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NATIONAL BUREAU OF STANDARDS REPORT

9884

A COMPENDIUM OF EVALUATED AND ESTIMATED RATE COEFFICIENTS

July 1968

This project is an activity of the Chemical Kinetics Information Center, N.B.S. The work was supported by the Naval Ordnance Systems Command ORD 3311 as part of a program to foster the production of tables of chemical kinetics.

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NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

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NATIONAL BUREAU OF STANDARDS REPORT

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A COMPENDIUM OF EVALUATED AND ESTIMATED RATE COEFFICIENTS

Edited By
David Garvin
Institute for Materials Research

July 1968

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CHAPTER 1: INTRODUCTION

This report is an annotated handbook on rates of elementary gas phase reactions. It is limited to rate evaluations. No attempt has been made to record all research papers pertinent to a particular reaction. There are two principal parts to the report, a compilation and a set of rate evaluations.

The compilation merges the information presented in several recent journal articles and reports that are devoted to the evaluation or estimation of rate coefficients for elementary reactions. A single table, arranged by reaction, lists the various recommended rates in a common format. Notes to the table show what data sources were used by each evaluator, and, where possible, how his recommended value was determined. The person requiring a rate for a specific reaction may compare the recommendations, compare their data bases and also extract a bibliography of the pertinent work.

The rate evaluations, which are presented in full, stand independent of the main table. They are for reactions of some importance to combustion and atmospheric chemistry. They are presented in a form suited to the reaction-by-reaction evaluation of rate data as opposed to that used in monographs. It is hoped that they will serve as models, albeit ones to be improved upon, for future rate data examinations.

It is also hoped that this technique for presenting rate evaluations, either one or a few reactions at a time, will find favor among kineticists. The labor involved is modest, particularly for the scientist who needs to review previous work during the design of his own experiments. Such evaluations would be welcome additions to later editions of this report. It is only by a cooperative effort that the basic kinetic data used in applied research and technology can be improved significantly in a reasonable time.

The restriction to evaluated material means that the values listed here are the results of a process of reexamination of available data. One may hope that there has been a detailed examination of the data and a comparison with the behavior of similar reactions. That is, that the purview of the evaluator may be broader than that of the experimenter. The results of such reexamination may be a selection, a composite of acceptable data, a calculation, or, in the absence of other guides, a guess. Evaluation, particularly when the data are few, seems to be a highly subjective process. The skills developed during the examination of many reactions are applied. The quality of the work and the reliability of the results are highly variable.

The reader must be warned that this compilation is incomplete. Worthy candidates for inclusion, both new and old continue to come to our attention. It became apparent that no reasonable terminal date could be set for the preparation of the material from all available sources. Arbitrarily, it was decided to issue the material prepared by the end of June 1968 and then continue the collection of data.

This implies that the report may be revised, expanded and reissued. That is our intention, should the work prove useful. It is also our hope to provide not only a current table of rate data but to offer an outlet for the presentation of rate evaluations. To these ends the principal table and the bibliography have been prepared in machine readable form and are stored on magnetic tape. Eventually most of the other material will be transcribed. It will be possible to produce upon demand a current version of the main table and the bibliography as computer printout, magnetic tape records or on cards. The numberical material is arranged in fixed locations so that it may be used directly for input to computation programs.

Suggestions for improvement and correction and contributions of evaluated material will be welcome. Without readers and readability a compilation of this type serves no purpose.

Acknowledgments

The proposal made by Dr. Charles W. Beckett and by the ad hoc committee chaired by Dr. Robert M. Fristrom that kinetics tables analogous to the JANAF Thermochemical Tables are needed provided the initial impetus for this work. Both Drs. Beckett and Fristrom have offered encouragement and valuable advice.

The work was made possible through financial support by the Naval Ordnance Systems Command, ORD 3311, for this project and by the Office of Standard Reference Data, NBS and the Advanced Research Projects Agency for the operation of the Chemical Kinetics Information Center.

Dr. Leroy Schieler gave us a punched card file of the contents of the extensive Aerospace Corporation compilation. This formed the starting point for our table of rate coefficients. Correspondence with Dr. Schieler, Dr. S. S. Cherry and Mr. G. S. Bahn has been of assistance in interpreting their reports. Dr. Wm. E. Wilson has provided the rate evaluations in Chapter 5. These are based on earlier reports but have been rewritten extensively for this collection.

The organization and preparation of the report has been the province of Mrs. M. C. Peter. Preparation of computer-based table in Chapter IV and of the bibliography was carried out in the Chemical Kinetics Information Center under the supervision of Mr. James G. Koch, Sr. The bibliography was typed and cross checked by Mrs. Robert M. Henderson. Computer programs for calculating and converting rate coefficients while controlling significant figures were designed and written by Clayton L. Albright and J. Robert Arms of the Computer Services Division, NBS.

To all of them go our thanks for able and good natured advice and aid.

CHAPTER 2: PRESENTATION OF RATE EVALUATIONS

This part records suggestions about the content of a rate evaluation and the form in which it is presented. No new features are suggested, each appears in some report, but all rarely appear in the same. The remarks are not based upon experience in making rate evaluations but on that accumulated in using them. As is so often true, it is the failures that lead the user to suggest.

Potential users have made suggestions. An ad hoc committee on chemical kinetics data dissemination sponsored by the JANAF Thermochemical Panel made the following suggestions in April 1967.[1] The committee had in mind the production of data sheets, each to be devoted to a single reaction. The model in view at the time was N. H. Pratt's compilation.[2]

a. That evaluations of both the forward and reverse reactions of a system be presented together.

b. That the results of each research paper be included in a table together with their temperature ranges and limits of error when known.

c. That all results be presented in a consistent form and the same set of units. The recommended form for rate expressions is $k = AT^B \exp(-C/T)$. The values of the rate parameters should be consistent with time in seconds, temperature in Kelvin, and concentration in molecules (particles) per cubic centimeter. It was recommended that the activation energy term be reported in the form $C = E^*/R$, where E^* is the activation energy and R the gas constant.

d. That each rate coefficient expression be accompanied by a value for a common reference temperature.

e. That the tabulated results and the recommended expression be displayed in graphical form.

f. That equilibrium data be included.

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1. "Report on the Establishment of Chemical Kinetics Tables", Chemical Propulsion Information Agency, unnumbered report, April 1967, p. 16.

2. Pratt, N. H., "Some Chemical Reaction Rate Data for Gas Dynamic Studies", National Gas Turbine Establishment (Pyestock, Hants, England), unnumbered report, October 1963.

These are good guides. They allow the evaluator ample scope. The ideas have been used effectively for some years. Kaskan and Browne[3] and Schofield[4] demonstrated the effective use of figures in rate evaluations. The latter provided easy to use tables. The recent report[5] from the University, Leeds, has an exemplary format. All of these merit study by the potential evaluator. A few additional suggestions are offered below.

Make an evaluation complete enough so the reader will have little need to examine the original papers. If this can be done, matters of form become secondary. Make it unnecessary for the next man to redo the work. With this in mind:

a. Tabulate data points where ever possible. If necessary, scale them from figures.

b. Base the evaluation on data points if possible. Rate coefficients are usually more reliable than rate parameters.

c. Summarize how the results were obtained in each study and record an opinion on the work. Comparison of several papers often reveals possible flaws. That not obvious to the casual reader comes to light.

d. Explain how the recommended value was obtained. Give temperature limits and uncertainties.

e. Graph the material. There is no more useful form of presentation. New data can be easily added and assessed.

f. Cite the sources actually used. Cite B, not A, if B's summary of A' work was consulted. Explain recalculations and non-trivial conversions.

g. Discuss the reaction at any suitable length. Spend space to save future effort.

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3. Kaskan, W. E. and Browne, W. G., General Electric Company Space Sciences Laboratory Report R64SD37, July 1964.

4. Schofield, K., Planet. Space Sci. 15, 643 (1967).

5. Baulch, D. L., Drysdale, D. D., and Lloyd, A. C., "Critical Evaluation of Rate Data for Homogeneous Gas-Phase Reactions of Interest in High Temperature Systems", Dept. of Physical Chemistry, The University, Leeds, England, High Temperature Reaction Rate Data Report No. 1, May 1968.

CHAPTER 3: ORGANIZATION OF THE REPORT

A. General Description

The bulk of the report is a table of rate coefficients (Chapter 4). This is the main entry point for the reader. A guide to the arrangement of the table is given at the beginning of Chapter 4. The table is followed by a group of "Reaction Summaries" (Chapter 5). Five of these are rate evaluations. The others are collections of notes about reactions that have received considerable attention. They are not single summaries, one per reaction, but are separate notes, one per evaluation. These notes are gathered together for convenience. Each collection shares a common reference list.

Chapters 6 and 7 contain notes to the main table. These are of two types: general and specific. The general notes in Chapter 6 are explanations of abbreviations used throughout the main table. These categorize the basis used by the evaluator in developing his recommendation. The specific notes, Chapter 7, are arranged in separate sets for each source quoted in the main table. A complete identification of the papers is given at the start of the section. The sets of notes are ordered alphabetically by author. Wherever practical the notes are those given in the papers, rewritten to meet the needs of this larger collection. In some cases they are interpretations of extensive material. In any case, the editor of this report, and not the original author, is responsible for errors of fact and interpretation. Each note has its own reference list. The citations identify the source, but are kept brief.

The references cited are those given by the original authors. The papers have not all been examined. Occasionally an obvious error has been corrected and occasionally a citation has been expanded to include companion papers. A few items remain for which the citations are incomplete or ambiguous.

Chapter 8 is a general bibliography, arranged by author. It lists the articles referred to throughout the report. These citations are intended to be unambiguous and complete. Most include titles.

B. Processing of the Original Data: Uncertainties and Significant Figures

The data tabulated here came from diverse sources. The conventions used by the authors varied. All data have been reduced to a common form. These rules have been followed in processing the numbers:

1. A tabulated number should reflect the precision to which the original number was stated.
2. Explicit uncertainties should be stated only when they were explicitly stated for the original number.
3. Numbers received without stated uncertainties should be treated as if they were precise to ±1 in the least significant figure.
4. Calculations of rate coefficients using the tabulated numbers should report results consonant with the uncertainties, explicit or implied, in the rate parameters.
5. The propagation of uncertainties, of whatever origin, through a calculation may be treated by the same rule as that used for standard errors:

$$W = f(x,y)$$

$$\sigma_w^2 = (\partial f/\partial x)^2\sigma_x^2 + (\partial f/\partial y)^2\sigma_y^2$$

where the sigma's are the absolute uncertainties.

The use of this last rule does not imply that the stated uncertainties are standard statistical errors. Most of them are personal estimates. The meaning of an uncertainty varies from source to source.

These rules pose no problems to the compiler who applies them in hand calculations. However, when computer technology is introduced the rules must be implemented explicitly case by case. This implementation has been made and applied in the construction of the table. Hopefully, it may be of use to others. The programming of this trivial problem revealed a number of machine-calculation pitfalls.

The rules stated above are an incomplete description of the process. In some cases the input number was rounded before it was accepted. These were cases for which the implied precision was unbelievable. Also, the dividing line for rounding up is .505 not .5. This assures that activation energy estimates of 5 and 6 kilocalories per mole (for example) will not, when divided by the gas constant, both become 3×10^3. The problem arises only for numbers for which uncertainties were not stated.

CHAPTER 4: TABLE OF RATE COEFFICIENTS

Part D of this chapter is a table of rate coefficients for elementary gas phase reactions. There are over 1600 entries for about 1450 reactions. Each entry is an evaluation, a calculation, an estimate or a selection recommended as the best available value.

The structure of the table is explained in Part A. Factors for converting the rate parameters are tabulated in Part B. The formulae for the molecules that appear in the rate coefficient table are listed in Part C in the order in which they appear. Chapters 6 and 7 contain supporting notes for the table.

Several points about the rate coefficients merit mention here.

(1) The form used for presenting the rate coefficients is

$$k = 10^{A}\ T^{B}\ \exp(-1000\ C/T)$$

Here the number C is related to the activation energy by $1000\ C = E/R$ where R is the gas constant. For the kineticist, who still compares activation energies in kcal mol^{-1}, the conversion $E = 1.987\ C$ will serve.

(2) The calculation of a rate coefficient at a particular temperature from the tabulated data is most easily done using

$$\log_{10}k = A + B\ \log_{10}T - 434.3\ C/T$$

(3) The preexponential term in the Arrhenius equation

$$k = \alpha\ \exp(-E/RT)$$

here becomes

$$\alpha = 10^{A}\ T^{B}$$

This term α is often used for rapid comparison of the kinetic behavior of reactions. For any set of units α has a typical range of values. These are shown below for the two common sets of concentration units used in the original papers.

	molecule cm^{-3}	mol cm^{-3}
First order	10^{10} - 10^{16}	10^{10} - 10^{16}
Second order	10^{-13} - 10^{-9}	10^{10} - 10^{14}
Third order	10^{-32} - 10^{-30}	10^{15} - 10^{17}

The table in Part D lists k's consistent with molecules/cm^3. These characteristic ranges are of help in interpreting a rate expression for which no units are stated. This situation occasionally arises in the notes quoted in Chapters 5 and 7. In passing it may be noted that molecule/cm^3 rate expressions have distinct ranges for values of α for reactions of different orders. The only other practical set of units for which α has distinguishable ranges is mol/m^3, which, to date, has been used very little.

A: Guide to the Rate Coefficient Table

Rate Parameters for $k = 10^{(A \pm A')} T^{(B \pm B')} \exp(-1000(C \pm C')/T)$ ①

	Reaction Source and Notes		Range T/1000	Order	A	±A'	B	±B'	C	±C'	Log K at T = 1000	±△
②	0 + 02 + M => 03 + M (M = 03)											
	BASCMB-1966 XP (7)	⑤		3rd	-34.0	.2	0		- .5		-33.78	.20
③	JONSTN-1968 Eval (2)		.2-1	3rd	-34.3	.2	0		-1.057		-33.84	.20
	SCOFLD-1967 XP (29)	⑥	⑦	3rd	-34.28		0		-1.01		-33.84	
④	See summary for reverse reaction						⑧				⑨	

1. Equation for which rate parameters are tabulated. A', B' and C' are uncertainties and are stated only when given explicitly in the original paper.

2. Reaction. Reactants on left. All reactants appear in rate equation. Subscripts printed on line. Electrical charges when present enclosed in square brackets: O^- = O[-].

3. Source quoted. See Chapter 7 for identification.

4. Specific notes on each evaluation are collected in Chapter 5 when this note appears.

5. General note describing basis for determining tabulated numbers. See Chapter 6.

6. Specific numbered note on this evaluation. In Chapter 7. All notes for a single source grouped together (unless item 4 appears in table).

7. Applicable temperature range.

8. Rate parameters consistent with temperature in Kelvin, time in seconds, concentration in molecules per cm^3.

9. Logarithm of rate coefficient at 1000 K. $\log_{10}k = A + B\log_{10}T - 434.3\ C/T$.

B. Conversion Factors

Conversion of $\log_{10}k$ or A to a different concentration basis for the equation: $k = 10^A\ T^B \exp(-1000\ C/T)$

To convert from X to Y <u>add</u> tabulated value.
To convert from Y to X, <u>substract</u>.

Y → X ↓	$\frac{\text{cm}^3}{\text{mole second}}$	$\frac{\text{liter}}{\text{mole second}}$	$\text{atm}^{-1}\text{s}^{-1}$	$\text{torr}^{-1}\text{s}^{-1}$
$\frac{\text{cm}^3}{\text{molecule-second}}$	23.780	20.780	21.86 -log T	18.98 -log T

Y → X ↓	$\frac{\text{cm}^6}{\text{mole second}}$	$\frac{\text{liter}^2}{\text{mole second}}$	$\text{atm}^{-2}\text{s}^{-1}$	$\text{torr}^{-2}\text{s}^{-1}$
$\frac{\text{cm}^6}{\text{molecule-second}}$	47.560	41.560	43.73 -2log T	37.96 -2log T

$$k(\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}) = k(\text{cm}^3\text{mol}^{-1}\text{s}^{-1})/N_{\text{Avog}} = k(\text{atm}^{-1}\text{s}^{-1})\cdot RT/N_{\text{Avog}}$$

$$k(\text{cm}^6\text{molecule}^{-2}\text{s}^{-1}) = k(\text{cm}^6\text{mol}^{-2}\text{s}^{-1})/N^2_{\text{Avog}} = K(\text{atm}^{-2}\text{s}^{-1})\cdot(RT/N_{\text{Avog}})^2$$

$$N_{\text{Avog}} = 6.02252 \times 10^{23} \text{ molecule mol}^{-1}$$

Conversion of "energy coefficient", C, in the exponential term of $k = 10^A\ T^B \exp(-1000\ C/T)$

To convert from X to Y <u>multiply</u> by the tabulated number. To convert from Y to X <u>divide</u>.

Y → X ↓	E^* kJ mol^{-1}	E^* J mol^{-1}	E^* kcal mol^{-1}	E^* cal mol^{-1}	E^* eV molecule^{-1}
C in Kelvin	8.314	8.314×10^3	1.987	1.987×10^3	8.617×10^{-2}
E^* kcal mol^{-1}	4.184	4.184×10^3	1	10^3	4.336×10^{-2}

$1000\ C = E^*/R$, $R = 8.3143\ \text{J mol}^{-1}\text{K}^{-1} = 1.9872\ \text{cal mol}^{-1}\text{K}^{-1} = 8.6170 \times 10^{-5}\ \text{eV K}^{-1}$

C. List of Chemical Formulae

The formulae used for molecules that appear in reactions in Part D are listed below. Barring error, each molecule is represented only one way.

The order in which the formulae are listed is related to the reactions in Part D in the following way:

(a) The sequence of first reactants is the same as in the list below.

(b) Reactants and products are ordered (separately) in the sequence shown below, with the exceptions

(1) The electron, E[-], the photon, PHOTON, and the generalized third body, M are always placed last within a set of reactants or products.

(2) Specific third bodies do not appear in reactions, they are identified in a following parenthetical expression.

This ordering scheme is strictly alphabetical, being produced by a character-by-character sort from left to right over the entire reaction. The sorting order is: blank, [, +, -, numerals, letters.

This arrangement is not chemical. The procedure makes no distinction between upper and lower case letters as in Ba, BC, Be, BO. Here, as in printing the table, we have surrendered and accepted the available computer technology.

