 3.81 \pm 0.95 \times 10^{-14}$	
			$k_b/(k_a + k_b) = 0.05$	(a)
	Atkinson, Pitts (1974)	300-392	$5.6 \times 10^{-12} \exp(-640 \pm 100/T)$ $(k_a + k_b)$	
			a) Calculated using above recommended value	
			for $(k_a + k_b)$	
1,58	$O + C_2H_6 \rightarrow$ products			
	*Herron, Huie (1973) evaluation	300-650	$4.1 \times 10^{-11} \exp(-3200/T)$	± 0.11

Reactions of O with CHO to C_2H_6

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
1,59	$O + C_3H_6 \rightarrow$ products			
	*Herron, Huie (1973) evaluation	200-500	$4.1 \times 10^{-12} \exp(-38/T)$	±0.08
	Atkinson, Pitts (1974)	300-392	$3.45 \times 10^{-12} \exp(0 \pm 150/T)$	
1,60	O + alkane $\rightarrow HO$ + alkyl radical			
	Herron, Huie (1969)	250-600	$k = [0.8 \exp(-2900/T) N_p + 2.2 \exp(-2250/T) N_s + 2.6 \exp(-1650/T) N_t] \times 10^{-11}$ Where N_p, N_s, and N_t are the number of primary, secondary, and tertiary hydrogen atoms, respectively. Do not use formula for CH_4.	
2,4	$O(^1D_2) + O_2 \rightarrow O_2(^1\Sigma_g^+) + O(^3P)$	298	7.4×10^{-11} $cm^3 molecule^{-1}s^{-1}$	±0.1 a
2,7	$O(^1D_2) + O_3 \rightarrow O_2(^3\Sigma_g^-) + O_2$ (?) (a)	"	5.3×10^{-10} $(k_a + k_b)$ $k_a/k_b \sim 1$	±0.3 a,c
	$\rightarrow O_2 + 2O(^3P)$ (b)	"		
2,9	$O(^1D_2) + NO \rightarrow NO + O(^3P)$	"	1.7×10^{-10}	±0.3 a
2,10	$O(^1D_2) + NO_2 \rightarrow NO + O_2$	"	2.8×10^{-10}	±0.1 a
2,12	$O(^1D_2) + N_2 \rightarrow N_2 + O(^3P)$	"	5.4×10^{-11}	±0.15 a
2,12M	$O(^1D_2) + N_2 + M \rightarrow N_2O + M$	"	2.8×10^{-36} $cm^6molecule^{-2}s^{-1}$	b
2,13	$O(^1D_2) + N_2O \rightarrow N_2 + O_2$ (a)	"	1.1×10^{-10} $cm^3molecule^{-1}s^{-1}$	±0.1 a
	$\rightarrow 2NO$ (b)	"	1.1×10^{-10}	±0.1 a
2,17	$O(^1D_2) + NH_3 \rightarrow NH_2 + HO$	298	$\sim 4 \times 10^{-10}$	(a,d)
2,21	$O(^1D_2) + H_2 \rightarrow HO + H$	"	2.9×10^{-10}	±0.1 a
2,22	$O(^1D_2) + H_2O \rightarrow 2HO$	"	3.5×10^{-10}	±0.1 a
2,23	$O(^1D_2) + H_2O_2 \rightarrow HO + HO_2$	"	$\sim 5 \times 10^{-10}$	a,d
2,39	$O(^1D_2) + HCl \rightarrow$ products		2×10^{-10}	e

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
2,45	$O(^1D_2) + CO \rightarrow CO + O(^3P)$	"	7.7×10^{-11}	±0.1 a
2,46	$O(^1D_2) + CO_2 \rightarrow CO_2 + O(^3P)$	"	1.8×10^{-10}	±0.1 a
2,56	$O(^1D_2) + CH_4 \rightarrow CH_3 + HO$ (a)	"	4.0×10^{-10} $(k_a + k_b)$	±0.1 a
	$\rightarrow CH_2O + H_2$ (b)		$k_a/k_b = 10$	
2,58	$O(^1D_2) + C_2H_6 \rightarrow C_2H_5 + HO$ (a)	"	6.2×10^{-10} $(k_a + k_b)$	±0.1 a
	$\rightarrow CH_3 + CH_2OH$ (b)			
2,61	$O(^1D_2) + CHF_2Cl \rightarrow$ products	298	3.5×10^{-10}	(f)
2,61	$O(^1D_2) + CFCl_3 \rightarrow$ products	"	5.8×10^{-10}	(f)
2,61	$O(^1D_2) + CF_2Cl_2 \rightarrow$ products	"	5.3×10^{-10}	(f)
2,61	$O(^1D_2) + CF_4 \rightarrow$ products	"	$< 2 \times 10^{-11}$	(f,g)
2,61	$O(^1D_2) + CF_2ClCFCl_2 \rightarrow$ products	"	5.5×10^{-10}	(f)
2,61	$O(^1D_2) + CF_2ClCF_2Cl \rightarrow$ products	"	3.3×10^{-10}	(f)

a. *Evaluation for this survey (R.J.C.).

b. Gaedtke, et al (1973)

c. Further determinations are desirable.

d. Roughly estimated by analogy, no measurements available.

e. Based on relative value of Gauthier and Snelling (1974) and value for $k(CO_2)$ in this table.

f. Based on relative values of Pitts, Sandoval, and Atkinson and value for $k(N_2O)$ in this table.

g. Upper limit based on estimated accuracy limit; no reaction was observed.

Reactions of $O(^1D)$ continued

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k	
3,1	$O(^1S) + O(^3P) \rightarrow ?$	300	7.5×10^{-12}	±0.2	a
3,4	$O(^1S) + O_2 \rightarrow ?$	200-377	$4.3 \times 10^{-12} \exp(-850/T)$	±0.15	a
3,7	$O(^1S) + O_3 \rightarrow ?$	300	5.8×10^{-10}	±0.07	a
3,9	$O(^1S) + NO \rightarrow ?$	200-291	$3.2 \times 10^{-11}(T)^{0.5}$	±0.05	a
3,10	$O(^1S) + NO_2 \rightarrow ?$	300	5×10^{-10}	±0.2	a
3,12	$O(^1S) + N_2 \rightarrow ?$	200-380	$< 5 \times 10^{-17}$		a
3,13	$O(^1S) + N_2O \rightarrow ?$	300	1.4×10^{-11}	±0.1	a
3,17	$O(^1S) + NH_3 \rightarrow ?$	300	5×10^{-10}	±0.2	a
3,22	$O(^1S) + H_2O \rightarrow ?$	300	$> 10^{-10}$	±1	a
3,46	$O(^1S) + CO_2 \rightarrow ?$	200-450	$3.1 \times 10^{-11} \exp(-1320/T)$	±0.15	a
3,56	$O(^1S) + CH_4 \rightarrow ?$	300	2×10^{-14}	±0.4	a

a) Rate constants evaluated for this survey by T. G. Slanger and K. H. Welge

Reactions of $O(^1S)$

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
4,hν	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$			
	Hampson, et al (1973a) review		Ø = 1 $175 < \lambda < 200$ nm	
4,hν	$O_2 + h\nu \rightarrow O(^3P) + O(^1D)$			
	Hampson, et al (1973a) review		Ø = 1 $133 < \lambda < 175$ nm	
4,hν	$O_2 + h\nu \rightarrow$ 2 oxygen atoms			
	Hampson, et al (1973a) review		Ø = 1 $106 < \lambda < 200$ nm	
4,hν	$O_2 + h\nu$			
	Hampson, et al (1973a) review		Recommended values of absorption cross section $135 < \lambda < 243$ nm	
4,8	$O_2 + N \rightarrow NO + O$		see reverse reaction	
4,9,9	$O_2 + NO + NO \rightarrow NO_2 + NO_2$			
	*Baulch, et al (1973) review	273-660	$3.3 \times 10^{-39} \exp(530/T)$ $cm^6 molecule^{-2} s^{-1}$ $k_1[NO]^2 [O_2] = -(1/2)d[NO]/dt$	±0.2
	Stedman, Niki (1973)	300	2.0×10^{-38} where $d[NO_2]/dt = 2k[NO]^2[O_2]$	±0.1
4,9,10	$O_2 + NO + NO_2 \rightarrow NO_2 + NO_3$		see reverse reaction	
4,9	$O_2 + NO \rightarrow NO_2 + O$		see reverse reaction	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Nntes and Reliability of log k
4,9M	$O_2 + NO + M \rightarrow NO_3 + M$			
	Baulch, et al (1973) review		No recommendation	
4,10	$O_2 + NO_2 \rightarrow NO + O_3$		see reverse reaction	
4,11	$O_2 + NO_3 \rightarrow NO_2 + O_3$		see reverse reaction	
4,12	$O_2 + N_2 \rightarrow N_2O + O$			
	*Baulch, et al (1973) review	1200-2000	$1.0 \times 10^{-10} \exp(-55.2 \times 10^3/T)$	±0.4 (a)
			(a) $k_f = k_r K_{eq}$	
4,18	$O_2 + H \rightarrow HO + O$		see reverse reaction	
4,18M	$O_2 + H + M \rightarrow HO_2 + M$			
	*This Survey (D.D.D.)	203-404	$6.7 \times 10^{-33} \exp(290/T)\ cm^6molecule^{-2}s^{-1}$	±.07 (a)
			M = Ar or He, $k(300) = 1.8 \times 10^{-32}$	
			Rel. M efficiencies: Ar(1.0), He(1.0), N_2(3.1), O_2(3.1), H_2O(25)	
		(a)	This evaluation is based on the 300 K data reviewed by Baulch, et al. (1972) and the recent studies by Hikida, et al (1971), Kurylo (1972) and Wong and Davis (1974).	
	Baulch, et al (1972) eval.	300-2000	$4.1 \times 10^{-33} \exp(500/T)$ M = Ar	±.2
			Rel. M eff.: Ar(1.0), He(1.0), N_2(1.3), O_2(1.3), H_2O(21)	
	Bishop, Dorfman (1970)	300	2.35×10^{-32} M = Ar	
	Hikida, Eyre, Dorfman (1971)	300	1.64×10^{-32} M = Ar	
	Ahumada, Michael, Osborne (1972)	300	0.75×10^{-32} M = He	
			Rel. M efficiencies: He(1.0), Ar(0.8)	
	Allen, Moortgat (1973)	115-300	$1.4(\pm0.14) \times 10^{-33} \exp(+700(\pm50)/T)$, M = Ar	
			Rel. M eff.: at 297K: Ar(1.0), He(0.97), H_2(1.28).	
	Kurylo (1972)	203-404	$6.7 \times 10^{-33} \exp(235/T)$	
			Rel. M eff.: Ar(1.0), He(1.0), N_2(3.4)	

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
	Wong, Davis (1974)	220-360	$6.8 \times 10^{-33} \exp(340/T)$	
			Rel. M efficiencies:	
			Ar(1.0), He(0.93) N_2(2.8), H_2(3.0), CH_4(21.5)	
	Westenberg, DeHaas (1972a)	300	1.9×10^{-32} M = Ar or He	
4,21	$O_2 + H_2 \rightarrow H + HO_2$		see reverse reaction	
4,21	$O_2 + H_2 \rightarrow HO + HO$			
	Baulch, et al (1972) review		no recommendation	
4,22	$O_2 + H_2O \rightarrow HO_2 + HO$			
	Baulch, et al (1972) review		no recommendation	
4,23	$O_2 + H_2O_2 \rightarrow HO_2 + HO_2$			
	Baulch, et al (1972) review		no recommendation	
4,24	$O_2 + HNO \rightarrow NO + HO_2$			
	Demerjian, et al (1974) review	300	$< 2.1 \times 10^{-20}$, $E/R > 5000K$	estimated
4,27	$O_2 + SO \rightarrow SO_2 + O$			
	*Breckenridge, Miller (1972) (WHB)	300	$< 8 \times 10^{-17}$	
	*Schofield (1973) review (WHB)	400-2500	$3.0 \times 10^{-13} \exp(-2800/T)$	±0.3
4,31	$O_2 + HS \rightarrow SO + HO$			
	Cupitt, Glass (1974)	295	$< 10^{-13}$	
4,35M	$O_2 + Cl + M \rightarrow ClOO + M$			
	Nicholas, Norrish (1968)	293	1.7×10^{-33} $cm^6molecule^{-2}s^{-1}$	
	Clyne and Coxon (1968)	300	$< 5.5 \times 10^{-33}$	
	Stedman (1968)	200-300	5.5×10^{-34}	(a)
			(a) As quoted by Clyne and Coxon (1968).	
4,47	$O_2 + CHO \rightarrow CO + HO_2$			
	*Washida, et al (1973)	297	$k/k(O + CHO) = 2.74 \pm 0.21 \times 10^{-2}$	
			yielding $k = 5.7 \pm 1.2 \times 10^{-12}$	
			(continued)	

Reactions of O_2 with H to CHO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Demerjian, et al (1974) review	300	1.7 x 10^{-13}	estimated
	Peeters, Mahnen (1973)	1400-1800	5 x 10^{-11}	
4.49	$O_2 + CH_3 \rightarrow CH_2O + HO$			
	Basco, et al (1972)	295	3 x 10^{-16}	estimated (a)
		a. Based on negative result and sensitivity limit. Other measurements at higher T suggest an appreciable activation energy.		
4.49M	$O_2 + CH_3(+M) \rightarrow CH_3O_2(+M)$			
	*Laufer, Bass (1974)	298	10^{12} x k P(N_2)/torr	(a)
			0.45 50	
			0.7 100	
			1.2 700	
	Basco, et al (1972)	295	5.1 x 10^{-13}	(b)
			2.6 x 10^{-31} cm^{6}molecule^{-2}s^{-1} $M = N_2$	(c)
	Van den Bergh, Callear (1971)	295	1.8 x 10^{-12} preliminary	(b)
			6 x 10^{-31} cm^{6}molecule^{-2}s^{-1} $M = C_3H_8$ preliminary	(c)
			(a) Values are based on k($CH_3 + CH_3$) = 9.5 x 10^{-11}, given in Bass, Laufer (1973).	
			(b) 2nd order high pressure limit.	
			(c) 3rd order low pressure limit.	
4.50	$O_2 + CH_3O \rightarrow . . .$		see $CH_3O + O_2$	
5.M	$O_2(^1\Delta) + M \rightarrow O_2 + M$			
	*Hampson, et al. (1973) review	285-322	2.2 x 10^{-18} $(T/300)^{0.8}$, $M = O_2$	±0.1
		300	<2 x 10^{-20}, $M = N_2$	
	*Breckenridge, Miller (1972) (WHB)	300	< 2 x 10^{-15} $M = SO_2$	(a)
			(continued)	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Collins, et al (1973)	300	1.4×10^{-19}, $M = N_2$	±0.06
	Fisher, McCarty (1966) (WHB)	300	$< 3 \times 10^{-16}$ $M = CO$	(a)
			(a) total rate, quenching and reaction	
	Huestis, et al. (1974)	77	$1.0 \pm 0.1 \times 10^{-18}$ $M = O_2$	(b)
			(b) Liquid phase. When combined with gas phase data of Findlay and Snelling (1971a) (summarized in Hampson, et al. (1973)	
			$k = 2.2 \times 10^{-18} (T/300)^{0.5}$	
5,7	$O_2(^1\Delta) + O_3 \rightarrow 2O_2 + O$			
	Clark, Jones, Wayne (1970)	195-439	$6.6 \times 10^{-13} \exp(-1560/T)$	±0.24
	Findlay, Snelling (1971)	283-321	$4.5 \times 10^{-11} \exp(-2830/T)$	±0.11
	Becker, et al (1972)	296-360	$6.0 \times 10^{-11} \exp(-2850/T)$	±0.17
	Collins, et al (1973)	300	4.4×10^{-15}	±0.11
	Schofield (1972) review	283-321	$4.5 \times 10^{-11} \exp(-2830/T)$	±0.11
5,27	$O_2(^1\Delta) + SO \rightarrow O_2 + SO(^1\Delta)$			
	Breckenridge, Miller (1972) (WHB)	300	$3.5 \pm 0.36 \times 10^{-13}$	
6,M	$O_2(^1\Sigma) + M \rightarrow O_2 + M$			
	*Hampson, et al. (1973) review	300	1.5×10^{-16}, $M = O_2$	±0.12
			$2.0 \times 10^{-15} = N_2$	±0.1
			4×10^{-12}, $M = H_2O$	±0.18
7,hv	$O_3 + h\nu \rightarrow O(^3P) + O_2(^3\Sigma^-)$			
	*Hampson, et al. (1973) review		$\phi = 1$, $450 < \lambda < 750$ nm - Chappuis bands	
			$\phi = 0$ $250 < \lambda < 350$ nm	
	Johnston (1973)		$k = 3.39 \times 10^{-4} s^{-1}$ (Daylight)	
			($450 < \lambda < 750$nm - Chappuis bands)	

Reactions of $O_2(^1\Delta)$, $O_2(^1\Sigma)$, and of O_3

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
7,hv	$O_3 + hv \to O(^3P) + O_2(^1\Delta$ or $^1\Sigma)$			
	*Hampson, et al. (1973) review		$\phi = 1$, 310< λ <350 nm - Huggins bands	
			$\phi = 0$, λ< 310 nm	
7,hv	$O_3 + hv \to O(^1D) + O_2(^1\Delta)$			
	*Hampson, et al. (1973) review		$\phi = 1$, 250< λ <310 nm - Hartley bands	
			$\phi = 0$, λ >310 nm	
	Lin, DeMore (1973)		Results consistent with above recommendation.	
7,hv	$O_3 + hv \to O(^1D) + O_2(^1\Sigma_g^+)$			
	*Hampson, et al. (1973) review		$\phi = 0$, 250< λ <350 nm	
7,M	$O_3 + M \to O + O_2 + M$		see reverse reaction	
7,8	$O_3 + N \to NO + O_2$			
	*Baulch, et al (1973) review	300	5.7×10^{-13}	±0.2
7,9	$O_3 + NO \to NO_2 + O_2$ (f)			
4,10	$O_2 + NO_2 \to NO + O_3$ (r)			
	*Hampson, et al (1973) review	198-330	$k_f = 9 \times 10^{-13} \exp(-1200/T)$ $cm^3 molecule^{-1} s^{-1}$	±0.11
	Stedman, Niki (1973)	298	$k_f = 1.73 \pm 0.1 \times 10^{-14}$	±0.2
	Baulch, et al (1973) review	200-350	$k_f = 1.5 \times 10^{-12} \exp(-1330/T)$	±0.2
		200-350	$k_r = k_f/K_{eq} = 2.8 \times 10^{-12} \exp(-25400/T)$	±0.2
	Ghormley, et al (1973)	298	$k_f = 1.41 \times 10^{-14}$	±0.01 precision
	Bemand, et al (1973)	300	$k_f = 1.81 \pm 0.13 \times 10^{-14}$	
	Becker, Schurath, Seitz (1974)	290	$k_f = 1.70 \times 10^{-14}$	
7,9	$O_3(001) + NO \to NO_2 + O_2$			
	Gordon, Lin (1973)	300	2.5×10^{-13}	(a)
	Kurylo, et al (1974)	300	2.7×10^{-13}	(a)

(a) Rate ~20 times faster than with $O_3(000)$. $O_3(010)$ may be reactive species

Reactions of O_3 with hν to NO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k	
7,10	$O_3 + NO_2 \rightarrow NO_3 + O_2$ (f)				
4,11	$O_2 + NO_3 \rightarrow O_3 + NO_2$ (r)				
	*This survey (R.F.H.)	220–340	$k_f = 1.2 \times 10^{-13} \exp(-2450/T)$	$\pm$0.1	
	Hampson, et al (1973) review	298	$k_f = 5 \times 10^{-17}$	$\pm$0.2	
	Johnston, Yost (1949)	286–302	$k_f = 9.8 \times 10^{-12} \exp(-3500/T)$		
	Baulch, et al (1973) review	286–302	$k_f = 9.8 \times 10^{-12} \exp(-3500/T)$	$\pm$0.3	
		300	$k_r = 7 \times 10^{-34}$ based on k_f	$\pm$0.3	
	Wu, Morris, and Niki (1973)	299	$k_f = 4.4 \times 10^{-17}$	$\pm$0.06	(a)
	Ghormley, et al (1973)	298	$k_f = 3.2 \times 10^{-17}$	$\pm$0.07	
	Davis, Prusazcyk, Dwyer, Kim (1974)	260–343	$k_f = 9.76 \pm 0.54 \times 10^{-14} \exp(-2427 \pm 140/T)$		
	Graham, Johnston (1974)	231–298	$k_f = 1.34 \pm 0.11 \times 10^{-13} \exp(-2466 \pm 30/T)$		
	Stedman, Niki (1973)	298	$k_f = 6.5 \pm 0.8 \times 10^{-17}$		
	Huie, Herron (1974a)	259–362	$k_f = 1.57 \pm 0.41 \times 10^{-13} \exp(-2509 \pm 76/T)$		
	Becker, Schurath, Seitz(1974)	289	$k_f = 3.24 \times 10^{-17}$		
		(a)	Revision, based on later experiments, of value reported by Stedman and Niki (1973)		
7,18	$O_3 + H \rightarrow HO + O_2$				
	*Hampson, et al (1973) review	300	2.6×10^{-11} cm^3 $molecule^{-1}s^{-1}$	$\pm$0.1 ?	
7,19	$O_3 + HO \rightarrow HO_2 + O_2$				
	*Hampson, et al (173) review	220–450	$1.6 \times 10^{-12} \exp(-1000/T)$	$\pm$0.3	
	DeMore (1973)	300	8×10^{-14}		
	DeMore (1974)	271–333	$k/k(HO + CO) = 16.8 \exp(-1230/T)$		
			$k = 2.4 \times 10^{-12} \exp(-1230/T)$	(b)	
	Anderson, Kaufman (1973)	220–450	$1.3 \times 10^{-12} \exp(-956/T)$		
			(continued)		

Reactions of O_3 with NO_2, H, and HO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
	Davis (1974)	300	$7.5 \pm 0.3 \times 10^{-14}$	
	Kurylo (1973)	298	6.5×10^{-14}	±0.06
	Simonaitis, Heicklen (1973c)	300	$k > 1.5 \times 10^{-14}$	(a)
			(a) Indirect; based on measurement of	
			$k\cdot[k(HO_2 + O_3)]/k(HO + HO_2)$	
			(b) Using value of k(HO + CO) from this survey.	
7.19	$O_3 + HO(v_1 > 0) \rightarrow$ products			
	Coltharp, Worley, Potter (1971)	300	$v_1(HO)$ $k/cm^3molecule^{-1}s^{-1}$	
			2 $1.9 \pm1.1 \times 10^{-12}$	
			3 $2.4 \pm0.9 \times 10^{-12}$	
			4 $2.8 \pm0.8 \times 10^{-12}$	
			5 $3.4 \pm0.7 \times 10^{-12}$	
			6 $5.3 \pm0.6 \times 10^{-12}$	
			7 $6.5 \pm0.5 \times 10^{-12}$	
			8 $6.7 \pm0.5 \times 10^{-12}$	
			9 $7.7 \pm0.3 \times 10^{-12}$	
7.20	$O_3 + HO_2 \rightarrow (HO + 2O_2)$			
	*This Survey (D.G.)	225-298	$1 \times 10^{-13} \exp(-1250/T)$	±0.3 a
	DeMore (1973)	300	3×10^{-15}	
	Anderson (1973)	220-450	$k/k(HO + O_3 \rightarrow HO_2 + O_2) \lesssim 0.1$	
	Lloyd (1974) review	200-500	$1.7 \times 10^{-13} \exp(-1400/T)$	$>\pm0.3$ a,b
	Simonaitis, Heicklen (1973b)	225-298	$k/(k_{ref})^{0.5} = 1.9 \times 10^{-8} \exp(-1000/T)$ $(cm^3molecule^{-1}s^{-1})^{0.5}$	±0.15 a
	DeMore, Tschuikow-Roux (1974)	273-332	$k/(k_{ref})^{0.5} = 1.1 \times 10^{-7} \exp(-1550 \pm 250/T)$	(a)