Al
Al[+]
Al_2O
$Al_2O[+]$
Al_2O_2
AlCl
$AlCl_2$
$AlCl_3$
AlClF
AlF
AlF_2
AlF_3
AlH
AlO
AlO_2
AlO_2H
AlOCl
AlOF
AlOH
B
B[+]
B_2O_2
B_2O_3
Be
Be[+]
Be_2O_2
Be_3O_3
Be_4O_4
BeCl
$BeCl_2$
BeClF
BeF
BeF_2
BeH
BeH_2
BeO
BeO_2H_2
BeOH
BF
BF_2

BF_3
BH
BH_2
BH_3
BO
BO[+]
BO_2
BO_2H
BOF
BOH
Br
C
C_2
C_2H
C_2H_2
C_2H_3
C_2H_4
C_2H_5
C_2H_6
C_2O
C_3
C_3H_7
C_3H_8
C_4H_9
C_4H_{10}
CH
CH_2
CH_2O
CH_3
CH_4
CHO
CHO[+]
Cl
Cl[-]
Cl_2
ClF
ClO
CN
CN[-]
CO
CO_2
Cs
Cs[+]
CsCl
CsOH
D
D_2
F
F[-]
F_2
H
H[-]
H_2
H_2O
H_2O_2
H_3O[+]
HBr
HCl
HCN
HD
HF
HI
HNO
HO_2
HOCl
I
K
K[+]
KH
KH_2O[+]
KO_2
KOH
Li
Li[+]
LiCl
LiH
LiH_2O[+]
LiO
LiO_2
LiOH
Mg
MgH
N
N_2
N_2O
N_2O_4
N_2O_5
Na
Na[+]
NaCl
NaF
NaH
NaH_2O[+]
NaO
NaO_2
NaOH
NH
NH_2
NH_3
NH_3[+]
NO
NO[+]
NO_2
NO_3
O
O[-]
O_2
O_2[-]
O_3
OH
OH[-]
P
PH
S
SH
Si
SiH

D. Table of Rate Coefficients

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
AL + AL2O[+] => AL2O + AL[+] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6
AL + ALCL2 => ALCL + ALCL TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
AL + ALF2 => ALF + ALF TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
AL + ALF3 => ALF + ALF2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8
AL + ALH => AL + ALH MAYER-1968 J+P		2ND	-13.48		+1.21		+1.91		-10.68
AL + ALO + M => AL2O + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
AL + BE[+] => AL[+] + BE TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7
AL + BEF => ALF + BE TUNDER-1967 OME		2ND	-12.1		+0.5		+4.0		-12.3
AL + BEH => ALH + BE MAYER-1968 J+P		2ND	-12.52		+0.72		+2.01		-11.23
AL + BEO => ALO + BE TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
AL + BH => ALH + B MAYER-1968 J+P		2ND	-12.15		+0.72		+8.35		-13.61
AL + CH => ALH + C MAYER-1968 J+P		2ND	-13.78		+1.07		+13.99		-16.64
AL + CL + M => ALCL + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
AL + CL[-] => ALCL + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6
AL + CL2 => ALCL + CL TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3
AL + CLF => ALCL + F TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3
AL + CLF => ALF + CL TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3
AL + F + M => ALF + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		+0.5		0		-29.6
AL + H2 => ALH + H MAYER-1968 J+P		2ND	-11.27		+0.73		+21.59		-18.45
AL + H3O[+] => AL[+] + H + H2O TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6
AL + HBR => ALH + BR MAYER-1968 J+P		2ND	-12.63		+0.76		+15.05		-16.88
AL + HCL => ALCL + H TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
AL + HCL => ALH + CL MAYER-1968 J+P		2ND	-12.50		+0.75		+22.95		-20.21
AL + HF => ALF + H TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1
AL + HF => ALH + F MAYER-1968 J+P		2ND	-12.14		+0.73		+38.25		-26.55
AL + HI => ALH + I MAYER-1968 J+P		2ND	-14.3		+1.40		+7.20		-13.2
AL + KCL => ALCL + K TUNDER-1967 OME		2ND	-12.1		+0.5		3.5		-12.1
AL + KF => ALF + K TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ EXP(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
AL + KH => ALH + K MAYER-1968 J+P		2ND	-13.06		+0.94		+3.62		-11.81
AL + LICL => ALCL + LI TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
AL + LIF => ALF + LI TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1
AL + LIH => ALH + LI MAYER-1968 J+P		2ND	-13.27		+1.14		+5.54		-12.25
AL + MGH => ALH + MG MAYER-1968 J+P		2ND	-12.46		+0.67		+1.51		-11.11
AL + NACL => ALCL + NA TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7
AL + NAF => ALF + NA TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
AL + NAH => ALH + NA MAYER-1968 J+P		2ND	-12.52		+0.75		+2.87		-11.52
AL + NH => ALH + N MAYER-1968 J+P		2ND	-12.22		+0.70		+10.97		-14.88
AL + O + M => ALO + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
AL + O[-] => ALO + E[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6
AL + O2 => ALO + O TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
AL + OH => ALH + O MAYER-1968 J+P		2ND	-12.67		+0.80		+22.80		-20.17

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
AL + OH => ALO + H TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
AL + OH + M => ALOH + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
AL + PH => ALH + P MAYER-1968 BEHO		2ND	-11.63		+0.5		+4.03		-11.9
AL + SH => ALH + S MAYER-1968 BEHO		2ND	-11.67		+0.5		+11.42		-15.1
AL + SIH => ALH + SI MAYER-1968 J+P		2ND	-12.60		+0.67		+1.11		-11.07
AL[+] + CL[-] + M => ALCL + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
AL[+] + E[-] + M => AL + M (M= ANY) TUNDER-1967 OMF		3RD	-23.9		-1.5		0		-28.4
AL[+] + F[-] + M => ALF + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
AL[+] + H[-] + M => ALH + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
AL[+] + K => AL + K[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL[+] + KCL => ALCL + K[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.5		-12.8
AL[+] + KF => ALF + K[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.5		-12.8
AL[+] + LI => AL + LI[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL[+] + LICL => ALCL + LI[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
AL[+] + LIF => ALF + LI[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.5		-12.8

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
AL[+] + NA => AL + NA[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL[+] + NACL => ALCL + NA[+] TUNDER-1967 OMF		2ND	-12.1		+0.5		+2.5		-11.7
AL[+] + NAF => ALF + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
AL[+] + O[-] + M => ALO + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
AL2O + ALO2H => AL2O2 + ALOH TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
AL2O + ALOCL => AL2O2 + ALCL TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
AL2O + BE[+] => AL2O[+] + BE TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL2O + F => ALF + ALO TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
AL2O + LI[+] => AL2O[+] + LI TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL2O + O[-] => AL2O2 + E[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
AL2O + O2[-] => AL2O2 + O[-] TUNDER-1967 OMF		2ND	-13.1		+0.5		+2.5		-12.7
AL2O + OH => AL2O2 + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
AL2O[+] + E[-] + M => AL2O + M (M= ANY) TUNDER-1967 OMF		3RD	-23.9		-1.5		0		-28.4

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±A AT T = 1000
AL2O[+] + K => AL2O + K[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
AL2O[+] + NA => AL2O + NA[+] TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6
AL2O[+] + O[-] => AL2O2 TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3
AL2O2 + CO => AL2O + CO2 TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
AL2O2 + N => AL2O + NO TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
AL2O2 + O => AL2O + O2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
ALCL + ALO => AL2O + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALCL + CL + M => ALCL2 + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
ALCL + CL[-] => ALCL2 + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3
ALCL + CL2 => ALCL2 + CL TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
ALCL + CLF => ALCL2 + F TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
ALCL + O[-] => ALO + CL[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
ALCL2 + H => ALCL + HCL TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALCL2 + K => ALCL + KCL TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7
ALCL2 + LI => ALCL + LICL TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
ALCL2 + NA => ALCL + NACL TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALCL3 + K => ALCL2 + KCL TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALCL3 + LI => ALCL2 + LICL TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALF + BEF => AL + BEF2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.5		-13.3
ALF + BEF => ALF2 + BE TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
ALF + CLF => ALF2 + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
ALF + F + M => ALF2 + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
ALF + NAF => ALF2 + NA TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALF2 + ALF2 => ALF + ALF3 TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALF2 + BEF => ALF + BEF2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALF2 + BEF => ALF3 + BE TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
ALF2 + F => ALF3 TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
ALF2 + H => ALF + HF TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6

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RATE PARAMETERS FOR $K = 10^{(A*A')} T^{(B*B')} EXP(-1000(C*C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A *A'	B *B'	C *C'	LOG K *A AT T = 1000
ALF2 + HF => ALF3 + H TUNDER-1967 OMF		2ND	-12.8	+0.5	+3.5	-12.8
ALF2 + K => ALF + KF TUNDER-1967 OME		2ND	-12.1	+0.5	+3.0	-11.9
ALF2 + LI => ALF + LIF TUNDER-1967 OMF		2ND	-12.8	+0.5	+4.5	-13.3
ALF2 + LIF => ALF3 + LI TUNDER-1967 OME		2ND	-12.8	+0.5	+3.5	-12.8
ALF2 + NAF => ALF3 + NA TUNDER-1967 OME		2ND	-12.8	+0.5	+3.0	-12.6
ALF3 + BEF => ALF2 + BEF2 TUNDER-1967 OMF		2ND	-12.8	+0.5	+4.0	-13.0
ALH + B => AL + BH MAYER-1968 J+P		2ND	-12.38	+0.72	+1.41	-10.83
ALH + BE => AL + BEH MAYER-1968 J+P		2ND	-12.07	+0.72	+7.75	-13.27
ALH + BR => AL + HBR MAYER-1968 J+P		2ND	-12.96	+0.71	+3.77	-12.47
ALH + C => AL + CH MAYER-1968 J+P		2ND	-13.04	+1.00	+6.14	-12.70
ALH + CL => AL + HCL MAYER-1968 J+P		2ND	-12.88	+0.70	+3.93	-12.49
ALH + F => AL + HF MAYER-1968 J+P		2ND	-12.83	+0.69	+2.82	-11.98
ALH + H => AL + H2 MAYER-1968 J+P		2ND	-12.04	+0.68	+2.01	-10.87
ALH + I => AL + HI MAYER-1968 J+P		2ND	-14.5	+1.34	+4.13	-12.3
ALH + K => AL + KH MAYER-1968 J+P		2ND	-12.89	+0.98	+14.29	-16.15

RATE PARAMETERS FOR K = $10^{(A\pm A')}$ $T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
ALH + LI => AL + LIH MAYER-1968 J+P		2ND	-13.32	+1.15	+9.01	-13.78
ALH + MG => AL + MGH MAYER-1968 J+P		2ND	-11.821	+0.67	+10.82	-14.51
ALH + N => AL + NH MAYER-1968 J+P		2ND	-12.40	+0.69	+1.46	-10.96
ALH + NA => AL + NAH MAYER-1968 J+P		2ND	-12.46	+0.77	+11.47	-15.13
ALH + O => AL + OH MAYER-1968 J+P		2ND	-12.74	+0.73	+4.18	-12.36
ALH + P => AL + PH MAYER-1968 BERO		2ND	-11.46	+0.5	+.35	-10.1
ALH + S => AL + SH MAYER-1968 BERO		2ND	-11.48	+0.5	+.55	-10.2
ALH + SI => AL + SIH MAYER-1968 J+P		2ND	-11.78	+0.67	+11.88	-14.93
ALO + AL[+] + M => AL2O[+] + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1	-0.5	0	-32.6
ALO + ALO => AL2O + O TUNDER-1967 OMF		2ND	-12.8	+0.5	+3.0	-12.6
ALO + CL => ALCL + O TUNDER-1967 OMF		2ND	-12.1	+0.5	+3.0	-11.9
ALO + CO => AL + CO2 TUNDER-1967 OMF		2ND	-12.8	+0.5	+3.0	-12.6
ALO + F => ALF + O TUNDER-1967 OMF		2ND	-12.1	+0.5	+3.0	-11.9

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM , TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/ . SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BERO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
ALO + H + M => ALOH + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
ALO + H[-] => AL + OH[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
ALO + H2O => ALOH + OH TUNDER-1967 OMF (36)		2ND	-11.86		+0.5		0		-10.4
ALO + HNO => ALOH + NO TUNDER-1967 OMF (36)		2ND	-12.27		+0.5		0		-10.8
ALO + N => AL + NO TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
ALO + NAH => ALOH + NA TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
ALO + NAOH => ALOH + NAO TUNDER-1967 OME (36)		2ND	-12.63		+0.5		0		-11.1
ALO + NH2 => ALOH + NH TUNDER-1967 OMF (36)		2ND	-12.74		+0.5		0		-11.2
ALO + NH3 => ALOH + NH2 TUNDER-1967 OME (36)		2ND	-11.96		+0.5		0		-10.5
ALO + OH[-] => ALO2H + E[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
ALO2 + H => ALOH + OH TUNDER-1967 OME		2ND	-13.1		+0.5		+3.0		-12.9
ALO2H + BE => ALO + BEOH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
ALO2H + BEOH => ALO + BEO2H2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALO2H + CL => ALOCL + OH TUNDER-1967 OME		2ND	-13.1		+0.5		+2.5		-12.7
ALO2H + CL[-] => ALOCL + OH[-] TUNDER-1967 OMF		2ND	-13.8		+0.5		+3.0		-13.6

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \; T^{(B \pm B')} \; \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
ALO2H + CO => ALOH + CO2 TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
ALO2H + F => ALOF + OH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALO2H + F[-] => ALOF + OH[-] TUNDER-1967 OMF		2ND	-13.1		+0.5		+2.5		-12.7
ALO2H + H => ALO + H2O TUNDER-1967 OMF		2ND	-13.8		+0.5		+2.5		-13.4
ALO2H + LI => ALO + LIOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALO2H + LI => ALOH + LIO TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALO2H + N => ALOH + NO TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
ALO2H + NA => ALO + NAOH TUNDER-1967 OMF		2ND	-13.1		+0.5		+2.5		-12.7
ALO2H + NA => ALOH + NAO TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
ALO2H + O => ALOH + O2 TUNDER-1967 OMF		2ND	-13.1		+0.5		+3.0		-12.9
ALOCL + BE => ALCL + BEO TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
ALOCL + F => ALCLF + O TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
ALOCL + H => ALCL + OH TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
ALOCL + K => ALO + KCL TUNDER-1967 OME		2ND	-12.8		+0.5		+4.0		-13.0
ALOCL + LI => ALO + LICL TUNDER-1967 OME		2ND	-12.8		+0.5		+4.0		-13.0
ALOF + BE => ALF + BEO TUNDER-1967 OME		2ND	-12.8		+0.5		+4.0		-13.0
ALOF + CO => ALF + CO2 TUNDER-1967 OME		2ND	-12.8		+0.5		+4.0		-13.0
ALOF + F => ALF2 + O TUNDER-1967 OMF		2ND	-13.8		+0.5		+4.0		-14.0
ALOF + N => ALF + NO TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALOF + O => ALF + O2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALOH + BEH => ALO + BEH2 TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + BEO => ALO + BEOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + BEO => ALO2H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
ALOH + BEOH => AL + BEO2H2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALOH + CH => ALO + CH2 TUNDER-1967 J+P		2ND	-13.2		+0.7		+1.0		-11.5
ALOH + CL => ALCL + OH TUNDER-1967 OME		2ND	-13.1		+0.5		+2.5		-12.7
ALOH + CL => ALO + HCL TUNDER-1967 OME (36)		2ND	-12.63		+0.5		0		-11.1
ALOH + CL => ALOCL + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2

RATE PARAMETERS FOR K = $10^{(A\pm A')}\ T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
ALOH + CN => ALO + HCN TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + F => ALF + OH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALOH + F => ALO + HF TUNDER-1967 OME (36)		2ND	-12.52		+0.5		0		-11.0
ALOH + F => ALOF + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + H => ALO + H2 TUNDER-1967 J+P		2ND	-12.70		+0.7		+2.5		-11.7
ALOH + K => ALO + KOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
ALOH + LIO => ALO + LIOH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + N => ALO + NH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + NAO => ALO + NAOH TUNDER-1967 OMF (36)		2ND	-12.29		+0.5		0		-10.8
ALOH + NH => ALO + NH2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + O => ALO + OH TUNDER-1967 OMF (36)		2ND	-12.21		+0.5		0		-10.7
ALOH + O[-] => ALO + OH[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2
ALOH + O[-] => ALO2H + E[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
ALOH + OH => ALO + H2O										
TUNDER-1967 OMF (36)		2ND	-12.46		+0.5		0		-11.0	
B + B2O3 => B2O2 + BO										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0	
B + BEH => BE + BH										
MAYER-1968 J+P		2ND	-12.38		+0.67		+1.21		-10.90	
B + BF2 => BF + BF										
CHERRY-1967 OMF		2ND	-12.8	2.0	+0.5		+3.4		-12.8	2.0
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
B + BF3 => BF + BF2										
CHERRY-1967 OMF		2ND	-12.8	3.0	+0.5		+4.4		-13.2	3.0
TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0	
B + BH => B + BH										
MAYER-1968 BERO		2ND	-11.52		+0.5		+2.92		-11.3	
B + BH2 => BH + BH										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
B + BH3 => BH + BH2										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
B + BO2 => BO + BO										
CHERRY-1967 OMF		2ND	-12.8	3.0	+0.5		+3.8		-12.9	3.0
B + BOF => BF + BO										
CHERRY-1967 OMF		2ND	-12.8	3.0	+0.5		+4.7		-13.3	3.0
TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.5		-13.3	
B + CH => BH + C										
MAYER-1968 J+P		2ND	-13.70		+1.06		+4.08		-12.29	
B + CL + M => BECL + M (M= ANY)										
TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6	
B + F + M => BF + M (M= ANY)										
CHERRY-1967 OMF		3RD	-31.1	1.4	-0.5		0		-32.6	1.4
TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6	
B + F[-] => BF + E[-]										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+5.5		-13.7	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
B + F2 => BF + F										
CHERRY-1967 OMF		2ND	-12.1	1.4	+0.5		+1.0		-11.0	1.4
B + H2 => BH + H										
MAYER-1968 J+P		2ND	-11.63		+0.73		+14.85		-15.88	
B + H2O => BOH + H										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
B + HBR => BH + BR										
MAYER-1968 J+P		2ND	-14.1		+1.27		+8.40		-13.9	
B + HCL => BH + CL										
MAYER-1968 J+P		2ND	-12.70		+0.77		+15.55		-17.14	
B + HF => BF + H										
CHERRY-1967 OMF		2ND	-12.1	2.0	+0.5		+3.8		-12.2	2.0
TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.5		-12.1	
B + HF => BH + F										
MAYER-1968 J+P		2ND	-12.02		+0.68		+30.30		-23.13	
B + HI => BH + I										
MAYER-1968 J+P		2ND	-12.89		+0.82		+3.88		-12.11	
B + KH => BH + K										
MAYER-1968 J+P		2ND	-12.30		+0.70		+1.11		-10.68	
B + LIH => BH + LI										
MAYER-1968 J+P		2ND	-13.04		+0.98		+3.62		-11.67	
B + MGH => BH + MG										
MAYER-1968 BEBO		2ND	-11.74		+0.5		+.15		-10.3	
B + NAF => BF + NA										
TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9	

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```
                                          (A±A')  (B±B')
           RATE PARAMETERS FOR K =  10       T         EXP(-1000(C±C')/T)

  REACTION                  RANGE  ORDER     A    ±A'      B  ±B'      C    ±C'       LOG  K  ±Δ
     SOURCE AND NOTES       T/1000                                                    AT T = 1000

 B + NAH => BH + NA
  MAYER-1968   J+P                  2ND  -12.17          +0.68       +1.11            -10.61

 B + NAO => BO + NA
  TUNDER-1967 OMF                   2ND  -12.1           +0.5        +2.0             -11.5

 B + NH => BH + N
  MAYER-1968   J+P                  2ND  -12.807         +0.91       +3.42            -11.56

 B + O + M => BO + M   (M= ANY)
  CHERRY-1967 OMF                   3RD  -31.1   1.4     -0.5         0               -32.6   1.4
  TUNDER-1967 OMF                   3RD  -31.1           -0.5         0               -32.6

 B + O[-] => BO + E[-]
  TUNDER-1967 OMF                   2ND  -12.8           +0.5        +5.5             -13.7

 B + O2 => BO + O
  CHERRY-1967 OMF                   2ND  -12.1   2.0     +0.5        +3.3             -12.0   2.0
  TUNDER-1967 OMF                   2ND  -12.1           +0.5        +3.0             -11.9

 B + O2[-] => BO + O[-]
  TUNDER-1967 OMF                   2ND  -12.1           +0.5        +2.5             -11.7

 B + OH => BH + O
  MAYER-1968   J+P                  2ND  -12.16          +0.67      +12.48            -15.57

 B + OH => BO + H
  CHERRY-1967 OMF                   2ND  -12.1   2.0     +0.5        +2.8             -11.8   2.0
  TUNDER-1967 OME                   2ND  -12.1           +0.5        +3.0             -11.9

 B + OH[-] => BO + H[-]
  TUNDER-1967 OMF                   2ND  -13.1           +0.5        +4.5             -13.6

 B + PH => BH + P
  MAYER-1968   J+P                  2ND  -12.52          +0.71       +1.31            -10.96

 B + SH => BH + S
  MAYER-1968   J+P                  2ND  -12.830         +0.81       +3.67            -11.99

 B + SIH => BH + SI
  MAYER-1968   BERO                 2ND  -11.97          +0.5         +.55            -10.7

 B[+] + E[-] + M => B + M   (M= ANY)
  TUNDER-1967 OMF                   3RD  -23.9           -1.5         0               -28.4
```

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
B[+] + F[-] + M => BF + M (M= ANY) TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5
B[+] + NA => B + NA[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
B[+] + NAF => BF + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
B[+] + NAO => BO + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
B[+] + NAO => BO[+] + NA TUNDER-1967 OMF		2ND	-12.1		+0.5		+2.0		-11.5
B[+] + O[-] + M => BO + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
B[+] + O2 => BO[+] + O TUNDER-1967 OME		2ND	-12.1		+0.5		+4.5		-12.6
B[+] + O2[-] => BO + O TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7
B2O2 + NAO => B2O3 + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2
B2O2 + O => B2O3 TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
B2O2 + O[-] => B2O3 + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3
B2O2 + O2 => B2O3 + O TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
B2O2 + O2[-] => B2O3 + O[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\, T^{(B \pm B')}\, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
B2O2 + OH => B2O3 + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
B2O3 + BF => B2O2 + BOF TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
BE + BEH => BE + BEH MAYER-1968 J+P		2ND	-13.18		+1.06		+5.99		-12.60
BE + BEO2H2 => BEOH + BEOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BE + BH => B + BEH MAYER-1968 J+P		2ND	-11.70		+0.67		+13.84		-15.70
BE + CH => BEH + C MAYER-1968 J+P		2ND	-12.74		+0.79		+17.72		-18.06
BE + CHO => BEH + CO TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.0		-11.7
BE + CL2 => BECL + CL TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
BE + CLF => BECL + F TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
BE + CLF => BEF + CL TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
BE + F + M => BEF + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
BE + F2 => BEF + F TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
BE + H + M => BEH + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
BE + H2 => BEH + H MAYER-1968 BERO		2ND	-10.816		+0.5		+25.82		-20.5
BE + H2O => BEOH + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
BE + HBR => BEH + BR MAYER-1968 J+P		2ND	-11.807	+0.68	+18.62	-17.85
BE + HCL => BEH + CL MAYER-1968 J+P		2ND	-11.63	+0.67	+26.02	-20.91
BE + HF => BEH + F MAYER-1968 J+P		2ND	-11.27	+0.67	+42.38	-27.65
BE + HI => BEH + I MAYER-1968 J+P		2ND	-11.74	+0.67	+9.96	-14.05
BE + KH => BEH + K MAYER-1968 BERO		2ND	-10.97	+0.5	+2.42	-10.5
BE + LIH => BEH + LI MAYER-1968 J+P		2ND	-12.88	+1.04	+10.72	-14.41
BE + LIO => BEO + LI TUNDER-1967 OME		2ND	-12.1	+0.5	+2.5	-11.7
BE + MGH => BEH + MG MAYER-1968 J+P		2ND	-12.94	+0.95	+3.27	-11.51
BE + NAH => BEH + NA MAYER-1968 J+P		2ND	-13.06	+1.12	+4.43	-11.62
BE + NAO => BEO + NA TUNDER-1967 OME		2ND	-12.1	+0.5	+2.0	-11.5
BE + NH => BEH + N MAYER-1968 BERO		2ND	-11.35	+0.5	+15.40	-16.5
BE + O + M => BEO + M (M= ANY) TUNDER-1967 OME		3RD	-31.1	-0.5	0	-32.6
BE + O[-] => BEO + E[-] TUNDER-1967 OME		2ND	-12.1	+0.5	0	-10.6

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
BE + O2[-] => BEO + O[-] TUNDER-1967 OMF		2ND	-12.1	+0.5	+2.5	-11.7
BE + OH => BEH + O MAYER-1968 BEHO		2ND	-11.40	+0.5	+24.66	-20.6
BE + OH => BEO + H TUNDER-1967 OMF		2ND	-12.1	+0.5	+3.0	-11.9
BE + OH + M => BEOH + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1	-0.5	0	-32.6
BE + PH => BEH + P MAYER-1968 BERO		2ND	-11.27	+0.5	+9.81	-14.0
BE + SH => BEH + S MAYER-1968 BERO		2ND	-11.30	+0.5	+16.86	-17.1
BE + SIH => BEH + SI MAYER-1968 J+P		2ND	-12.70	+0.74	+2.92	-11.75
BE[+] + CL[-] + M => BECL + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0	-0.5	0	-31.5
BE[+] + E[-] + M => BE + M (M= ANY) TUNDER-1967 OMF		3RD	-23.9	-1.5	0	-28.4
BE[+] + LI => BE + LI[+] TUNDER-1967 OMF		2ND	-12.2	+0.5	0	-10.7
BE[+] + LICL => BECL + LI[+] TUNDER-1967 OMF		2ND	-12.8	+0.5	+3.0	-12.6
BE[+] + LIF => BEF + LI[+] TUNDER-1967 OMF		2ND	-12.8	+0.5	+3.5	-12.8
BE[+] + LIH => BEH + LI[+] TUNDER-1967 OMF		2ND	-12.8	+0.5	+1.5	-12.0
BE[+] + LIO => BEO + LI[+] TUNDER-1967 OMF		2ND	-12.8	+0.5	+2.5	-12.4
BE[+] + NA => BE + NA[+] TUNDER-1967 OMF		2ND	-12.2	+0.5	0	-10.7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±A AT T = 1000
BE[+] + NACL => BECL + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BE[+] + NAF => BEF + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BE[+] + NAH => BEH + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BE[+] + NAO => BEO + NA[+] TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.0		-12.2
BE[+] + NO => BE + NO[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7
BE[+] + O[-] + M => BEO + M (M= ANY) TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5
BE[+] + O2[-] => BE[+] + O TUNDER-1967 OMF		2ND	-12.1		+0.5		+2.5		-11.7
BE2O2 + BEO => BE3O3 TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
BE2O2 + BEOH => BE3O3 + H TUNDER-1967 OMF		2ND	-13.1		+0.5		+2.0		-12.5
BE3O3 + BEO => BE4O4 TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
BE3O3 + BEOH => BE4O4 + H TUNDER-1967 OMF		2ND	-13.1		+0.5		+2.0		-12.5
BECL + BECL => BE + BECL2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BECL + BEF => BF + BECLF TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BECL + CL + M => BECL2 + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
BECL + CL[-] => BECL2 + E[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3
BECL + CL2 => BECL2 + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BECL + CLF => BECL2 + F TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BECL + CLF => BECLF + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BECL + E[-] => BE + CL[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6
BECL + F + M => BECLF + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
BECL + F2 => BECLF + F TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.0		-11.7
BECL + H => BE + HCL TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
BECL + HCL => BECL2 + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BECL + HF => BECLF + H TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.5		-12.8
BECL + LICL => BECL2 + LI TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BECL + LI => BE + LICL TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
BECL + LIF => BECLF + LI TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.5		-12.8
BECL + NA => BE + NACL TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BECL + NACL => BECL2 + NA TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BECL + NAF => BECLF + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BECL + O => BEO + CL TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9
BECL + O[-] => BEO + CL[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BECL + OH => BEOH + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BEF + BEF => BE + BEF2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
BEF + CL + M => BECLF + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		+0.5		0		-29.6
BEF + CLF => BECLF + F TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEF + CLF => BEF2 + CL TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEF + F + M => BEF2 + M (M= ANY) TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6
BEF + F2 => BEF2 + F TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.0		-11.7
BEF + H => BE + HF TUNDER-1967 OME		2ND	-12.2		+0.5		+4.0		-12.4
BEF + HCL => BECLF + H TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6

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RATE PARAMETERS FOR K = $10^{(A*A')}\ T^{(B*B')}$ EXP(-1000(C*C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	*A'	B	*B'	C	*C'	LOG K *Δ AT T = 1000
BEF + HF => BEF2 + H TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8
BEF + LI => BE + LIF TUNDER-1967 OME		2ND	-12.1		+0.5		+4.0		-12.3
BEF + LICL => BECLF + LI TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEF + LIF => BEF2 + LI TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8
BEF + NA => BE + NAF TUNDER-1967 OME		2ND	-12.1		+0.5		+4.0		-12.3
BEF + NACL => BECLF + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEF + NAF => BEF2 + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEF + O => BEO + F TUNDER-1967 OME		2ND	-12.1		+0.5		+4.0		-12.3
BEF + OH => BEOH + F TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEH + BEH => BE + BEH2 TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
BEH + BR => BE + HBR MAYER-1968 J+P		2ND	-12.67		+0.67		+1.66		-11.38
BEH + C => BE + CH MAYER-1968 J+P		2ND	-12.55		+0.76		+4.13		-12.06
BEH + CHO => BEH2 + CO TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7
BEH + CL => BE + HCL MAYER-1968 J+P		2ND	-12.48		+0.67		+1.21		-11.00
BEH + CL => BECL + H TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BEH + CN => BE + HCN TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
BEH + F => BE + HF MAYER-1968 J+P		2ND	-12.67		+0.67		+1.26		-11.21
BEH + H => BE + H2 MAYER-1968 BEBO		2ND	-11.58		+0.5		+.65		-10.4
BEH + H + M => BEH2 + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
BEH + I => BE + HI MAYER-1968 J+P		2ND	-12.52		+0.67		+1.16		-11.01
BEH + K => BE + KH MAYER-1968 BEBO		2ND	-11.58		+0.5		+7.35		-13.3
BEH + LI => BE + LIH MAYER-1968 J+P		2ND	-13.44		+1.08		+8.45		-13.87
BEH + LIH => BEH2 + LI TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEH + LIO => BE + LIOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEH + MG => BE + MGH MAYER-1968 J+P		2ND	-12.74		+0.96		+6.89		-12.85
BEH + N => BE + NH MAYER-1968 BEBO		2ND	-11.789		+0.5		+.25		-10.4
BEH + NA => BE + NAH MAYER-1968 J+P		2ND	-13.46		+1.16		+7.25		-13.13
BEH + NAH => BEH2 + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BEH + NAO => BE + NAOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH + NH => BE + NH2 TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEH + NH => BEH2 + N TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH + NH2 => BEH2 + NH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH + O => BE + OH MAYER-1968 BERO		2ND	-11.811		+0.5		+.30		-10.4
BEH + O => BEO + H TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6
BEH + O[-] => BE + OH[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
BEH + OH => BE + H2O TUNDER-1967 OMF		2ND	-12.8		+0.5		+1.5		-12.0
BEH + P => BE + PH MAYER-1968 BERO		2ND	-11.70		+0.5		+.40		-10.4
BEH + S => BE + SH MAYER-1968 BERO		2ND	-11.74		+0.5		+.25		-10.3
BEH + SI => BE + SIH MAYER-1968 J+P		2ND	-12.29		+0.74		+8.00		-13.54
BEH2 + BEO => BEH + BEOH TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + CL => BEH + HCL TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + CN => BEH + HCN TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + F => BEH + HF TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BEH2 + H => BEH + H2 TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + LIO => BEH + LIOH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + O => BEH + OH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + O[-] => BEH + OH[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEH2 + OH => BEH + H2O TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEO + BEO => BE2O2 TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3
BEO + BEOH => BE2O2 + H TUNDER-1967 OME		2ND	-13.1		+0.5		+2.0		-12.5
BEO + CH2O => BEOH + CHO TUNDER-1967 J+P		2ND	-12.00		+0.6		+1.0		-10.6
BEO + CH3 => BEOH + CH2 TUNDER-1967 J+P		2ND	-12.58		+0.7		+.5		-10.7
BEO + CH4 => BEOH + CH3 TUNDER-1967 J+P		2ND	-11.727		+0.6		+2.0		-10.8
BEO + CHO => BEOH + CO TUNDER-1967 OME (36)		2ND	-12.67		+0.5		0		-11.2
BEO + CHO => BOH + CO TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7
BEO + CO => BE + CO2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BEO + H + M => BEOH + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
BEO + H2 => BEOH + H TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEO + H2O => BEOH + OH TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEO + HCL => BEOH + CL TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEO + HCN => BEOH + CN TUNDER-1967 J+P		2ND	-12.19		+0.7		+7.5		-13.3
BEO + HNO => BEOH + NO TUNDER-1967 OME (36)		2ND	-12.24		+0.5		0		-10.7
BEO + LIH => BEOH + LI TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
BEO + LIOH => BEOH + LIO TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BEO + N => BE + NO TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
BEO + NAH => BEOH + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0
BEO + NAOH => BEOH + NAO TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8
BEO + NH => BEOH + N TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BEO + NH2 => BEOH + NH TUNDER-1967 OME (36)		2ND	-11.55		+0.5		0		-10.0
BEO + NH3 => BEOH + NH2 TUNDER-1967 OME (36)		2ND	-11.67		+0.5		0		-10.2
BEO + O => BE + O2 TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BEO + OH => BEOH + O TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6
BEO + OH[-] => BEOH + O[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		+4.0		-13.0
BEO2H2 + H => BEOH + H2O TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEOH + CH => BEO + CH2 TUNDER-1967 J+P		2ND	-12.5		+0.7		+1.0		-10.8
BEOH + CL => BEO + HCL TUNDER-1967 OMF (36)		2ND	-12.83		+0.5		0		-11.3
BEOH + F => BEO + HF TUNDER-1967 OMF (36)		2ND	-12.8		+0.5		0		-11.3
BEOH + H => BEO + H2 TUNDER-1967 J+P		2ND	-12.1		+0.7		+2.5		-11.1
BEOH + KOH => BEO2H2 + K TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEOH + LIOH => BEO2H2 + LI TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEOH + NAO => BEO + NAOH TUNDER-1967 OMF (36)		2ND	-12.52		+0.5		0		-11.0
BEOH + NAOH => BEO2H2 + NA TUNDER-1967 OMF		2ND	-12.8		+0.5		+2.5		-12.4
BEOH + O => BEO + OH TUNDER-1967 OMF (36)		2ND	-12.48		+0.5		0		-11.0
BEOH + OH => BEO + H2O TUNDER-1967 OMF (36)		2ND	-12.74		+0.5		0		-11.2

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RATE PARAMETERS FOR K = $10^{(A±A')}$ $T^{(B±B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
BEOH + OH => BEO2H2										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BF2 + F2 => BF3 + F										
CHERRY-1967 OME		2ND	-12.8	1.4	+0.5		+1.		-11.7	1.5
BF + BO2 => BO + BOF										
CHERRY-1967 OME		2ND	-12.8	2.0	+0.5		+3.8		-12.9	2.0
BF + F + M => BF2 + M (M= ANY)										
CHERRY-1967 OME (26)		3RD	-32.6	1.4	-0.5		0		-34.1	1.4
BF + F[-] => BF2 + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BF + F2 => BF2 + F										
CHERRY-1967 OME		2ND	-12.8	1.7	+0.5		+1.		-11.7	1.8
BF + O => BO + F										
CHERRY-1967 OME		2ND	-12.1	3.0	+0.5		+5.0		-12.8	3.0
BF + O + M => BOF + M (M= ANY)										
CHERRY-1967 OME (26)		3RD	-32.6	1.4	-0.5		0		-34.1	1.4
BF + O[-] => BO + F[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		+8.1		-14.8	
BF + O[-] => BOF + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BF + O2 => BOF + O										
CHERRY-1967 (26)		2ND	-11.937		+0.5		0		-10.4	
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BF + O2[-] => BOF + O[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
BF + OH => BO + HF										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+39.3		-29.1	3.0
BF + OH => BOF + H										
CHERRY-1967 OME		2ND	-12.8	2.0	+0.5		+2.8		-12.5	2.0
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
BF2 + BF2 => BF + BF3										
CHERRY-1967 (26)		2ND	-14.90		+0.48		+.74		-13.78	
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
BF2 + BO => BF + BOF										
CHERRY-1967 OMF		2ND	-12.8	1.4	+0.5		+3.4		-12.8	1.4
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
BF2 + BO2 => BOF + BOF										
CHERRY-1967 OMF		2ND	-13.5	2.0	+0.5		+36.5		-27.8	2.0
BF2 + F => BF3										
TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3	
BF2 + F + M => BF3 + M (M= ANY)										
CHERRY-1967 OMF (26)		3RD	-32.6	1.4	-0.5		0		-34.1	1.4
BF2 + F[-] => BF3 + E[-]										
TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3	
BF2 + H => BF + HF										
CHERRY-1967 OMF		2ND	-12.8	2.0	+0.5		+3.4		-12.8	2.0
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
BF2 + HF => BF3 + F										
CHERRY-1967 OMF		2ND	-12.8	2.0	+0.5		+3.8		-12.9	2.0
BF2 + NA => BF + NAF										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
BF2 + NAF => BF3 + NA										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
BF2 + O => BOF + F										
CHERRY-1967 OMF		2ND	-12.8	2.0	+0.5		+3.4		-12.8	2.0
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	

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```
                                      (A±A')  (B±B')
                 RATE PARAMETERS FOR K =  10         T        EXP(-1000(C±C')/T)

  REACTION                   RANGE  ORDER    A    ±A'      B  ±B'       C     ±C'         LOG  K  ±Δ
    SOURCE AND NOTES         T/1000                                                       AT T = 1000

BF2 + OH => BOF + HF
 CHERRY-1967 OME (26)               2ND  -13.5  3.0     +0.5         +31.5                -25.7   3.0

BF3 + BO => BF2 + BOF
 CHERRY-1967 OME                    2ND  -12.8  1.7     +0.5          +4.4                -13.2   1.7

BH + BH3 => BH2 + BH2
 TUNDER-1967 OME                    2ND  -12.8          +0.5          +2.0                -12.2

BH + BR => B + HBR
 MAYER-1968  J+P                    2ND  -14.2          +1.25         +4.08               -12.2

BH + C => B + CH
 MAYER-1968  J+P                    2ND  -12.87         +1.06         +3.12               -11.04

BH + CH2 => BH2 + CH
 TUNDER-1967 J+P                    2ND  -11.759        +0.7          +1.36               -10.2

BH + CH2O => BH2 + CHO
 TUNDER-1967 J+P                    2ND  -11.734        +0.6          +4.5                -11.9

BH + CH3 => BH2 + CH2
 TUNDER-1967 J+P                    2ND  -12.15         +0.7          +2.0                -10.9

BH + CH4 => BH2 + CH3
 TUNDER-1967 J+P                    2ND  -11.46         +0.6           +.50                -9.9

BH + CHO => BH2 + CO
 TUNDER-1967 OME (36)               2ND  -12.46         +0.5           0                  -11.0

BH + CL => B + HCL
 MAYER-1968  J+P                    2ND  -12.92         +0.74         +3.47               -12.21

BH + F => B + HF
 MAYER-1968  J+P                    2ND  -12.58         +0.67         +1.81               -11.36

BH + H => B + H2
 MAYER-1968  J+P                    2ND  -12.19         +0.71         +2.21               -11.02

BH + H + M => BH2 + M  (M= ANY)
 TUNDER-1967 OME                    3RD  -31.1          -0.5           0                  -32.6

BH + HCN => BH2 + CN
 TUNDER-1967 J+P                    2ND  -11.70         +0.6           +.96               -10.3
```

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BH + HNO => BH2 + NO TUNDER-1967 OME (36)		2ND	-11.70		+0.5		0		-10.2
BH + I => B + HI MAYER-1968 J+P		2ND	-12.99		+0.82		+7.70		-13.87
BH + K => B + KH MAYER-1968 J+P		2ND	-12.46		+0.89		+19.48		-18.24
BH + LI => B + LIH MAYER-1968 J+P		2ND	-12.89		+1.01		+14.04		-15.95
BH + MG => B + MGH MAYER-1968 BEBO		2ND	-11.15		+0.5		+16.41		-16.8
BH + N => B + NH MAYER-1968 J+P		2ND	-12.784		+0.91		+.86		-10.43
BH + NA => B + NAH MAYER-1968 J+P		2ND	-12.78		+0.91		+16.61		-17.26
BH + NH2 => BH2 + NH TUNDER-1967 J+P		2ND	-12.06		+0.6		+3.0		-11.6
BH + NH3 => BH2 + NH2 TUNDER-1967 J+P		2ND	-11.93		+0.6		+2.0		-11.0
BH + O => B + OH MAYER-1968 J+P		2ND	-12.16		+0.67		+.75		-10.48
BH + P => B + PH MAYER-1968 J+P		2ND	-12.22		+0.71		+4.53		-12.06
BH + S => B + SH MAYER-1968 J+P		2ND	-12.55		+0.81		+.25		-10.23
BH + SI => B + SIH MAYER-1968 BEBO		2ND	-11.07		+0.5		+18.32		-17.5

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
BH2 + H => BH + H2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BH2 + H => BH3 TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BH2 + H2 => BH3 + H TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BO + B[+] => B + BO[+] TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7	
BO + BO => B2O2 TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BO + CH2 => BOH + CH TUNDER-1967 OME (36)		2ND	-12.17		+0.5		0		-10.7	
BO + CH2O => BOH + CHO TUNDER-1967 J+P		2ND	-12.04		+0.6		+.81		-10.6	
BO + CH3 => BOH + CH2 TUNDER-1967 J+P		2ND	-11.98		+0.6		+3.0		-11.5	
BO + CH4 => BOH + CH3 TUNDER-1967 J+P		2ND	-11.70		+0.6		+.81		-10.3	
BO + CHO => BOH + CO TUNDER-1967 OME (36)		2ND	-12.63		+0.5		0		-11.1	
BO + F => BF + O TUNDER-1967 OME		2ND	-12.8		+0.5		+5.5		-13.7	
BO + F + M => BOF + M (M= ANY) CHERRY-1967 OME (26)		3RD	-32.6	1.4	-0.5		0		-34.1	1.4
BO + F[-] => BOF + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BO + F2 => BOF + F CHERRY-1967 OME		2ND	-12.8	1.7	+0.5		+1.		-11.7	1.8
BO + H[-] => BOH + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
BO + H2 => BOH + H										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BO + H2O => BOH + OH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BO + HF => BOF + H										
CHERRY-1967 OME		2ND	-12.8	3.0	+0.5		+3.8		-12.9	3.0
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
BO + NAF => BOF + NA										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BO + NAH => BOH + NA										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
BO + NAOH => BO2H + NA										
TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
BO + NAOH => BOH + NAO										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
BO + O + M => BO2 + M (M= ANY)										
CHERRY-1967 OME (26)		3RD	-32.6	1.4	-0.5		0		-34.1	1.4
BO + O2 => BO2 + O										
CHERRY-1967 OME		2ND	-12.8	1.7	+0.5		+3.3		-12.7	1.7
BO + OH => BO2 + H										
CHERRY-1967 OME		2ND	-12.8	2.0	+0.5		+2.8		-12.5	2.0
BO + OH => BO2H										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BO + OH => BOH + O										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	