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
			(a) Reference reaction: $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$. Preferred value is based on meas. of Simonaitis and Heicklen and k_{ref} given in these tables. (b) Pre-exponential factor increased	
7,27	$O_3 + SO \rightarrow O_2 + SO_2$			
	Schofield (1973) review	223-303	$2.5 \times 10^{-12} \exp(-1050/T)$	±0.5
7,28	$O_3 + SO_2 \rightarrow SO_3 + O_2$			
	Daubendiek, Calvert (1974)	300	$k < 8 \times 10^{-24}$	
	Davis, Prusazcyk, Dwyer, Kim (1974)	300	$k < 2 \times 10^{-22}$	
7,32	$O_3 + H_2S \rightarrow$ products			
	Becker, Inocencio, Schurath (1974)	300	$< 2 \times 10^{-20}$	
	Glavas, Toby (1974)	298-343	$2 \times 10^{-12} \exp(-4000/T)$	
7,35	$O_3 + Cl \rightarrow ClO + O_2$			
	Watson (1974) review	300	$1.85 \pm 0.36 \times 10^{-11}$	±0.1
7,36	$O_3 + ClO \rightarrow OClO + O_2$ $\rightarrow ClOO + O_2$			
	Watson (1974) review	300	$< 5 \times 10^{-15}$	
7,45	$O_3 + CO \rightarrow CO_2 + O_2$			
	Arin, Warneck (1972)	296	$< 4 \times 10^{-25}$	
7,56	$O_3 + CH_4 \rightarrow$ products			
	Dillemuth, et al (1960)	310-340	$2.7 \times 10^{-13} \exp(-7700/T)$	
7,57	$O_3 + C_2H_4 \rightarrow$ products			
	*Herron, Huie (1974)	235-362	$9.0 \times 10^{-15} \exp(-2560/T)$	±0.1
	Demerjian, et al (1974) review	300	2.7×10^{-18}	

(continued)

Reactions of O_3 with HO_2 to C_2H_4

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k
	DeMore (1969)	178-233	$3.2 \times 10^{-15} \exp(-2400/T)$	
	Stedman, et al (1973)	300	$1.55 \pm 0.15 \times 10^{-18}$	
	Davis (1974)	300	$1.6 \pm 0.2 \times 10^{-18}$	
	Becker, Schurath, Seitz (1974)	280-360	$1.2 \times 10^{-14} \exp(-2490 \pm 100/T)$	
7,59	$O_3 + C_3H_6$ -> products			
	*Herron, Huie (1974)	235-362	$6.1 \times 10^{-15} \exp(-1900/T)$	±0.1
	Demerjian et al (1974) review	300	1.0×10^{-17}	
	DeMore (1969)	183, 193, 300	$1.6 \times 10^{-15} \exp(-1600/T)$	(a)
	Stedman, et al (1973)	300	$1.25 \pm 0.1 \times 10^{-17}$	
	Becker, Schurath, Seitz (1974)	280-360	$1.1 \times 10^{-14} \exp(-1970 \pm 100/T)$	
			a) Includes 300 K point of Hanst et al (1958).	
7,59	O_3 + allene -> products			
	Toby, Toby (1974b)	273-343	$1.6 \times 10^{-15} \exp(-2750/T)$	±0.7 (a)
			(a) Mechanism reconsidered. Data in Toby and Toby (1974a)	
7,5	O_3 + 1-butene -> products			
	Huie, Herron (1974b)	225-363	$2.9 \pm 0.2 \times 10^{-15} \exp(-1686 \pm 20/T)$	
7,59	O_3 + cis-2-butene -> products			
	Huie, Herron (1974b)	225-363	$3.1 \pm 0.7 \times 10^{-15} \exp(-956 \pm 54/T)$	
7,59	O_3 + trans-2-butene -> products			
	Huie, Herron (1974b)	225-363	$6.0 \pm 1.0 \times 10^{-15} \exp(-1051 \pm 43/T)$	
7,59	O_3 + 1,3-butadiene -> products			
	Toby, Toby (1974b)	273-343	$1 \times 10^{-13} \exp(-2900/T)$	±0.5
	Becker, Schurath, Seitz (1974)	280-360	$5.4 \times 10^{-14} \exp(-2680/T)$	

Reactions of O_3 with C_2H_4 to 1,3-butadiene

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k
8,8M	$N + N + M \rightarrow N_2 + M$			
	*Baulch, et al (1973) review	100-600	$8.3 \times 10^{-34} \exp(+500/T) cm^6 molecule^{-2}s^{-1}$, $(M = N_2)$	± 0.2 (200-600) <0.2 ($T<200K$)
			where $-d[N]/dt = 2k[N]^2[M]$	
	Taylor (1974) review	2000-10000	$7.6 \times 10^{-32}\ T^{-1/2}$ $M = N_2$ $3.0 \times 10^{-32}\ T^{-1/2}$ $M = O_2, O, NO$ $6.5 \times 10^{-27}\ T^{-3/2}$ $M = N$	
8,9	$N + NO \rightarrow N_2 + O$ (f)			
1,12	$O + N_2 \rightarrow N + NO$ (r)			
	*Baulch, et al (1973) review	300-5000	$k_f = 2.7 \times 10^{-11}$	± 0.1 (a)
		2000-5000	$k_r = 1.3 \times 10^{-10} \exp(-38000/T)$	± 0.3
			(a) Uncertainty increases to ± 0.3 for $T > 2000$. k_f based on 300 K data and $k_r(T > 2000)$.	
	Taylor (1974) review	2000-10000	$k_f = 2.7 \times 10^{-11}$	
8,10	$N + NO_2 \rightarrow N_2O + O$			
	Clyne (1974)	300	1.4×10^{-12}	tentative (a,b)
			(a) Believed to be sole reaction channel. (b) Preferred over earlier work reviewed in Baulch, et al (1973), which suggested several reaction channels.	
8,19	$N + HO \rightarrow NO + H$			
	*Baulch, et al (1973) review	300	5.3×10^{-11}	± 0.3 (a)
			(a) Based on $k/k(O + HO \rightarrow O_2 + H) = 1.4$	
8,37	$N + OClO \rightarrow NO + ClO$			
	Watson (1974) review	298	$k < 6 \times 10^{-13}$	preliminary value

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and reliability of log k
9,hv	$NO + h\nu$			
	Hampson, et al (1973a) review		Recommended values of oscillator strengths	
			from which absorption cross sections can be	
			derived are given for β, γ, δ, and ϵ bands.	
			Recommended values of absorption cross section	
			$106 < \lambda < 135$ nm.	
			No recommended quantum yield values.	
9,M	$NO + M \rightarrow N + O + M$			
	*Baulch, et al (1973) review	4200–6700	Insufficient data for a reliable recommendation.	
			Use, with caution:	
			$6.6 \times 10^{-4} T^{-1.5} \exp(-75.5 \times 10^{3}/T)$ cm^3 $molecule^{-1}s^{-1}$	
			($M = Ar, O_2, N_2$)	
			$k(M = NO, N, O)/k(Ar) \sim 18$	
9,9	$NO + NO \rightarrow N + NO_2$			
	Baulch, et al (1973) review		Endothermic. Unimportant compared to	
			$NO + NO \rightarrow N_2O + O$	
9,9	$NO + NO \rightarrow N_2O + O$		see reverse reaction	
9,9,4	$NO + NO + O_2 \rightarrow NO_2 + NO_2$		see $O_2 + NO + NO \rightarrow NO_2 + NO_2$	
9,10,22	$NO + NO_2 + H_2O \rightarrow 2HNO_2$			
	Hampson, et al (1973) review	300	$<1.1 \times 10^{-55}$ cm^9 $molecule^{-3}s^{-1}$	
			where k is defined as:	
			$-d[NO_2]/dt = k[NO][NO_2][H_2O]^2$	
			main reaction probably is heterogeneous	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9.11	$NO + NO_3 \rightarrow 2NO_2$			
	*Harker, Johnston (1972)	300	8.7×10^{-12}	
	(D.G., D.D.D.)			
	Baulch, et al (1973) review	300	$\sim 2 \times 10^{-11}$	±0.7 estimate
	Johnston (1966) review	300	8.3×10^{-12}	
		Temperature effect is probably zero or very small.		
9.16	$NO + NH_2 \rightarrow N_2 + H_2O^*$			
	Gehring, et al (1973)	300	8×10^{-12}	±0.1
	Gordon, et al (1971)	300	2.7×10^{-11}	
9.18M	$NO + H + M \rightarrow HNO + M$			
	*This survey (DG)	220-400	$2.1 \times 10^{-32} \exp(300/T)$	±0.2
	Baulch, et al (1973) review	230-700	$1.5 \times 10^{-32} \exp(300/T)$ $cm^6 molecule^{-2} s^{-1}$ $M = H_2$	±0.2
	Atkinson, Cvetanovic (1973)	286-390	$2.5 \times 10^{-32} \exp(270/T)$ $M = H_2$	
	Allen, Moortgat (1973)	180-300	$5.6(\pm 0.6) \times 10^{-33} \exp(+375(\pm 65)/T)$, $M = Ar$	
	Thrush (1973) review	230-700	$2 \times 10^{-32} \exp(+300/T)$, $M = H_2$	
9.19	$NO + HO \rightarrow NO_2 + H$			
	Baulch, et al (1973) review	298-633	$5.2 \times 10^{-12} \exp(-15.1 \times 10^3/T)$	±0.2 (298K) (a)
		based on $k = 5.8 \times 10^{-10} \exp(-740/T)$ for reverse reaction		increasing to
			(a) corrected expression	±0.3(633K)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9,19M	$NO + HO(+M) \rightarrow HNO_2(+M)$			
	Hampson, et al (1973a) review		Elevation/km k(T,M)	
		220	15 2.4×10^{-12}	±0.5 Relative
		217	20 1.5×10^{-12}	values from one
		222	25 8.9×10^{-13}	elevation to
		227	30 4.8×10^{-13}	another ±10%
		235	35 2.6×10^{-13}	$M = N_2$
		250	40 1.1×10^{-13}	
		260	45 5.9×10^{-14}	
	Baulch, et al (1973) review	273-395	$2.2 \times 10^{-32} \exp(+1110/T)$ $cm^6 molecule^{-2} s^{-1}$ M=He (3rd order low pressure limit)	±0.2 at 300K inc. to ±0.3 at 395 K
		300	2×10^{-12} $cm^3 molecule^{-1} s^{-1}$ (2d order high pressure limit)	±0.3
	Anderson, et al. (1974)	295,439	$5.8 \pm 1.2 \times 10^{-31} \times (295/T)^{+2.4}$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2$ (3rd order low pressure limit) Relative efficiencies: N_2(1.0), Ar(0.58), He(0.57)	
	Howard, Evenson (1974)	296	$7.8 \pm 1.2 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2$ (3rd order low pressure limit) Relative efficiencies: N_2(1.0), Ar(0.56), He(0.51)	
	Cox (1974a)	294	$k/k(HO + CO) = 40 \pm 7$ $k = 5.6 \pm 1 \times 10^{-12}$ $cm^3 molecule\ s^{-1}$ (a) 2nd order rate constant, [M] = 1 atm $N_2 + O_2$ (b) Based on k(HO + CO), this survey	(a,b)

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Wayne (1974)	300	$7 \pm 2 \times 10^{-31}$ cm^{6}molecule^{-2}s^{-1}, M = Ar	
			$15 \pm 5 \times 10^{-31}$, M = N_2	
			(3rd order low pressure limits)	
	Gordon, Mulac (1974)	435	$7.5 \pm 0.3 \times 10^{-12}$ cm^{3}molecule^{-1}s^{-1}	
			(2nd order rate constant at 1 atm. H_2O vapor)	
9.20	$NO + HO_2 \rightarrow NO_2 + OH$			
	* This survey (D.D.D.)	300	2×10^{-13}	±0.5
	Lloyd (1974) review	300	1.7×10^{-13}, $E/R < 2000$	±0.3
	Payne, Stief, and Davis (1973)	300	4×10^{-13}	±0.5 (a,b,c)
	Simonaitis and Heicklen (1973a)	300	$> 1.5 \times 10^{-13}$	±0.5 (a)
	Baulch, et al (1973) review	300	3×10^{-13}	±0.8
	Cox (1974b)	298	$1.6 \pm 0.4 \times 10^{-12}$	(a,c)
		(a)	Relative rate measurement. Value based on $k(HO_2 + HO_2)$ this survey.	
		(b)	Relative rate measurement. Reference reaction: $HO_2 + SO_2 \rightarrow SO_3 + HO$ (and ultimately $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$).	
		(c)	Recalculated.	
9.20M	$NO + HO_2 + M \rightarrow HONO_2 + M$			
	Cox (1974b)	298	$1.8 \pm 0.4 \times 10^{-13}$ cm^{3}molecule^{-1}s^{-1}	(a,b,c)
			(a) 2d order rate constant, [M] = 1 atm. $N_2 + O_2$	
			(b) Relative rate measurement. Value based on $k(HO_2 + HO_2)$ this survey.	
			(c) Recalculated.	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9,21	$NO + H_2 \rightarrow HNO + H$			
	Baulch, et al (1973) review	2000	5.3×10^{-18} cm^3 $molecule^{-1} s^{-1}$	± 0.2 (a)
			(a) No data. Value based on reverse rate	
9,22	$NO + H_2O \rightarrow HNO + HO$			
	Baulch, et al (1973) review	2000	4×10^{-18}	± 0.2 (a)
			(a) No data. Value based on reverse rate. (corrected)	
9,23	$NO + H_2O_2 \rightarrow HO + HNO_2$			
	*Hampson, et al (1973) review	300	$< 5 \times 10^{-20}$	
		500	$\sim 2 \times 10^{-20}$	
	Gray, et al (1972)	300	$< 5 \times 10^{-20}$	
9,35M	$NO + Cl + M \rightarrow ClNO + M$			
	*Watson (1974) review	300	$1.1 \pm 0.2 \times 10^{-31}$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2$	
			Rel. efficiencies: $N_2(1.0)$, $O_2(1.2)$	
9,36	$NO + ClO \rightarrow NO_2 + Cl$			
	*Watson (1974) review	298	$1.7 \pm 0.2 \times 10^{-11}$	
9,37	$NO + OClO \rightarrow NO_2 + ClO$			
	*Watson (1974) review	298	$3.4 \pm 0.5 \times 10^{-13}$	

Reactions of NO with H_2 to OClO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
9,49M	NO + CH_3 (+M) -> CH_3NO (+M)			
	Laufer, Bass (1974)	298	10^{11} x k $P(N_2)$/torr	(a)
			.3 50	
			.45 100	
			1.1 700	
	Basco, et al (1970)	298	4 x 10^{-12}	(b)
	Van den Bergh, Callear (1971)	295	1.7 x 10^{-11}	(b)
			(a) Values are based on $k(CH_3 + CH_3)$ = 9.5 x 10^{-11} given in Bass, Laufer (1973).	
			(b) 2nd order high pressure limit.	
9,50	NO + CH_3O -> . . .		see CH_3O + NO -> . . .	
9,51	NO + CH_3O_2 -> CH_3O_2NO (a) -> CH_2O + HONO (b) -> CH_3O + NO_2 (c)			
	Demerjian, et al (1974) review	300	k_c = 3.3 x 10^{-12} exp(-500/T)	estimate
	Pate, Finlayson, Pitts (1974)	296	Reaction proceeds exclusively through channel (c)	
	Simonaitis, Heicklen (1974)	298	$k_c/k = 0.80 \pm 0.15$ $(k = k_a + k_b + k_c)$	

Reactions of NO with CH_3 and CH_3O_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
10,hv	NO_2 + hv -> NO + O			
	*Bayes (1974)		λ/nm $\phi(O(^3P))$	
			295-398 1.0 - 0.0008(λ - 275)	(a)
			398 0.90 ± 0.05	
			400 0.76 ± 0.04	
			405 0.37 ± 0.02	
			410 0.14 ± 0.01	
			(a) Based on analysis of data in Jones and Bayes (1973)	
	*Hampson, et al (1973a) review		absorption cross section data 108 < λ < 500 nm	
10,M	NO_2 + M -> NO + O + M		see reverse reaction	
10,10	NO_2 + NO_2 -> NO + NO_3			
	Baulch, et al (1973) review		No recommendation	
10,10	NO_2 + NO_2 -> NO + NO + O_2			
	Baulch, et al (1973) review	600-2000	$3.3 \times 10^{-12} \exp(-13540/T)$	±0.15 (600-1000 K)
			$k_1[NO_2]^2 = -(1/2)d[NO_2]/dt$	increasing to 0.3 at 2000 K
10,10M	NO_2 + NO_2 + M -> N_2O_4 + M (f)			
	N_2O_4 + M -> NO_2 + NO_2 + M (r)			
	Baulch, et al (1973) review	250-350	$k_f = 4.7 \times 10^{-35} \exp(-860/T)$ cm^{6}molecule^{-2}s^{-1} M = N_2	±0.15 (a)
			(a) $k_f = k_r K_{eq}$	
	Baulch, et al (1973) review	250-350	$k_r = 4.2 \times 10^{-7} \exp(-5550/T)$ M = N_2	±0.15
	Schofield (1973) review	250-350	$k_r = 3.3 \times 10^{-7} \exp(-5540/T)$ M = N_2	±0.15
10,11	NO_2 + NO_3 -> NO_2 + O_2 + NO (f)			
4,9,10	O_2 + NO + NO_2 -> NO_2 + NO_3 (r)			
	*Baulch, et al (1973) review	300-850	$k_f = 2.3 \times 10^{-13} \exp(-1000/T)$	±0.4 (a)
		300-500	$k_r = k_f/K_{eq} = 8 \times 10^{-41} \exp(400/T)$cm^{6}molecule^{-2}s^{-1}	±0.4

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Johnston (1966) review	300–1100	$k_f = 3.8 \times 10^{-13} \exp(-2200/T)$	
			(a) Based on $N_2O_5 + M \rightarrow NO_2 + NO_3 + M$ and $2NO_2 \rightarrow 2NO + O_2$	
10,11M	$NO_2 + NO_3 (+M) \rightarrow N_2O_5 (+M)$			
	*This survey (HSJ)		Elevation/km k (T,M) Log (M)	
			cm^{3}molecule^{-1}s^{-1}	
		220	15 1.9×10^{-12} 18.60	
		217	20 1.1×10^{-12} 18.27	
		222	25 6.6×10^{-13} 17.93	
		227	30 4.5×10^{-13} 17.53	
		235	35 2.7×10^{-13} 17.26	
		250	40 1.5×10^{-13} 16.92	
		260	45 7.1×10^{-14} 16.60	
10,11M	$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$ (f)			
14,M	$N_2O_5 + M \rightarrow NO_2 + NO_3 + M$ (r)			
	Baulch, et al (1973) review	300	$k_f = 2.8 \times 10^{-30}$ cm^{6}molecule^{-2}s^{-1}	±0.3 (a)
		300	3.8×10^{-12} cm^{3}molecule^{-1}s^{-1}	±0.4 (a)
			(2d order high pressure limit)	
		300–340	$k_r^{\cdot} = 2.2 \times 10^{-5} \exp(-9700/T)$ cm^{3}molecule^{-1}s^{-1}	±0.3 (a)
		273–300	$5.7 \times 10^{14} \exp(-10600/T)$ s^{-1}	±0.4 (a)
			(limiting first order expression)	
			(a) $k_f = K_{eq} k_r$. $M = N_2O_5 + NO$	
10,17	$NO_2 + NH_3 \rightarrow NH_2 + HNO_2$			
	Bedford, Thomas (1972)	615–660	$6.7 \times 10^{-12} \exp(-13900/T)$	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$		Notes and Reliability of log k
10.18	$NO_2 + H \rightarrow HO + NO$				
	*Hampson, et al (1973) review	300	4.8×10^{-11}		±0.1
	Baulch, et al (1973) review	298-633	$5.8 \times 10^{-10} \exp(-740/T)$		±0.2 at 298K
					increasing to ±0.3
					at 633K
10.19M	$NO_2 + HO (+M) \rightarrow HNO_3 (+M)$				
	*Tsang (1973) review		Elevation/km	k(T,M)	
	Summarized in Hampson (1973a)				
		220	15	3.0×10^{-12}	±0.3 Relative
		217	20	2.2×10^{-12}	values from one
		222	25	1.4×10^{-12}	elevation to
		227	30	8.9×10^{-13}	another ±5%
		235	35	5.2×10^{-13}	$M = N_2$
		250	40	2.6×10^{-13}	
		260	45	1.4×10^{-13}	
	For tabulated values of k(T,M) at intervals of 20 degrees Kelvin and 0.5 in $\log_{10}[M]$. see separate table				
10.19M	$NO_2 + HO + M \rightarrow HNO_3 + M$ (f)				
26,M	$HNO_3 + M \rightarrow HO + NO_2 + M$ (r)				
	Baulch, et al (1973) review	273-400	$k_f = 3.6 \times 10^{-32} \exp(+1100/T) cm^6 molecule^{-2}s^{-1}$		±0.2
			M = He		
		800-1200	$k_r = 2.7 \times 10^{-9} \exp(-15400/T) cm^3 molecule^{-1}s^{-1}$		±0.4
			M = Ar		
		300	$k_f = 8 \times 10^{-12} cm^3 molecule^{-1}s^{-1}$		±0.4
			(2d order high pressure limit)		

(continued)

Reactions of NO_2 with H and HO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k
	Anderson, et al. (1974)	295–450	$k_f = 2.3 \pm 0.5 \times 10^{-30} \times (295/T)^{+2.5}$ $cm^6 molecule^{-2}s^{-1}$	
			$M = N_2$	
			Relative efficiencies: $N_2(1.0)$, Ar(0.43), He(0.43)	
	Howard, Evenson (1974)	296	$k_f = 2.9 \pm 0.4 \times 10^{-30}$ $M = N_2$	
	Gordon, Mulac (1974)	435	$k_f = 5.3 \times 10^{-12}$ $cm^3 molecule^{-1}s^{-1}$	
			(2nd order rate constant at 1 atm. H_2O vapor)	
	Wayne (1974)	300	$15 \pm 5 \times 10^{-31}$ $cm^6 molecule^{-2}s^{-1}$, $M = Ar$	
			$26 \pm 10 \times 10^{-31}$, $M = N_2$	
10,20	$NO_2 + HO_2 \rightarrow HNO_2 + O_2$			
	*This survey (D.G.)	300	$\sim 3 \times 10^{-14}$	(a)
	Simonaitis, Heicklen (1974)	298	$k/k(HO_2 + NO) = 0.14 \pm 0.02$	
			$k > 3 \times 10^{-13}$	(b)
	Cox (1974b)	298	$1.6 \pm 0.4 \times 10^{-13}$	(b,c)
			(a) Recommendation based on ratio in Simonaitis, Heicklen (1974) and $k(HO_2 + NO)$ from this survey.	
			(b) Interpretation of photolysis experiments. Value based on $k(HO_2 + HO_2)$ this survey.	
			(c) Recalculated.	
10,28	$NO_2 + SO_2 \rightarrow SO_3 + NO$			
	Davis (1974)	300	$k < 2 \times 10^{-24}$	
10,35M	$NO_2 + Cl + M \rightarrow NO_2Cl + M$			
	Watson (1974) review	298	7.2×10^{-31}	preliminary value