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RATE PARAMETERS FOR K = $10^{(A \pm A')}$ $T^{(B \pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
BO + OH[-] => BO2H + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BO + OH[-] => BOH + O[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
BO[+] + E[-] + M => BO + M (M= ANY) TUNDER-1967 OME		3RD	-23.9		-1.5		0		-28.4	
BO[+] + F[-] + M => BOF + M (M= ANY) TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
BO[+] + H[-] + M => BOH + M (M= ANY) TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
BO[+] + NA => BO + NA[+] TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
BO[+] + OH[-] => BO2H TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
BO2 + F => BOF + O CHERRY-1967 OME		2ND	-12.8	2.0	+0.5		+1.91		-12.1	2.0
BO2H + F => BOF + OH TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
BO2H + F[-] => BOF + OH[-] TUNDER-1967 OME		2ND	-13.1		+0.5		+3.5		-13.1	
BO2H + H => BO + H2O TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
BO2H + H => BOH + OH TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
BOF + OH => BO2 + HF CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+38.2		-28.6	3.0
BOH + CH => BO + CH2 TUNDER-1967 OME (36)		2ND	-12.14		+0.5		0		-10.6	
BOH + CN => BO + HCN TUNDER-1967 OME (36)		2ND	-12.29		+0.5		0		-10.8	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
BOH + F => BF + OH TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BOH + F => BO + HF TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BOH + F => BOF + H TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BOH + NAO => BO2H + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2
BOH + O2 => BO2H + O TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
BOH + O2[-] => BO2H + O[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
BR + CH => C + HBR MAYER-1968 J+P		2ND	-14.5		+1.22		+1.63		-11.5
BR + H2 => H + HBR MAYER-1968 J+P		2ND	-11.46		+0.68		+9.66		-13.61
BR + HBR => BR + HBR MAYER-1968 BEBO		2ND	-11.845		+0.5		+.20		-10.4
BR + HCL => CL + HBR MAYER-1968 BEBO		2ND	-11.784		+0.5		+8.00		-13.8
BR + HF => F + HBR MAYER-1968 BEBO		2ND	-11.811		+0.5		+24.41		-20.9
BR + HI => HBR + I MAYER-1968 BEBO		2ND	-11.830		+0.5		+.15		-10.4
BR + KH => HBR + K MAYER-1968 J+P		2ND	-13.24		+0.77		+6.39		-13.70

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
BR + LIH => HBR + LI MAYER-1968 J+P		2ND	-13.06	+0.82	+5.84	-13.13
BR + MGH => HBR + MG MAYER-1968 J+P		2ND	-12.87	+0.67	+1.71	-11.60
BR + NAH => HBR + NA MAYER-1968 J+P		2ND	-12.90	+0.71	+4.53	-12.74
BR + NH => HBR + N MAYER-1968 BERO		2ND	-11.95	+0.5	0	-10.4
BR + OH => HBR + O MAYER-1968 BERO		2ND	-12.02	+0.5	+7.50	-13.8
BR + PH => HBR + P MAYER-1968 J+P		2ND	-12.55	+0.67	+.91	-10.93
BR + SH => HBR + S MAYER-1968 BERO		2ND	-12.00	+0.5	+.05	-10.5
BR + SIH => HBR + SI MAYER-1968 BERO		2ND	-12.27	+0.5	+.81	-11.1
C + C + M => C2 + M (M= ANY) TUNDER-1967 OME		3RD	-31.6	-0.5	0	-33.1
C + C2 + M => C3 + M (M= ANY) TUNDER-1967 OMF		3RD	-31.6	-0.5	0	-33.1
C + C2H => C2 + CH TUNDER-1967 OME		2ND	-12.1	+0.5	+2.0	-11.5
C + CH => C + CH MAYER-1968 J+P		2ND	-13.67	+1.13	+4.03	-12.03
C + CH2 => CH + CH TUNDER-1967 OME		2ND	-12.1	+0.5	+9.1	-14.5
C + CH2O => CH + CHO TUNDER-1967 EST (11)		2ND	-13.3	+0.5	+1.5	-12.5
C + CH4 => CH + CH3 TUNDER-1967 OME		2ND	-12.1	+0.5	+3.0	-11.9

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
C + CHO => CH + CO										
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
C + CO2 => CO + CO										
CHERRY-1967 OME		2ND	-12.8	3.0	+0.5		+3.5		-12.8	3.0
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
C + H + M => CH + M (M= ANY)										
TUNDER-1967 (1)		3RD	-31.3		-0.5		0		-32.8	
C + H2 => CH + H										
MAYER-1968 J+P		2ND	-10.98		+0.68		+12.88		-14.53	
C + HBR => BR + CH										
MAYER-1968 J+P		2ND	-13.48		+1.22		+5.03		-12.00	
C + HCL => CH + CL										
MAYER-1968 BEBO		2ND	-11.06		+0.5		+11.42		-14.5	
C + HF => CH + F										
MAYER-1968 J+P		2ND	-11.40		+0.67		+28.49		-21.75	
C + HI => CH + I										
MAYER-1968 J+P		2ND	-11.95		+0.69		+1.76		-10.64	
C + KH => CH + K										
MAYER-1968 J+P		2ND	-12.85		+0.94		+6.09		-12.67	
C + LIH => CH + LI										
MAYER-1968 J+P		2ND	-12.98		+1.04		+8.91		-13.73	
C + MGH => CH + MG										
MAYER-1968 J+P		2ND	-12.20		+0.68		+1.46		-10.79	
C + NAH => CH + NA										
MAYER-1968 J+P		2ND	-12.63		+0.86		+5.39		-12.39	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
C + NH => CH + N										
MAYER-1968 J+P		2ND	-12.97		+1.05		+3.07		-11.15	
C + NO => CO + N										
CHERRY-1967 OME		2ND	-12.1	2.0	+0.5		+4.2		-12.4	2.0
C + O + M => CO + M (M= ANY)										
CHERRY-1967 OME		3RD	-31.1	1.4	-0.5		0		-32.6	1.4
TUNDER-1967 OME		3RD	-31.6		-0.5		0		-33.1	
C + O2 => CO + O										
CHERRY-1967 OME		2ND	-12.1	2.0	+0.5		+3.3		-12.0	2.0
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
C + OH => CH + O										
MAYER-1968 J+P		2ND	-11.793		+0.67		+11.47		-14.76	
C + OH => CO + H										
CHERRY-1967 OME		2ND	-12.1	.7	+0.5		+2.8		-11.82	.72
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
C + OH + M => CHO + M (M= ANY)										
TUNDER-1967 OME		3RD	-32.1		-0.5		0		-33.6	
C + PH => CH + P										
MAYER-1968 J+P		2ND	-12.70		+0.84		+3.22		-11.58	
C + SH => CH + S										
MAYER-1968 J+P		2ND	-13.36		+1.11		+3.57		-11.58	
C + SIH => CH + SI										
MAYER-1968 J+P		2ND	-12.44		+0.68		+2.32		-11.41	
C2 + C2 => C + C3										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
C2 + CH => C3 + H										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
C2 + CH2O => C2H + CHO										
TUNDER-1967 EST (11)		2ND	-13.5		+0.5		+3.0		-13.3	
C2 + CHO => C2H + CO										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	

RATE PARAMETERS FOR $K = 10^{(A*A')} T^{(B*R')} EXP(-1000(C*C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
C2 + H => C + CH TUNDER-1967 (1)		2ND	-12.1		+0.5		+5.0		-12.8
C2 + H => C2H TUNDER-1967 (1)		2ND	-12.1		+0.5		0		-10.6
C2 + O => C + CO TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
C2H + C2H => C2 + C2H2 TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6
C2H + CH => C + C2H2 TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
C2H + CH => C2 + CH2 TUNDER-1967 (1)		2ND	-12.8		+0.5		+20.1		-20.0
C2H + CH2 => C2 + CH3 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
C2H + CH2 => C2H2 + CH TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
C2H + CH2O => C2H2 + CHO TUNDER-1967 EST (11)		2ND	-13.3		+0.5		+3.0		-13.1
C2H + CH3 => C2 + CH4 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
C2H + CH3 => C2H2 + CH2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
C2H + CH4 => C2H2 + CH3 TUNDER-1967 EST (11)		2ND	-13.8		+0.5		+3.0		-13.6
C2H + CHO => C2H2 + CO TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
C2H + H => C2 + H2 TUNDER-1967 (1)		2ND	-12.1		+0.5		+17.6		-18.2
C2H + H => C2H2 TUNDER-1967 (1)		2ND	-12.1		+0.5		0		-10.6
C2H + H => CH + CH TUNDER-1967 OME		2ND	-12.1		+0.5		+25.2		-21.5
C2H + H2O => C2H2 + OH TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6
C2H + O => C2 + OH TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
C2H + O => CH + CO TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
C2H + OH => C2 + H2O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
C2H + OH => C2H2 + O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
C2H2 + H => C2H + H2 TUNDER-1967 (1)		2ND	-12.1		+0.5		+7.5		-13.9
C2H4 + H => C2H3 + H2 SCOFLD-1967 XP (22)	.8-.95	2ND	-10.54		0		+3.47		-12.05
C2H4 + H => C2H5 SCOFLD-1967 XP (23)	.3-.8	2ND	-10.35		0		+2.26		-11.33
C2H6 + H => C2H5 + H2 SCOFLD-1967 XP (18)	.3-1.4	2ND	-9.66		0		+5.25		-11.94
C2H6 + O => C2H5 + OH SCOFLD-1967 XP (26)	.3-.9	2ND	-10.37		0		+2.97		-11.66
C2O + CO => C2 + CO2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
C2O + M => C + CO + M (M= ANY) TUNDER-1967 OME		2ND	-6.8		0		+50		-28.5

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
C2O + O => CO + CO									
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
C3 + O => C2 + CO									
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
C3 + OH => C2 + CHO									
TUNDER-1967 OME		2ND	-13.8		+0.5		+5.0		-14.5
C3H8 + H => C3H7 + H2									
SCOFLD-1967 XP (19)	.3-1.2	2ND	-10.17		0		+3.79		-11.81
C4H10(ISO) + H => C4H9(ISO)									
SCOFLD-1967 XP (21)	.3-.9	2ND	-10.38		0		+3.27		-11.80
C4H10(N) + H => C4H9(N) + H									
SCOFLD-1967 XP (20)	.3-.8	2ND	-10.046		0		+3.72		-11.660
CH + CH => C2H2									
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH + CH2 => C + CH3									
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH + CH2O => CH2 + CHO									
TUNDER-1967 EST (11)		2ND	-13.5		+0.5		+2.5		-13.1
TUNDER-1967 J+P		2ND	-12.74		+0.7		+2.0		-11.5
CH + CH3 => CH2 + CH2									
TUNDER-1967 J+P		2ND	-12.70		+0.7		+2.5		-11.7
CH + CH4 => CH2 + CH3									
TUNDER-1967 J+P		2ND	-12.40		+0.7		+3.0		-11.6
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH + CHO => CH2 + CO									
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
TUNDER-1967 J+P		2ND	-13.3		+0.7		+.5		-11.4

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
CH + CL => C + HCL MAYER-1968 BERO		2ND	-12.27		+0.5		+.30		-10.9
CH + CO2 => CHO + CO TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6
CH + F => C + HF MAYER-1968 J+P		2ND	-12.78		+0.67		+.91		-11.16
CH + H => C + H2 MAYER-1968 J+P		2ND	-12.40		+0.67		+1.21		-10.92
CH + H => CH2 TUNDER-1967 (1)		2ND	-12.1		+0.5		0		-10.6
CH + HCN => CH2 + CN TUNDER-1967 J+P		2ND	-12.26		+0.6		+4.0		-12.2
CH + HO2 => CH2 + O2 TUNDER-1967 OME		2ND	-13.8		+0.5		+7.5		-15.6
CH + HO2 => CHO + OH TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH + I => C + HI MAYER-1968 J+P		2ND	-12.87		+0.68		+6.54		-13.67
CH + K => C + KH MAYER-1968 J+P		2ND	-13.55		+1.09		+24.61		-20.96
CH + LI => C + LIH MAYER-1968 J+P		2ND	-13.83		+1.15		+20.23		-19.16
CH + MG => C + MGH MAYER-1968 J+P		2ND	-12.17		+0.69		+18.72		-18.22
CH + N => C + NH MAYER-1968 J+P		2ND	-13.74		+1.04		+1.51		-11.28
CH + NA => C + NAH MAYER-1968 J+P		2ND	-13.42		+0.99		+21.84		-19.93
CH + NAOH => CH2 + NAO TUNDER-1967 J+P		2ND	-11.784		+0.6		+2.5		-11.1

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CH + NH2 => CH2 + NH TUNDER-1967 J+P		2ND	-13.3		+0.7		+1.0		-11.6	
CH + NH3 => CH2 + NH2 TUNDER-1967 J+P		2ND	-13.1		+0.7		+1.0		-11.4	
CH + O => C + OH MAYER-1968 J+P		2ND	-12.60		+0.67		+.75		-10.92	
CH + O => CHO[+] + E[-] JENSEN-1967 EST (61)	1-3.5	2ND	-11.3	1.0	0		0		-11.3	1.0
CH + O => CO + H TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
CH + O + M => CHO + M (M= ANY) TUNDER-1967 OME		3RD	-31.6		-0.5		0		-33.1	
CH + O[-] => CHO + E[-] TUNDER-1967 OMF		2ND	-12.8		+0.5		0		-11.3	
CH + O2 => CHO + O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
CH + OH => C + H2O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
CH + OH => CHO + H TUNDER-1967 OME		2ND	-12.1		+0.5		+5.0		-12.8	
CH + P => C + PH MAYER-1968 J+P		2ND	-13.25		+0.85		+7.35		-13.89	
CH + S => C + SH MAYER-1968 J+P		2ND	-13.9		+1.11		+.55		-10.8	
CH + SI => C + SIH MAYER-1968 J+P		2ND	-12.19		+0.68		+20.99		-19.26	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
CH2 + CH2 => CH + CH3 TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH2 + CH20 => CH3 + CHO TUNDER-1967 EST (11)		2ND	-13.3		+0.5		+3.0		-13.1
CH2 + CH4 => CH3 + CH3 TUNDER-1967 J+P (11)		2ND	-11.697		+0.7		+10.1		-14.0
CH2 + CHO => CH3 + CO TUNDER-1967 J+P		2ND	-13.3		+0.7		+.5		-11.4
CH2 + CL => CH + HCL TUNDER-1967 J+P		2ND	-12.22		+0.7		+1.46		-10.8
CH2 + F => CH + HF TUNDER-1967 J+P		2ND	-12.9		+0.7		+2.5		-11.9
CH2 + H => CH + H2 TUNDER-1967 J + P (1)		2ND	-12.32		+0.7		+13.1		-15.9
CH2 + H2 => CH3 + H TUNDER-1967 EST (11)		2ND	-13.8		+0.5		+5.0		-14.5
CH2 + H20 => CH3 + OH TUNDER-1967 OME		2ND	-13.8		+0.5		+5.0		-14.5
CH2 + HNO => CH3 + NO TUNDER-1967 OME (36)		2ND	-12.1		+0.5		0		-10.6
CH2 + O => CH + OH TUNDER-1967 OME		2ND	-12.27		+0.7		+13.1		-15.9
CH2 + O => CHO + H TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
CH2 + O2 => CH20 + O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1
CH2 + OH => CH + H20 TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9
CH2 + OH => CH3 + O TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
CH20 => CHO + H TUNDER-1967 (7)		1ST	+17.5		0		+43.8		-1.5
CH20 + CH3 => CH4 + CHO TUNDER-1967 SEL (6)		2ND	-13.8		+0.5		+3.0		-13.6
CH20 + CN => CHO + HCN TUNDER-1967 J+P		2ND	-12.70		+0.7		+1.5		-11.3
CH20 + H => CHO + H2 TUNDER-1967 SEL (6)		2ND	-10.8		0		+1.0		-11.2
CH20 + O => CHO + OH TUNDER-1967 J+P		2ND	-12.2		+0.6		+2.0		-11.3
CH20 + OH => CHO + H20 TUNDER-1967 J+P		2ND	-13.1		+0.7		+.5		-11.2
CH3 + CHO => CH2 + CH20 TUNDER-1967 J+P		2ND	-12.60		+0.7		+2.0		-11.4
CH3 + CHO => CH4 + CO TUNDER-1967 OME (36)		2ND	-12.30		+0.5		0		-10.8
CH3 + CL => CH2 + HCL TUNDER-1967 J+P		2ND	-12.44		+0.7		+4.0		-12.1
CH3 + CN => CH2 + HCN TUNDER-1967 J+P		2ND	-11.83		+0.7		+1.5		-10.4
CH3 + F => CH2 + HF TUNDER-1967 J+P		2ND	-13.0		+0.7		+.5		-11.1
CH3 + H => CH2 + H2 TUNDER-1967 J+P		2ND	-12.52		+0.7		+1.5		-11.1
CH3 + H => CH4 TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
CH3 + H2 => CH4 + H									
TUNDER-1967 SEL (6)		2ND	-13.8		+0.5		+5.0		-14.5
CH3 + HNO => CH4 + NO									
TUNDER-1967 OME (36)		2ND	-12.08		+0.5		0		-10.6
CH3 + HO2 => CH4 + O2									
TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6
CH3 + NAO => CH2 + NAOH									
TUNDER-1967 OME (36)		2ND	-11.67		+0.5		0		-10.2
CH3 + NH => CH2 + NH2									
TUNDER-1967 J+P		2ND	-12.83		+0.7		+1.0		-11.2
CH3 + NH2 => CH2 + NH3									
TUNDER-1967 J+P		2ND	-12.55		+0.7		+1.0		-10.9
CH3 + O => CH2 + OH									
TUNDER-1967 OME		2ND	-12.8		+0.5		+.86		-11.7
CH3 + O => CH2O + H									
TUNDER-1967 SEL (16)		2ND	-10.50		0		0		-10.50
CH3 + OH => CH2 + H2O									
TUNDER-1967 J+P		2ND	-13.0		+0.7		+1.0		-11.3
CH4 + CHO => CH2O + CH3									
TUNDER-1967 J+P		2ND	-11.845		+0.6		+4.5		-12.0
CH4 + CL => CH3 + HCL									
TUNDER-1967 J+P		2ND	-11.94		+0.6		+.65		-10.4
CH4 + CN => CH3 + HCN									
TUNDER-1967 J+P		2ND	-12.32		+0.7		+2.5		-11.3
CH4 + F => CH3 + HF									
TUNDER-1967 J+P		2ND	-12.83		+0.7		+.5		-10.9
CH4 + H => CH3 + H2									
SCOFLD-1967 EVAL (17)	.4-2	2ND	-10.17		0		+5.84		-12.70
TUNDER-1967 J+P		2ND	-12.14		+0.7		+3.5		-11.6
CH4 + NAO => CH3 + NAOH									
TUNDER-1967 J+P		2ND	-12.58		+0.7		+.5		-10.7

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CH4 + NH => CH3 + NH2										
TUNDER-1967 J+P		2ND	-12.01		+0.6		+3.5		-11.7	
CH4 + NH2 => CH3 + NH3										
TUNDER-1967 J+P		2ND	-11.802		+0.6		+4.0		-11.7	
CH4 + O => CH3 + OH										
SCOFLD-1967 EVAL (25)	.3-1	2ND	-10.28		0		+4.00		-12.02	
TUNDER-1967 SEL (37)		2ND	-12.2		+0.5		+4.0		-12.4	
CH4 + OH => CH3 + H2O SEE REACTION SUMMARY										
SCOFLD-1967 EVAL (24)	.3-1.8	2ND	-9.92		0		+2.97		-11.21	
TUNDER-1967 SEL (16)		2ND	-9.24		0		+4.5		-11.19	
WILSON-1968 EVAL (2)	.3-2	2ND	-10.3	.7	0		2.50		-11.38	.70
CH4 + OH => CO + H2O (OVERALL)										
JENSEN-1967 XP (59)	1-3.5	2ND	-10.3	.7	0		+2.5		-11.38	.70
CH4 + OH => CO2 + H3O[+] + E[-] (OVERALL)										
JENSEN-1967 XP (60)	1-3.5	2ND	-16.3	1.0	0		+2.5		-17.4	1.0
CHO + CHO => CH2O + CO										
TUNDER-1967 OME (36)		2ND	-12.63		+0.5		0		-11.1	
CHO + CL => CO + HCL										
TUNDER-1967 OME (36)		2ND	-11.83		+0.5		0		-10.3	
CHO + CN => CO + HCN										
TUNDER-1967 OME (36)		2ND	-12.50		+0.5		0		-11.0	
CHO + F => CO + HF										
TUNDER-1967 OME (36)		2ND	-12.74		+0.5		0		-11.2	
CHO + H => CO + H2										
JENSEN-1967 EST (57)	1-3.5	2ND	-11.0	2.0	0		0		-11.0	2.0
TUNDER-1967 OME (36)		2ND	-11.60		+0.5		0		-10.1	

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CHO + HNO => CH2O + NO										
TUNDER-1967 OME (36)		2ND	-12.27		+0.5		0		-10.8	
CHO + LI => CO + LIH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7	
CHO + LI[+] => CHO[+] + LI										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
CHO + M => CO + H + M (M= ANY)										
TUNDER-1967 SEL (6)		2ND	-8.8		+0.5		+11.6		-12.3	
CHO + N => CO + NH										
TUNDER-1967 OME		2ND	-12.5		+0.5		+1.0		-11.4	
CHO + NA => CO + NAH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7	
CHO + NAO => CO + NAOH										
TUNDER-1967 OME (36)		2ND	-12.52		+0.5		0		-11.0	
CHO + NH => CO + NH2										
TUNDER-1967 OME (36)		2ND	-12.63		+0.5		0		-11.1	
CHO + NH2 => CH2O + NH										
TUNDER-1967 J+P		2ND	-12.67		+0.6		+2.0		-11.7	
CHO + NH2 => CO + NH3										
TUNDER-1967 OME (36)		2ND	-12.36		+0.5		0		-10.9	
CHO + NH3 => CH2O + NH2										
TUNDER-1967 J+P		2ND	-12.30		+0.6		+1.5		-11.2	
CHO + NO => CO + HNO										
TUNDER-1967 OME		2ND	-12.5		+0.5		+1.0		-11.4	
CHO + O => CO + OH										
JENSEN-1967 EST (57)	1-3.5	2ND	-11.0	1.5	0		0		-11.0	1.5
TUNDER-1967 OME (36)		2ND	-12.52		+0.5		0		-11.0	
CHO + O[-] => CO + OH[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7	
CHO + OH => CO + H2O										
JENSEN-1967 EST (57)	1-3.5	2ND	-11.0	2.0	0		0		-11.0	2.0
TUNDER-1967 OME (36)		2ND	-12.74		+0.5		0		-11.2	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CHO[+] + E[-] + M => CHO + M (M= ANY)										
TUNDER-1967 OME		3RD	-23.9		+1.5		0		-19.4	
CHO[+] + H2O => CO + H3O[+]										
JENSEN-1967 EST (62)	1-3.5	2ND	-8.0	.7	0		0		-8.00	.70
CL + CL + M => CL2 + M (M= ANY)										
JENSEN-1967 REV (22)	1-3.5	3RD	-28.5	1.0	-1.0		0		-31.5	1.0
CL + CL[-] => CL2 + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CL + CS + M => CSCL + M (M= ANY)										
JENSEN-1967 EST (26)	1-3.5	3RD	-28.0	2.0	-1.0		0		-31.0	2.0
CL + E[-] + M => CL[-] + M (M= ANY)										
JENSEN-1967 EST (35)	1-3.5	3RD	-29.5	1.5	0		0		-29.5	1.5
TUNDER-1967 OME		3RD	-27.6		-1.0		0		-30.6	
CL + F + M => CLF + M (M= ANY)										
CHERRY-1967 OME		3RD	-31.1	1.4	-0.5		0		-32.6	1.4
CL + F2 => CLF + F										
CHERRY-1967 J+P		2ND	-10.9	1.4	+0.68		+.15		-8.9	1.4
CL + H + M => HCL + M (M= ANY)										
CHERRY-1967 OMF (16)		3RD	-31.1	1.4	-0.5		0		-32.6	1.4
JENSEN-1967 EST (21)	1-3.5	3RD	-28.5	1.5	-1.0		0		-31.5	1.5
TUNDER-1967 OMF		3RD	-31.1		-0.5		0		-32.6	
CL + H[-] => CL[-] + H										
TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7	
CL + H[-] => HCL + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CL + H2 => H + HCL										
JENSEN-1967 XP (12)	1-3.5	2ND	-9.8	.7	0		+2.82		-11.02	.70
MAYER-1968 J+P		2ND	-12.11		+0.79		+2.97		-11.03	
TUNDER-1967 SEL (31)		2ND	-9.87		0		+3.0		-11.17	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±A
CL + H20 => HCL + OH										
JENSEN-1967 EST (13)	1-3.5	2ND	-10.3	1.5	0		+9.6		-14.5	1.5
CL + HBR => BR + HCL										
MAYER-1968 BEHO		2ND	-11.78		+0.5		+.20		-10.4	
CL + HCL => CL + HCL										
MAYER-1968 BEHO		2ND	-11.74		+0.5		+.30		-10.4	
CL + HCN => CN + HCL										
TUNDER-1967 J+P		2ND	-12.13		+0.6		+1.01		-10.8	
CL + HF => F + HCL										
MAYER-1968 BEHO		2ND	-11.816		+0.5		+16.71		-17.6	
CL + HI => HCL + I										
MAYER-1968 BEHO		2ND	-11.74		+0.5		+.25		-10.3	
CL + HNO => HCL + NO										
TUNDER-1967 OME (36)		2ND	-11.38		+0.5		0		-9.9	
CL + HO2 => HCL + O2										
JENSEN-1967 EST (51)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
CL + K + M => KCL + M	(M= ANY)									
JENSEN-1967 EST (26)	1-3.5	3RD	-28.0	2.0	-1.0		0		-31.0	2.0
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
CL + KH => HCL + K										
MAYER-1968 J+P		2ND	-13.16		+0.76		+6.34		-13.63	
CL + KO2 => KCL + O2										
JENSEN-1967 EST (49)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
CL + LI + M => LICL + M	(M= ANY)									
JENSEN-1967 EST (26)	1-3.5	3RD	-28.0	2.0	-1.0		0		-31.0	2.0
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
CL + LIH => H + LICL										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CL + LIH => HCL + LI										
MAYER-1968 J+P		2ND	-12.63		+0.70		+3.72		-12.14	

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CL + LIO => LICL + O										
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	
CL + LIO2 => LICL + O2										
JENSEN-1967 EST (49)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
CL + MGH => HCL + MG										
MAYER-1968 BEBO		2ND	-12.02		+0.5		+.55		-10.8	
CL + NA + M => NACL + M	(M= ANY)									
JENSEN-1967 EST (26)	1-3.5	3RD	-28.0	2.0	-1.0		0		-31.0	2.0
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
CL + NAH => H + NACL										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CL + NAH => HCL + NA										
MAYER-1968 J+P		2ND	-12.89		+0.71		+4.93		-12.90	
CL + NAO => NACL + O										
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
CL + NAO2 => NACL + O2										
JENSEN-1967 EST (49)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
CL + NAOH => HCL + NAO										
TUNDER-1967 OME (36)		2ND	-12.78		+0.5		0		-11.3	
CL + NH => HCL + N										
MAYER-1968 BEBO		2ND	-11.97		+0.5		+.15		-10.5	
CL + NH2 => HCL + NH										
TUNDER-1967 OME (36)		2ND	-12.07		+0.5		0		-10.6	
CL + NH3[+] => +HCL + NH2										
TUNDER-1967 OME (36)		2ND	-12.13		+0.5		0		-10.6	

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RATE PARAMETERS FOR K = $10^{(A\pm A')}\ T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CL + O + M => CLO + M (M= ANY)										
JENSEN-1967 EST (42)	1-3.5	3RD	-28.7	1.5	-1.0		0		-31.7	1.5
CL + O[-] => CL[-] + O + O										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
CL + O2[-] => CL[-] + O2										
TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6	
CL + OH => HCL + O										
JENSEN-1967 EST (14)	1-3.5	2ND	-10.5	1.5	0		+2.5		-11.6	1.5
MAYER-1968 J+P		2ND	-12.48		+0.67		+.05		-10.49	
CL + OH + M => HOCL + M (M= ANY)										
JENSEN-1967 EST (67)	1-3.5	3RD	-28.5	1.5	-1.0		0		-31.5	1.5
CL + OH[-] => CL[-] + OH										
TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7	
CL + PH => HCL + P										
MAYER-1968 J+P		2ND	-12.55		+0.67		+1.16		-11.04	
CL + SH => HCL + S										
MAYER-1968 BERO		2ND	-11.97		+0.5		+.45		-10.7	
CL + SIH => HCL + SI										
MAYER-1968 BERO		2ND	-12.26		+0.5		+.86		-11.1	
CL[-] + CN => CL + CN										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CL[-] + CS[+] => CL + CS										
JENSEN-1967 EST (31)	1-3.5	2ND	-7.5	2.0	-0.5		0		-9.0	2.0
CL[-] + H => HCL + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CL[-] + H3O[+] => H + HCL + OH										
JENSEN-1967 XP (66)	1-3.5	2ND	-7.5	1.0	0		0		-7.5	1.0
CL[-] + H3O[+] => H2O + HCL										
TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6	
CL[-] + K[+] => CL + K										
JENSEN-1967 XP (33)	1-3.5	2ND	-8.0	2.0	-0.5		0		-9.5	2.0

RATE PARAMETERS FOR K = $10^{(A\pm A')}$ $T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CL[-] + K[+] + M => KCL + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
CL[-] + KH2O[+] => CL + H2O + K										
JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
CL[-] + LI[+] => CL + LI										
JENSEN-1967 EST (31)	1-3.5	2ND	-6.7	2.0	-0.5		0		-8.2	2.0
CL[-] + LI[+] + M => LICL + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
CL[-] + LIH2O[+] => CL + H2O + LI										
JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
CL[-] + NA => NACL + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CL[-] + NA[+] => CL + NA										
JENSEN-1967 XP (32)	1-3.5	2ND	-6.7	1.0	-0.5		0		-8.2	1.0
CL[-] + NA[+] + M => NACL + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
CL[-] + NAH2O[+] => CL + H2O + NA										
JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
CL2 + F => CL + CLF										
CHERRY-1967 J+P		2ND	-11.0	1.4	+0.68		+.25		-9.1	1.4
CL2 + F2 => CLF + CLF										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+13.5		-17.9	3.0
CL2 + H => CL + HCL										
CHERRY-1967 SEL (3)		2ND	-9.3	1.4	0		+1.5		-10.0	1.4
JENSEN-1967 SEL (11)	1-3.5	2ND	-9.2	.7	0		+1.5		-9.85	.70

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CL2 + H2 => HCL + HCL										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+11.6		-17.0	3.0
CL2 + K => CL + KCL										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CL2 + NA => CL + NACL										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CLF + H => CL + HF										
CHERRY-1967 J+P (5)		2ND	-11.5	1.4	+0.68		+1.61		-10.2	1.4
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CLF + H => F + HCL										
CHERRY-1967 J+P (5)		2ND	-11.0	1.4	+0.68		+.96		-9.4	1.4
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CLF + H2 => HCL + HF										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+23.3		-22.1	3.0
CLF + HCL => CL2 + HF										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+23.1		-22.0	3.0
CLF + NA => CL + NAF										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CLF + NA => F + NACL										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
CLO + H => HCL + O										
JENSEN-1967 EST (44)	1-3.5	2ND	-10.5	1.5	0		0		-10.5	1.5
CLO + K => KCL + O										
JENSEN-1967 EST (43)	1-3.5	2ND	-9.7	2.0	0		+1.5		-10.4	2.0
CLO + LI => LICL + O										
JENSEN-1967 (02)		2ND	-9.7	1.5	0		+1.5		-10.4	1.5
CLO + NA => NACL + O										
JENSEN-1967 EST (43)	1-3.5	2ND	-9.7	2.0	0		+1.5		-10.4	2.0
CLO + O => CL + O2										
JENSEN-1967 EST (45)	1-3.5	2ND	-10.7	1.5	0		+1.5		-11.4	1.5

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \; T^{(B \pm B')} \; \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CLO + OH => CL + HO2 JENSEN-1967 EST,REV (46)	1-3.5	2ND	-9.3	2.0	0		0		-9.3	2.0
CN + H + M => HCN + M (M= ANY) TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
CN + H[-] => CN[-] + H TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
CN + H[-] => HCN + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
CN + H2 => H + HCN TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
CN + HCL => CL + HCN TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
CN + HNO => HCN + NO TUNDER-1967 OME (36)		2ND	-12.20		+0.5		0		-10.7	
CN + NAH => HCN + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
CN + NH => HCN + N TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7	
CN + NH2 => HCN + NH TUNDER-1967 J+P		2ND	-13.1		+0.7		+1.0		-11.4	
CN + NH3 => HCN + NH2 TUNDER-1967 J+P		2ND	-12.9		+0.7		+1.0		-11.2	
CN + O[-] => CN[-] + O TUNDER-1967 OME		2ND	-12.1		+0.5		+4.5		-12.6	
CN + O2[-] => CN[-] + O2 TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	

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RATE PARAMETERS FOR K = $10^{(A\pm A')}\ T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CN + OH => HCN + O TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
CN + OH[-] => CN[-] + OH TUNDER-1967 OMF		2ND	-12.2		+0.5		0		-10.7	
CN + OH[-] => HCN + O[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+4.5		-13.3	
CN[-] + F => CN + F[-] TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
CN[-] + H => HCN + E[-] TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
CN[-] + H3O[+] => H2O + HCN TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
CO + H + M => CHO + M (M= ANY) JENSEN-1967 EST (58)	1-3.5	3RD	-28.5	.5	-1.0		0		-31.50	.52
CO + H[-] => CHO + E[-] TUNDER-1967 OMF		2ND	-12.1		+0.5		0		-10.6	
CO + HNO => CO2 + NH TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	
CO + HO2 => O2 + OH JENSEN-1967 EST (56)	1-3.5	2ND	-11.0	2.0	0		+5.0		-13.2	2.0
CO + LIO => CO2 + LI TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
CO + N2O => CO2 + N2 TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
CO + NAO => CO2 + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+2.0		-12.2	
CO + NO2 => CO2 + NO TUNDER-1967 OME		2ND	-12.5		+0.5		+2.5		-12.1	
CO + O => CO2 BAULCH-1968 EVAL (2)	.4-.55	2ND	-13.53		0		+1.26		-14.08	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\, T^{(B \pm B')}\, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CO + O => CO2 + PHOTON										
BAULCH-1968 EVAL (2)		2ND	-17.86		0		-1.30	0.25	-17.30	.11
CO + O + M => CO2 + M (M= ANY)										
CHERRY-1967 SEL (14)		3RD	-31.6	2.5	0		+1.76		-32.4	2.5
JENSEN-1967 XP (5)	1-3.5	3RD	-28.3	1.5	-1.0		+2.0		-32.2	1.5
TUNDER-1967 SEL (26)		3RD	-31.6		-0.5		+1.8		-33.9	
CO + O[-] => CO2 + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
CO + O2 => CO2 + O										
CHERRY-1967 SEL (6)		2ND	-11.2	3.0	0		+25.7		-22.4	3.0
CO + OD => CO2 + D										
BAULCH-1968 XP (1)	.3	2ND	-13.26	.01						
CO + OH => CO2 + H SEE REACTION SUMMARY										
BAHN-1968 SEL (1)		2ND	-12.29		0		+.30		-12.42	
BAULCH-1968 EVAL (1)		2ND	-12.03	0.3	0		+0.54	.25	-12.26	.32
CHERRY-1967 SEL (24)		2ND	-12.3	.7	0		+.30		-12.43	.70
JENSEN-1967 SEL (10)	1-3.5	2ND	-12.3	.7	0		+.30		-12.43	.70
KASKAN-1964 EVAL(10)		2ND	-11.27		0		+3.17		-12.65	
SCOFLD-1967 EVAL (28)	.3-2	2ND	-11.96		0		+.51		-12.18	
TUNDER-1967 SEL (38)		2ND	-12.3		0		+.3		-12.4	
WILSON-1968 EVAL (3)	.3-2	2ND	-12.3	.7	0		+.30		-12.43	.70
CO2 + H => CO + OH										
BAULCH-1968 REV (1)		2ND	-10.03	.12	0		+11.8	0.5	-15.15	.25
KASKAN-1964 REV (10)		2ND	-6.35		+0.79		+15.45		-10.69	
CO2 + H2 => CO + H2O										
TUNDER-1967 OME		2ND	-14.8		+0.5		+7.5		-16.6	
CO2 + M => CO + O + M										
BAHN-1968 EVAL (2)		2ND	+8.65		-4.5		+64.19		-32.7	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
CO2 + N => CO + NO										
CHERRY-1967 (25)		2ND	-12.8	3.0	+0.5		+30.		-24.3	3.0
TUNDER-1967 OME		2ND	-12.5		+0.5		+4.0		-12.7	
CO2 + O => CO + O2										
BAULCH-1968 XP (3)		2ND	-10.50		0		+27.25		-22.33	
TUNDER-1967 OME		2ND	-12.1		+0.5		+4.0		-12.3	
CS + H2O => CSOH + H										
JENSEN-1967 XP,EST (20)	1-3.5	2ND	-10.5	1.5	0		+15.6		-17.3	1.5
CS + H3O[+] => CS[+] + H + H2O										
JENSEN-1967 EST (63)	1-3.5	2ND	-8.0	.7	0		0		-8.00	.70
CS + HCL => CSCL + H										
JENSEN-1967 EST (17)	1-3.5	2ND	-9.5	1.5	0		0		-9.5	1.5
CS + OH + M => CSOH + M (M= ANY)										
JENSEN-1967 XP (25)	1-3.5	3RD	-27.5	1.5	-1.0		0		-30.5	1.5
CS[+] + E[-] + M => CS + M (M= ANY)										
JENSEN-1967 REV (30)	1-3.5	3RD	-21.7	.7	-1.5		0		-26.20	.72
CS[+] + OH[-] => CS + OH										
JENSEN-1967 EST (34)	1-3.5	2ND	-7.0	2.0	-0.5		0		-8.5	2.0
D + H2 => H + HD										
SCOFLD-1967 EVAL (1)	.3-1	2ND	-10.37		0		+3.41		-11.85	
D2 + H => D + H2										
SCOFLD-1967 EVAL (1)	.3-1	2ND	-10.27		0		+4.30		-12.14	
F + E[-] + M => F[-] + M (M= ANY)										
TUNDER-1967 OME		3RD	-27.6		-1.0		0		-30.6	
F + F + M => F2 + M (M= ANY)										
JENSEN-1967 REV (24)	1-3.5	3RD	-29.5	1.0	-1.5		0		-34.0	1.0
F + H + M => HF + M (M= ANY)										
CHERRY-1967 EST (19)		3RD	-28.7	1.5	-1.0		0		-31.7	1.5
JENSEN-1967 XP (23)	1-3.5	3RD	-28.0	1.0	-1.0		0		-31.0	1.0
F + H + M => HF + M (M= H2O)										
TUNDER-1967 OME (19)		3RD	-28.9		-0.5		0		-30.4	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
F + H + M => HF + M (M= H2)										
TUNDER-1967 OME (19)		3RD	-29.7		-0.5		0		-31.2	
F + H + M => HF + M (M= H)										
TUNDER-1967 OME (19)		3RD	-30.02		-0.5		0		-31.5	
F + H + M => HF + M (M= OH)										
TUNDER-1967 OME (19)		3RD	-28.9		-0.5		0		-30.4	
F + H[-] => F[-] + H										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
F + H2 => H + HF										
CHERRY-1967 EST (2)		2ND	-11.1	1.7	0		+2.87		-12.3	1.7
MAYER-1968 J+P		2ND	-11.70		+0.67		+1.31		-10.26	
F + H2O => HF + OH										
CHERRY-1967 J+P		2ND	-13.6	1.4	+0.68		+.30		-11.7	1.4
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
F + HBR => BR + HF										
MAYER-1968 BEBO		2ND	-11.802		+0.5		+.20		-10.4	
F + HCL => CL + HF										
CHERRY-1967 J+P		2ND	-11.5	1.4	+0.68		+.30		-9.6	1.4
MAYER-1968 BEBO		2ND	-11.811		+0.5		+.30		-10.4	
F + HCN => CN + HF										
TUNDER-1967 J+P		2ND	-13.167		+0.7		+.5		-11.3	
F + HF => F + HF										
MAYER-1968 J+P		2ND	-13.24		+0.99		+.55		-10.51	
F + HI => HF + I										
MAYER-1968 BEBO		2ND	-11.74		+0.5		+.20		-10.3	
F + HNO => HF + NO										
TUNDER-1967 OME (36)		2ND	-11.40		+0.5		0		-9.9	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
F + K + M => KF + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
F + KH => HF + K									
MAYER-1968 J+P		2ND	-13.15		+0.77		+4.98		-13.00
F + LI + M => LIF + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
F + LIH => H + LIF									
TUNDER-1967 OMF		2ND	-12.1		+0.5		+1.5		-11.3
F + LIH => HF + LI									
MAYER-1968 J+P		2ND	-12.821		+0.72		+4.28		-12.52
TUNDER-1967 J+P		2ND	-12.40		+0.7		+4.0		-12.0
F + LIO => LIF + O									
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7
F + LIOH => HF + LIO									
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8
F + MGH => HF + MG									
MAYER-1968 BERO		2ND	-12.06		+0.5		+.30		-10.7
F + NA + M => NAF + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
F + NAH => H + NAF									
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3
F + NAH => HF + NA									
MAYER-1968 J+P		2ND	-12.95		+0.73		+4.03		-12.51
F + NAO => NAF + O									
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5
F + NAOH => HF + NAO									
TUNDER-1967 OME (36)		2ND	-12.70		+0.5		0		-11.2
F + NH => HF + N									
MAYER-1968 BERO		2ND	-12.06		+0.5		+.50		-10.8
F + NH2 => HF + NH									
TUNDER-1967 OME (36)		2ND	-11.99		+0.5		0		-10.5