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
10,49	$NO_2 + CH_3 \rightarrow CH_3O + NO$			
	Glanzer, Troe (1973) review	300-1400	3.3×10^{-11} (a) Based on $k/k(CH_3 + NO) = 3.3$ at room temperature and on shock wave pyrolysis of CH_3NO_2	±0.25 (a)
10,49M	$NO_2 + CH_3 (+M) \rightarrow CH_3NO_2 (+M)$			
	Glanzer, Troe (1973) review	295	2.8×10^{-11} $cm^3molecule^{-1}s^{-1}$ (a) Based on high pressure limit rate ratio $k/k(CH_3 + NO) = 1.7$	±0.1 (a)
10,49M	$NO_2 + CH_3 + M \rightarrow CH_3NO_2 + M$			
	Glanzer, Troe (1973) review	900-1400	6.9×10^{-31} $cm^6molecule^{-2}s^{-1}$, M = Ar (a) $k_f = k_r K_{eq}$	(a)
10,50	$NO_2 + CH_3O \rightarrow . . .$		see $CH_3O + NO_2 \rightarrow . . .$	
10,51	$NO_2 + CH_3O_2 \rightarrow CH_3O_2NO_2$ (a) $\rightarrow CH_2O + HONO_2$ (b) $\rightarrow CH_3O + NO_3$ (c)			
	*Heicklen (1973) review	298	$k_a/k = 0.75 \pm 0.05$ $k_b/k = 0.25 \pm 0.1$ $k_c/k < 0.1$	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
11,hv	$NO_3 + hv \rightarrow NO + O_2$			
	*Johnston (1974) review		Very strong absorption spectrum 600-700nm. Pre-dissociated spectra. Alternative products (NO_2 + O) energetically impossible at wave lengths above 576 nm. Destruction of NO_3 observed; primary products not observed.	
	See ERRATA			
	Johnston (1973)		$2.64 \times 10^{-2}s^{-1}$ (450-578nm) Daylight	
			$4.34 \times 10^{-2}s^{-1}$ (579-680nm) Daylight	
11,M	$NO_3 + M \rightarrow NO_2 + O + M$		see reverse reaction	
11,11	$NO_3 + NO_3 \rightarrow 2NO_2 + O_2$			
	*Johnston (1966) review	600-1100	$4.3 \times 10^{-12} \exp(-3850/T)$	± 0.3 (a)
	*Baulch, et al (1973) review	293-309	$5 \times 10^{-12} \exp(-3000/T)$	± 0.5 (a)
			(a) $-d[NO_3]/d4 = 2k[NO_3]^2$. Based on rate of O_3 decomp. in presence of N_2O_5	
11,22	$NO_3 + H_2O \rightarrow HNO_3 + HO$			
	Baulch, et al (1973) review	300	2.3×10^{-26}	± 0.3 (a)
			(a) $k_f = k_r K_{eq}$	
11,28	$NO_3 + SO_2 \rightarrow NO_2 + SO_3$			
	Daubendiek, Calvert (1974)	300	$k < 7 \times 10^{-21}$	
	Davis (1974)	300	$k < 1 \times 10^{-14}$	preliminary
12,M	$N_2 + M \rightarrow N + N + M$			
	*Baulch, et al (1973) review	6000-15000	$6.1 \times 10^{-3}T^{-1.6}\exp(-113{,}200/T)$cm^{3}molecule^{-1}s^{-1} $M = N_2$	± 0.5
12,19	$N_2 + HO \rightarrow N_2O + H$			
	*Baulch, et al (1973) review	700-2500	$5.4 \times 10^{-12} \exp(-40.4 \times 10^3/T)$	± 0.2 (a)
			(a) $k_f = k_r K_{eq}$ (corrected expression)	

Reactions of NO_3 and N_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
13,M	$N_2O + M \rightarrow N_2 + O + M$		see reverse reaction	
13,18	$N_2O + H \rightarrow N_2 + HO$			
	Baulch, et al (1973) review	700-2500	$1.26 \times 10^{-10} \exp(-7600/T)$	± 0.2
	Baldwin, et al (1973)	773	4.3×10^{-15}	± 0.15
13,19	$N_2O + HO \rightarrow$ products			
	Gordon, Mulac (1974)	440	$< 2 \times 10^{-14}$	
13,36	$N_2O + ClO \rightarrow$ products			
	Walker (1972)	587	$k < 7 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1974) review.	
13,45	$N_2O + CO \rightarrow$ products			
	Milks, Matula (1973)	1169-1655	$3.5 \times 10^{-13} \exp(-8650/T)$	
14,hν	$N_2O_5 + h\nu \rightarrow . . .$			
	*Jones, Wulf (1937)		λ/nm Absn. cross sect./cm^{2}molecule^{-1}, base e	Scatter: 25%
			285 4.6×10^{-20}	Reliability
			290 3.8×10^{-20}	unknown
			300 2.3×10^{-20}	
			310 1.2×10^{-20}	
			320 0.69×10^{-20}	
			330 0.39×10^{-20}	
			340 0.24×10^{-20}	
			350 0.17×10^{-20}	
			360 0.095×10^{-20}	
	Holmes, Daniels (1934)		265 $18. \times 10^{-20}$	
			280 8.3×10^{-20}	
			>302 Zero	

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}		Notes and Reliability of log k
	Murphy (1969)		$0.5 \times \phi(-N_2O_5) = \phi(0) = 0.31$ $\lambda = 280$ nm		
			Meas. by Holmes, Daniels (1934) are consistent		
	Hampson, et al (1973a) review		Survey of photochemistry including data listed above.		
	Daubendiek, Calvert (1974)		Figure giving molar extinction coefficient vs λ. $250 < \lambda/\mathrm{nm} < 350$		
14,M	N_2O_5 (+M) -> NO_2 + NO_3 (+M)		Elevation/km	k/s^{-1}	
	*This survey (HSJ)	220	15	5.0×10^{-7}	±0.5
		217	20	1.8×10^{-7}	
		222	25	3.0×10^{-7}	
		227	30	5.5×10^{-7}	
		235	35	1.9×10^{-6}	
		250	40	1.6×10^{-5}	
		260	45	4.4×10^{-5}	
		Extrapolated from data taken between 273 and 353 K.			
14,M	N_2O_5 + M -> NO_2 + NO_3 + M		see reverse reaction		
14,22	N_2O_5 + H_2O -> 2HNO_3				
	Hampson, et al (1973) review	300	$k < 1 \times 10^{-20}$		
	Morris, Niki (1973)	298	$< 1.3 \times 10^{-20}$		
14,28	N_2O_5 + SO_2 -> products				
	Daubendiek, Calvert (1974)	300	$k < 4 \times 10^{-23}$		
	Davis (1974)	300	$k < 8 \times 10^{-24}$		
16,18M	NH_2 + H + M -> NH_3 + M				
	Baulch, et al (1973) review	2000-3000	1.2×10^{-33} exp(11200/T) cm^6 molecule^{-2}s^{-1}, M = Ar		±0.3 (a)
			(a) $k_f = K_{eq} k_r$		

Reactions of N_2O_5 and NH_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
16,19	$NH_2 + HO \rightarrow NH_3 + O$		see reverse reaction	
16,21	$NH_2 + H_2 \rightarrow NH_3 + H$			
	Baulch, et al (1973) review	800	$< 10^{-16}$ $k_f = k_{eq} k_r$	approximate
16,22	$NH_2 + H_2O \rightarrow NH_3 + HO$			
	Baulch, et al (1973) review		no data, no recommendation	
17,M	$NH_3 + M = NH_2 + H + M$			
	Baulch, et al (1973) review	2000-3000	$k = 1.5 \times 10^{-8} \exp(-42400/T)$ (M = Ar)	±0.3 (a)
			(a) To be used when $P(M) < 4$ atm.	
17,18	$NH_3 + H \rightarrow NH_2 + H_2$			
	Baulch, et al (1973) review	800	$< 10^{-16}$	approximate
17,19	$NH_3 + HO \rightarrow NH_2 + H_2O$			
	Hack, et al. (1974)	298-669	$5.3 \pm 0.8 \times 10^{-12} \exp(-920/T)$	
	Stuhl (1973a)	298	1.5×10^{-13}	±0.1
	Kurylo (1973)	298	4.1×10^{-14}	±0.06
	Gordon, Mulac (1974)	418	$4.3 \pm 0.5 \times 10^{-13}$	
	Smith, Zellner (1974b)	228-472	$2.3 \times 10^{-12} \exp(-800/T)$	(a)
			(a) Preliminary results were reported in Zellner and Smith (1974)	
17,36	$NH_3 + ClO \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1974) review.	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
18.18M	$H + H + M \rightarrow H_2 + M$ (f)			
21,M	$H_2 + M \rightarrow H + H + M$ (r)			
	Baulch, et al (1972) review	300	$k_f = 8.3 \times 10^{-33}\ cm^6molecule^{-2}s^{-1}$ $M = H_2$	±0.2
		1700-5000	$= 1.8 \times 10^{-30}\ T^{-1}$ $M = Ar$	±0.3
			Rel. efficiencies: $H_2(1.0)$, $Ar(0.25)$	
			$-d[H]/dt = 2k[H]^2[M]$	
		2500-5000	$k_r = 3.7 \times 10^{-10}\ exp(-48300/T) cm^3molecule^{-1}s^{-1}$,	±0.3
			$M = Ar$	
18,19	$H + HO \rightarrow H_2 + O$		see reverse reaction	
18,19M	$H + HO + M \rightarrow H_2O + M$ (f)			
22,M	$H_2O + M \rightarrow H + HO + M$ (r)			
	*Baulch, et al (1972) review	1000-3000	$k_f = 6.1 \times 10^{-26} T^{-2} cm^6molecule^{-2}s^{-1}$, $M = N_2$	±0.3
		2000-6000	$k_r = 5.8 \times 10^{-9}\ exp(-52900/T)\ cm^3molecule^{-1}s^{-1}$	±0.2
			$M = N_2$	
18,20	$H + HO_2 \rightarrow HO + HO$ (1f)			
19,19	$HO + HO \rightarrow H + HO_2$ (1r)			
18,20	$H + HO_2 \rightarrow H_2 + O_2$ (2)			
18,20	$H + HO_2 \rightarrow H_2O + O$ (3)			
	Baulch, et al (1972) review	290-800	$k_{1f} = 4.2 \times 10^{-10}\ exp(-950/T)$	±0.3 (a)
			$k_{1r} = k_{1f}/K_{eq} = 2.0 \times 10^{-11} exp(-20200/T)$	±0.3
		290-800	$k_2 = 4.2 \times 10^{-11}\ exp(-350/T)$	±0.4
			$k_{2r} = k_{2f}/K_{eq} = 9.1 \times 10^{-11}\ exp(-29100/T)$	±0.4
			k_3 = no recommendation	
	Lloyd (1974) review	300-1000	k_{1f} and k_2 - same as Baulch, et al	>±0.3 (a)
			$k_3 = 8.3 \times 10^{-11}\ exp(-500/T)$	>±0.5 (b)
			(continued)	

Reactions of H with H, HO, and HO_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Moortgat, Allen (1973)	297	$k_{1f} = 8.3 \times 10^{-12}$	? (c)
			$k_2 = 1 \times 10^{-11}$	? (c)
			$k_3 = 6.7 \times 10^{-12}$	? (c)
			(a) Reaction 1 and rate ratios control values for reactions 2 and 3.	
			(b) Temperature coefficient estimated.	
			(c) Secondary reaction in $H + O_2 + M$ systems, fit of concentration vs. time plots.	
18,22	$H + H_2O \rightarrow H_2 + HO$			
	Baulch, et al (1972) review	300-2500	$1.5 \times 10^{-10} \exp(-10250/T)$	±0.06 at 300K increasing to ±0.2 at high temp.
18,23	$H + H_2O_2 \rightarrow H_2 + HO_2$ (a) $\rightarrow HO + H_2O$ (b)			
	*Klemm, Payne, Stief (1974)	283-353	$k_a + k_b = 5.2 \pm 2.0 \times 10^{-12} \exp(-1400 \pm 140/T)$	
	Gorse, Volman (1974)	300	$k_a = 3.1 \pm 0.8 \times 10^{-15}$	
			$k_b = 5.7 \pm 1.4 \times 10^{-15}$	
	Hampson, et al (1973)	300-800	$k_a = 2.8 \times 10^{-12} \exp(-1900/T)$	(a)
			k_b no recommendation	(a)
			(a) Accepts recommendations of Baulch, et al (1972).	
	Meagher, Heicklen (1974)	298	$k_b/k_a = 1.3$	
18,24	$H + HNO \rightarrow H_2 + NO$			
	Hampson, et al (1973) review	211-703	$> 5 \times 10^{-14}$	±0.3
		2000	7×10^{-12}	±0.3

(continued)

Reactions of H with HO_2 to HNO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
	Baulch, et al (1973) review	300	$10^{-13} < k < 10^{-12}$	
		2000	8×10^{-12}	±0.2
18,25	$H + HNO_2 \rightarrow$ products			
	Hampson, et al (1973) review		No data	
	Baulch, et al (1973) review		No recommendation	
18,26	$H + HNO_3 \rightarrow$ products			
	Hampson, et al (1973) review	300	$< 1 \times 10^{-13}$	
	Chapman, Wayne (1974)	300	$< 2 \times 10^{-15}$	
	Baulch, et al (1973) review	300	$< 10^{-13}$	approximate upper limit
18,31	$H + HS \rightarrow H_2 + S$			
	Cupitt, Glass (1974)	295	$2.5 \pm 0.8 \times 10^{-11}$	
18,32	$H + H_2S \rightarrow H_2 + HS$			
	Kurylo, Peterson, Braun (1971)	190-464	$1.29 \times 10^{-11} \exp(-860/T)$	
18,37	$H + OClO \rightarrow HO + ClO$			
	*Watson (1974) review	298	$5.7 \pm 1.2 \times 10^{-11}$	
18,48	$H + CH_2O \rightarrow H_2 + CHO$			
	Ridley, et al (1972)	297	5.4×10^{-14}	±0.04
	Westenberg, de Haas (1972b)	297-652	$2.2 \times 10^{-11} \exp(-1890/T)$	
19,M	$HO + M \rightarrow H + O + M$			
	Baulch, et al (1972) review		no recommendation ($E/R > 50000$ K)	
19,19	$HO + HO \rightarrow H + HO_2$		see reverse reaction	
19,19	$HO + HO \rightarrow H_2 + O_2$			
	Baulch, et al (1972) review		no recommendation	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	Notes and Reliability of log k
19,19	$HO + HO \rightarrow H_2O + O$ (f)			
1,22	$O + H_2O \rightarrow HO + HO$ (r)			
	*Baulch, et al (1972) review	300-2000	$k_f = 1.0 \times 10^{-11} \exp(-550/T)$	±0.2
		300-2000	$k_r = 1.1 \times 10^{-10} \exp(-9240/T)$	±0.2
	Rawlins, Gardiner (1974)	1500-2000	$k_f = 9.1 \times 10^{-11} \exp(-3500/T)$	
	Westenberg, de Haas (1973a)	300	$k_f = 2.3 \times 10^{-12}$	±0.06
	McKenzie, et al. (1973)	298	$k_f = 2.1 \pm 0.5 \times 10^{-12}$	
	Clyne and Down (1974)	300	$k_f = 1.4 \pm 0.2 \times 10^{-12}$	
		300	$k_f = 1.7 \pm 0.6 \times 10^{-12}$	(a)
	Trainor, von Rosenberg (1974)	300	$k_f = 2.1 \pm 0.2 \times 10^{-12}$	
	Wilson (1972) review	300	$k_f = 2.57 \times 10^{-12}$	+0.1, −0.5
			(a) Evaluation based on authors' work and other recent data	
19,19M	$HO + HO + M \rightarrow H_2O_2 + M$ (f)			
23,M	$H_2O_2 + M \rightarrow HO + HO + M$ (r)			
	Baulch, et al (1972) review	700-1500	$k_f = 2.5 \times 10^{-33} \exp(+2550/T)\text{cm}^6\text{molecule}^{-2}\text{s}^{-1}$	±0.1 $700<T<950$K
			$M = N_2$; $-d[OH]/dt = 2k[OH]^2[M]$	increasing to
			$k_r = 2.0 \times 10^{-7} \exp(-22900/T)\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$,	±0.3 at 1500K
			$M = N_2$; $k_f = k_r K_{eq}$	
	Trainor, von Rosenberg (1974)	300	$k_f = 2.5 \pm 0.3 \times 10^{-31}$ $M = N_2$	
19,20	$HO + HO_2 \rightarrow H_2O + O_2$			
	*This survey (H.S.J.)		The range of values $2 \times 10^{-11} < k < 2 \times 10^{-10}$ $\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$ should be considered in models of the stratosphere	
	Baulch, et al (1972) review		no recommendation	
			(continued)	

Reactions of HO with HO and HO_2

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/\mathrm{cm^3 molecule^{-1} s^{-1}}$	Notes and Reliability of log k
	Kaufman (1964) review	300	$k > 1 \times 10^{-11}$	estimate
	Lloyd (1974) review	300-1000	$8.3 \times 10^{-11} \exp(-500/T)$	±0.3
	Hochanadel, et al (1972)	300	2×10^{-10}	
	DeMore, Tschuikow-Roux (1974)	300	2×10^{-10}	± 0.5 (a)
			(a) Adjusted value - based on reported ratio and values of $k(O_3 + HO)$ and $k(HO_2 + HO_2)$ in this survey.	
19.20	$HO + HO_2 \rightarrow H_2O_2 + O$			
	Baulch, et al (1972) review		no recommendation	
19.21	$HO + H_2 \rightarrow H_2O + H$			
	Baulch, et al (1972) review	300-2500	$3.6 \times 10^{-11} \exp(-2590/T)$ $\mathrm{cm^3 molecule^{-1} s^{-1}}$	±0.08 at 300 K ±0.2 at high temp.
	Wilson (1972) review	300-2000	$3.8 \times 10^{-11} \exp(-2600/T)$	±0.3
	Stuhl, Niki (1972)	298	7.1×10^{-15}	+0.06
	Westenberg (1973a)	298	7.6×10^{-15}	±0.04
		352	1.8×10^{-14}	
		403	3.2×10^{-14}	
		518	1.4×10^{-13}	
		628	3.6×10^{-13}	
		745	6.6×10^{-13}	
	Smith, Zellner (1974a)	210-460	$1.8 \times 10^{-11} \exp(-2330/T)$	
	Overend, et al. (1974)	300	$5.79 \pm 0.26 \times 10^{-15}$	
	Gardiner, et al (1974)	1350-1600	$8.7 \times 10^{-11} \exp(-3250/T)$	
	Greiner (1969)	300-500	$6.8 \times 10^{-12} \exp(-2020/T)$	±0.15

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
19,21	$HO + D_2 \rightarrow HDO + D$			
	Smith, Zellner (1974a)	210–460	$1.25 \times 10^{-11} \exp(-2590/T)$	
19,22	$HO + H_2O \rightarrow H_2O_2 + H$			
	Baulch, et al (1972) review		no recommendation	
19,23	$HO + H_2O_2 \rightarrow H_2O + HO_2$			
	*Hampson (1973) quoting	300–800	$1.7 \times 10^{-11} \exp(-910/T)$	± 0.2
	Baulch, et al (1972) review			
	Gorse, Volman (1972)	300	$k/k(HO + CO) = 8.13$	
	Meagher, Heicklen (1974)	298	$k/k(HO + CO) = 4.1 \pm 0.6$	
19,24	$HO + HNO \rightarrow H_2O + NO$			
	Hampson, et al (1973) review	1600–2100	7×10^{-11}	± 0.7
	Baulch, et al (1973) review	2000	6×10^{-11}	± 0.2
19,25	$HO + HNO_2 \rightarrow H_2O + NO_2$			
	Cox (1974a)	294	$k/k(HO + CO) = 15 \pm 1$	(a)
			$k = 2.1 \pm 0.2 \times 10^{-12}$	
			(a) Based on k(HO + CO), this survey.	
	Demerjian, et al (1974) review	300	6.8×10^{-12}	estimated, no data
	Baulch, et al (1973) review	300	1.3×10^{-13}	± 0.6 estimated
19,26	$HO + HNO_3 \rightarrow H_2O + NO_3$			
	*This survey (H.S.J.)	220–270	1.3×10^{-13}	
	Hampson, et al (1973) review	300–650	$6 \times 10^{-13} \exp(-400/T)$	± 0.5
	Johnston (1974) review	300–700	$(1.5 \text{ to } 2.0) \times 10^{-13}$	± 0.2
	Wayne (1974)	300	1.5×10^{-13}	approximate
	Baulch, et al (1973) review	300	1.3×10^{-13}	± 0.3

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}		Notes and Reliability of log k
	Smith, Zellner (1974b)	240-406	$8 \pm 2 \times 10^{-14}$		(a,b)
			(a) Value recommended by authors for T ≤ 298K.		
			(b) Preliminary results were reported in Zellner and Smith (1974).		
19,28M	$HO + SO_2 + M \rightarrow HSO_3 + M$				
	Davis (1974)	300	10^{13} x k	P(He)/torr	
			0.87 ± 0.06	50	
			1.6 ± 0.1	150	
			2.7 ± 0.2	500	
			10^{13} x k	P(Ar)/torr	
			1.37 ± 0.06	50	
			2.50 ± 0.3	150	
			3.71 ± 0.3	500	
			10^{13} x k	P(N_2)/torr	
			0.80 ± 0.08	5	
			1.43 ± 0.14	10	
			2.44 ± 0.3	20	
			~ 9 (a)	760	
			Effective bimolecular rate constant in cm^{3}molecule^{-1}s^{-1}		
			(a) Extrapolated value.		
	Wayne (1974)	300	$4.5 \pm 1.5 \times 10^{-31}$ cm^{6}molecule^{-2}s^{-1}	, M = Ar	
			$7.2 \pm 2.6 \times 10^{-31}$	, M = N_2	
	Cox (1974a)	294	$k/k(HO + CO) = 4 \pm 0.5$		(a,b)
			$k = 5.6 \pm 0.8 \times 10^{-13}$		
			(a) 2nd order rate constant, [M] = 1 atm. $N_2 + O_2$		
			(b) Based on k(HO + CO), this survey.		
			(continued)		