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
F + NH3 => HF + NH2										
TUNDER-1967 OME (36)		2ND	-12.15		+0.5		0		-10.6	
F + O[-] => F[-] + O										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
F + O2[-] => F[-] + O2										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
F + OH => HF + O										
CHERRY-1967 J+P		2ND	-11.3	1.4	+0.68		+.10		-9.3	1.4
MAYER-1968 BEBO		2ND	-12.12		+0.5		+.15		-10.7	
F + OH + M => HF + O + M (M= HF)										
TUNDER-1967 OME (19)		3RD	-28.9		-0.5		+3.0		-31.7	
F + OH[-] => F[-] + OH										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
F + PH => HF + P										
MAYER-1968 J+P		2ND	-12.55		+0.67		+.96		-10.96	
F + SH => HF + S										
MAYER-1968 BEBO		2ND	-12.02		+0.5		+.30		-10.7	
F + SIH => HF + SI										
MAYER-1968 BEBO		2ND	-12.30		+0.5		+.96		-11.2	
F[-] + H3O[+] => H2O + HF										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
F[-] + K[+] + M => KF + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
F[-] + LI[+] + M => LIF + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	

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RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
F[-] + LIO => LIF + O[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
F[-] + NA[+] + M => NAF + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
F2 + H => F + HF										
CHERRY-1967 CT (1)		2ND	-11.1	1.4	+0.5		+2.0		-10.5	1.4
JENSEN-1967 EST (16)	1-3.5	2ND	-9.2	1.0	0		+1.5		-9.9	1.0
F2 + H => F + HF (M= AR)										
TUNDER-1967 (23)		2ND	-11.057		+0.5		+2.0		-10.4	
F2 + H2 => HF + HF										
CHERRY-1967 OME (26)		2ND	-13.5	3.0	+0.5		+20.		-20.7	3.0
F2 + HCL => CLF + HF										
CHERRY-1967 OMF (26)		2ND	-13.5	3.0	+0.5		+19.8		-20.6	3.0
F2 + K => F + KF										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.0		-11.0	
F2 + LI => F + LIF										
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.0		-11.0	
F2 + M => F + F + M (M= ANY)										
TUNDER-1967 SEL (35)		2ND	-7.93		0		+15.		-14.4	
H + E[-] + M => H[-] + M (M= ANY)										
TUNDER-1967 OMF		3RD	-27.6		-1.0		0		-30.6	
H + H + M => H2 + M (M= ANY) SEE SUMMARY FOR REVERSE REACTION										
CHERRY-1967 XP (21)		3RD	-28.7	1.0	-1.0		0		-31.7	1.0
JENSEN-1967 XP (3)	1-3.5	3RD	-29.0	.7	-1.0		0		-32.00	.72
TUNDER-1967 SEL (26)		3RD	-29.3		-1.0		0		-32.3	
H + H + M => H2 + M (M= H2O) SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (5)	.3-5	3RD	-33.5	.1	0		-.70	.23	-33.20	.14
KASKAN-1964 EVAL (5)	.3-5	3RD	-28.38		-1.0		0		-31.4	
H + H + M => H2 + M (M= H2) SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (5)	.3-5	3RD	-32.74	.01	0		-.70	.23	-32.44	.10
KASKAN-1964 EVAL (5)	-5	3RD	-28.9		-1.0		0		-31.9	

$$\text{RATE PARAMETERS FOR } K = 10^{(A*A')}\, T^{(B*B')}\, \mathrm{EXP}(-1000(C*C')/T)$$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	*A'	B	*B'	C	*C'	LOG K AT T = 1000	*Δ
H + H + M => H2 + M (M= HF)										
SEE SUMMARY FOR REVERSE REACTION										
TUNDER-1967 OME (19)		3RD	-28.6		-0.5		0		-30.1	
H + H + M => H2 + M (M= H)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (5)	.3-5	3RD	-31.60	.09	0		-.08	.2	-31.57	.13
KASKAN-1964 EVAL (5)	.3-5	3RD	-28.26		-1.0		0		-31.3	
H + H + M => H2 + M (M= N2)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (5)	.3-5	3RD	-33.5	.1	0		-.70	.23	-33.20	.14
H + H + M => H2 + M (M= OH)										
SEE SUMMARY FOR REVERSE REACTION										
TUNDER-1967 OME (19)		3RD	-28.9		-0.5		0		-30.4	
H + H[-] => H2 + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H + H2 => H + H2										
MAYER-1968 J+P		2ND	-12.02		+0.78		+4.48		-11.62	
H + H2O => H2 + OH										
SEE SUMMARY FOR REVERSE REACTION										
BAHN-1965 SEL (12)		2ND	-9.3	1.0	0		+10.57	.75	-13.9	1.1
BASCMB-1965 EVAL (1)	.3-3	2ND	-10.18		0		+10.0	.3	-14.52	.13
KASKAN-1964 REV (1)		2ND	-9.40		0		+10.42		-13.92	
SCOFLD-1967 REV (4)	.3-2.5	2ND	-9.52		0		+10.40		-14.03	
TUNDER-1967 J+P		2ND	-12.32		+0.7		+9.1		-14.2	
H + H2(PARA) => H + H2(ORTHO)										
SCOFLD-1967 EVAL (1)	.3-1	2ND	-10.10		0		+3.89		-11.79	
H + HBR => BR + H2										
MAYER-1968 J+P		2ND	-11.86		+0.67		+1.36		-10.44	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H + HCL => CL + H2										
CHERRY-1967 XP (4)		2ND	-12.0	1.0	+0.5		+1.56		-11.2	1.0
MAYER-1968 J+P		2ND	-12.38		+0.77		+2.42		-11.12	
H + HCN => CN + H2										
TUNDER-1967 J+P		2ND	-12.36		+0.7		+.91		-10.7	
H + HF => F + H2										
JENSEN-1967 SEL (15)	1-3.5	2ND	-10.7	.7	0		+17.6		-18.34	.70
MAYER-1968 J+P		2ND	-11.74		+0.67		+17.21		-17.20	
TUNDER-1967 XP (23,28)		2ND	-10.8		0		+17.6		-18.4	
H + HI => H2 + I										
MAYER-1968 J+P		2ND	-11.60		+0.67		+.81		-9.94	
H + HNO => H2 + NO										
SCOFLD-1967 XP (12)	.2-2	2ND	-10.7		0		+1.26		-11.2	
TUNDER-1967 (13,36)		2ND	-11.19		+0.5		0		-9.7	
H + HNO => NH + OH										
TUNDER-1967 OME		2ND	-12.5		+0.5		+6.5		-13.8	
H + HO2 => H2 + O2										
JENSEN-1967 EST (54)	1-3.5	2ND	-10.5	1.0	0		0		-10.5	1.0
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H + HO2 => OH + OH										
JENSEN-1967 XP (53)	1-3.5	2ND	-10.0	1.0	0		0		-10.0	1.0
H + HOCL => CLO + H2										
JENSEN-1967 EST (57)	1-3.5	2ND	-11.0	2.0	0		0		-11.0	2.0
H + KCL => HCL + K										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1	
H + KF => HF + K										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.5		-12.1	
H + KH => H2 + K										
MAYER-1968 J+P		2ND	-12.03		+0.70		+2.32		-10.94	
H + LI + M => LIH + M (M= ANY)										
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
H + LIF => HF + LI									
TUNDER-1967 (7)		2ND	-12.8		+0.5		+3.5		-12.8
H + LIH => H2 + LI									
MAYER-1968 J+P		2ND	-12.17		+0.71		+3.07		-11.37
H + LIO => LIH + O									
TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
H + MGH => H2 + MG									
MAYER-1968 BERO		2ND	-11.46		+0.5		+.91		-10.4
H + N + M => NH + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
H + N2O => N2 + OH									
SCOFLD-1967 XP (6)	.4-2	2ND	-10.31		0		+5.42		-12.66
TUNDER-1967 SEL (40)		2ND	-9.3		0		+8.1		-12.8
H + N2O => NH + NO									
TUNDER-1967 OME		2ND	-12.8		+0.5		+15.1		-17.9
H + NA + M => NAH + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
H + NAF => HF + NA									
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6
H + NAH => H2 + NA									
MAYER-1968 J+P		2ND	-11.97		+0.68		+2.01		-10.80
H + NAO + M => NAOH + M (M= ANY)									
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6
H + NAOH => H2 + NAO									
TUNDER-1967 J+P		2ND	-11.704		+0.7		+9.6		-13.8

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RATE PARAMETERS FOR $K = 10^{(A\pm A')} T^{(B\pm B')} \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±A
H + NH => H? + N										
MAYER-1968 J+P		2ND	-11.93		+0.67		+.75		-10.25	
H + NH + M => NH2 + M (M= ANY)										
TUNDER-1967 EST (13)		3RD	-31.3		-0.5		0		-32.8	
H + NH2 => H2 + NH										
TUNDER-1967 J+P		2ND	-12.63		+0.7		+2.0		-11.4	
H + NH2 => NH3										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H + NH3 => H2 + NH2										
TUNDER-1967 J+P		2ND	-12.50		+0.7		+1.5		-11.1	
TUNDER-1967 EST (13)		2ND	-12.1		+0.5		+1.0		-11.0	
H + NO + M => HNO + M (M= ANY)										
TUNDER-1967 XP (15)		3RD	-30.6		-0.5		+.35		-32.3	
H + NO2 => NO + OH										
SCOFLD-1967 XP (8)	.3-.6	2ND	-8.92		0		+.97		-9.34	
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	
H + O + M => OH + M (M= ANY)										
CHERRY-1967 SEL (22)		3RD	-29.3	.7	-1.0		0		-32.30	.72
JENSEN-1967 EST (2)	1-3.5	3RD	-29.0	1.0	-1.0		0		-32.0	1.0
KASKAN-1964 EST (6)		3RD	-32.8		0		0		-32.8	
H + O + M => OH + M (M= H2O)										
TUNDER-1967 OME,(4)		3RD	-28.9		-0.5		0		-30.4	
H + O + M => OH + M (M= H2)										
TUNDER-1967 OME,(4)		3RD	-29.7		-0.5		0		-31.2	
H + O + M => OH + M (M= H)										
TUNDER-1967 OME,(4)		3RD	-30.02		-0.5		0		-31.5	
H + O + M => OH + M (M= OH)										
TUNDER-1967 OME,(4)		3RD	-28.9		-0.5		0		-30.4	
H + O[-] => OH + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H + O[-] + M => OH[-] + M (M= ANY)										
TUNDER-1967 OME		3RD	-29.8		-0.5		0		-31.3	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H + O2 => O + OH SEE REACTION SUMMARY										
BAHN-1965 SEL (13)	1.5-1.7	2ND	-8.7	.8	0		+8.96	.50	-12.59	.83
BAHN-1965 SEL (13)	.3-.5	2ND	-8.9	.8	0		+8.51	.50	-12.59	.83
BALDWN-1963 EVAL,XP	.3-1.5	2ND	-9.4	.3	0		+8.4	.4	-13.05	.35
BASCMB-1965 EVAL (2)	.3-3	2ND	-9.35	.24	0		+8.4	.4	-13.00	.30
JENSEN-1967 XP (9)	1-3.5	2ND	-9.5	.2	0		+8.30		-13.10	.20
KASKAN-1964 EVAL (2)	.3-1.5	2ND	-9.40		0		+8.43		-13.06	
SCOFLD-1967 EVAL (2)	.3-2.5	2ND	-9.378		0		+8.44		-13.041	
TUNDER-1967 SEL (26)		2ND	-9.5		0		+8.6		-13.2	
H + O2 + M => HO2 + M (M= ANY)										
JENSEN-1967 XP (52)	1-3.5	3RD	-28.5	.7	-1.0		0		-31.50	.72
KASKAN-1964 EST (9)		3RD	-31.1		0		0		-31.1	
TUNDER-1967 OME,(26)		3RD	-32.6		-0.5		0		-34.1	
H + O2 + M => HO2 + M (M= AR)										
SCOFLD-1967 EVAL (30)	.2-1.5	3RD	-32.520		0		-.61		-32.255	
SCOFLD-1967 EVAL (30)	.2-1.5	3RD	-28.39		-1.29		0		-32.26	
H + O2 + M => HO2 + M (M= H2O)										
BASCMB-1965 EVAL (4)	.3-3	3RD	-31.51	.18	0		-.8	.4	-31.16	.25
H + O2 + M => HO2 + M (M= H2)										
BASCMB-1965 EVAL (4)	.3-3	3RD	-32.32	.18	0		-.8	.4	-31.97	.25
H + O2 + M => HO2 + M (M= N2)										
BASCMB-1965 EVAL (4)	.3-3	3RD	-32.8	.2	0		-.8	.4	-32.45	.26
H + O2 + M => HO2 + M (M= O2)										
BASCMB-1965 EVAL (4)	.3-3	3RD	-32.44	.18	0		-.3	.4	-32.31	.25
H + O2[-] => O + OH[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
H + O2[-] => OH + O[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H + O3 => O2 + OH										
SCOFLD-1967 (4-1)		2ND	-10.59		0		0		-10.59	
H + OH => H2 + O										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (3)	.3-3	2ND	-11.046		0		+3.7	.3	-12.65	.13
CHERRY-1967 XP,REV (11)		2ND	-11.6	.7	0		+2.62		-12.74	.70
KASKAN-1964 REV (3)		2ND	-11.63		0		+2.61		-12.76	
MAYER-1968 J+P		2ND	-12.58		+0.79		+2.16		-11.15	
SCOFLD-1967 REV (3)	.4-2.5	2ND	-11.032		0		+3.79		-12.677	
H + OH + M => H2O + M (M= ANY)										
CHERRY-1967 XP (20)		3RD	-28.6	3.0	-1.0		0		-31.6	3.0
JENSEN-1967 XP (4)	1-3.5	3RD	-28.0	1.0	-1.0		0		-31.0	1.0
KASKAN-1964 EVAL (5)		3RD	-25.91		-1.5		0		-30.4	
H + OH + M => H2O + M (M= H2O)										
BASCMB-1965 EVAL (6)	.3-3	3RD	-30.18	.15	0		-.93	.23	-29.78	.18
KASKAN-1964 EVAL (5)	.3-5	3RD	-25.30		-1.5		0		-29.8	
H + OH + M => H2O + M (M= N2)										
BASCMB-1965 EVAL (6)	.3-3	3RD	-30.9	.2	0		-.93	.23	-30.50	.22
H + OH[-] => H2O + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
H + PH => H2 + P										
MAYER-1968 J+P		2ND	-11.94		+0.67		+.96		-10.35	
H + SH => H2 + S										
MAYER-1968 J+P		2ND	-12.12		+0.67		+1.41		-10.72	
H + SIH => H2 + SI										
MAYER-1968 BEHO		2ND	-11.67		+0.5		+.20		-10.3	
H[-] + LI => LIH + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H[-] + LI[+] + M => LIH + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
H[-] + LIO => LI + OH[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H[-] + NA => NAH + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H[-] + NA[+] + M => NAH + M (M= ANY) TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
H[-] + NAO => NA + OH[-] TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
H[-] + NAO => NAOH + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H[-] + NH => NH2 + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H[-] + O => H + O[-] TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
H[-] + O => OH + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H[-] + O + M => OH[-] + M (M= ANY) TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
H[-] + O2 => H + O2[-] TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
H[-] + OH => H + OH[-] TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
H[-] + OH => H2O + E[-] TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
H2 + HO2 => H2O + OH JENSEN-1967 XP (55)	1-3.5	2ND	-11.0	1.7	0		+12.6		-16.5	1.7
H2 + I => H + HI MAYER-1968 J+P		2ND	-11.00		+0.67		+17.21		-16.46	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H2 + K => H + KH										
MAYER-1968 J+P		2ND	-11.16		+0.79		+32.56		-22.92	
H2 + KO2 => KOH + OH										
JENSEN-1967 EST (50)	1-3.5	2ND	-11.0	1.7	0		+5.0		-13.2	1.7
H2 + LI => H + LIH										
MAYER-1968 J+P		2ND	-11.58		+0.80		+26.07		-20.49	
H2 + LIO => H + LIOH										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
H2 + LIO2 => LIOH + OH										
JENSEN-1967 EST (50)	1-3.5	2ND	-11.0	1.7	0		+5.0		-13.2	1.7
H2 + M => H + H + M (M= ANY)										
BAHN-1965 SEL (9)		2ND	-2.8		-1.5		+51.95		-29.8	
H2 + M => H + H + M (M= AR)										
BAHN-1965 SEL (9)		2ND	-1.238		-2.0		+54.4		-30.8	
H2 + M => H + H + M (M= H2O)										
SEE REACTION SUMMARY										
BAHN-1965 SEL (9)		2ND	+.063		-2.0		+54.4		-29.5	
BASCMB-1965 EVAL (5)	.3-5	2ND	-9.328	.092	0		+51.73	.23	-31.78	.14
KASKAN-1964 EVAL (5)	.3-5	2ND	-4.74		-0.82		+51.94		-29.74	
H2 + M => H + H + M (M= H2)										
SEE REACTION SUMMARY										
BAHN-1965 SEL (9)		2ND	-3.52		-1.5		+51.97		-30.6	
BASCMB-1965 EVAL (5)	.3-5	2ND	-8.55	.09	0		+51.73	.23	-31.00	.13
KASKAN-1964 EVAL (5)	.3-5	2ND	-5.22		-0.82		+51.94		-30.22	
H2 + M => H + H + M (M= H)										
SEE REACTION SUMMARY										
BAHN-1965 SEL (9)		2ND	-5.70		-0.5		+51.97		-29.8	
BASCMB-1965 EVAL (5)	.3-5	2ND	-7.41	.09	0		+52.3	.2	-30.11	.13
KASKAN-1964 EVAL (5)	.3-5	2ND	-4.63		-0.82		+51.94		-29.63	
H2 + M => H + H + M (M= N2)										
SEE REACTION SUMMARY										
BASCMB-1965 EVAL (5)	.3-5	2ND	-9.328	.092	0		+51.73	.23	-31.78	.14
H2 + M => H + H + M (M= XE)										
BAHN-1965 SEL (9)		2ND	-6.52		-0.5		+51.97		-30.6	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±A
H2 + MG => H + MGH										
MAYER-1968 BERO		2ND	-10.690		+0.5		+29.69		-22.1	
H2 + N => H + NH										
MAYER-1968 J+P		2ND	-11.30		+0.67		+10.87		-14.01	
H2 + NA => H + NAH										
MAYER-1968 J+P		2ND	-11.16		+0.75		+30.15		-22.00	
H2 + NAO => H + NAOH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H2 + NAO2 => NAOH + OH										
JENSEN-1967 EST (50)	1-3.5	2ND	-11.0	1.7	0		+5.		-13.2	1.8
H2 + O => H + OH SEE REACTION SUMMARY										
BAHN-1965 SEL (12)		2ND	-11.4	.7	0		+3.88	.50	-13.08	.73
BASCMB-1965 EVAL (3)	.3-3	2ND	-10.70		0		+4.6	.3	-12.70	.13
JENSEN-1967 XP (8)	1-3.5	2ND	-10.5	.7	0		+4.13		-12.29	.70
KASKAN-1964 EVAL (3)		2ND	-11.26		0		+3.59		-12.82	
MAYER-1968 J+P		2ND	-11.99		+0.80		+3.07		-10.92	
SCOFLD-1967 EVAL (3)	.4-2.5	2ND	-10.68		0		+4.73		-12.73	
TUNDER-1967 SEL (37)		2ND	-10.2		0		+5.		-12.4	
H2 + O + M => H + OH + M (M= H2O)										
TUNDER-1967 OME (19)		3RD	-28.86		-0.5		+3.0		-31.7	
H2 + O[-] => H + OH[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
H2 + O2 => OH + OH										
BAHN-1965 SEL (10)		2ND	-9.382		0		+33.7		-24.01	
BASCMB-1965 REV (11)	.3-3	2ND	-10.15		0		+22.6		-19.96	
TUNDER-1967 XP (9,23)		2ND	-9.8		0		+35.2		-25.1	
H2 + OH => H + H2O SEE REACTION SUMMARY										
BASCMB-1965 XP (1)		2ND	-10.85		0		+2.4	.3	-11.89	.13
CHERRY-1967 XP (10)		2ND	-12.0	1.0	+0.5		+2.5		-11.6	1.0

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RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H2 + OH => H + H2O										
JENSEN-1967 XP,REV (7)	1-3.5	2ND	-10.4	.5	0		+2.77		-11.60	.50
KASKAN-1964 EVAL (1)	.3-2	2ND	-9.98		0		+2.97		-11.27	
SCOFLD-1967 EVAL (4)	.3-2.5	2ND	-10.20		0		+2.76		-11.40	
TUNDER-1967 SEL (38)		2ND	-12.0		+0.5		+2.5		-11.6	
WILSON-1968 EVAL (5)	.3-1.5	2ND	-10.43	.7	0		+2.6		-11.56	.70
H2 + P => H + PH										
MAYER-1968 J+P		2ND	-11.039		+0.67		+16.76		-16.30	
H2 + S => H + SH										
MAYER-1968 J+P		2ND	-11.25		+0.68		+10.07		-13.58	
H2 + SI => H + SIH										
MAYER-1968 BERO		2ND	-10.618		+0.5		+30.60		-22.4	
H2O + HO2 => H2O2 + OH										
BAHN-1965 SEL (17)		2ND	-15.70		0		+4.0		-17.44	
H2O + K => H + KOH										
JENSEN-1967 XP,EST (20)	1-3.5	2ND	-10.5	1.5	0		+20.1		-19.2	1.5
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H2O + LI => H + LIOH										
JENSEN-1967 XP,EST (20)	1-3.5	2ND	-10.5	1.5	0		+10.1		-14.9	1.5
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H2O + LIO => LIOH + OH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H2O + M => H + OH + M (M= ANY)										
KASKAN-1964 REV (5)	.3-2	2ND	-1.55		-1.31		+59.4		-31.26	
H2O + M => H + OH + M (M= AR)										
BAHN-1965 SEL (14)		2ND	+.817		-2.0		+62.00		-32.1	
H2O + M => H + OH + M (M= H2O)										
BAHN-1965 SEL (14)		2ND	+2.118		-2.0		+62.00		-30.8	
BASCMB-1965 REV (6)	.3-3	2ND	-5.8	.2	0		+59.03	.23	-31.42	.22
KASKAN-1964 REV (5)	.3-2	2ND	-.95		-1.31		+59.4		-30.66	
H2O + M => H + OH + M (M= HE)										
BAHN-1965 SEL (14)		2ND	-2.8		-1.5		+57.73		-32.4	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\, T^{(B \pm B')}\, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H2O + M => H + OH + M (M= N2)										
BASCMB-1965 REV (6)	.3-3	2ND	-6.47	.15	0		+59.03	.23	-32.09	.18
H2O + M => H + OH + M (M= XE)										
BAHN-1965 SEL (14)		2ND	-.8		-1.5		+57.73		-30.4	
H2O + NA => H + NAOH										
JENSEN-1967 XP,EST (20)	1-3.5	2ND	-10.5	1.5	0		+22.1		-20.1	1.5
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
H2O + NAO => NAOH + OH										
TUNDER-1967 OME (36)		2ND	-11.67		+0.5		0		-10.2	
H2O + O => OH + OH SEE SUMMARY FOR REVERSE REACTION										
BAHN-1965 SEL (12)		2ND	-9.9	.8	0		+9.06	.50	-13.83	.83
BASCMB-1965 EVAL (10)	.3-3	2ND	-10.15	.19	0		+9.1	.1	-14.10	.19
KASKAN-1964 EVAL (4)		2ND	-9.94		0		+8.93		-13.82	
SCOFLD-1967 REV (5)	.3-.9	2ND	-9.85		0		+9.1		-13.80	
TUNDER-1967 SEL (41)		2ND	-10.16		0		+9.1		-14.11	
H2O2 + M => OH + OH + M (M= ANY)										
BAHN-1965 SEL (15)		2ND	-6.55		0		+23.30		-16.66	
BAHN-1965 SEL (15)		2ND	+3.10		-3.		+25.21		-17.	
H2O2 + M => OH + OH + M (M= H2O2)										
BASCMB-1965 SEL (12)	.3-3	2ND	-6.55		0		+23.30		-16.66	
H2O2 + M => OH + OH + M (M= H2O)										
BASCMB-1965 SEL (12)	.3-3	2ND	-6.64		0		+23.30		-16.75	
H2O2 + M => OH + OH + M (M= N2)										
BASCMB-1965 SEL (12)	.3-3	2ND	-7.32		0		+23.30		-17.43	
H2O2 + M => OH + OH + M (M= O2)										
BASCMB-1965 SEL (12)	.3-3	2ND	-7.47		0		+23.30		-17.58	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
H3O[+] + E[-] => H + H + OH										
JENSEN-1967 XP (65)	1-3.5	2ND	-6.7	.2	0		0		-6.70	.20
H3O[+] + E[-] => H + H2O										
TUNDER-1967 OME (17)		2ND	-8.3		-0.5		0		-9.8	
H3O[+] + K => H + H2O + K[+]										
JENSEN-1967 EST (63)	1-3.5	2ND	-8.0	.7	0		0		-8.00	.70
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
H3O[+] + LI => H + H2O + LI[+]										
JENSEN-1967 EST (63)	1-3.5	2ND	-8.0	.7	0		0		-8.00	.70
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
H3O[+] + NA => H + H2O + NA[+]										
JENSEN-1967 SEL (64)	1-3.5	2ND	-8.0	.7	0		0		-8.00	.70
TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6	
H3O[+] + O[-] => H2O + OH										
TUNDER-1967 OME		2ND	-13.8		+0.5		+3.0		-13.6	
H3O[+] + OH[-] => H + H2O + OH										
JENSEN-1967 XP (66)	1-3.5	2ND	-7.1	1.0	0		0		-7.1	1.0
H3O[+] + OH[-] => H2O + H2O										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
HBR + I => BR + HI										
MAYER-1968 BERO		2ND	-11.830		+0.5		+8.35		-14.0	
HBR + K => BR + KH										
MAYER-1968 J+P		2ND	-12.95		+0.94		+28.33		-22.43	
HBR + LI => BR + LIH										
MAYER-1968 J+P		2ND	-12.94		+0.93		+20.53		-19.06	
HBR + MG => BR + MGH										
MAYER-1968 J+P		2ND	-11.60		+0.67		+22.04		-19.16	
HBR + N => BR + NH										
MAYER-1968 BERO		2ND	-11.46		+0.5		+1.21		-10.5	
HBR + NA => BR + NAH										
MAYER-1968 J+P		2ND	-12.60		+0.82		+24.36		-20.71	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
HBR + O => BR + OH										
MAYER-1968 BEBO		2ND	-11.50		+0.5		+.15		-10.1	
HBR + P => BR + PH										
MAYER-1968 J+P		2ND	-12.05		+0.67		+8.40		-13.69	
HBR + S => BR + SH										
MAYER-1968 BEBO		2ND	-11.48		+0.5		+.45		-10.2	
HBR + SI => BR + SIH										
MAYER-1968 BEBO		2ND	-11.06		+0.5		+22.80		-19.5	
HCL + E[-] => CL[-] + H										
JENSEN-1967 XP (37)	1-3.5	2ND	-1.0	2.5	0		+10.		-5.3	2.5
HCL + I => CL + HI										
MAYER-1968 BEBO		2ND	-11.74		+0.5		+16.16		-17.3	
HCL + K => CL + KH										
MAYER-1968 J+P		2ND	-12.811		+0.94		+36.03		-25.63	
HCL + K => H + KCL										
JENSEN-1967 XP (19)	1-3.5	2ND	-9.5	1.5	0		0		-9.5	1.5
HCL + LI => CL + LIH										
MAYER-1968 J+P		2ND	-12.32		+0.78		+26.22		-21.36	
HCL + LI => H + LICL										
JENSEN-1967 EST (17)	1-3.5	2ND	-9.5	1.5	0		0		-9.5	1.5
TUNDER-1967 SEL (6)		2ND	-12.8		+0.5		+3.0		-12.6	
HCL + LIO => CL + LIOH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
HCL + MG => CL + MGH										
MAYER-1968 BEBO		2ND	-11.12		+0.5		+28.94		-22.2	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
HCL + N => CL + NH										
MAYER-1968 BERO		2ND	-11.48		+0.5		+9.71		-14.2	
HCL + NA => CL + NAH										
MAYER-1968 J+P		2ND	-12.55		+0.83		+32.56		-24.19	
HCL + NA => H + NACL										
JENSEN-1967 XP (18)	1-3.5	2ND	-9.5	1.5	0		+2.5		-10.6	1.5
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
HCL + NAO => CL + NAOH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
HCL + O => CL + OH										
MAYER-1968 J+P		2ND	-12.20		+0.67		+.40		-10.36	
HCL + O[-] => CL[-] + OH										
TUNDER-1967 OME		2ND	-12.1		+0.5		+6.5		-13.4	
HCL + OH => CL + H2O										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
HCL + P => CL + PH										
MAYER-1968 J+P		2ND	-11.738		+0.67		+16.26		-16.78	
HCL + S => CL + SH										
MAYER-1968 BERO		2ND	-11.48		+0.5		+8.56		-13.7	
HCL + SI => CL + SIH										
MAYER-1968 BERO		2ND	-11.06		+0.5		+30.65		-22.9	
HCN + LIO => CN + LIOH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
HCN + NAO => CN + NAOH										
TUNDER-1967 J+P		2ND	-12.22		+0.6		+1.0		-10.9	
HCN + O => CN + OH										
TUNDER-1967 J+P		2ND	-12.33		+0.7		+.86		-10.6	
HCN + OH => CN + H2O										
TUNDER-1967 J+P		2ND	-12.48		+0.6		+2.5		-11.8	
HF + I => F + HI										
MAYER-1968 BERO		2ND	-11.78		+0.5		+32.56		-24.4	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
HF + K => F + KH MAYER-1968 J+P		2ND	-12.52	+0.95	+50.28	-31.49
HF + LI => F + LIH MAYER-1968 J+P		2ND	-12.33	+0.83	+43.18	-28.58
HF + M => F + H + M (M= ANY) TUNDER-1967 (2A)		2ND	-1.07	-2.0	+67.4	-36.3
HF + MG => F + MGH MAYER-1968 BERO		2ND	-11.17	+0.5	+45.14	-29.3
HF + N => F + NH MAYER-1968 BERO		2ND	-11.58	+0.5	+26.42	-21.5
HF + NA => F + NAH MAYER-1968 J+P		2ND	-12.36	+0.86	+48.11	-30.66
HF + O => F + OH MAYER-1968 BERO		2ND	-11.60	+0.5	+16.96	-17.5
HF + O[-] => F[-] + OH TUNDER-1967 OME		2ND	-12.8	+0.5	+3.5	-12.8
HF + P => F + PH MAYER-1968 BERO		2ND	-11.501	+0.5	+32.46	-24.1
HF + S => F + SH MAYER-1968 BERO		2ND	-11.52	+0.5	+24.86	-20.8
HF + SI => F + SIH MAYER-1968 BERO		2ND	-11.10	+0.5	+47.11	-30.0
HI + I => HI + I MAYER-1968 BERO		2ND	-11.835	+0.5	+.05	-10.4
HI + K => I + KH MAYER-1968 J+P		2ND	-12.87	+0.88	+19.83	-18.84

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} \; T^{(B \pm B')} \; \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
HI + LI => I + LIH MAYER-1968 J+P		2ND	-13.78		+1.26		+12.13		-15.26	
HI + MG => I + MGH MAYER-1968 BEHO		2ND	-11.10		+0.5		+13.69		-15.5	
HI + N => I + NH MAYER-1968 BEHO		2ND	-11.42		+0.5		+.20		-10.0	
HI + NA => I + NAH MAYER-1968 J+P		2ND	-12.55		+0.77		+15.50		-16.97	
HI + O => I + OH MAYER-1968 BEHO		2ND	-11.44		+0.5		+.05		-10.0	
HI + P => I + PH MAYER-1968 J+P		2ND	-12.26		+0.67		+1.06		-10.71	
HI + S => I + SH MAYER-1968 BEHO		2ND	-11.46		+0.5		+.05		-10.0	
HI + SI => I + SIH MAYER-1968 BEHO		2ND	-11.03		+0.5		+14.39		-15.8	
HNO + N => H + N2O TUNDER-1967 OME		2ND	-13.1		+0.5		+1.5		-12.3	
HNO + N => NH + NO TUNDER-1967 OME		2ND	-12.8		+0.5		+1.0		-11.7	
HNO + NAO => NAOH + NO TUNDER-1967 OME (36)		2ND	-12.11		+0.5		0		-10.6	
HNO + NH => NH2 + NO TUNDER-1967 EST (13)		2ND	-12.5		+0.5		+1.0		-11.4	
HNO + NH2 => NH3 + NO TUNDER-1967 (13,36)		2ND	-12.99		+0.5		0		-11.5	
HNO + O => H + NO2 TUNDER-1967 OME		2ND	-13.1		+0.5		+1.5		-12.3	
HNO + O => NH + O2 TUNDER-1967 OME		2ND	-12.8		+0.5		+3.5		-12.8	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
HNO + O => NO + OH										
TUNDER-1967 OME (36)		2ND	-12.08		+0.5		0		-10.6	
HNO + OH => H2O + NO										
TUNDER-1967 XP (3)		2ND	-12.5		+0.5		+1.0		-11.4	
HO2 + HO2 => H2O2 + O2										
BASCMB-1965 SEL (13)		2ND	-11.5		0		0		-11.5	
HO2 + M => H + O2 + M (M= ANY)										
BAHN-1965 SEL (16)		2ND	-1.058		-2.0		+25.2		-18.0	
KASKAN-1964 REV (9)		2ND	-7.8		+0.21		+23.10		-17.2	
HO2 + O => O2 + OH										
JENSEN-1967 EST (51)	1-3.5	2ND	-11.0	2.0	0		0		-11.0	2.0
HO2 + OH => H2O + O2										
JENSEN-1967 EST (51)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
HOCL + O => CLO + OH										
JENSEN-1967 EST (57)	1-3.5	2ND	-10.7	2.0	0		0		-10.7	2.0
HOCL + OH => CLO + H2O										
JENSEN-1967 EST (57)	1-3.5	2ND	-11.0	2.0	0		0		-11.0	2.0
I + KH => HI + K										
MAYER-1968 J+P		2ND	-13.11		+0.74		+6.09		-13.53	
I + LIH => HI + LI										
MAYER-1968 J+P		2ND	-13.83		+1.16		+5.59		-12.78	
I + MGH => HI + MG										
MAYER-1968 BEBO		2ND	-12.01		+0.5		+1.36		-11.1	
I + NAH => HI + NA										
MAYER-1968 J+P		2ND	-12.789		+0.69		+3.82		-12.38	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
I + NH => HI + N										
MAYER-1968 BERO		2ND	-11.90		+0.5		+6.54		-13.2	
I + OH => HI + O										
MAYER-1968 BERO		2ND	-11.96		+0.5		+15.60		-17.2	
I + PH => HI + P										
MAYER-1968 J+P		2ND	-12.63		+0.67		+1.71		-11.36	
I + SH => HI + S										
MAYER-1968 BERO		2ND	-11.97		+0.5		+7.75		-13.8	
I + SIH => HI + SI										
MAYER-1968 BERO		2ND	-12.25		+0.5		+.45		-10.9	
K + KH => K + KH										
MAYER-1968 J+P		2ND	-13.52		+1.32		+6.24		-12.27	
K + LIH => KH + LI										
MAYER-1968 J+P		2ND	-13.10		+1.18		+13.03		-15.22	
K + MGH => KH + MG										
MAYER-1968 J+P		2ND	-13.78		+1.30		+5.64		-12.33	
K + NAH => KH + NA										
MAYER-1968 J+P		2ND	-13.40		+1.29		+6.24		-12.24	
K + NH => KH + N										
MAYER-1968 J+P		2ND	-12.46		+0.85		+23.10		-19.94	
K + NO[+] => K[+] + NO										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
K + O2 + M => KO2 + M	(M= ANY)									
JENSEN-1967 EST (47)	1-3.5	3RD	-30.0	1.0	-1.0		0		-33.0	1.0
K + OH => KH + O										
MAYER-1968 J+P		2ND	-12.52		+0.87		+31.96		-23.78	
K + OH + M => KOH + M	(M= ANY)									
JENSEN-1967 XP (25)	1-3.5	3RD	-27.5	1.5	-1.0		0		-30.5	1.5
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
K + PH => KH + P										
MAYER-1968 J+P		2ND	-12.70		+0.84		+18.62		-18.26	

RATE PARAMETERS FOR $K = 10^{(A±A')} \, T^{(B±B')} \, EXP(-1000(C±C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
K + SH => KH + S										
MAYER-1968 J+P		2ND	-12.67		+0.83		+26.62		-21.73	
K + SIH => KH + SI										
MAYER-1968 J+P		2ND	-14.1		+1.28		+4.73		-12.3	
K[+] + E[-] + M => K + M (M= ANY)										
JENSEN-1967 REV (29)	1-3.5	3RD	-21.7	.5	-1.5		0		-26.20	.52
TUNDER-1967 OME		3RD	-23.9		-1.5		0		-28.4	
K[+] + OH[-] => K + OH										
JENSEN-1967 EST (34)	1-3.5	2ND	-7.0	2.0	-0.5		0		-8.5	2.0
K[+] + OH[-] + M => KOH + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
KH + LI => K + LIH										
MAYER-1968 J+P		2ND	-13.29		+1.14		+5.84		-12.40	
KH + MG => K + MGH										
MAYER-1968 J+P		2ND	-13.35		+1.27		+4.33		-11.42	
KH + N => K + NH										
MAYER-1968 J+P		2ND	-12.70		+0.76		+2.97		-11.71	
KH + NA => K + NAH										
MAYER-1968 J+P		2ND	-13.52		+1.28		+4.18		-11.49	
KH + O => K + OH										
MAYER-1968 J+P		2ND	-12.70		+0.73		+2.67		-11.67	
KH + P => K + PH										
MAYER-1968 J+P		2ND	-12.70		+0.75		+4.18		-12.26	
KH + S => K + SH										
MAYER-1968 J+P		2ND	-12.67		+0.73		+5.08		-12.68	