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
	Gordon, Mulac (1974)	435	1.8×10^{-12} $cm^3molecule^{-1}s^{-1}$ (2d order rate constant at 1 atm. H_2O vapor)	
	Castleman, et al (1974)	298	6.0×10^{-13} $cm^3molecule^{-1}s^{-1}$ (a) 2nd order rate constant, $[M] = 1$ atm. (mostly N_2) (b) Relative rate measurement. Reference reaction: $HO + CO \rightarrow CO_2 + H$	(a,b)
19,32	$HO + H_2S \rightarrow H_2O + HS$			
	Stuhl, F. (1974)	298	$3.1 \pm 0.5 \times 10^{-12}$	
19,39	$HO + HCl \rightarrow H_2O + Cl$			
	*Watson (1974) review	220-300	$2.8 \times 10^{-12} \exp(-400 \pm 100/T)$	
	Smith, Zellner (1974a)	210-460	$4.1 \times 10^{-12} \exp(-530/T)$	
	Takacs, Glass (1973)	295	$6.4 \pm 1.5 \times 10^{-13}$	±0.1
	Davis (1974)	300	$6.5 \pm 0.4 \times 10^{-13}$	
	Zahniser, et al (1974)	224-460	$2.0 \pm 0.1 \times 10^{-12} \exp(-312 \pm 10/T)$	
- - -	$HO + DCl \rightarrow HDO + Cl$			
	Smith, Zellner (1974a)	210-460	$4.7 \times 10^{-12} \exp(-780/T)$	
19,45	$HO + CO \rightarrow CO_2 + H$			
	*This survey (D.G.)	200-400	1.4×10^{-13}	±0.1 (a)
	Wilson (1972) review	300-2000	$5.1 \times 10^{-13} \exp(-300/T)$	±0.3
	Stuhl, Niki (1972)	300	1.35×10^{-13}	±0.06

(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Westenberg, de Haas (1973a)	298	1.33×10^{-13}	±0.04
		396	1.38×10^{-13}	
		523	1.44×10^{-13}	
		707	1.69×10^{-13}	
		915	2.17×10^{-13}	
	Davis, Fischer, Schiff (1974)	220-373	$2.15 \pm 0.19 \times 10^{-13} \exp(-80 \pm 40/T)$	±0.04
	Greiner (1969)	300-500	$2.1 \times 10^{-13} \exp(-115/T)$	±0.1
	Smith, Zellner (1973)	300	1.45×10^{-13}	(b)
	Peeters, Mahnen (1973)	1600-1900	4.7×10^{-13}	
	Gardiner, et al (1973)	1500-2000	$6.7 \times 10^{-12} \exp(-4000/T)$	
	Howard, Evenson (1974)	296	$1.56 \pm 0.2 \times 10^{-13}$	
	Gordon, Mulac (1974)	298	1.50×10^{-13}	
	Baulch, Drysdale (1974) review	250-2500	$\log k = -12.95 + 3.94 \times 10^{-4} \times T$	
			(a) Small temperature coef. at low temperatures. Ignore in models	
			(b) Data reported 210 $<T<$ 460 K. Slight positive temperature dependence, possibly curved.	
19,48	$HO + CH_2O \rightarrow H_2O + CHO$			
	*Morris, Niki (1971)	300	1.4×10^{-11}	±0.1
	Wilson (1972) review	300-1600	8×10^{-11}	±1
	Peeters, Mahnen (1973)	1400-1800	3.8×10^{-11}	
19,56	$HO + CH_4 \rightarrow CH_3 + H_2O$			
	*Davis, Fischer, Schiff (1974)	240-373	$2.36 \pm 0.21 \times 10^{-12} \exp(-1710 \pm 88/T)$	±0.04
	Wilson (1972) review	300-2000	$4.7 \times 10^{-11} \exp(-2500/T)$	±0.7

(continued)

Reactions of HO with CO, CH_2O, and CH_4

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$		Notes and Reliability of log k
	Overend, et al. (1974)	300	$6.51 \pm 0.26 \times 10^{-15}$		
	Peeters, Mahnen (1973)	1100-1900	5×10^{-11} exp(-3000/T)		
	Greiner (1970)	300-500	5.5×10^{-12} exp(-1900/T)		±0.1
	Margitan, et al (1974)	290-440	3.83×10^{-12} exp(-1840 ± 20/T)		±0.06
	Gordon, Mulac (1974)	381	2.6×10^{-14}	(1 atm H_2O vapor)	
		416	5.5×10^{-14}	(1 atm H_2O vapor)	
19.57	HO + C_2H_4 -> products				
	Stuhl (1973c)	298	3×10^{-12}		±0.12
	Smith, Zellner (1973)	210-460	7.5×10^{-12} exp(-110/T)		
			10^{12}x k	P(He)/torr	
	Davis (1974)	300	2.24	3	
			2.78	5	
			3.63	10	
			4.06	20	
			4.72	100	
			4.98	300	
		300	3.64×10^{-12} at 3 torr N_2		
	Morris, et al. (1971)	300	1.8×10^{-12}		
	Bradley, et al. (1973)	300	$1.7 \pm 0.5 \times 10^{-12}$		
	Greiner (1970a)	300-500	1.26×10^{-12} exp(454/T)		
	Gordon, Mulac (1974)	381	6.2×10^{-12}	(1 atm H_2O vapor)	
		416	7.3×10^{-12}	(1 atm H_2O vapor)	
19.58	HO + C_2H_6 -> products				
	Overend, et al. (1974)	300	$2.64 \pm 0.17 \times 10^{-13}$		
	Greiner (1970)	300-500	1.86×10^{-11} exp(-1230/T)		

Reactions of HO with CH_4, C_2H_4, and C_2H_6

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$		Notes and Reliability of log k
19,59	$HO + C_3H_6 \rightarrow$ products				
	Stuhl (1973c)	298	1.45×10^{-11}		±0.06
	Morris, et al. (1971)	300	1.7×10^{-11}		
	Bradley, et al. (1973)	300	$5.0 \pm 1.7 \times 10^{-12}$		
	Gorse, Volman (1974)	300	$k/k(CO + HO) = 89.3$		
			$k = 1.2 \times 10^{-11}$		(a)
			(a) $k(CO + HO)$ from this survey		
	Davis (1974)	300	$1.53 \pm 0.06 \times 10^{-11}$		
	Gordon, Mulac (1974)	381	1.4×10^{-11}	(1 atm H_2O vapor)	
		416	2.0×10^{-11}	(1 atm H_2O vapor)	
19,59	$HO + C_2H_2 \rightarrow$ products				
	Smith, Zellner (1973)	210-460	$2.0 \times 10^{-12} \exp(-250/T)$		
	Pastrana, Carr (1974)	300	$2.0 \pm 0.6 \times 10^{-13}$		
	Davis (1974)	300	$1.80 \pm 0.09 \times 10^{-13}$		
19,59	$HO + C_6H_6 \rightarrow$ products				
	Davis (1974)	300	$\underline{10^{12} \times k}$	$\underline{P(He)/torr}$	
			0.85	3	preliminary
			1.46	20	
			1.70	100	
19,59	$HO + C_6H_5CH_3 \rightarrow$ products				
	Davis (1974)	300	$\underline{10^{12} \times k}$	$\underline{P(He)/torr}$	
			3.7	3	preliminary
			4.9	20	
			5.8	100	

Reactions of HO with C_3H_6 to $C_6H_5CH_3$

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability o log k
19.60	$HO + C_4H_{10} \rightarrow$ products			
	Stuhl (1973b)		2.35×10^{-12}	±0.06
	Greiner (1970)	300-500	$1.41 \times 10^{-11} \exp(-524/T)$	
	Gorse, Volman (1974)	300	$k/k(CO + HO) = 19.4$	
			$k = 2.7 \times 10^{-12}$	(a)
			(a) k(CO + HO) from this survey	
19.60	HO + alkane $\rightarrow H_2O$ + alkyl radical			
	Greiner (1970)	300-500	$k = [1.0 \exp(-820/T) N_p + 2.3 \exp(-430/T) N_s + 2.1 \exp(+95/T) N_t] \times 10^{-12}$ Where N_p, N_s, and N_t are the number of primary secondary, and tertiary hydrogen atoms respectively. Do not use formula for CH_4 and C_2H_6.	

Reactions of HO with C_4H_{10} and alkane

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1}s^{-1}$	Notes and Reliability of log k
20,M	$HO_2 + M \rightarrow H + O_2 + M$			
	Baulch, et al (1972) review	300-2000	$3.5 \times 10^{-9} \exp(-23000/T)$, M = Ar	±0.2 (a)
	Lloyd (1974) review		same recommendation	
			(a) $k_f = k_r K_{eq}$	
20,M	$HO_2 + M \rightarrow HO + O + M$			
	Baulch, et al (1972) review		no recommendation	
20,20	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$			
	*Hampson (1973) review	300-1000	$3 \times 10^{-11} \exp(-500/T)$ cm^3 $molecule^{-1}s^{-1}$	±0.3 at 300 K
	Baulch, et al (1972) review	300	3.3×10^{-12}	
	Lloyd (1974) review	300-1000	$1.7 \times 10^{-11} \exp(-500/T)$	±0.3 at 300 K
			$-d[HO_2]/dt = 2k[HO_2]^2$. Temperature coefficient estimated	larger at higher T
20,21	$HO_2 + H_2 \rightarrow H_2O_2 + H$			
	Baulch, et al (1972) review	300-800	$1.2 \times 10^{-12} \exp(-9400/T)$	±0.3
	Lloyd (1974) review	300-1000	same recommendation.	
			$k_f = k_r K_{eq}$	
20,22	$HO_2 + H_2O \rightarrow H_2O_2 + HO$			
	Baulch, et al (1972) review	300-800	$4.7 \times 10^{-11} \exp(-16{,}500/T)$	±0.2
	Lloyd (1974) review	300-1000	same recommendation	
			$k_f = k_r K_{eq}$	
20,28	$HO_2 + SO_2 \rightarrow SO_3 + HO$			
	*Payne, Stief, Davis (1973)	300	9×10^{-16} $cm^3 molecule^{-1}s^{-1}$	±0.3 (a,b)
			(a) Relative rate measurement. Value based on $k(HO_2 + HO_2)$ this survey.	
			(b) Recalculated.	
20,35	$HO_2 + Cl \rightarrow ClO + HO$			
	This survey (D.D.D., H.S.J., D.G.)		1.5×10^{-11}	(a)
			(a) Estimate. No data. Modellers should consider the range 2×10^{-12} to 2×10^{-10}.	

Reactions of HO_2 with M to Cl

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
20,45	$HO_2 + CO \rightarrow CO_2 + HO$			
	*This survey (D.D.D., H.I.S.)	300	$<10^{-19}$	a
	Lloyd (1974) eval.	300-1000	$1.7 \times 10^{-13} \exp(-5000/T)$	b
	Westenberg, de Haas (1972a)	300	$\sim 1 \times 10^{-12}$	c,d
	Davis, Payne, Stief (1973)	300	$<10^{-20}$	e
	Wyrsch, et al (1974)	300	$<3 \times 10^{-18}$	
	Simonaitis, Heicklen (1973a)	373-473	$<5 \times 10^{-18}$	e
	Volman, Gorse (1972)	330	$<10^{-15}$	f
	Baldwin, Walker, Webster (1970)	713-773	$1 \times 10^{-10} \exp(-11500/T)$	e
	Vardanyan, Dangyan, Sachyan (1972)	878-952	$2.2 \times 10^{-10} \exp(-11500/T)$	

NOTE: a. The low value of k selected in this evaluation is based on the evaluation by Lloyd and the measurements by Davis, Payne, Stief and Simonaitis, Heicklen.

b. Based on Davis, Payne and Stief (1972) and high T results. Temperature coef. probably maximum value.

c. Indirect measurement using a low-pressure discharge flow system.

d. Relative rate measurement - reference reaction: $H + HO_2 \rightarrow HO + HO$

e. Relative rate measurement - reference reaction: $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$

f. Relative rate measurement - reference reaction: $HO + CO \rightarrow CO_2 + H$

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
20,48	$HO_2 + CH_2O \rightarrow H_2O_2 + CHO$			
	*Lloyd (1974) review	300-800	$1.7 \times 10^{-12} \exp(-4000/T)$	$>\pm 1$ at 300K, ± 0.2 at 800K
	Baldwin, et al (1972)	773	1.6×10^{-15}	(a)

(a) Derived by computer fit to data. Based on $k(HO_2 + HO_2 \rightarrow H_2O_2 + O_2) = 3.0 \times 10^{-12}\ cm^3 molecule^{-1} s^{-1}$

Reactions of HO_2 with CO and CH_2O

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
20,51	$HO_2 + CH_3O_2 \rightarrow CH_3O_2H + O_2$			
	Demerjian et al (1974) review	300	6.7×10^{-14}	estimate
20,57	$HO_2 + C_2H_4 \rightarrow C_2H_4O + HO$?			
	Walker (1973)	773	2.5×10^{-17}	(a)
			(a) Relative to k $(HO_2 + HCHO) = 1.6 \times 10^{-15}$	
20,57	$HO_2 + C_2H_4 \rightarrow$ addition products			
	Lloyd (1974) review	300	$\sim 1.7 \times 10^{-17}$	> ±1 (a)
			(a) Suggestion. Data are irreconcilable.	
20,58	$HO_2 + C_2H_6 \rightarrow H_2O_2 + C_2H_5$			
	Lloyd (1974) review	300-1000	$\sim 1.7 \times 10^{-12} \exp(-7000/T)$	±1 (a)
			(a) Relative rate data versus $2HO_2 \rightarrow H_2O_2 + O_2$ and $HO_2 + CO \rightarrow HO + CO_2$. Temp. coef. estimated.	
20,60	$HO_2 + C_3H_8 \rightarrow H_2O_2 + i\text{-}C_3H_7$			
	Lloyd (1974) review	300-1000	$<3.3 \times 10^{-13} \exp(-5300/T)$	±1 (a)
			(a) Based on upper limit meas. Temp. coef. estimated.	
20,60	$HO_2 + n\text{-}C_4H_{10} \rightarrow H_2O_2 + s\text{-}C_4H_9$ (primarily)			
	Lloyd (1974) review	300-1000	$8.3 \times 10^{-13} \exp(-5300/T)$	±1 (a)
			(a) Based on upper limit meas. Temp. coef. estimated.	
20,60	$HO_2 + i\text{-}C_4H_{10} \rightarrow H_2O_2 + t\text{-}C_4H_9$			
	Lloyd (1974) review	300-1000	$1.7 \times 10^{-13} \exp(-3500/T)$	±1 (a)
			(a) Based on upper limit meas. Temp. coef. estimated.	

Reactions of HO_2 with CH_3O_2 to $i\text{-}C_4H_{10}$

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
21,M	$H_2 + M \rightarrow H + H + M$		see reverse reaction	
21,35	$H_2 + Cl \rightarrow HCl + H$			
	*Watson (1974) review	298	$1.4 \pm 0.1 \times 10^{-14}$	(a)
			(a) For temp. dependence, use E/R = 2655 ± 200 K.	
21,36	$H_2 + ClO \rightarrow$ products			
	Walker (1972)	670	$< 8 \times 10^{-16}$	(a)
	Clyne, Coxon (1968)	294	$< 5 \times 10^{-16}$	
			(a) As quoted by Watson (1974) review.	
22,29	$H_2O + SO_3 \rightarrow$ products			
	Castleman, et al (1974)	298	$9.1 \pm 2.9 \times 10^{-13}$	
23,hν	$H_2O_2 + h\nu \rightarrow HO + HO$			
	*Hampson (1973) review		Absorption coefficient (cross section)	
			λ/nm — σ/cm^2 molecule^{-1}, base e	
			190 — 80×10^{-20}	
			195 — 60×10^{-20}	
			200 — 54×10^{-20}	
			205 — 46×10^{-20}	
			210 — 40×10^{-20}	
			215 — 34×10^{-20}	
			220 — 28×10^{-20}	
			225 — 24×10^{-20}	
			254 — 7.4×10^{-20}	
			Quantum yields (primary)	
			$\phi(-H_2O_2) = 1.0$ $\lambda > 200$nm.	
			See ref. for other, minor, channels pertinent for $\lambda < 200$nm.	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
23,M	$H_2O_2 + M \rightarrow HO + HO + M$		see reverse equation	
24,M	$HNO + M \rightarrow H + NO + M$			
	*Baulch, et al (1973) review	230–700	$5 \times 10^{-8} \exp(-24{,}500/T)$ $M = H_2$	±0.2 (a)
			(a) No data. Value based on reverse rate	
24,24	$HNO + HNO \rightarrow H_2O + N_2O$			
	*Baulch, et al (1973) review	300	4×10^{-15}	±0.3
25,hv	$HNO_2 + h\nu \rightarrow HO + NO$ (a)			
	$\rightarrow H + NO_2$ (b)			
	Cox (1974b)		$\phi_a \geq 0.97$	(a)
	Johnston (1973)		$k = 6.45 \times 10^{-4}$s^{-1}	(b)
			(a) Photolysis $330 < \lambda/nm < 380$	
			(b) Specific rate of photodissociation by daylight.	
26,hv	$HNO_3 + h\nu \rightarrow HO + NO_2$		Elevation/km k(noon)/s^{-1} k(24 hr. av.)/s^{-1}	
	*Johnston (1974) review	220	15 5.1×10^{-7} 1.5×10^{-7}	±0.15
		217	20 7.7×10^{-7} 2.3×10^{-7}	Rates are for
		222	25 2.8×10^{-6} 6.8×10^{-7}	45° latitude,
		227	30 1.4×10^{-5} 3.5×10^{-6}	solar equinox
		235	35 4.1×10^{-5} 1.2×10^{-5}	standard ozone
		250	40 7.6×10^{-5} 2.7×10^{-5}	background
		260	45 1.1×10^{-4} 4.2×10^{-5}	
	*Hampson, et al (1973) review		Absorption coefficients. See also Text.	
	Johnston, et al. (1974)		$\phi = 1$ $200 < \lambda < 315$nm	(a)
			(a) Products probably those shown above.	
			(continued)	

Reactions of HNO, HNO_2, and HNO_3

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	Biaume (1973)		Absorption cross section data for for $185 < \lambda < 325$ nm in good agreement with that of Johnston and Graham (1973) which is quoted in Hampson, et al. (1973).	
26,M	$HNO_3 + M \rightarrow HO + NO_2 + M$		see reverse reaction	
27,27	$SO + SO \rightarrow SO_2 + S$ or $(SO)_2$			
	*Schofield (1973) review (WHB)	300	$< 3 \times 10^{-15}$	
		1000	$< 2 \times 10^{-13}$	
	Chung, Calvert, Bottenheim (1974)	300	$8.3 \pm 6.7 \times 10^{-16}$	
27,29	$SO + SO_3 \rightarrow 2SO_2$			
	Chung, Calvert, Bottenheim (1974)	300	$2 \pm 1.2 \times 10^{-15}$	
28,49M	$SO_2 + CH_3\ (+M) \rightarrow CH_3SO_2\ (+M)$			
	James, et al (1973)	300	$3 \times 10^{-13}\ cm^3 molecule^{-1} s^{-1}$	± 0.1
35,35M	$Cl + Cl + M \rightarrow Cl_2 + M$			
	*Watson (1974) review	200-500	$6 \times 10^{-34} \exp(900 \pm 250/T)\ cm^6 molecule^{-2} s^{-1}$	M = Ar
35,37	$Cl + OClO \rightarrow 2ClO$			
	Watson (1974) review	300	$5.9 \pm 0.9 \times 10^{-11}$ ($E = 0 \pm 1$ kJ/mol)	± 0.1
35,37	$Cl + ClOO \rightarrow Cl_2 + O_2$ (a) $\rightarrow 2ClO$ (b)			
	Johnston, et al (1969)	298	$k_a = 1.56 \times 10^{-10}$ $k_a/k_b = 108$	
	Nicholas, Norrish (1968)	298	$k_a/k_b = 15$	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
35,40	$Cl + Cl_2O \rightarrow Cl_2 + ClO$			
	*Watson (1974) review	300	6.8×10^{-13}	
35,42	$Cl + NOCl \rightarrow NO + Cl_2$			
	*Watson (1974) review	298	$3 \pm 0.5 \times 10^{-11}$	
35,43	$Cl + NO_2Cl \rightarrow NO_2 + Cl_2$			
	Watson (1974) review	298	$k > 3 \times 10^{-14}$	
35,56	$Cl + CH_4 \rightarrow HCl + CH_3$			
	*Watson (1974) review	300-686	$5.6 \times 10^{-11} \exp(-1790/T)$	
	Davis, et al (1970)	300	$1.5 \pm 0.1 \times 10^{-13}$	
	Pettis, Knox (1964)		$4 \times 10^{-11} \exp(-1930/T)$	
	Clyne, Walker (1973)	300-686	$5.1 \times 10^{-11} \exp(-1790/T)$	
36,hv	$ClO + h\nu \rightarrow Cl + O$			
	*Watson (1974) review		absorption cross section data $225 < \lambda < 300$ nm	
36,36	$ClO + ClO \rightarrow Cl_2 + O_2$ $\rightarrow Cl + ClOO$			
	*Watson (1974) review	298	$2.4 \pm 0.4 \times 10^{-14}$ (low pressure, 1-3 torr)	(a)
			4.6×10^{-14} (high pressure, > 75 torr)	(a)
			(a) $-d[ClO]/dt = k[ClO]^2$, (sum of both paths).	
36,36	$ClO + ClO \rightarrow Cl + OClO$			
	Watson (1974) review	298	$k < 2.2 \times 10^{-15}$	provisional upper limit
36,45	$ClO + CO \rightarrow CO_2 + Cl$			
	*Watson (1974) review	587	1.7×10^{-15}	
36,56	$ClO + CH_4 \rightarrow$ products			
	Walker (1972)	670	$\sim 4 \times 10^{-15}$	(a)
			(a) As quoted by Watson (1974) review.	

Reactions of Cl and ClO

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
36,57	$ClO + C_2H_4 \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1974) review.	
36,59	$ClO + C_2H_2 \rightarrow$ products			
	Walker (1972)	670	$k < 5 \times 10^{-16}$	(a)
			(a) As quoted by Watson (1974) review.	
37,M	$ClOO + M \rightarrow Cl + O_2 + M$			
	Watson (1974) review		Table of values of rate constant as a function of altitude.	
37,hv	$ClOO + h\nu \rightarrow ClO + O(^1D)$			
	Watson (1974) review		absorption cross section data $225 < \lambda < 280$ nm	
39,hv	$HCl + h\nu \rightarrow H + Cl$			
	Watson (1974) review		absorption cross section data $140 < \lambda < 200$ nm	
44,hv	$Cl_2 + h\nu \rightarrow 2Cl$			
	Watson (1974) review		absorption cross section data $240 < \lambda < 450$ nm	
45,50	$CO + CH_3O \rightarrow$ . . .		see $CH_3O + CO$	

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
48.hν	$CH_2O + h\nu \rightarrow CHO + H$ (a) $\rightarrow CO + H_2$ (b)			
	Calvert, et al (1972)		$\phi_a + \phi_b = 1$, $290 < \lambda < 360$ nm	(a)

λ/nm	ϕ_a	ϕ_b	absn. cross section cm^2 $molecule^{-1}$ base e**
290	0.81	0.19	31.8×10^{-21}
300	0.66	0.34	32.5
310	0.52	0.48	31.4
320	0.40	0.60	23.4
330	0.29	0.71	23.6
340	0.18	0.82	19.7
350	0.09	0.91	8.37
360	0.01	0.99	1.77

**Averaged for 10 nm bands. See McQuigg, Calvert (1969) for graph of absn. coefficient vs. wave length.

Sperling, Toby (1973)

λ/nm	ϕ_a	ϕ_b
313	0.8	0.2
334	0.45	0.25
366	0.2	0.45

(a) The two sets of measurements upon which ϕ's are based are inconsistent. Channels (a) and (b) may not be elementary. No recommendation (D.G.)

Reactions of CH_2O with hν

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
50.4	$CH_3O + O_2 \rightarrow CH_2O + HO_2$ (1)			
50.9	$CH_3O + NO \rightarrow CH_3ONO$ (2a)			
	$\rightarrow CH_2O + HNO$ (2b)			
50.10	$CH_3O + NO_2 \rightarrow CH_3ONO_2$ (3a)			
	$\rightarrow CH_2O + HNO_2$ (3b)			
50.45	$CH_3O + CO \rightarrow$ products (4)			
	*Heicklen (1973)	298	$k_1 \sim 3 \times 10^{-18}$	
			$\sim 1.6 \times 10^{-13} \exp(-3300/T)$	
			$k_2 \sim 8 \times 10^{-14}$	
		298	$k_1/k_2 = 4.7 \times 10^{-5}$ ±20%	ratio probably is smaller at 220 K
			$k_{2b}/k_2 = 0.145$ ±0.015	
			$k_2/k_3 = 1.2$ ±0.1	
		298	$k_{2a}/k_{3a} = 1.1$	
		363	$= 1.8$	
		403	$= 2.7$	
		298	$k_{3a}/k_3 = 0.9$ ±0.1	k_{3a}/k_{3b} probably constant 300–400 K
		298	$k_{3b}/k_3 = 0.1$ ±0.01	
		298–423	$k_4/k_2 = 5 \times 10^{-4}$	

Reactions of CH_3O

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant k/cm^{3}molecule^{-1}s^{-1}	Notes and Reliability of log k
	Demerjian, et al (1974) review	300	$k_1 = 1.6 \times 10^{-17}$	
			$\sim 4.2 \times 10^{-13} \exp(-3000/T)$	
			adjusted to fit C_4H_{10}/NO_x simulation studies	
			$k_{2a} = 1.7 \times 10^{-13}$	
			$k_{2b}/k_{2a} = 0.17$	
			$k_{3a} = 3.3 \times 10^{-13}$	
			$k_{3b}/k_{3a} = 0.1$	
	Batt, McCulloch, Milne (1974)	393-473	$k_{2a} \sim 3 \times 10^{-11}$	±0.4
			$k_{2b} \sim 7 \times 10^{-12}$	±0.5
51,51	$CH_3O_2 + CH_3O_2 \rightarrow CH_3OOH + CH_2O_2$ (a)			
	$\rightarrow 2CH_3O + O_2$ (b)			
	Demerjian, et al (1974) review	300	$k_a = 6.8 \times 10^{-14}$, $k_a = k_b$	estimate
	Parkes, et al (1973)	300	$3.3 \pm 1.1 \times 10^{-13}$ $k_a + k_b$	
54,hv	$CH_3ONO + h\nu \rightarrow CH_3O^* + NO$ (a)			
	$\rightarrow$ isomer (b)			
	$\rightarrow CH_2O + HNO$ (c)			
	$\rightarrow CH_2O + H + NO$ (d)			
	*Heicklen (1973) review	298	$k_a/k = 0.76 \pm 0.02$, $\lambda = 366nm$	
		298	$k_b/k = 0.24 \pm 0.04$, $\lambda = 366nm$	
		298	$(k_c + k_d)/k < 0.02$, $\lambda = 366nm$	
			$k = k_a + k_b + k_c + k_d$	
61,hv	$CFCl_3 + h\nu$			
	$CF_2Cl_2 + h\nu$			
	Watson (1974) review		Tabulated values of absorption cross sections for $186 < \lambda/nm < 226$.	

4. Rate constant for the reaction $HO + NO_2$ $(+ N_2) \rightarrow HNO_3$ $(+ N_2)$ as a function of temperature and total gas concentration.

W. Tsang

National Bureau of Standards

May, 1974

Rate constants for this reaction are provided here in tabular form covering the temperature range 190-350 K and the total concentration range 10^{16} - 3×10^{19} molecule cm^{-3}. They are recommended for use in modelling of the atmosphere.

These numbers were obtained using the correlation developed by W. Tsang, Int. J. Chem. Kinetics 5, 947, (1973), and also presented in R. F. Hampson, editor, "Chemical Kinetics Data Survey. VI", NBSIR 73-207 (Aug. 1973). The calculations have been made with the same parameters as used for the graphs and tables presented earlier.

This correlation is rated as good to a factor of 2 in k on an absolute scale throughout the range tabulated. It is, however, fitted to the room temperature data and is presumably better in this region than the rating stated above. Relative values throughout the table may be good to 25% in k. Thus the second decimal place in log k should be considered a guard digit. Linear interpolation should be used.

The correlation passes through the low pressure data of Anderson, Margitan, and Kaufman, J. Chem. Phys. 60, 3310-3317 (1974) but has a smaller pressure dependence than they found.

Reaction rate constant correlation for $HO + NO_2\ (+N_2) \rightarrow HNO_3\ (+N_2)$.

The tabulated nos. are $\log_{10}(k/\mathrm{cm}^3\ \mathrm{molecule}^{-1}\mathrm{s}^{-1})$ for the bimolecular formulation,

$d[HNO_3]/dt = k\ [HO]\ [NO_2]$, for the inert gas in large excess

T/K	$\log_{10}([N_2]/\mathrm{molecule\ cm}^{-3})$							
	16.0	16.5	17.0	17.5	18.0	18.5	19.0	19.5
190	-12.92	-12.55	-12.22	-11.92	-11.67	-11.46	-11.31	-11.21
210	-13.06	-12.69	-12.34	-12.02	-11.76	-11.53	-11.37	-11.25
230	-13.18	-12.79	-12.43	-12.11	-11.83	-11.59	-11.41	-11.27
250	-13.28	-12.88	-12.52	-12.18	-11.89	-11.64	-11.44	-11.29
270	-13.36	-12.96	-12.59	-12.24	-11.94	-11.67	-11.46	-11.30
290	-13.44	-13.03	-12.65	-12.30	-11.98	-11.71	-11.48	-11.31
300	-13.47	-13.06	-12.68	-12.32	-12.00	-11.72	-11.49	-11.31
310	-13.51	-13.09	-12.70	-12.34	-12.02	-11.73	-11.50	-11.31
330	-13.57	-13.15	-12.75	-12.39	-12.05	-11.76	-11.51	-11.32
350	-13.62	-13.20	-12.80	-12.43	-12.09	-11.78	-11.53	-11.32

To obtain log k' for the termolecular formulation, $d\ [HNO_3] = k'\ [HO][NO_2][N_2]$ with k' in $\mathrm{cm}^6\ \mathrm{molecule}^{-2}\mathrm{s}^{-1}$, subtract the log of the concentration of N_2 at the head of each column from each number in its column, e.g. $\log k' = -12.92-16.0 = -28.92$ for T = 190 K and $\log [N_2] = 16.0$.

5. Reference List

Ahumada, J. J., Michael, J. V., and Osborne, D. T., "Pressure Dependence and Third Body Effects on The Rate Constants for $H + O_2$, $H + NO$, and $H + CO$," J. Chem. Phys. 57, 3736-3745 (1972)

Albers, E. A., Hoyermann, K., Wagner, H. Gg., and Wolfrum J., "Study of the Reaction of Ammonia with Oxygen Atoms," Symp. Combust. 12th (Combustion Institute, Pittsburgh, 1969) 313-321

Albers, E. A., Hoyermann, K., Wagner, H. Gg., and Wolfrum J., "Absolute Measurements of Rate Coefficients for the Reactions of H and O Atoms with H_2O_2 and H_2O," Symp. Combust. 13th (Combustion Institute, Pittsburgh, 1970) 81-88

Allen, E. R., and Moortgat, G. K., "Kinetic Studies of the Termolecular Reactions of Hydrogen Atoms with Nitric Oxide and with Molecular Oxygen," Third Intern. Symp. Gas Kinetics, Brussels (1973), Abstract D1

Anderson, J. G., and Kaufman, F., "Kinetics of the Reaction $OH(v = 0) + O_3 \rightarrow HO_2 + O_2$," Chem. Phys. Lett. 19, 483-486 (1973)

Anderson, J. G., Margitan, J. J., and Kaufman, F., "Gas Phase Recombination of OH with NO and NO_2," J. Chem. Phys. 60, 3310-3317 (1974)

Arin, L. M., and Warneck, P., "Reaction of Ozone with Carbon Monoxide," J. Phys. Chem. 76, 1514-1515 (1972)

Arnoldi, D., and Wolfrum, J., "The Reaction of Vibrationally Excited HCl with Oxygen and Hydrogen Atoms," Chem. Phys. Lett. 24, 234-238 (1974)

Atkinson, R., and Cvetanović, R. J., "Determination of the Rates of Hydrogen Atom Reaction with NO by a Modulation Technique," Can. J. Chem. 51, 370-372 (1973)

Atkinson, R., and Pitts, J. N., Jr., "Temperature Dependence of the Reaction Rate Constants for $O(^3P)$ Atoms with C_2H_4, C_3H_6 and $NO(M = N_2O)$, Determined by a Modulation Technique," Chem. Phys. Lett. 27, 467-470 (1974)

Balakhnin, V. P., Egorov, V. I., and Intezarova, E. I., "Kinetics Investigation of the Elemental Reactions of Oxygen Atoms in the Gas Phase by EPR. II. The Reaction $O + HCl = OH + Cl$," Kinetics and Catalysis 12, 258 (1971); tr. of: Kinetika i Kataliz 12, 299 (1971)

Baldwin, R. R., Gethin, A., and Walker, R. W., "Reaction of Hydrogen Atoms with Nitrous Oxide," J. Chem. Soc. Faraday Trans. I 69, 352-358 (1973)

Baldwin, R. R., Fuller, A. R., Longthorn, D., and Walker, R. W., "Addition of Formaldehyde to Slowly Reacting Hydrogen + Oxygen Mixtures," J. Chem. Soc. Faraday Trans. I 68, 1362-1367 (1972)

Baldwin, R. R., Walker, R. W., and Webster, S. J., "The Carbon Monoxide-Sensitized Decomposition of Hydrogen Peroxide," Combust. Flame 15, 167-172 (1970)

Ball, M. J., and Larkin, G. S., "Determination of the Rates of Atomic Reactions by the Discharge-Flow Method," Nature Phys. Sci. 245; 63-64 (1973)

Basco, N., James, D. G. L., and James, F. C., "A Quantitative Study of Alkyl Radical Reactions by Kinetic Spectroscopy. II. Combination of the Methyl Radical with the Oxygen Molecule," Intern. J. Chem. Kinet. 4, 129-149 (1972)

Basco, N., James, D. G. L., and Suart, R. D., "A Quantitative Study of Alkyl Radical Reactions by Kinetic Spectroscopy. Part I. Mutual Combination of Methyl Radicals and Combination of Methyl Radicals with Nitric Oxide," Intern. J. Chem. Kinet. 2, 215-234 (1970)

Bass, A. M., and Laufer, A. H., "The Methyl Radical Combination Rate Constant as Determined by Kinetic Spectroscopy," Intern. J. Chem. Kinet. 5, 1053-1065 (1973)

Batt, L., McCulloch, R. D., and Milne, R. T., "Thermochemical and Kinetic Studies of Alkyl Nitrites (RONO) - D(RO-NO), The Reactions between RO and NO, and the Decomposition of RO," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton, Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Baulch, D. L., and Drysdale, D. D., "An Evaluation of the Rate Data for the Reaction $CO + OH \rightarrow CO_2 + H$," Combust. Flame 23, 215-225 (1974)

Baulch, D. L., Drysdale, D. D., Horne, D. G., and Lloyd, A. C., "Evaluated Kinetic Data for High Temperature Reactions, Vol. 1: Homogeneous Gas Phase Reactions of the H_2-O_2 System," (Butterworths, London, 1972)

Baulch, D. L., Drysdale, D. D., and Horne, D. G., [unpublished data sheets prepared for this survey] University of Leeds, 1973

Baulch, D. L., Drysdale, D. D., and Horne, D. G., "Rate Constants for Reactions of the H_2-N_2-O_2 System," in Chemical Kinetics Data Survey V. Sixty-six Contributed Rate and Photochemical Data Evaluations on Ninety-four Reactions, NBSIR 73-206, D. Garvin, Ed., National Bureau of Standards, Washington, D. C. (1973) pages 49-115

Bayes, K. D., letter to RFH, March 11, 1974

Becker, K. H., Groth, W., and Schurath, U., "Reactions of $O_2(^1\Delta_g)$ with Ozone," Chem. Phys. Letts. 14, 489-492 (1972)

Becker, K. H., Groth, W., and Thran, D., "Mechanism of the Air Afterglow $NO + O \rightarrow NO_2 + h\nu$," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 353-363

Becker, K. H., Inocencio, M., and Schurath, U., "The Reaction of Ozone with Hydrogen Sulfide and its Organic Derivatives," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Becker, K. H., Schurath, U., and Seitz, H., "Ozone-Olefin Reactions in the Gas Phase. 1. Rate Constants and Activation Energies," Intern. J. Chem. Kinet. 6, 725-739 (1974)

Bedford, G., and Thomas, J. H., "Reaction between Ammonia and Nitrogen Dioxide," J. Chem. Soc. Faraday Trans. I 68, 2163-2170 (1972)

Bemand, P. P., Clyne, M. A. A., and Watson, R. T., "Atomic Resonance Fluorescence and Mass Spectrometry for Measurements of the Rate Constants for Elementary Reactions: $O(^3P_J) + NO_2 \rightarrow NO + O_2$ and $NO + O_3 \rightarrow NO_2 + O_2$," J. Chem. Soc. Faraday Trans. II 70, 564-576 (1974)

Benson, S. W., and O'Neal, H. E., "Kinetic Data on Gas Phase Unimolecular Reactions," NBS-NSRDS-21 (1970). (Supt. Doc., U.S. Govt. Printing Office, Washington, D.C. 20402)

Bevan, P. L., and Johnson, G. R. A., "Kinetics of Ozone Formation in the Pulse Radiolysis of Oxygen Gas," J. Chem. Soc. Faraday Trans. I 69, 216-227 (1973)

Biaume, F., "Nitric Acid Vapour Absorption Cross-Section Spectrum and Its Photodissociation in the Stratosphere," J. Photochem. 2, 139-149 (1973)

Bishop, W. P., and Dorfman, L. M., "Pulse Radiolysis Studies. XVI. Kinetics of the Reaction of Gaseous Hydrogen Atoms with Molecular Oxygen by Fast Lyman-α Absorption Spectrophotometry," J. Chem. Phys. 52, 3210-3216 (1970)

Bradley, J. N., Hack, W., Hoyermann, K., and Wagner, H. Gg., "Kinetics of the Reaction of Hydroxyl Radicals with Ethylene and with C_3 Hydrocarbons," J. Chem. Soc. Faraday Trans. I 69, 1889-1898 (1973)

Breckenridge, W. H., and Miller, T. A., "Kinetic Study by EPR of the Production and Decay of $SO(^1\Delta)$ in the Reaction of $O_2(^1\Delta_g)$ with $SO(^3\Sigma^-)$," J. Chem. Phys. 56, 465-474 (1972)

Brown, R. D. H., and Smith, I. W. M., "Absolute Rate Constants for the Reactions of $O(^3P)$ Atoms with HCl and HBr," Intern. J. Chem. Kinet., in press (1974)

Brown, R. D. H., Glass, G. P., and Smith, I. W. M., "Relaxation of HCl(v = 1) and DCl(v = 1) by Cl and O Atoms," Abstract of paper given at 4th Conference on Chemical and Molecular Lasers, St. Louis Missouri, October 1974. Proceedings of meeting to be published IEEE J. Quantum Electronics.

Calvert, J. G., Kerr, J. A., Demerjian, K. L., and McQuigg, R. D., "Photolysis of Formaldehyde as a Hydrogen Atom Source in the Lower Atmosphere, Science 175, 751-752 (1972)

Campbell, I. M., and Gray, C. N., "Rate Constants for $O(^3P)$ Recombination and Association with $N(^4S)$," Chem. Phys. Letts. 18, 607-609 (1973)

Castleman, A. W., Jr., Davis, R. E., Munkelwitz, H. R., Tang, I. N., and Wood, W. P., "Kinetics of Association Reactions Pertaining to H_2SO_4 Aerosol Formation," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton, Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Chapman, C. J., and Wayne, R. P., "The Reaction of Atomic Oxygen and Hydrogen with Nitric Acid," Intern. J. Chem. Kinet. 6, 617-630 (1974)

Chung, K., Calvert, J. G., and Bottenheim, J. W., "The Photochemistry of Sulfur Dioxide Excited within its First Allowed Band (3130 Å) and the 'Forbidden' Band (3700-4000 Å)," Intern. J. Chem. Kinet., in press (1974)

Clark, I. D., Jones, I. T. N., and Wayne, R. P., "The Kinetics of the Reaction between $O_2(^1\Delta_g)$ and Ozone," Proc. Roy. Soc. London A 317, 407-416 (1970)

Clyne, M. A. A., Private communication (1974)

Clyne, M. A. A., and Coxon, J. A., "Kinetics Studies of Oxyhalogen Radical Systems," Proc. Roy. Soc., (London) A 303, 207-231 (1968)

Clyne, M. A. A., and Cruse, H. W., "Studies of Ground-State $^2P_{3/2}$ Halogen Atoms Using Atomic Resonance Absorption," Trans. Faraday Soc. 67, 2869-2885 (1971)

Clyne, M. A. A., and Cruse, H. W., "Atomic Resonance Fluorescence Spectrometry for Rate Constants of Rapid Bimolecular Reactions. Part 1. Reactions $O + NO_2$, $Cl + ClNO$, $Br + ClNO$," J. Chem. Soc. Faraday Trans. II 68, 1281-1299 (1972)

Clyne, M. A. A., and Down, S., "Kinetic Behaviour of OH $X^2\Pi$ and $A^2\Sigma^+$ using Molecular Resonance Fluorescence Spectrometry," J. Chem. Soc. Faraday Trans. II 70, 253-266 (1974)

Clyne, M. A. A., and Walker, R. F., "Absolute Rate Constants for Elementary Reactions in the Chlorination of CH_4, CD_4, CH_3Cl, CH_2Cl_2, $CHCl_3$, $CDCl_3$ and $CBrCl_3$," J. Chem. Soc. Faraday Trans. I 69, 1547-1567 (1973)

Collins, R. J., Husain, D., and Donovan, R. J., "Kinetic and Spectroscopic Studies of $O_2(a^1\Delta_g)$ by Time-Resolved Absorption Spectroscopy in the Vacuum Ultra-violet," J. Chem. Soc. Faraday Trans. II 69, 145-157 (1973)

Coltharp, R. N., Worley, S. D., and Potter, A. E., "Reaction Rate of Vibrationally Excited Hydroxyl with Ozone," Appl. Optics 10, 1786-1789 (1971)

Cox, R. A., "The Photolysis of Nitrous Acid in the Presence of Carbon Monoxide and Sulphur Dioxide," J. Photochem., in press (1974a)

Cox, R. A., "The Photolysis of Gaseous Nitrous Acid - A Technique for Obtaining Kinetic Data on Atmospheric Photo-Oxidation Reactions," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974b. Proceedings to be published Intern. J. Chem. Kinet.

Cupitt, L. T., and Glass, G. P., "Reactions of SH with Atomic Oxygen and Hydrogen," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Daubendiek, R. L., and Calvert, J. G., "A Study of the N_2O_5-SO_2-O_3 Reaction System, Environ. Lett., in press (1974)

Davis, D. D., "Absolute Rate Constants for Elementary Reactions of Atmospheric Importance: Results from the University of Maryland's Gas Kinetics Laboratory, Report #I, Chemistry Department, University of Maryland, July 1974

Davis, D. D., Braun, W., and Bass, A. M., "Reactions of $Cl^2P_{3/2}$: Absolute Rate Constants for Reaction with H_2, CH_4, C_2H_6, CH_2Cl_2, C_2Cl_4, and c-C_6H_{12}," Intern. J. Chem. Kinet. 2, 101-114 (1970)

Davis, D. D., Fischer, S., and Schiff, R., "Flash Photolysis-Resonance Fluorescence Kinetics Study: Temperature Dependence of the Reactions $OH + CO \rightarrow CO_2 + H$ and $OH + CH_4 \rightarrow H_2O + CH_3$," J. Chem. Phys. 61, 2213-2219 (1974)

Davis, D. D., Herron, J. T., and Huie, R. E., "Absolute Rate Constants for the Reaction $O(^3P) + NO_2 \rightarrow NO + O_2$ Over the Temperature Range 230-339K," J. Chem. Phys. 58, 530-535 (1973)

Davis, D. D., Payne, W., and Stief, L., "The Hydroperoxyl Radical in Atmospheric Chemical Dynamics: Reaction with Carbon Monoxide," Science 179, 280-282 (1973)

Davis, D. D., Prusazcyk, J., Dwyer, M., and Kim, P., "A Stop-Flow Time of Flight Mass Spectrometry Kinetics Study. Reaction of Ozone with Nitrogen Dioxide and Sulfur Dioxide," J. Phys. Chem. 78, 1775-1779 (1974)

Davis, D. D., Wong, W., and Lephardt, J., "A Laser Flash Photolysis-Resonance Fluorescence Kinetic Study: Reaction of $O(^3P)$ with O_3." Chem. Phys. Lett. 22, 273-278 (1973)

Davis, D. D., Wong, W., and Schiff, R., "A Dye Laser Flash Photolysis Kinetics Study of the Reaction of Ground-State Atomic Oxygen with Hydrogen Peroxide," J. Phys. Chem. 78, 463-464 (1974)

Demerjian, K. L., Kerr, J. A., and Calvert, J. G., "The Mechanism of Photochemical Smog Formation," Adv. Environ. Sci. and Technology 4, 1-262 (1974) J. N. Pitts, Jr., and R. L. Metcalf, editors, Wiley-Interscience

DeMore, W. B., "Rate Constants for the Reactions of Hydroxyl and Hydroperoxyl with Ozone," Science 180, 735-737 (1973)

DeMore, W. B., "Arrhenius Constants for the Reactions of Ozone with Ethylene and Acetylene," Intern. J. Chem. Kinet. 1, 209-220 (1969)

DeMore, W. B., "Rate Constant Ratio for the Reactions of OH with O_3 and CO." Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

DeMore, W. B., and Tschuikow-Roux, E., "Temperature Dependence of the Reactions of OH and HO_2 with O_3." J. Phys. Chem. 78, 1447-1451 (1974)

Dillemuth, F. J., Skidmore, D. R., and Schubert, C. C., "The Reaction of Ozone with Methane," J. Phys. Chem. 64, 1496-1499 (1960)

Donovan, R. J., Husain, D., and Kirsch, L. J., "Reactions of Atomic Oxygen. Part 1: The Rate of the Reaction $O + O_2 + M \rightarrow O_3 + M$ (M = He, Ar and Kr)," Trans. Faraday Soc. 66, 2551-2559 (1970)

Fettis, G. C., and Knox, J. H., "Rate Constants of Halogen Atom Reactions," G. Porter, Ed., Progress in Reaction Kinet. (Pergamon Press) 2, 1-38 (1964)

Findlay, F. D., and Snelling, D. R., "Temperature Dependence of the Rate Constant for the Reaction $O_2(^1\Delta_g) + O_3 \rightarrow 2O_2 + O$," J. Chem. Phys. 54, 2750-2755 (1971)

Findlay, F. D., and Snelling, D. R., "Collisional Deactivation of $O_2(^1\Delta_g)$," J. Chem. Phys. 55, 545-551 (1971a)

Fisher, E. R., and McCarty, M., Jr., "Study of the Reaction of Electronically Excited Oxygen Molecules with Carbon Monoxide," J. Chem. Phys. 45, 781-784 (1966)

Foner, S. N., and Hudson, R. L., "Mass Spectrometry of the HO_2 Free Radical," J. Chem. Phys. 36, 2681-2688 (1962)

Francis, P. D., "The Production of Oxygen Atoms in a Microwave Discharge and the Recombination Kinetics in a Gas Flow System," Brit. J. Appl. Phys. 2, 1717-1730 (169)

Gaedtke, H., Glanzer, K., Hippler, H., Luther, K., and Troe, J., "Addition Reactions of Oxygen Atoms at High Pressures," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 295-303

Gardiner, W. C., Jr., Mallard, W. G., McFarland, M., Morinaga, L., Owen, J. H., Rawlins, W. T., Takeyama, T., and Walker, B. F., "Elementary Reaction Rates from Post-Induction-Period Profiles in Shock-Initiated Combustion," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 61-72

Gardiner, W. C., Jr., Mallard, W. G., and Owen, J. H., "Rate Constant of $OH + H_2 = H_2O + H$ from 1350 to 1600 K," J. Chem. Phys. 60, 2290-2295 (1974)

Gauthier, M., and Snelling, D. R., "Production et Désexcitation de $O(^1D)$, $O_2(^1\Delta_g)$, et $O_2(^1\Sigma_g^+)$ dans la Photolyse de l'Ozone À 253.7 nm," Centre de Recherches Pour la Defense Valcartier, Quebec, Canada, DREV R-704/74 (February, 1974)

Gehring, M., Hoyermann, K., Schacke, H., and Wolfrum, J., "Direct Studies of Some Elementary Steps for the Formation and Destruction of Nitric Oxide in the H-N-O System," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 99-105

Ghormley, J. A., Ellsworth, R. L., and Hochanadel, C. J., "Reaction of Excited Oxygen Atoms with Nitrous Oxide. Rate Constants for Reaction of Ozone with Nitric Oxide and with Nitrogen Dioxide," J. Phys. Chem. 77, 1341-1345 (1973). Erratum: 78, 2698 (1974)

Glanzer, K., and Troe, J., [unpublished data sheets prepared for this survey] Ecole Polytechnique Federale de Lausanne (1973)

Glavas, S., and Toby, S., "The Reaction between Ozone and Hydrogen Sulfide," typescript, School of Chemistry, Rutgers University, New Brunswick, N.J., and private communication from S. Toby (1974)

Gordon, R. J., and Lin, M. C., "The Reaction of Nitric Oxide with Vibrationally Excited Ozone," Chem. Phys. Lett. 22, 262-268 (1973)

Gordon, S., and Mulac, W. A., "Reaction of the $OH(X^2\pi)$ Radical Produced by the Pulse Radiolysis of Water Vapor," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Gordon, S., Mulac, W., and Nangia, P., "Pulse Radiolysis of Ammonia Gas. II. Rate of Disappearance of the $NH_2(X^2B_1)$ Radical," J. Phys. Chem. 75, 2087-2093 (1971)

Gorse, R. A., and Volman, D. H., "Photochemistry of the Gaseous Hydrogen Peroxide-Carbon Monoxide System: Rate Constants for Hydroxyl Radical Reactions with Hydrogen Peroxide and Isobutane by Competitive Kinetics," J. Photochem. 1, 1-10 (1972)

Gorse, R. A., and Volman, D. H., "Photochemistry of the Gaseous Hydrogen Peroxide-Carbon Monoxide System II: Rate Constants for Hydroxyl Radical Reactions with Hydrocarbons and for Hydrogen Atom Reactions with Hydrogen Peroxide," J. Photochem. 3, 115-122 (1974)

Graham, R. A., and Johnston, H. S., "Kinetics of the Gas-Phase Reaction between Ozone and Nitrogen Dioxide," J. Chem. Phys. 60, 4628-4629 (1974)

Gray, D., Lissi, E., and Heicklen, J., "The Reaction of Hydrogen Peroxide with Nitrogen Dioxide and Nitric Oxide," J. Phys. Chem. 76, 1919-1924 (1972)

Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. V. Reactions with H_2 and CO in the Range 300-500°K," J. Chem. Phys. 51, 5049-5051 (1969)

Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. VI. Reactions with Alkanes in the Range 300-500°K," J. Chem. Phys. 53, 1070-1076 (1970)

Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. VII. The Reaction with Ethylene in the Range 300-500°K," J. Chem. Phys. 53, 1284-1285 (1970a)

Hack, W., Hoyermann, K., and Wagner, H. Gg., "Reaktionen des Hydroxylradikals mit Ammoniak und Hydrazin in der gasphase," Ber. Bunsenges. Physik. Chem. 78, 386-391 (1974)

Hampson, R. F., (editor), "Survey of Photochemical and Rate Data for Twenty-Eight Reactions of Interest in Atmospheric Chemistry," J. Phys. Chem. Ref. Data 2, No. 2 pgs. 267-312 (1973). These are revised versions of data sheets originally distributed as NBS Reports 10692 and 10828.

Hampson, R. F., (editor), "Chemical Kinetics Data Survey VI. Photochemical and Rate Data for Twelve Gas Phase Reactions of Interest for Atmospheric Chemistry," NBSIR 73-207 (1973a)

Hanst, P. L., Stephens, E. R., Scott, W. E., and Doerr, R. C., "Atmospheric Ozone-Olefin Reactions," (The Franklin Institute, Philadelphia, Pa. 1958)

Harker, A., and Johnston, H. S., "Photolysis of Nitrogen Dioxide to Produce Transient O, NO_3 and N_2O_5," J. Phys. Chem. 77, 1153-1156 (1973)

Heicklen, J., "Gas-Phase Reactions of Alkylperoxy and Alkoxy Radicals," Adv. Chem. Ser. (Amer. Chem. Soc., Washington) 76, 23-39 (1968)

Heicklen, J., "Photochemical and Rate Data for Methyl Nitrite, Methoxy and Methylperoxy," Chemical Kinetics Data Survey V. Sixty-six Contributed Rate and Photochemical Data Evaluations on Ninety-four Reactions, NBSIR 73-206, D. Garvin, Ed., National Bureau of Standards, Washington, D.C. (1973) pages 43-48

Herron, J. T., and Huie, R. E., "Rate Constants for the Reactions of Ozone with Ethene and Propene, from 235.0 to 362.0 K," J. Phys. Chem. 78, 2085-2088 (1974)

Herron, J. T., and Huie, R. E., "Rate Constants for the Reactions of Atomic Oxygen (O^3P) with Organic Compounds in the Gas Phase," J. Phys. Chem. Ref. Data 2, 467-518 (1973)

Herron, J. T., and Huie, R. E., "Rates of Reaction of Atomic Oxygen. II. Some C_2 to C_8 Alkanes," J. Phys. Chem. 73, 3327-3337 (1969)

Hikida, T., Eyre, J. A., and Dorfman, L. M., "Pulse Radiolysis Studies. XX. Kinetics of Some Addition Reactions of Gaseous Hydrogen Atoms by Fast Lyman-α Absorption Spectrophotometry," J. Chem. Phys. 54, 3422-3428 (1971)

Hippler, H., and Troe, J., "Hochdruckbereich der Rekombination $O + O_2 \rightarrow O_3$," Ber. Bunsenges. Physik. Chem. 75, 27-32 (1971)

Hippler, H., Schippert, C., and Troe, J., "Photolysis of NO_2 and Collisional Energy Transfer in the Reactions $O + NO \rightarrow NO_2$ and $O + NO_2 \rightarrow NO_3$," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Hochanadel, C. J., Ghormley, J. A., and Ogren, P. J., "Absorption Spectrum and Reaction Kinetics of HO_2 Radical in the Gas Phase," J. Chem. Phys. 56, 4426-4432 (1972)

Hollinden, G. A., Kurylo, M. J., and Timmons, R. B., "Electron Spin Resonance Study of the Kinetics of the Reaction of $O(^3P)$ Atoms with H_2S," J. Phys. Chem. 74, 988-991 (1970)

Holmes, H. H., and Daniels, F., "The Photolysis of Nitrogen Oxides: N_2O_5 N_2O_4 and NO_2," J. Amer. Chem. Soc. 56, 630-637 (1934)

Howard, C. J., and Evenson, K. M., "Laser Magnetic Resonance Study of the Gas Phase Reactions of OH with CO, NO, and NO_2," J. Chem. Phys. 61, 1943-1952 (1974)

Huestis, D. L., Black, G., Edelstein, S. A., and Sharpless, R. L., "Fluorescence and Quenching of $O_2(^1\Delta_g)$ and $[O_2(^1\Delta_g)]_2$ in Liquid Oxygen," J. Chem. Phys. 60, 4471-4474 (1974)

Huie, R. E., and Herron, J. T., "Temperature Dependence of the Rate Constants for Reactions of Ozone with Some Olefins," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Huie, R. E., and Herron, J. T., "The Rate Constant for the Reaction $O_3 + NO_2 \rightarrow O_2 + NO_3$ Over the Temperature Range 259-362° K," Chem. Phys. Lett. 27, 411-414 (1974a)

Huie, R. E., Herron, J. T., and Davis, D. D., "Absolute Rate Constants for the Reaction $O + O_2 + M \rightarrow O_3 + M$ Over the Temperature Range 200-346°K," J. Phys. Chem. 76, 2653-2658 (1972)

Husain, D., Kirsch, L. J., and Donovan, R. J., "A Kinetic Study of $O(2^3P_J)$ by Atomic Absorption Spectroscopy Following the Flash Photolysis of Ozone," J. Photochem. 1, 69-73 (1972)

Jacob, A., and Winkler, C. A., "Kinetics of the Reactions of Oxygen Atoms and Nitrogen Atoms with Sulphur Trioxide," J. Chem. Soc. Faraday Trans. I 68, 2077-2082 (1972)

James, F. C., Kerr, J. A., and Simons, J. P., "A Direct Measurement of the Rate of Reaction of the Methyl Radical with Sulphur Dioxide," J. Chem. Soc. Faraday Trans. I 69, 2124-2129 (1973)

Johnston, H. S., "Gas Phase Reaction Rate Theory," The Ronald Press Co., New York (1966), Chapter 1

Johnston, H. S., "Gas Phase Reaction Kinetics of Neutral Oxygen Species," NBS-NSRDS-20, 1968. (Supt. of Documents, U.S. Govt. Printing Office, Washington, D.C. 20402)

Johnston, H. S., "Catalytic Reduction of Stratospheric Ozone by Nitrogen Oxides," Adv. Environ. Sci. and Technology 4, 263-380 (1974), J. N. Pitts, Jr., and R. L. Metcalf, editors, Wiley-Interscience

Johnston, H. S., private communication (1973)

Johnston, H. S., Chang, S.-G., and Whitten, G., "Photolysis of Nitric Acid Vapor," J. Phys. Chem. 78, 1-7 (1974)

Johnston, H. S., and Graham, R., "Gas Phase Ultraviolet Absorption Spectrum of Nitric Acid Vapor," J. Phys. Chem. 77, 62-63 (1973)

Johnston, H. S., Morris, E. D., Jr., and Van den Bogaerde, J., "Molecular Modulation Kinetic Spectrometry. ClOO and ClO_2 Radicals in the Photolysis of Chlorine in Oxygen," J. Amer. Chem. Soc. 91, 7712-7727 (1969)

Jones, I. T. N., and Bayes, K. D., "Photolysis of Nitrogen Dioxide," J. Chem. Phys. 59, 4836-4844 (1973)

Jones, E. J., and Wulf, O. R., "Absorption Coefficient of Nitrogen Pentoxide in the Ultraviolet and the Visible Absorption Spectrum of NO_3," J. Chem. Phys. 5, 873-877 (1937)

Kaufman, F., "Aeronomic Reactions Involving Hydrogen. A Review of Recent Laboratory Studies," Ann. Geophys. 20, 106-114 (1964)

Kerr, J. A., and Parsonage, M. J., "Evaluated Kinetic Data on Gas Phase Addition Reactions: Reactions of Atoms and Radicals with Alkenes, Alkynes and Aromatic Compounds," (Butterworths, 1972)

Klemm, R. B., Payne, W. A., and Stief, L. J., "Absolute Rate Parameters for the Reaction of Atomic Hydrogen with H_2O_2," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Kondratiev, V. N., "Konstanty Skorosti Gazofaznykh Reaktsij Spravochnik," (Izdatelstvo "Nauka", Moskva, 1970); also issued as "Rate Constants of Gas Phase Reactions, Reference Book," R. M. Fristrom, Ed., Translated by L. J. Holtschlag COM-72-10014, Office of Standard Reference Data, NBS (1972) (Distributed by National Technical Information Service, Springfield, Va. 22151)

Kurylo, M. J., Hollinden, G. A., LeFevre, H. F., and Timmons, R. B., "ESR Study of the Kinetics of the Reactions of D Atoms and O Atoms with NH_3," J. Chem. Phys. 51, 4497-4501 (1969)

Kurylo, M. J., "Absolute Rate Constants for the Reaction $H + O_2 + M \rightarrow HO_2 + M$ Over the Temperature Range 203-404 K," J. Phys. Chem. 76, 3518-3526 (1972)

Kurylo, M. J., "Kinetics of the Reactions $OH(v = 0) + NH_3 \rightarrow H_2O + NH_2$ and $OH(v = 0) + O_3 \rightarrow HO_2 + O_2$ at 298^{o}K," Chem. Phys. Letts. 23, 467-471 (1973)

Kurylo, M. J., Braun, W., Kaldor, A., Freund, S. M., and Wayne, R. P., "Infra-red Laser Enhanced Reactions: Chemistry of Vibrationally Excited O_3 with NO and $O_2(^1\Delta)$," J. Photochem. 3, 71-87 (1974)

Kurylo, M. J., Peterson, N. C., and Braun, W., "Absolute Rate of the Reaction $H + H_2S$," J. Chem. Phys. 54, 943-946 (1971)

Laufer, A. H., and Bass, A. M., "Rate Constants of the Combination of Methyl Radicals with Nitric Oxide and Oxygen," typescript, National Bureau of Standards, Washington, D. C. (1974)

Lin, C. L., and DeMore, W. B., "$O(^1D)$ Production in Ozone Photolysis Near 3100Å," J. Photochem. 2, 161-164 (1973)

Lloyd, A. C., "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," Intern. J. Chem. Kinet. 6, 169-228 (1974) Supersedes NBS Report 10447

Lundell, O. R., Ketcheson, R. D., and Schiff, H. I., "The Production of $O(^3P)$ Atoms, Free From Excited Molecules, and Their Reaction with O_3," Symp. Combust. 12th (Combustion Institute, Pittsburgh, 1969) 307-311

Mack, G. P. R., and Thrush, B. A., "Reaction of Oxygen Atoms with Carbonyl Compounds. Part 1. Formaldehyde," J. Chem. Soc. Faraday Trans. I 69, 208-215 (1973)

Margitan, J. J., Kaufman, F., and Anderson, J. G., "The Reaction of OH with CH_4," Geophys. Res. Lett. 1, 80-81 (1974)

McCrumb, J. L., and Kaufman, F., "Kinetics of the O + O_3 Reaction," J. Chem. Phys. 57, 1270-1276 (1972)

McKenzie, A., Mulcahy, M. F. R., and Steven, J. R., "Kinetics of Decay of Hydroxyl Radicals at Low Pressure," J. Chem. Phys. 59, 3244-3254 (1973)

McQuigg, R. D., and Calvert, J. G., "The Photodecomposition of CH_2O, CD_2O, CHDO and CH_2O-CD_2O Mixtures at Xenon Flash Lamp Intensities," J. Amer. Chem. Soc. 91, 1590-1599 (1969)

Meaburn, G. M., Perner, D., LeCalve, J., and Bourene, M., "A Pulsed-Radiolysis Study of Atomic Oxygen Reactions in the Gas Phase," J. Phys. Chem. 72, 3920-3925 (1968)

Meagher, J. F., and Heicklen, J., "The Photolysis of Hydrogen Peroxide in the Presence of Carbon Monoxide," Dept. of Chemistry and Center for Air Environment Studies, The Pennsylvania State University, University Park Pennsylvania, CAES Publication No. 370-74 May, 1974

Milks, D., and Matula, R. A., "A Single-Pulse Shock-Tube Study of the Reaction between Nitrous Oxide and Carbon Monoxide," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 33-96

Moortgat, G. K., and Allen, E. R., "The Room Temperature Reactions of Hydrogen-Atoms in Molecular Oxygen," National Center for Atmospheric Research, Boulder (1973). Abstract of unpublished work.

Morley, C., and Smith, I. W. M., "Rate Measurements of Reactions of OH by Resonance Absorption. Part I. Reactions of OH with NO_2 and NO," J. Chem. Soc. Faraday Trans. II 68, 1016-1030 (1972)

Morris, E. D., Jr., and Niki, H., "Mass Spectrometric Study of the Reaction of Hydroxyl Radical with Formaldehyde," J. Chem. Phys. 55, 1991-1992 (1971)

Morris, E. D., Jr., and Niki, H., "Reaction of Methyl Radicals with Atomic Oxygen," Intern. J. Chem. Kinet. 5, 47-53 (1972)

Morris, E. D., Jr., and Niki, H., "Reaction of Dinitrogen Pentoxide with Water," J. Phys. Chem. 77, 1929-1932 (1973)

Morris, E. D., Jr., Stedman, D. H., and Niki, H., "Mass Spectrometric Study of the Reactions of the Hydroxyl Radical with Ethylene, Propylene, and Acetaldehyde in a Discharge-Flow System," J. Amer. Chem. Soc. 93, 3570-3572 (1971)

Mulcahy, M. F. R., and Williams, D. J., "Kinetics of Combination of Oxygen Atoms with Oxygen Molecules," Trans. Faraday Soc. 64, 59-70 (1968)

Nicholas, J. E., and Norrish, R. G. W., "Some Reactions in the Chlorine and Oxygen System Studied by Flash Photolysis," Proc. Roy. Soc. (London) A 307, 391-397 (1968)

Overend, R., Paraskevopoulos, G., and Cvetanović, R. J., "Hydroxyl Radical Rate Measurement for Simple Species by Flash Photolysis Kinetic Spectroscopy," Eleventh Informal Conference on Photochemistry, Vanderbilt Univ., June 1974

Parkes, D. A., Paul, D. M., Quinn, C. P., and Robson, R. C., "The Ultraviolet Absorption by Alkylperoxy Radicals and Their Mutual Reactions," Chem. Phys. Lett. 23, 425-429 (1973)

Pastrana, A., and Carr, R. W., Jr., "Rate of the Reaction of Hydroxyl Radical with Acetylene," Intern. J. Chem. Kinet. 6, 587-595 (1974)

Pate, C. T., Finlayson, B. J., and Pitts, J. N., Jr., "A Long Path Infrared Spectroscopic Study of the Reaction of Methylperoxy Free Radicals with Nitric Oxide," J. Am. Chem. Soc. 96, 6554-6558 (1974)

Payne, W. A., Stief, L. J., and Davis, D. D., "A Kinetics Study of the Reaction of HO_2 with SO_2 and NO," J. Amer. Chem. Soc. 95, 7614-7619 (1973)

Peeters, J., and Mahnen, G., "Reaction Mechanisms and Rate Constants of Elementary Steps in Methane-Oxygen Flames," Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 133-141

Pitts, J. N., Jr., Sandoval, H. L., and Atkinson, R., "Relative Rate Constants fo the Reaction of $O(^1D)$ Atoms with Fluorocarbons and N_2O," Chem. Phys. Lett. 29, 31-34 (1974)

Pruss, F. J., Jr., Slagle, I. R., and Gutman, D., "Determination of Branching Ratios for the Reaction of Oxygen Atoms with Ethylene," J. Phys. Chem. 78, 663-665 (1974)

Rawlins, W. T., and Gardiner, W. C., Jr., "Rate Constant of OH + OH = H_2O + O from 1500 to 2000 K," J. Chem. Phys. 60, 4676-4681 (1974)

Ridley, B. A., Davenport, J. A., Stief, L. J., and Welge, K. H., "Absolute Rate Constant for the Reaction H + H_2CO," J. Chem. Phys. 57, 520-523 (1972)

Sauer, M. C., Jr., "A Pulse-Radiolysis Study of the Dependence of the Reaction of Atomic Oxygen with Oxygen on the Nature of the Third Body," J. Phys. Chem. 71, 3311-3313 (1967)

Schofield, K., "The Rate of Destruction of $O_2(^1\Delta_g)$ by Atomic Hydrogen," Intern. J. Chem. Kinet. 4, 255-263 (1972)

Schofield, K., "Evaluated Chemical Kinetic Rate Constants for Various Gas Phase Reactions," J. Phys. Chem. Ref. Data 2, 25-84 (1973)

Simonaitis, R., and Heicklen, J., "The Reactions of HO_2 with Carbon Monoxide and Nitric Oxide and the Reaction of $O(^1D)$ with Water," J. Phys. Chem. 77, 1096-1102 (1973a)

Simonaitis, R., and Heicklen, J., "The Reaction of HO_2 with O_3," J. Phys. Chem. 77, 1932-1935 (1973b)

Simonaitis, R., and Heicklen, J., "The Mechanism of the H_2O-Catalyzed Chain Photodecomposition of O_3 and the Reaction of HO with O_3," J. Photochem. 2, 309-314 (1973c)

Simonaitis, R., and Heicklen, J., "The Reaction of HO_2 with NO and NO_2," J. Phys. Chem. 78, 653-657 (1974)

Simonaitis, R., and Heicklen, J., "Reactions of CH_3O_2 with NO and NO_2," J. Phys. Chem. 78, 2417-2421 (1974)

Slagle, I. R., Pruss, F. J., Jr., and Gutman, D., "Kinetics into the Steady State. I. Study of the Reaction of Oxygen Atoms with Methyl Radicals," Intern. J. Chem. Kinet. 6, 111-123 (1974)

Slanger, T. G., and Black, G., "Reaction Rate Measurements of $O(^3P)$ Atoms by Resonance Fluorescence. I. $O(^3P) + O_2 + M \rightarrow O_3 + M$ and $O(^3P) + NO + M \rightarrow NO_2 + M$," J. Chem. Phys. 53, 3717-3721 (1970)

Slanger, T. G., Wood, B. J., and Black, G., "Investigation of the Rate Coefficient for $O(^3P) + NO_2 \rightarrow O_2 + NO$," Intern. J. Chem. Kinet. 5, 615-620 (1973)

Slanger, T. G., and Welge, K. H., "Rate Constants for Reactions of $O(^1S)$," in Chemical Kinetics Data Survey V. Sixty-six Contributed Rate and Photochemical Data Evaluations on Ninety-four Reactions, NBSIR 73-206, D. Garvin, Ed., National Bureau of Standards, Washington, D.C., (1973) pages 22-32

Smith, I. W. M., and Zellner, R., "Rate Measurements of Reactions of OH by Resonance Absorption Part 2. Reactions of OH with CO, C_2H_4 and C_2H_2," J. Chem. Soc. Faraday Trans. II 69, 1617-1627 (1973)

Smith, I. W. M., and Zellner, R., "Rate Measurements of Reactions of OH by Resonance Absorption. Part 3. Reactions of OH with H_2, D_2, Hydrogen and Deuterium Halides," J. Chem. Soc. Faraday Trans. II 70, 1045-1056 (1974a)

Smith, I. W. M., and Zellner, R., "Rate Measurements of Reactions of OH by Resonance Absorption. Part 4. - Reactions of OH with NH_3 and HNO_3," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Sperling, H. P., and Toby, S., "The Photochemical Decomposition of Gaseous Formaldehyde," Can. J. Chem. 51, 471-475 (1973)

Stedman, D. H., and Niki, H., "Kinetics and Mechanism for the Photolysis of Nitrogen Dioxide in Air," J. Phys. Chem. 77, 2604-2609 (1973)

Stedman, D. H., Wu, C. H., and Niki, H., "Kinetics of Gas-Phase Reactions of Ozone with Some Olefins," J. Phys. Chem. 77, 2511-2514 (1973)

Stuhl, F., "Absolute Rate Constant for the Reaction $OH + NH_3 \rightarrow NH_2 + H_2O$," J. Chem. Phys. 59, 535-537 (1973a)

Stuhl, F., "Rate Constant for the Reaction of OH with $n\text{-}C_4H_{10}$," Z. Naturforsch. Pt A 28, 1383-1384 (1973b)

Stuhl, F., "Determination of Rate Constants for the Reactions of OH with Propylene and Ethylene by a Pulsed Photolysis-Resonance Fluorescence Method," Ber. Bunsenges. Physik. Chem. 77, 674-677 (1973c).

Stuhl, F., "Determination of the Rate Constant for the Reaction $OH + H_2S$ by a Pulsed Photolysis - Resonance Fluorescence Method," Ber. Bunsenges. Physik. Chem. 78, 230-232 (1974)

Stuhl, F., and Niki, H., "Detection of Oxygen (^3P) Atoms in Pulsed Vacuum UV Photolysis of NO and Its Application to O Atom Reactions," Chem. Phys. Lett. 7, 197-200 (1970)

Stuhl, F., and Niki, H., "Measurements of Rate Constants for Termolecular Reactions of $O(^3P)$ with NO, O_2, CO, N_2, and CO_2 Using a Pulsed Vacuum-uv Photolysis-Chemiluminescent Method," J. Chem. Phys. 55, 3943-3953 (1971)

Stuhl, F., and Niki, H., "Pulsed Vacuum-uv Photochemical Study of Reactions of OH with H_2, D_2, and CO Using a Resonance-Fluorescent Detection Method," J. Chem. Phys. 57, 3671-3677 (1972)

Takacs, G. A., and Glass, G. P., "Reactions of Hydroxyl Radicals with Some Hydrogen Halides," J. Phys. Chem. 77, 1948-1951 (1973)

Taylor, R. L., "High Temperature Air Reactions," in NBSIR 74-430 Chemical Kinetics Data Survey VII. Tables of Rate and Photochemical Data for Modelling of the Stratosphere (Revised), D. Garvin and R. F. Hampson, Eds., National Bureau of Standards, Washington, D.C., January 1974

Thrush, B. A., Letter to D. Garvin (Sept. 1973) reevaluating work in his laboratory

Toby, F. S., and Toby, S., "Reaction between Ozone and Allene in the Gas Phase," Intern. J. Chem. Kinet. 6, 417-428 (1974)

Toby, F. S., and Toby, S., "The Reaction of Ozone with 1,3-Butadiene and with Allene," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Trainor, D. W., and von Rosenberg, C. W., Jr., "Flash Photolysis Study of the Gas Phase Recombination of Hydroxyl Radicals," J. Chem. Phys. 61, 1010-1015 (1974)

Tsang, W., "Comparison between Experimental and Calculated Rate Constants for Dissociation and Combination Reactions Involving Small Polyatomic Molecules," Intern. J. Chem. Kinet. 5, 947-963 (1973)

Vardanyan, I. A., Dangyan, T. M., and Sachyan, G. A., "Rate Constants for the Reaction $HO_2 + CO \rightarrow CO_2 + OH$," Dokl. Phys. Chem. 205, 632-634 (1972); tr. of Dokl. Akad. Nauk SSSR 205, 619-621 (1972)

van den Bergh, H. E., and Callear, A. B., "Spectroscopic Measurement of the Rate of the Gas-Phase Combination of Methyl Radicals with Nitric Oxide and Oxygen at 295 K," Trans. Faraday Soc. 67, 2017-2024 (1971)

Volman, D. H., and Gorse, R. A., "Rate Constant for the Reaction of HO_2 with Carbon Monoxide," J. Phys. Chem. 76, 3301-3302 (1972)

von Rosenberg, C. W., Jr., and Trainor, D. W., "Vibrational Excitation of Ozone Formed by Recombination," J. Chem. Phys. 61, 2442-2456 (1974)

Walker, R. W., Ph.D., thesis, Univ. of London, Queen Mary College, 1973

Walker, R. W., "Activation Energies of the Reversible Reaction between Hydrogen Atoms and Methane to give Hydrogen and Methyl Radicals," J. Chem. Soc., Sect. A, 2391-2398 (1968)

Walker, R. W., Comments on "Gas-Phase Oxidation of Butene-2: The Role of Acetaldehyde in the Reaction," by Ray, D. J. M., Diaz, R. R., and Wassington, D. J., Symp. Combust. 14th (Combustion Institute, Pittsburgh, 1973) 265-266

Washida, N., and Bayes, K. D., "The Rate of Reaction of Methyl Radicals with Atomic Oxygen," Chem. Phys. Letts. 23, 373-375 (1973)

Washida, N., Martinez, R. I., and Bayes, K. D., "The Oxidation of Formyl Radicals," typescript, Univ. of California (Los Angeles) (1973)

Watson, R. T., "Chemical Kinetics Data Survey VIII. Rate Constants of ClO_x of Atmospheric Interest," NBSIR 74-516 (1974) (distributed by Chemical Kinetics Information Center, National Bureau of Standards, Washington, D.C. 20234)

Wayne, R. P., private communication (1974)

Westenberg, A. A., and deHaas, N., "Steady-State Intermediate Concentrations and Rate Constants. Some HO_2 Results," J. Phys. Chem. 76, 1586-1593 (1972a)

Westenberg, A. A., and deHaas, N., "Measurement of the Rate Constant for $H + H_2CO \rightarrow H_2 + HCO$ at 297-652°K," J. Phys. Chem. 76, 2213-2214 (1972b)

Westenberg, A. A., and deHaas, N., "Rates of $CO + OH$ and $H_2 + OH$ Over an Extended Temperature Range," J. Chem. Phys. 58, 4061-4065 (1973a)

Westenberg, A. A., and deHaas, N., "Rate of the Reaction $OH + OH \rightarrow H_2O + O$," J. Chem. Phys. 58, 4066-4071 (1973b)

Wilson, Wm. E., Jr., "A Critical Review of the Gas-Phase Reaction Kinetics of the Hydroxyl Radical," J. Phys. Chem. Ref. Data 1, 535-573 (1972)

Wong, E. L., and Belles, F. E., "Rate Measurements for the Reaction of Hydrogen Chloride and Deuterium Chloride with Atomic Oxygen," Lewis Research Center, NASA, Cleveland, Ohio, NASA Tech. Note, NASA TN-D-6495 (1971); Chem. Abstr. 76:18326q (1972)

Wong, W., and Davis, D. D., "A Flash Photolysis-Resonance Fluorescence Study of the Reaction of Atomic Hydrogen with Molecular Oxygen: $H + O_2 + M \rightarrow HO_2 + M$," Intern. J. Chem. Kinet. 6, 401-416 (1974)

Wu, C. H., Morris, E. D., Jr., and Niki, H., "The Reaction of Nitrogen Dioxide with Ozone," J. Phys. Chem. 77, 2507-2511 (1973)

Wyrsch, D., Wendt, H. R., and Hunziker, H. E., "Modulation Kinetic Spectroscopy of $Hg/H_2/O_2/CO$ Mixtures: Reactions of HgH and HO_2," XI. Intern. Symp. on Free Radicals (Berchtesgaden-Konigssee, Sept. 4-7, 1973) Paper No. 36; see also, Ber. Bunsenges. Physik. Chem. 78, 204 (1974)

Zahniser, M. S., Kaufman, F., and Anderson, J. G., "Kinetics of the Reaction of OH with HCl," Chem. Phys. Lett. 27, 507-510 (1974)

Zellner, R., and Smith, I. W. M., "Rate Constants for the Reactions of OH with NH_3 and HNO_3," Chem. Phys. Lett. 26, 72-74 (1974)

APPENDIX 1.

Chemical Thermodynamic Properties of Selected Molecular Species

E. S. Domalski, D. Garvin, and D. D. Wagman

Two tables are provided showing chemical thermodynamic properties of selected molecular species of interest in stratospheric chemistry. In these tables there are sufficient data for the usual calculations of heats of reaction and equilibria.

The first table lists enthalpy and Gibbs energy of formation, entropy and heat capacity data. The information was extracted from "Selected Values of Chemical Thermodynamic Properties" (D. D. Wagman, et. al., NBS Technical Note 270-3, January 1968) except as indicated in the Notes. The thermodynamic properties tabulated are:

1. enthalpy of formation at 0K and 298.15K,
2. Gibbs energy of formation at 298.15K,
3. enthalpy increment between 0K and 298.15K,
4. entropy at 298.15K,
5. heat capacity at constant pressure at 298.15K.

The values given for the heats of formation are based on experimental thermodynamic and spectroscopic measurements except where otherwise indicated; the values of S°, $C_p{}^\circ$ and $H^\circ_{298}-H^\circ_0$ for the gaseous species were calculated by standard statistical-mechanical equations, using corrections for vibrational anharmonicities, rotational stretching, and rotation-vibration interactions where these data were available.

The second table presents bond dissociation energies or bond strengths. These usually are the enthalpies of simple bond scission reactions. However, there are some cases in which there is a substantial contribution from rearrangement of electronic structure in the products (reducing the bond energy).

The values given here for some molecules will differ slightly from values adopted by the CODATA Task Group on Key Values for Thermodynamics (see CODATA Bulletin 10, published by the International Council of Scientific Unions Committee on Data for Science and Technology, December 1973). These differences will have no significant effect on the enthalpies or free energies of reaction calculated from the tables.

National Bureau of Standards CHEMICAL THERMODYNAMIC PROPERTIES OF SELECTED MOLECULAR SPECIES Washington, D. C.

Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity *

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p	
Formula and Description	State	Formula Weight	0 °K	298.15 °K (25 °C)					
			kcal/mol				cal/deg mol		
O oxygen, atomic	g	15.9994	58.983	59.553	55.389	1.607	38.467	5.237	
$O(^1D)$	g	15.9994	104.34	104.78		1.481			(1)
$O(^1S)$	g	15.9994	155.60	156.04		1.481			(1)
O_2 oxygen, molecular, $(^3\Sigma_g^-)$	g	31.9988	0	0	0	2.0746	49.003	7.016	(2)
$O_2(^1\Delta)$	g	31.9988	22.54	22.54					(1)
$O_2(^1\Sigma)$	g	31.9988	37.51	37.51					(1)
O_3 ozone	g	47.9982	34.74	34.1	39.0	2.4736	57.08	9.37	
H hydrogen, atomic	g	1.0080	51.626	52.095	48.581	1.481	27.391	4.9679	
H_2 hydrogen, molecular	g	2.0159	0	0	0	2.0238	31.208	6.889	
OH hydroxyl	g	17.0074	9.25	9.31	8.18	2.1070	43.890	7.143	
HO_2 hydroperoxyl	g	33.0068	6.	5.		2.39	54.38	8.34	(3)
H_2O water	g	18.0153	-57.102	-57.796	-54.634	2.3667	45.104	8.025	
H_2O_2 hydrogen peroxide	g	34.0147	-31.08	-32.58	-25.24	2.594	55.6	10.3	
N nitrogen, atomic	g	14.0067	112.534	112.979	108.883	1.481	36.622	4.968	
N_2 nitrogen, molecular	g	28.0134	0	0	0	2.072	45.77	6.961	
NO nitric oxide	g	30.0061	21.45	21.57	20.69	2.197	50.347	7.133	
NO_2 nitrogen dioxide	g	46.0055	8.60	7.93	12.26	2.438	57.35	8.89	
NO_3 nitrogen trioxide	g	62.008	18.5	17.0	27.7	2.62	60.4	11.2	(3)
N_2O nitrous oxide	g	44.0128	20.435	19.61	24.90	2.284	52.52	9.19	
N_2O_4 dinitrogen tetroxide	g	92.0110	4.49	2.19	23.38	3.918	72.70	18.47	

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
				kcal/mol			cal/deg mol		
N_2O_5 dinitrogen pentoxide	g	108.0104	5.7	2.7	27.5	4.237	85.0	20.2	
NH imino (imidogen)	g	15.0147	90.	90.	88.6	2.060	43.29	6.97	(5)
NH_2 amino	g	16.0226	46.2	45.5	47.8	2.37	46.51	8.02	(4)
NH_3 ammonia	g	17.0306	-9.34	-11.02	-3.94	2.388	45.97	8.38	
HNO nitroxyl hydride	g	31.0142	24.5	23.8	26.859	2.387	52.729	8.279	(3)
HNO_2 cis,nitrous acid	g	47.0135	-17.12	-18.64	-10.27	2.608	59.43	10.70	
trans, nitrous acid	g	47.0135	-17.68	-19.15	-10.82	2.652	59.54	11.01	
cis-trans mixture, equil.	g	47.0135		-19.0	-11.0		60.7	10.9	
HNO_3 nitric acid	g	63.0129	-29.94	-32.28	-17.87	2.815	63.64	12.75	
S sulfur, rhombic	c	32.064	0	0	0	1.054	7.60	5.41	
	g	32.064	66.1	66.636	56.949	1.591	40.094	5.658	
SO monosulfur monoxide	g	48.0634	1.5	1.496	-4.741	2.087	53.02	7.21	
SO_2 sulfur dioxide	g	64.0628	-70.336	-70.944	-71.748	2.521	59.30	9.53	
SO_3 sulfur trioxide	c	80.0622		-108.63	-88.19		12.5		
	liq	80.0622		-105.41	-88.04		22.85		
	g	80.0622	-93.21	-94.58	-88.69	2.796	61.34	12.11	
H_2SO_4 sulfuric acid	c	98.0775	-194.069						
	liq	98.0775		-194.548	-164.938	6.748	37.501	33.20	
S_2O disulfur monoxide	g	80.1274				2.66	63.8	10.5	(3)
HS sulfur monohydride	g	33.0720	33.1	33.3	26.3	2.22	46.73	7.76	(5)

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
			kcal/mol				cal/deg mol		
H_2S hydrogen sulfide	g	34.0799	-4.232	-4.93	-8.02	2.379	49.16	8.18	
C graphite, Acheson spectroscopic	c	12.0112	0	0	0	0.251	1.372	2.038	
CO carbon monoxide	g	28.0106	-27.199	-26.416	-32.780	2.0716	47.219	6.959	
CO_2 carbon dioxide	g	44.0100	-93.963	-94.051	-94.254	2.2378	51.06	8.87	
CH_3 methyl	g	15.0351	35.6	34.8	35.3	2.49	46.38	9.25	(3)
CH_4 methane	g	16.0430	-15.970	-17.88	-12.13	2.388	44.492	8.439	
HCO formyl	g	29.0185	-4.2	-4.12	-7.76	2.386	53.68	8.26	
$HCHO$ formaldehyde	g	30.0265	-25.03	-25.95	-24.51	2.394	52.26	8.46	(6)
CH_3O methoxy	g	31.0345		3.9		2.41	64.2	8.9	(7) (24)
CH_3O_2 methylperoxyl	g	47.0339		22.					(8)
CH_3OOH methylhydroperoxide	g	48.0347		-30.8	-17.4		67.9	15.	(9)
CH_3NO_2 nitromethane	g	61.0406	-14.546	-17.86	-1.65	3.083	65.69	13.70	
CH_3ONO methyl nitrite	g	61.0406		-16.5		3.36	69.7	16.5	(10)(24)
CH_3NO_3 methyl nitrate	g	77.0400		-29.8	-9.4	3.55	76.1	16.1	(11, 12)(24)
$COCl_2$ phosgene	g	98.9166	-52.195	-52.61	-49.20	3.067	67.74	13.78	(13)

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table

Substance			ΔHf°_0	ΔHf°	ΔGf°	$H^\circ_{298} - H^\circ_0$	S°	C°_p	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
			kcal/mol				cal/deg mol		
C_2H_2 acetylene	g	26.0382	54.324	54.19	50.00	2.392	48.00	10.50	
C_2H_4 ethylene	g	28.0542	14.515	12.49	16.28	2.525	52.45	10.41	
C_2H_5 ethyl radical	g	29.0627		25.7	32.0		59.6	10.9	(14)
C_2H_6 ethane	g	30.0701	-16.323	-20.04	-7.66	2.856	54.85	12.58	(15,16)
C_3H_6 propylene	g	42.0816	8.467	4.88	15.00	3.237	63.80	15.27	(15)
C_3H_8 propane	g	44.0976	-19.684	-25.02	-5.81	3.512	64.51	17.57	(15,16)
C_4H_{10} n-butane	g	58.1248	-23.552	-30.03	-3.97	4.645	74.12	23.29	(15,16)
C_4H_{10} isobutane	g	58.1248	-25.223	-32.07	-4.91	4.276	70.42	23.14	(15,16)
CH_2CO ketene	g	42.0376	-10.66	-11.4	-11.6	2.819	59.16	12.37	(17)
CH_3CO acetyl radical	g	43.0456		-5.8	-3.0		64.5	12.7	(19)
CH_3CHO acetaldehyde	g	44.0536	-37.14	-39.72	-30.31	3.01	59.8	13.7	
CH_3COCl acetyl chloride	g	78.4986	-57.93	-60.07	-51.08	3.529	70.56	16.25	(18)
Cl chlorine, atomic	g	35.453	28.68	29.082	25.262	1.499	39.457	5.220	
ClO chlorine monoxide	g	51.4524	24.33	24.47	23.68	2.278	53.78	8.23	(20)
ClO_2 chlorine dioxide (sym.)	g	67.4518	25.09	24.5	28.8	2.580	61.36	10.03	

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Table

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
				kcal/mol			cal/deg mol		
ClO_2 chlorine dioxide (unsym.)	g	67.4518	21.7	21.3	25.1	2.78	63.0	11.0	(21)
ClO_3 chlorine trioxide	g	83.4512		37					
HCl hydrogen chloride	g	36.4610	-22.020	-22.062	-22.777	2.066	44.646	6.96	
HOCl hypochlorous acid	g	52.4604				2.440	56.54	8.88	
NOCl nitrosyl chloride	g	65.4591	12.81	12.36	15.77	2.716	62.52	10.68	
NO_2Cl nitryl chloride	g	81.4585	4.29	3.0	13.0	2.915	65.02	12.71	
Cl_2 chlorine, molecular	g	70.906	0	0	0	2.193	53.288	8.104	
Cl_2O dichlorine monoxide	g	86.9054	19.62		23.3	2.806	64.07	11.48	(22)
Cl_2O_4 chlorine perchlorate	g	134.9036				4.16	78.21	20.56	(23)
CF_4 carbon tetrafluoride	g	88.0048	-221.61	-223.04	-212.37	3.043	62.45	14.59	(3)
$CClF_3$ chlorotrifluoromethane	g	104.4594	-168.0	-169.2	-159.5	3.294	68.17	15.99	(3)
CF_2Cl_2 dichlorodifluoromethane	g	120.9140	-116.5	-117.5	-108.2	3.553	71.91	17.31	(3)
CCl_3F trichlorofluoromethane	g	137.3686	-68.24	-69.0	-59.6	3.838	74.00	18.65	(3)
CCl_4 carbon tetrachloride	g	153.8232	-22.42	-22.94	-12.83	4.120	74.02	19.93	(3, 25, 26)

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Enthalpy and Gibbs Energy of Formation; Entropy and Heat Capacity

Table

Substance			ΔHf_0°	ΔHf°	ΔGf°	$H_{298}^\circ - H_0^\circ$	S°	C_p°	
Formula and Description	State	Formula Weight	0°K	298.15°K (25°C)					
			kcal/mol				cal/deg mol		
CH_3Cl methyl chloride	g	50.4881	-17.69	-19.59	-13.98	2.489	55.99	9.73	(3, 27)
CH_2Cl_2 methylene dichloride	g	84.9331	-21.19	-22.83	-16.49	2.830	64.57	12.16	(3, 25)
$CHCl_3$ chloroform	g	119.3781	-23.49	-24.66	-16.83	3.383	70.63	15.63	(3, 25)
CF_3 trifluoromethyl radical	g	69.0064	-111.7	-112.4	-109.21	2.754	63.33	11.90	(3)
CCl_3 trichloromethyl radical	g	118.3702	19.15	19.	22.09	3.392	70.92	15.21	(3)
C_2Cl_4 tetrachloroethylene	g	165.8343	-2.83	-2.97	5.15	4.759	82.05	22.84	(3)
C_2HCl_3 trichloroethylene	g	131.3893	-1.032	-1.86	4.31	3.975	77.6	19.18	
CH_3CCl_3 1,1,1-trichloroethane (methyl chloroform)	g	133.4052	-34.65	-34.01	-18.21	4.30	76.49	22.07	(28)

Notes

1. Hampson, R. F. et al, J. Phys. Chem. Ref. Data 2, 267-312 (1973) [Data sheet on O_3 + hν (u.v.) p. 303.

2. Contributions of the higher electronic states of molecular oxygen to the enthalpy, entropy, and heat capacity at 298 K are insignificant.

3. Stull, D. R. and Prophet, H. "JANAF Thermochemical Tables" 2nd. ed. NSRDS-NBS 37 (1971).

4. Tsang, W. Estimated from kinetic data on the decomposition of N_2H_4. Chapter 12, NBS Report 10904, 1 July 1972.

5. NBS Report 10904, 1 July 1972, pp. 239-307.

6. R. A. Fletcher and G. Pilcher, Trans. Faraday Soc. 66, 794-799 (1970) provide more recent data for ΔHf°, 298.15 K.

7. Data obtained from Benson and O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, page 55).

8. We estimated the $\Delta Hf^{\circ}[CH_3O_2(g)]$ by assuming that: (a) the breaking of the O-O bond in CH_3O_2 was equivalent to the O-O bond scission (37 kcal mol^{-1}) in CH_3OOCH_3 and (b) the breaking of the O-H bond in CH_3O_2H was equivalent to the O-H bond scission (104 kcal mol^{-1}) in CH_3OH.

9. Values for ΔHf°, S°, and Cp° at 298.15 K were calculated using the group additivity method described by Benson and O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, ppg. 40-42).

10. The value for ΔHf° [$CH_3ONO(g)$] = -16.5 kcal mol^{-1} was derived from the combustion data of Geiseler and Thierfelder (Z. physik. Chem., N. F., 29, 248-257 (1961)), and the equilibrium data of Leermakers and Ramsperger (J. Am. Chem. Soc. 54, 1837-1845 (1932)) for: $CH_3OH(g) + NOC\ell(g) = CH_3ONO(g) + HC\ell(g)$.

11. The value for ΔHf° ($CH_3ONO_2(g)$) = -29.8 kcal mol^{-1} was derived from the work of Ray and Ogg (J. Phys. Chem. 63, 1522-1523 (1959)) on the enthalpy of reaction of N_2O_5 with CH_3ONO.

12. We have chosen S° [$CH_3ONO_2(g)$] = 76.1 cal $mol^{-1}K^{-1}$ based upon low temperature thermal data of Gray and Smith (J. Chem. Soc. 1953, 2380-2385). Calculations from microwave studies by Dixon and Wilson (J. Chem. Phys. 35, 191-198 (1961)) give S° = 72.15 cal $mol^{-1}K^{-1}$.

13. Davies, J. V., and Pritchard, H. O., J. Chem. Thermodynamics 4, 23-29 (1972) provide more recent ΔHf° data.

14. Data on ΔHf°, S°, C_p° obtained from S. W. Benson and H. E. O'Neal ("Kinetic Data on Gas Phase Unimolecular Reactions", NSRDS-NBS-21, Feb. 1970, page 567).

15. Rossini, F. D., Pitzer, K. S., Arnett, R. L., Braun, R. M. and Pimentel, G. C., "Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds", API Research Project 44, Carnegie Press, Pittsburgh, 1953.

16. $\Delta Hf°$ data from Pittam and Pilcher (J. Chem. Soc., Faraday Trans. I, 68, 2224-2229 (1972).

17. $\Delta Hf°$ data from R. L. Nuttall, A. H. Laufer and M. V. Kilday., J. Chem. Thermodynamics 3, 167-174 (1971).

18. Devore, J. A., and O'Neal, H. E., J. Phys. Chem. 73, 2644-2648 (1969).

19. Data on S° and $C_p°$ were obtained from Note (14), page 589; data on $\Delta Hf°$ came from Note (18).

20. Spectroscopic studies of N. Basco and R. D. Morse, J. Molec. Spectros. 45, 35 (1973); R. A. Durie and D. A. Ramsay, Can. J. Phys. 36, 35 (1958); P. A. G. O'Hare and A. C. Wahl, J. Chem. Phys. 54, 3770 (1971); L. Andrews and J. I. Raymond, J. Chem. Phys. 55, 3087 (1971); D. R. Johnson and F. X. Powell, Bull. Am. Phys. Soc. 13, 594 (1968); A. Carrington, P. N. Dyer, and D. H. Levy, J. Chem. Phys. 47, 1756 (1967) were examined and used to calculate the thermodynamic properties.

21. Arkell, A., and Schwager, I., J. Am. Chem. Soc. 89, 5999 (1967); Johnston, H., Morris, E. D., and Vanden Bogaerde, J., J. Am. Chem. Soc. 91, 7712 (1969), Clyne, M. A. A. and White, I. F., Trans. Faraday Soc. 67, 2068 (1971).

22. Studies by D. J. Gardiner, J. Mol. Spectroscopy 38, 476 (1971) and G. E. Herberich, R. H. Jackson, and D. J. Miller, J. Chem. Soc. (A) 1966, 336 were examined and the data used to calculate the thermodynamic properties.

23. The spectroscopic data of K. O. Christe, C. J. Schack and E. C. Curtis, Inorg. Chem. 10, 1589 (1971) were used.

24. Thermal Constants of Substances (Termichesky Konstanty Veshchestv), Vol. IV, V. P. Glushko, Editor, Moscow (1970).

25. The combustion data of A. T. Hu and G. C. Sinke, J. Chem. Thermodynamics 1, 507-513 (1969) were used to derive ∆Hf° 298.15 K values for CCl_4, $CHCl_3$, and CH_2Cl_2 in the liquid state.

26. The vaporization data of D. L. Hildenbrand and R. A. McDonald, J. Phys. Chem. 63, 1521-1522 (1959) were used.

27. The combustion data of R. A. Fletcher and G. Pilcher, Trans. Faraday Soc. 67, 3191-3201 (1971) were used to calculate ∆Hf° [$CH_3Cl(g)$].

28. J. Chao, A. S. Rodgers, R. C. Wilhoit, and B. J. Zwolinski, J. Phys. & Chem. Ref. Data 3, 141-162 (1974) provide a recent evaluation of the thermodynamic properties of CH_3CCl_3.

Bond Dissociation Energies, D_0^{o} at 0 K

Reaction	kJ/mol	kcal/mol	Note (1)
$O_2 \rightarrow 2O$	493.59±0.4	117.97±0.1	
$O_3 \rightarrow O_2 + O$	101.4±2.1	24.24±0.5	(2)
$H_2 \rightarrow 2H$	432.00±0.04	103.25±0.01	
$HO \rightarrow H + O$	423.8±2.1	101.3±0.5	
$HO_2 \rightarrow HO + O$	264.4±4	63.2±1	
$\rightarrow H + O_2$	192±13	46±3	
$H_2O \rightarrow HO + H$	493.7±0.8	118.0±0.2	
$H_2O_2 \rightarrow 2HO$	207.1±2.1	49.5±0.5	
$H_2O_2 \rightarrow H + HO_2$	370.3±8.4	88.5±2.0	
$N_2 \rightarrow N + N$	941.69±0.04	225.07±0.01	
$NO \rightarrow N + O$	627.9	150.1	(2)
$NO_2 \rightarrow NO + O$	300.5	71.83	(2)
$NO_3 \rightarrow NO_2 + O$	205±21	49±5	(2) N-O
$N_2O \rightarrow N + NO$	474.9±4	113.5±1	
$\rightarrow N_2 + O$	161.3	38.58	(2)
$N_2O_3 \rightarrow NO + NO_2$	35.1±0.8	8.4±0.2	N-O
$N_2O_4 \rightarrow NO_2 + NO_2$	53.2	12.7	(2) N-N
$N_2O_5 \rightarrow NO_2 + NO_3$	89.5	21.4	(2) N-O
$HNO \rightarrow H + NO$	203	48.6	(2)
$\rightarrow NH + O$	475	113.5	
trans-$HNO_2 \rightarrow HO + NO$	209.07	49.07	(2) N-O
$HNO_3 \rightarrow HO + NO_2$	200	47.8	(2) N-O
$NH \rightarrow H + N$	356±8	85±2	
$NH_2 \rightarrow H + HN$	360	86	(2,3)

Bond Dissociation Energies, D_0^o at 0 K

Reaction	kJ/mol	kcal/mol	Note (1)
$NH_3 \rightarrow NH_2 + H$	453	108	(2,3)
$CO \rightarrow C + O$	1071.94 ± 0.4	256.2 ± 0.1	
$CO_2 \rightarrow CO + O$	525.9 ± 0.4	125.7 ± 0.1	
$CHO \rightarrow CH + O$	859	205	(2)
$\rightarrow CO + H$	119.7	28.6	
$CH_2O \rightarrow CHO + H$	314	75	
$CH_3O \rightarrow CH_3 + O$	378	90.4	(2,3)
$\rightarrow H + H_2C = O$	88.2	21.1	(2,3)
$CH_3O_2 \rightarrow CH_3O + O$	173.	41.5	(2,3)
$\rightarrow CH_3 + O_2$	53.6	12.8	(2,3)
$CH_3 \rightarrow CH_2 + H$	469.9 ± 0.4	112.3 ± 0.1	
$CH_4 \rightarrow CH_3 + H$	425.1 ± 8.4	101.6 ± 2.0	
$CH_3OOH \rightarrow CH_3O + HO$	184.	44.0	(2,3)
$\rightarrow CH_3 + HO_2$	295.	70.6	(2,3)
$CH_3ONO \rightarrow CH_3 + NO_2$	248	59.2	(2,3)
$CH_3NO_2 \rightarrow CH_3 + NO_2$	254	60.6	(2,3)
$CH_3ONO_2 \rightarrow CH_3O + NO_2$	174	41.6	(2,3)
$\rightarrow CH_3 + NO_3$	341	81.6	(2,3)
$SO \rightarrow S + O$	517.1 ± 8	123.6 ± 2	
$SO_2 \rightarrow SO + O$	547.3 ± 8	130.8 ± 2.0	
$SO_3 \rightarrow SO_2 + O$	342.7 ± 4	81.9 ± 1	

Notes

1. Unless another source is indicated, the values are those recommended by Darwent, B. deB., "Bond Dissociation Energies in Simple Molecules," Natl. Stand. Ref. Data Series - Natl. Bur. Standards <u>31</u> (January 1970).
2. Calculated from heats of formation in the accompanying table "Chemical Thermodynamic Properties of Selected Molecular Species". Sources of data are indicated in notes to that table.
3. Calculated for 298 K, values at OK not being available.

ADDENDA March 1975

The editors learned of the following data too late for inclusion in the main body of the table:

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1,28M	$O + SO_2 + M \rightarrow SO_3 + M$			
	Atkinson, Pitts (1974)	299-392	$9.2 \times 10^{-32} \exp(-1000/T)$ $cm^6 molecule^{-2} s^{-1}$ $M = N_2O$	
5,M	$O_2(^1\Delta) + M \rightarrow O_2 + M$			
	Penzhorn, et al. (1974)	300	$3.9 \pm 0.9 \times 10^{-20}$ $M = SO_2$	
		300	$2.1 \pm 0.2 \times 10^{-19}$ $M = H_2S$	
8,9	$N + NO \rightarrow N_2 + O$			
	Clyne, McDermid (1975)	298-670	$7.7 \pm 1.5 \times 10^{-11} \exp(-367 \pm 54/T)$	
9,20	$NO + HO_2 \rightarrow NO_2 + OH$			
	Hack, et al (1974)	298-670	$2.0 \pm 0.5 \times 10^{-11} \exp(-1200 \pm 150/T)$	
19,20	$HO + HO_2 \rightarrow H_2O + O_2$			
	Hack, et al (1974)	298	$k < 3 \times 10^{-11}$	
19,23	$HO + H_2O_2 \rightarrow H_2O + HO_2$			
	Hack, et al (1974)	298-670	$8.0 \pm 1.7 \times 10^{-12} \exp(-670 \pm 70/T)$	
25,hv	$HNO_2 + h\nu$			
	Johnston, Graham (1974)		Tabulated values of absorption cross section 300-400nm	

The following rate constants for reactions of bromine species are taken from Table 5.25 of Section 5.7.5 "Chlorine, the Chlorine Oxides and other Halogen Species," by R. T. Watson, in Chapter 5. "Chemistry of the Stratosphere" of "The Natural Stratosphere of 1974", E. Reiter, editor, C.I.A.P. Monograph 1: The numbering scheme for the bromine species corresponds to that used for the chlorine species with the letter "B" as a suffix.

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
1,36B	$O + BrO \rightarrow Br + O_2$	300	8×10^{-11}	
7,35B	$O_3 + Br \rightarrow BrO + O_2$	300	1.2×10^{-12} $E/R \lesssim 1320K$	
9,36B	$NO + BrO \rightarrow NO_2 + Br$	300	2.0×10^{-11}	
19,39B	$HO + HBr \rightarrow H_2O + Br$	300	5.1×10^{-12}	

ADDENDA
(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
		220	2.4×10^{-12}	
21,35B	$H_2 + Br \rightarrow HBr + H$	300	1.7×10^{-27}	
		220	6.5×10^{-33}	
35B,56	$Br + CH_4 \rightarrow HBr + CH_3$	300	7.9×10^{-24}	
		220	1.1×10^{-28}	
36B,hv	$BrO + h\nu \rightarrow Br + O$		Photodissociation rate is unknown	(a)
			(a) An order of magnitude estimate, $J(BrO) \sim 10^{-2}s^{-1}$, is given by Watson.	
36B,36B	$BrO + BrO \rightarrow 2Br + O_2$	300	6.4×10^{-12}	

The following preliminary values of rate constants for reactions of hydroxyl radicals with halogenated methanes, ethanes, and ethylenes were very recently communicated to the editors by C. J. Howard.

$HO + M \rightarrow$ products

M	$10^{15} \times k$	
CH_4	9.5	preliminary
CH_3F	15	preliminary
CH_3Cl	36	preliminary
CH_2F_2	7.8	preliminary
CH_2FCl	37	preliminary
CH_2Cl_2	150	preliminary
CHF_3	2.9	preliminary
CHF_2Cl	3.4	preliminary
$CHFCl_2$	26	preliminary
$CHCl_3$	120	preliminary
CF_4	< 0.4	preliminary

(continued)

ADDENDA
(continued)

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3 molecule^{-1} s^{-1}$	Notes and Reliability of log k
	HO + M -> products (continued)			
	M		$10^{15} \times k$	
	CF_3Cl		< 0.7	preliminary
	CF_2Cl_2		< 0.4	preliminary
	$CFCl_3$		< 0.5	preliminary
	CCl_4		< 4	preliminary
	C_2H_6		290	preliminary
	C_2H_5Cl		390	preliminary
	CH_3CF_2H		33	preliminary
	CH_3CF_2Cl		7.3	preliminary
	C_2H_4		2500 $(p > 3 \text{ torr})$	preliminary
	C_2H_3Cl		5800 $(p > 2 \text{ torr})$	preliminary
	CH_2CF_2		2100 $(p > 1.5 \text{ torr})$	preliminary
	CF_2CFCl		5400 $(p > 0.7 \text{ torr})$	preliminary

ERRATA March 1975

The following changes should be made to the entries now given in the main body of the table:

No.	Reaction/Reference * = Preferred Value	Temp. Range/K	Reaction Rate Constant $k/cm^3molecule^{-1}s^{-1}$	Notes and Reliability of log k
1,48	$O + CH_2O \rightarrow CHO + OH$			
	Delete entry by Demerjian, et al (1974) and replace with following entry:			
	*Herron, Huie (1973) review	300	1.5×10^{-13}	±0.15
1,49	$O + CH_3 \rightarrow CH_2O + H$ (a) $\rightarrow CHO + H_2$ (b)			
	Change entry by Morris, Niki (1972) to the following form:			
	Morris, Niki (1972)	300	$k_a/k(O + \text{tetramethylethylene}) = 1.5$	
4,49M	$O_2 + CH_3(+M) \rightarrow CH_3O_2(+M)$			
	Delete asterisk beside entry by Laufer, Bass (1974)			
11,hv	$NO_3 + hv \rightarrow NO + O_2$			
	Replace entire entry with the following entry:			
	$NO_3 + hv$			
	Johnston (1975)		For $\lambda < 580$ nm, dissociates to $NO_2 + O$ with unknown q.y. Does <u>not</u> dissociate to $NO + O_2$ at any wavelength. Tabulated values of absorption cross section from 450-680nm given in Johnston, Graham (1974). Specific photodissociation rates in daylight are $2.6 \times 10^{-2}s^{-1}$ (450-578 nm) and $4.34 \times 10^{-2}s^{-1}$ (579-680nm)	

Reference List for Addenda and Errata

Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of O(^{3}P) Atoms with SO_2(M = N_2O) over the Temperature Range 299-392 K," Chem. Phys. Lett. 29, 28-30 (1974)

Clyne, M. A. A., and McDermid, L. S., "Mass Spectrometric Determinations of the Rates of Elementary Reactions of NO and of NO_2 with Ground State N^4S Atoms," Typescript (1975)

Hack, W., Hoyermann, K., and Wagner, H. Gg., "The Reaction $NO + HO_2 \rightarrow NO_2 + OH$ with $OH + H_2O_2 \rightarrow HO_2 + H_2O$ as an HO_2 Source," Presented at Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere, Airlie House, Warrenton, Virginia, September 1974. Proceedings to be published Intern. J. Chem. Kinet.

Howard, C. J., private communication, March 1975

Johnston, H. S., and Graham, R., "Photochemistry of NO_x and HNO_x Compounds," Can. J. Chem. 52, 1415-1423 (1974)

Penzhorn, R.-D., Gusten, H., Schurath, U., and Becker, K. H., "Quenching of Singlet Molecular Oxygen by Some Atmospheric Pollutants," Environ. Sci. Technology 8, 907-909 (1974)

APPENDIX 3. CONVERSION TABLES

EQUIVALENT SECOND ORDER RATE CONSTANTS

A ╲ B	$cm^3 mol^{-1} s^{-1}$	$dm^3 mol^{-1} s^{-1}$	$m^3 mol^{-1} s^{-1}$	$cm^3 molecule^{-1} s^{-1}$	$(mm\ Hg)^{-1} s^{-1}$	$atm^{-1} s^{-1}$	$ppm^{-1} min^{-1}$	$m^2 kN^{-1} s^{-1}$
$1\ cm^3 mol^{-1} s^{-1}$ =	1	10^{-3}	10^{-6}	1.66×10^{-24}	$1.604 \times 10^{-5} T^{-1}$	$1.219 \times 10^{-2} T^{-1}$	2.453×10^{-9}	$1.203 \times 10^{-4} T^{-1}$
$1\ dm^3 mol^{-1} s^{-1}$ =	10^3	1	10^{-3}	1.66×10^{-21}	$1.604 \times 10^{-2} T^{-1}$	$12.19\ T^{-1}$	2.453×10^{-6}	$1.203 \times 10^{-1} T^{-1}$
$1\ m^3 mol^{-1} s^{-1}$ =	10^6	10^3	1	1.66×10^{-18}	$16.04\ T^{-1}$	$1.219 \times 10^4 T^{-1}$	2.453×10^{-3}	$120.3\ T^{-1}$
$1\ cm^3 molecule^{-1} s^{-1}$ =	6.023×10^{23}	6.023×10^{20}	6.023×10^{17}	1	$9.658 \times 10^{18} T^{-1}$	$7.34 \times 10^{21} T^{-1}$	1.478×10^{15}	$7.244 \times 10^{19} T^{-1}$
$1\ (mm\ Hg)^{-1} s^{-1}$ =	$6.236 \times 10^4 T$	$62.36\ T$	$6.236 \times 10^{-2} T$	$1.035 \times 10^{-19} T$	1	760	4.56×10^{-2}	7.500
$1\ atm^{-1} s^{-1}$ =	$82.06\ T$	$8.206 \times 10^{-2} T$	$8.206 \times 10^{-5} T$	$1.362 \times 10^{-22} T$	1.316×10^{-3}	1	6×10^{-5}	9.869×10^{-3}
$1\ ppm^{-1} min^{-1}$ = at 298K, 1 atm. total pressure	4.077×10^8	4.077×10^5	407.7	6.76×10^{-16}	21.93	1.667×10^4	1	164.5
$1\ m^2 kN^{-1} s^{-1}$ =	$8314\ T$	$8.314\ T$	$8.314 \times 10^{-3} T$	$1.38 \times 10^{-20} T$	0.1333	101.325	6.079×10^{-3}	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under Column B and multiply the old value by it, e.g. to convert $cm^3 molecule^{-1} s^{-1}$ to $m^3 mol^{-1} s^{-1}$ multiply by 6.023×10^{17}

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the H_2-O_2 System, Butterworths, London, 1972.

EQUIVALENT THIRD ORDER RATE CONSTANTS

A \ B	$cm^6 mol^{-2} s^{-1}$	$dm^6 mol^{-2} s^{-1}$	$m^6 mol^{-2} s^{-1}$	$cm^6 molecule^{-2} s^{-1}$	$(mm\ Hg)^{-2} s^{-1}$	$atm^{-2} s^{-1}$	$ppm^{-2} min^{-1}$	$m^4 kN^{-2} s^{-1}$
1 $cm^6 mol^{-2} s^{-1}$ =	1	10^{-6}	10^{-12}	2.76 x 10^{-48}	2.57 x $10^{-10} T^{-2}$	1.48 x $10^{-4} T^{-2}$	1.003 x 10^{-19}	1.447 x $10^{-8} T^{-2}$
1 $dm^6 mol^{-2} s^{-1}$ =	10^6	1	10^{-6}	2.76 x 10^{-42}	2.57 x $10^{-4} T^{-2}$	148 T^{-2}	1.003 x 10^{-13}	1.447 x $10^{-2} T^{-2}$
1 $m^6 mol^{-2} s^{-1}$ =	10^{12}	10^6	1	2.76 x 10^{-36}	257 T^{-2}	1.48 x $10^8 T^{-2}$	1.003 x 10^{-7}	1.447 x $10^4 T^{-2}$
1 $cm^6 molecule^{-2} s^{-1}$ =	3.628 x 10^{47}	3.628 x 10^{41}	3.628 x 10^{35}	1	9.328 x $10^{37} T^{-2}$	5.388 x $10^{43} T^{-2}$	3.64 x 10^{28}	5.248 x $10^{39} T^{-2}$
1 $(mm\ Hg)^{-2} s^{-1}$ =	3.89 x $10^9 T^2$	3.89 x $10^3 T^2$	3.89 x $10^{-3} T^2$	1.07 x $10^{-38} T^2$	1	5.776 x 10^5	3.46 x 10^{-5}	56.25
1 $atm^{-2} s^{-1}$ =	6.733 x $10^3 T^2$	6.733 x $10^{-3} T^2$	6.733 x $10^{-9} T^2$	1.86 x $10^{-44} T^2$	1.73 x 10^{-6}	1	6 x 10^{-11}	9.74 x 10^{-5}
1 $ppm^{-2} min^{-1}$ = at 298K, 1 atm. total pressure	9.97 x 10^{18}	9.97 x 10^{12}	9.97 x 10^6	2.75 x 10^{-29}	2.89 x 10^4	1.667 x 10^{10}	1	1.623 x 10^6
1 $m^4 kN^{-2} s^{-1}$ =	6.91 x $10^7 T^2$	69.1 T^2	6.91 x $10^{-5} T^2$	1.904 x $10^{-40} T^2$	0.0178	1.027 x 10^4	6.16 x 10^{-7}	1

See note to Table for Second Order Rate Constants

CONVERSION FACTORS FOR UNITS OF OPTICAL ABSORPTION COEFFICIENTS

B A	(cross section σ) $cm^2 molecule^{-1}$ base e	$(atm\ at\ 273)^{-1} cm^{-1}$ base e	$dm^3 mol^{-1} cm^{-1}$ base 10	$cm^2 mol^{-1}$ base 10
1 $(atm\ at\ 298)^{-1} cm^{-1}$ base e =	4.06×10^{-20}	1.09	10.6	1.06×10^4
1 $(atm\ at\ 298)^{-1} cm^{-1}$ base 10 =	9.35×10^{-20}	2.51	24.4	2.44×10^4
1 $(mm\ Hg\ at\ 298)^{-1} cm^{-1}$ base 10 =	7.11×10^{-17}	1.91×10^3	1.86×10^4	1.86×10^7
1 $(atm\ at\ 273)^{-1} cm^{-1}$ base e =	3.72×10^{-20}	1	9.73	9.73×10^3
1 $(atm\ at\ 273)^{-1} cm^{-1}$ base 10 =	8.57×10^{-20}	2.303	22.4	2.24×10^4
1 $dm^3\ mol^{-1} cm^{-1}$ base 10 =	3.82×10^{-21}	0.103	1	10^3
1 $cm^2\ mol^{-1}$ base 10 =	3.82×10^{-24}	1.03×10^{-4}	10^{-3}	1
1 $cm^2\ molecule^{-1}$ base e =	1	2.69×10^{19}	2.62×10^{20}	2.62×10^{23}

To convert an absorption coefficient from one set of units A to a new set B, multiply by the value tabulated for row A under column B, e.g. to convert the value of the absorption coefficient expressed in $dm^3\ mol^{-1} cm^{-1}$ base 10 to $(atm\ at\ 273)^{-1} cm^{-1}$ base e, multiply by 0.103.

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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

A table of data for gas phase chemical reactions and photochemistry of neutral species is presented. Specifically, it gives preferred values for reaction rate constants, photoabsorption cross sections, and quantum yields of primary photochemical processes and also cites recent experimental work. It is intended to provide the basic physical chemical data needed as input data for calculations modelling atmospheric chemistry. An auxiliary table of thermochemical data for the pertinent chemical species is given in the appendix.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Atmospheric chemistry; chemical kinetics; data evaluation; gas phase; photoabsorption cross section; photochemistry; quantum yield; rate constant

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