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(A±A') (B±B')
RATE PARAMETERS FOR K = 10 T EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
KH + SI => K + SIH										
MAYER-1968 J+P		2ND	-13.32		+1.19		+4.83		-11.85	
KH2O[+] + E[-] => H2O + K										
JENSEN-1967 EST (40)	1-3.5	2ND	-7.0	1.5	0		0		-7.0	1.5
KH2O[+] + M => H2O + K[+] + M (M= ANY)										
JENSEN-1967 EST (39)	1-3.5	2ND	-9.0	1.5	0		+10.		-13.3	1.6
KH2O[+] + OH[-] => H2O + K + OH										
JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
KO2 + OH => KOH + O2										
JENSEN-1967 EST (51)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
LI + LIH => LI + LIH										
MAYER-1968 J+P		2ND	-13.15		+1.10		+10.32		-14.33	
LI + MGH => LIH + MG										
MAYER-1968 J+P		2ND	-13.24		+1.00		+4.03		-11.99	
LI + NAH => LIH + NA										
MAYER-1968 J+P		2ND	-13.20		+1.11		+5.13		-12.10	
LI + NH => LIH + N										
MAYER-1968 J+P		2ND	-13.55		+1.15		+19.28		-18.47	
LI + NO[+] => LI[+] + NO										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
LI + O + M => LIO + M (M= ANY)										
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
LI + O2 + M => LIO2 + M (M= ANY)										
JENSEN-1967 EST (47)	1-3.5	3RD	-30.0	1.0	-1.0		0		-33.0	1.0
LI + OH => LIH + O										
MAYER-1968 J+P		2ND	-12.29		+0.76		+24.51		-20.65	
LI + OH + M => LIOH + M (M= ANY)										
JENSEN-1967 XP (25)	1-3.5	3RD	-27.5	1.5	-1.0		0		-30.5	1.5
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
LI + PH => LIH + P										
MAYER-1968 J+P		2ND	-13.70		+1.19		+12.63		-15.61	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
LI + SH => LIH + S										
MAYER-1968 J+P		2ND	-12.78		+0.83		+18.27		-18.22	
LI + SIH => LIH + SI										
MAYER-1968 J+P		2ND	-13.46		+0.96		+8.10		-14.10	
LI[+] + E[-] + M => LI + M (M= ANY)										
JENSEN-1967 REV (27)	1-3.5	3RD	-19.7	.5	-2.0		0		-25.70	.52
TUNDER-1967 OMF		3RD	-23.9		-1.5		0		-28.4	
LI[+] + O[-] + M => LIO + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
LI[+] + O2[-] => LIO + O										
TUNDER-1967 OME		2ND	-11.1		+0.5		+2.5		-10.7	
LI[+] + OH[-] => LI + OH										
JENSEN-1967 EST (34)	1-3.5	2ND	-7.0	2.0	-0.5		0		-8.5	2.0
LI[+] + OH[-] + M => LIOH + M (M= ANY)										
TUNDER-1967 OME		3RD	-30.0		-0.5		0		-31.5	
LICL + O[-] => CL[-] + LIO										
TUNDER-1967 OMF		2ND	-12.8		+0.5		+3.0		-12.6	
LIH + LIO => LI + LIOH										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
LIH + MG => LI + MGH										
MAYER-1968 J+P		2ND	-12.58		+1.00		+9.96		-13.90	
LIH + N => LI + NH										
MAYER-1968 J+P		2ND	-13.36		+1.00		+6.39		-13.13	
LIH + NA => LI + NAH										
MAYER-1968 J+P		2ND	-13.11		+1.13		+10.27		-14.18	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±A
LIH + NAO => LI + NAOH TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
LIH + NH => LI + NH2 TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
LIH + O => LI + OH MAYER-1968 J+P		2ND	-12.40		+0.71		+2.42		-11.32	
LIH + OH => H2O + LI TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
LIH + P => LI + PH MAYER-1968 J+P		2ND	-13.44		+1.11		+5.44		-12.47	
LIH + S => LI + SH MAYER-1968 J+P		2ND	-12.55		+0.76		+3.98		-12.00	
LIH + SI => LI + SIH MAYER-1968 J+P		2ND	-12.50		+0.91		+15.45		-16.48	
LIH2O[+] + E[-] => H2O + LI JENSEN-1967 EST (40)	1-3.5	2ND	-7.0	1.5	0		0		-7.0	1.5
LIH2O[+] + M => H2O + LI[+] + M (M= ANY) JENSEN-1967 XP (38)	1-3.5	2ND	-9.0	1.5	0		+25.		-19.8	1.6
LIH2O[+] + OH[-] => H2O + LI + OH JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
LIO + N => LI + NO TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	
LIO + NAH => LIOH + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
LIO + NH => LIOH + N TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
LIO + NH2 => LIOH + NH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
LIO + O => LI + O2 TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\,T^{(B\pm B')}\,\mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
LIO + O[-] => LI + O2[-] TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	
LIO + OH => LIOH + O TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
LIO + OH[-] => LIOH + O[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+4.5		-13.3	
LIO2 + OH => LIOH + O2 JENSEN-1967 EST (51)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
MG + MGH => MG + MGH MAYER-1968 J+P		2ND	-13.40		+1.20		+1.71		-10.54	
MG + NAH => MGH + NA MAYER-1968 J+P		2ND	-13.15		+1.20		+3.98		-11.28	
MG + NH => MGH + N MAYER-1968 J+P		2ND	-11.60		+0.67		+19.68		-18.13	
MG + OH => MGH + O MAYER-1968 BEBO		2ND	-11.38		+0.5		+28.54		-22.3	
MG + PH => MGH + P MAYER-1968 J+P		2ND	-12.02		+0.69		+14.80		-16.37	
MG + SH => MGH + S MAYER-1968 J+P		2ND	-11.93		+0.68		+21.74		-19.33	
MG + SIH => MGH + SI MAYER-1968 J+P		2ND	-13.58		+1.07		+4.33		-12.25	
MGH + N => MG + NH MAYER-1968 J+P		2ND	-12.46		+0.67		+.86		-10.82	
MGH + NA => MG + NAH MAYER-1968 J+P		2ND	-13.70		+1.22		+3.22		-11.44	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
MGH + O => MG + OH MAYER-1968 BERO		2ND	-11.78		+0.5		+.65		-10.6	
MGH + P => MG + PH MAYER-1968 J+P		2ND	-12.58		+0.67		+1.66		-11.29	
MGH + S => MG + SH MAYER-1968 J+P		2ND	-12.52		+0.67		+1.51		-11.17	
MGH + SI => MG + SIH MAYER-1968 J+P		2ND	-13.30		+1.04		+5.79		-12.69	
N + N + M => N2 + M (M= ANY) CHERRY-1967 SEL (15)		3RD	-29.6	1.0	-1.0		0		-32.6	1.0
N + N + M => N2 + M (M= N2) SCOFLD-1967 XP (31)	.3	3RD	-32.027		0		0		-32.027	
N + N + NA => N2 + NA + E[-] TUNDER-1967 SEL (42)		3RD	-32.0		0		0		-32.0	
N + NA + O => NA[+] + NO + E[-] TUNDER-1967 SEL (42)		3RD	-32.0		0		0		-32.0	
N + NAH => NA + NH MAYER-1968 J+P		2ND	-12.70		+0.75		+3.82		-12.11	
N + NAO => NA + NO TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
N + NH => H + N2 TUNDER-1967 EST (13)		2ND	-12.1		+0.5		+1.0		-11.0	
N + NH => N + NH MAYER-1968 J+P		2ND	-12.821		+0.91		+.05		-10.11	
N + NH2 => NH + NH TUNDER-1967 EST (13)		2ND	-12.1		+0.5		+1.0		-11.0	
N + NH3 => NH + NH2 TUNDER-1967 EST (13)		2ND	-12.1		+0.5		+1.0		-11.0	
N + NO => N2 + O CHERRY-1967 SEL (7)		2ND	-10.6	.7	0		0		-10.60	.70

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')} \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
N + NO2 => N2 + O + O										
BAHN-1964 SEL (19)		2ND	-13.7	.5	0		0		-13.70	.50
N + O + M => NO + M (M= ANY)										
CHERRY-1967 SEL (15)		3RD	-30.8	1.0	-0.5		0		-32.3	1.0
N + O[-] => NO + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
N + O2 => NO + O SEE REACTION SUMMARY										
CHERRY-1967 SEL (9)		2ND	-15.5	.7	+1.5		+3.0		-12.30	.72
SCOFLD-1967 EVAL (10)	.4-1.7	2ND	-10.599		0		+3.92		-12.300	
SCOFLD-1967 EVAL (10)	.4-5	2ND	-15.609		+1.5		+2.85		-12.3	
TUNDER-1967 (25)		2ND	-13.656		+1.0		+3.5		-12.2	
WILSON-1968 EVAL (1)	.3-5	2ND	-14.00	.30	+1.0		+3.2		-12.39	.34
N + O2[-] => NO + O[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
N + O3 => NO + O2										
SCOFLD-1967 (4-3)		2ND	-12.24		0		0		-12.24	
N + OH => H + NO										
CHERRY-1967 OME		2ND	-12.1	2.0	+0.5		+2.8		-11.8	2.0
TUNDER-1967 OMF		2ND	-12.1		+0.5		+2.5		-11.7	
N + OH => NH + O										
MAYER-1968 BEBO		2ND	-11.793		+0.5		+9.21		-14.3	
N + PH => NH + P										
MAYER-1968 J+P		2ND	-12.78		+0.73		+3.37		-12.05	
N + SH => NH + S										
MAYER-1968 BEBO		2ND	-11.70		+0.5		+.60		-10.5	
N + SIH => NH + SI										
MAYER-1968 J+P		2ND	-12.821		+0.67		+2.67		-11.97	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\, T^{(B \pm B')}\, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±A AT T = 1000
N2 + M => N + N + M (M= ANY)									
BAHN-1964 SEL (2)		2ND	-2.307		-1.5		+113.19		-55.9
TUNDER-1967 SEL (5)		2ND	-4.50		-1.0		+113.2		-56.6
N2 + M => N + N + M (M= AR)									
BAHN-1964 SEL (2)		2ND	-6.496		-0.5		+113.19		-57.1
TUNDER-1967 EST (30)		2ND	-7.2		-0.5		+113.2		-57.8
N2 + M => N + N + M (M= N2)									
BAHN-1964 SEL (2)		2ND	-6.103		-0.5		+113.9		-57.0
TUNDER-1967 EST (30)		2ND	-6.05		-0.5		+113.2		-56.7
N2 + M => N + N + M (M= NO)									
BAHN-1964 SEL (2)		2ND	-6.496		-0.5		+113.9		-57.4
TUNDER-1967 EST (30)		2ND	-7.60		-0.5		+113.2		-58.2
N2 + M => N + N + M (M= N)									
BAHN-1964 SEL (2)		2ND	-1.167		-1.5		+113.9		-55.1
TUNDER-1967 EST (30)		2ND	-7.2		-0.5		+113.2		-57.8
N2 + M => N + N + M (M= O2)									
BAHN-1964 SEL (2)		2ND	-6.496		-0.5		+113.9		-57.4
TUNDER-1967 EST (30)		2ND	-7.60		-0.5		+113.2		-58.2
N2 + M => N + N + M (M= O)									
BAHN-1964 SEL (2)		2ND	-6.496		-0.5		+113.9		-57.4
TUNDER-1967 EST (30)		2ND	-7.60		-0.5		+113.2		-58.2
N2 + NO => N + N2O									
TUNDER-1967 SEL (5)		2ND	-15.9		0		+60.9		-42.3
N2 + NO2 => N2O + NO									
BAHN-1964 SEL (17)		2ND	-9.11		0		+41.92		-27.30
N2 + NO2 => NO + N2O									
TUNDER-1967 SEL (5)		2ND	-9.63		0		+41.8		-27.77
N2 + O => N + NO									
BAHN-1964 SEL (5)		2ND	-12.04		+0.5		+36.2		-26.3
TUNDER-1967 SEL (5)		2ND	-9.95		0		+37.7		-26.31
N2 + O + E[-] => N2 + O[-]									
TUNDER-1967 SEL (42)		3RD	-31.1		0		0		-31.1

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\,T^{(B\pm B')}\,\mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
N2 + O2 => N + NO2										
BAHN-1964 SEL (11)		2ND	-11.78		0		+60.4		-37.99	
TUNDER-1967 SEL (5)		2ND	-12.55		0		+68.4		-42.24	
N2 + O2 => N2O + O										
BAHN-1964 SEL (8)		2ND	-14.18		0		+46.8		-34.49	
TUNDER-1967 SEL (5)		2ND	-11.2		0		+53.3		-34.3	
N2 + O2 => NO + NO										
BAHN-1964 SEL (3)		2ND	+1.179		-2.5		+64.67		-34.4	
TUNDER-1967 SEL (5)		2ND	-9.5		0		+61.4		-36.1	
N2O + M => N + NO + M (M= ANY)										
TUNDER-1967 SEL (5)		2ND	-9.8		-1.0		+57.9		-37.9	
N2O + NH => HNO + N2										
TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
N2O + NO2 => N2 + NO + O2										
BAHN-1964 SEL (20)		2ND	-12.0		0		0		-12.0	
N2O + O => N + NO2										
BAHN-1964 SEL (11)		2ND	-11.8		0		+26.7		-23.4	
TUNDER-1967 (5,29)		2ND	-10.8		0		+25.2		-21.7	
N2O + O => NO + NO										
BAHN-1964 SEL (7)		2ND	-9.5		0		+14.	2.	-15.58	.87
SCOFLD-1967 XP (7)	1.4-2.3	2ND	-10.12		0		+12.13		-15.38	
N2O + O2 => N + NO3										
BAHN-1965 OME (1)		2ND	-9.0		-1.5		+53.25		-36.6	
N2O + O2 => NO + NO2										
BAHN-1964 SEL (12)		2ND	-9.0		-1.5		+4.98		-15.7	
TUNDER-1967 SEL (5)		2ND	-10.8		0		+35.2		-26.1	
N2O4 => NO2 + NO2										
BAHN-1965 SEL (6)		1ST	+16.00		0		+6.59		+13.14	

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RATE PARAMETERS FOR K = $10^{(A \pm A')}$ $T^{(B \pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
N2O4 + M => NO2 + NO2 + M										
BAHN-1965 SEL (6)		2ND	-6.48		0		+5.5		-8.87	
N2O5 => NO2 + NO3 (400 MM HG)										
BAHN-1965 SEL (8)		1ST	+14.097		0		+10.6		+9.50	
N2O5 => NO2 + NO3 (57 MM HG)										
BAHN-1965 SEL (8)		1ST	+13.097		0		+10.1		+8.71	
N2O5 + M => NO2 + NO3 + M										
BAHN-1965 SEL (7)		2ND	-7.08		0		+8.3	.4	-10.68	.17
NA + E[-] => NA[+] + E[-] + E[-]										
TUNDER-1967 SEL (5)		2ND	-10.37		+0.5		+59.9		-34.9	
NA + NAH => NA + NAH										
MAYER-1968 J+P		2ND	-13.44		+1.25		+4.18		-11.50	
NA + NH => N + NAH										
MAYER-1968 J+P		2ND	-12.60		+0.85		+21.84		-19.53	
NA + NO[+] => NA[+] + NO										
TUNDER-1967 SEL (42)		2ND	-10.3		-0.5		0		-11.8	
NA + O + M => NAO + M (M= ANY)										
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	
NA + O + O => NA[+] + O2 + E[-]										
TUNDER-1967 SEL (5)		3RD	-31.0		0		0		-31.0	
NA + O[-] => NAO + E[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
NA + O2 + M => NAO2 + M (M= ANY)										
JENSEN-1967 XP (48)	1-3.5	3RD	-30.0	1.0	-1.0		0		-33.0	1.0
TUNDER-1967 SEL (42)		3RD	-34.0		0		0		-34.0	
NA + OH => NAH + O										
MAYER-1968 BEHO		2ND	-11.63		+0.5		+27.68		-22.1	
NA + OH + M => NAOH + M (M= ANY)										
JENSEN-1967 XP (25)	1-3.5	3RD	-27.5	1.5	-1.0		0		-30.5	1.5
TUNDER-1967 OME		3RD	-31.1		-0.5		0		-32.6	

RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NA + OH[-] => NAOH + E[-]										
TUNDER-1967 OME		2ND	-12.8		+0.5		0		-11.3	
NA + PH => NAH + P										
MAYER-1968 J+P		2ND	-12.58		+0.77		+15.45		-16.98	
NA + SH => NAH + S										
MAYER-1968 J+P		2ND	-12.40		+0.73		+21.99		-19.75	
NA + SIH => NAH + SI										
MAYER-1968 J+P		2ND	-13.55		+0.99		+2.87		-11.83	
NA[+] + E[-] => NA + PHOTON										
TUNDER-1967 SEL (5)		2ND	-9.70		-0.75		0		-11.95	
NA[+] + E[-] + M => NA + M (M= ANY)										
JENSEN-1967 REV (28)	1-3.5	3RD	-19.8	.5	-2.0		0		-25.80	.52
TUNDER-1967 SEL (44)		3RD	-22.9		-2.5		0		-30.4	
NA[+] + O[-] => NA + O										
TUNDER-1967 SEL (42)		2ND	-5.2		-1.0		0		-8.2	
NA[+] + O[-] + M => NAO + M (M= ANY)										
TUNDER-1967 SEL (42)		3RD	-29.0		0		0		-29.0	
NA[+] + O2[-] => NA + O2										
TUNDER-1967 SEL (42)		2ND	-5.2		-1.0		0		-8.2	
NA[+] + O2[-] => NAO + O										
TUNDER-1967 OMF		2ND	-12.1		+0.5		+3.0		-11.9	
NA[+] + OH[-] => NA + OH										
JENSEN-1967 EST (34)	1-3.5	2ND	-7.0	2.0	-0.5		0		-8.5	2.0
NA[+] + OH[-] + M => NAOH + M (M= ANY)										
TUNDER-1967 OMF		3RD	-30.0		-0.5		0		-31.5	

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RATE PARAMETERS FOR $K = 10^{(A\pm A')}\ T^{(B\pm B')}\ \mathrm{EXP}(-1000(C\pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NACL + O[-] => CL[-] + NAO TUNDER-1967 OME		2ND	-12.1		+0.5		+1.0		-11.0	
NAF + O[-] => F[-] + NAO TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
NAH + NAO => NA + NAOH TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
NAH + NH => NA + NH2 TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
NAH + O => H + NAO TUNDER-1967 OME		2ND	-12.1		+0.5		+1.5		-11.3	
NAH + O => NA + OH MAYER-1968 BEBO		2ND	-11.42		+0.5		+.50		-10.1	
NAH + OH => H2O + NA TUNDER-1967 OME		2ND	-12.8		+0.5		+1.5		-12.0	
NAH + P => NA + PH MAYER-1968 J+P		2ND	-12.50		+0.71		+3.07		-11.70	
NAH + S => NA + SH MAYER-1968 J+P		2ND	-12.36		+0.68		+2.52		-11.41	
NAH + SI => NA + SIH MAYER-1968 J+P		2ND	-12.70		+0.93		+5.08		-12.11	
NAH2O[+] + E[-] => H2O + NA JENSEN-1967 EST (40)	1-3.5	2ND	-7.0	1.5	0		0		-7.0	1.5
NAH2O[+] + M => H2O + NA[+] + M (M= ANY) JENSEN-1967 EST (39)	1-3.5	2ND	-9.0	1.5	0		+17.6		-16.6	1.5
NAH2O[+] + OH[-] => H2O + NA + OH JENSEN-1967 EST (41)	1-3.5	2ND	-7.0	2.0	0		0		-7.0	2.0
NAO + NH => N + NAOH TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4	
NAO + NH2 => NAOH + NH TUNDER-1967 OME (36)		2ND	-11.70		+0.5		0		-10.2	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \; T^{(B \pm B')} \; \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NAO + NH3 => NAOH + NH2 TUNDER-1967 OME (36)		2ND	-10.798		+0.5		0		-9.3	
NAO + O => NA + O2 TUNDER-1967 OME		2ND	-12.1		+0.5		+3.0		-11.9	
NAO + O[-] => NA + O2[-] TUNDER-1967 OME		2ND	-12.1		+0.5		+2.0		-11.5	
NAO + OH => NAOH + O TUNDER-1967 OME		2ND	-12.8		+0.5		+3.0		-12.6	
NAO + OH[-] => NAOH + O[-] TUNDER-1967 OME		2ND	-12.8		+0.5		+4.5		-13.3	
NAO2 + OH => NAOH + O2 JENSEN-1967 EST (51)	1-3.5	2ND	-10.7	1.7	0		0		-10.7	1.7
NAOH + O => NAO + OH TUNDER-1967 OME (36)		2ND	-12.36		+0.5		0		-10.9	
NAOH + OH => H2O + NAO TUNDER-1967 OME (36)		2ND	-12.70		+0.5		0		-11.2	
NH + NO2 => HNO + NO TUNDER-1967 OME		2ND	-12.5		+0.5		+2.5		-12.1	
NH + O => H + NO TUNDER-1967 EST (13)		2ND	-12.1		+0.5		+2.5		-11.7	
NH + O => N + OH MAYER-1968 BEBO		2ND	-11.78		+0.5		+.05		-10.3	
NH + O + M => HNO + M (M= ANY) TUNDER-1967 OME		3RD	-31.6		-0.5		0		-33.1	
NH + O[-] => N + OH[-] TUNDER-1967 OME		2ND	-12.1		+0.5		+2.5		-11.7	

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RATE PARAMETERS FOR K = $10^{(A\pm A')} T^{(B\pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K ±Δ AT T = 1000
NH + OH => H2O + N									
TUNDER-1967 OME		2ND	-12.1		+0.5		+1.0		-11.0
NH + P => N + PH									
MAYER-1968 J+P		2ND	-12.52		+0.74		+9.06		-14.23
NH + S => N + SH									
MAYER-1968 BERO		2ND	-11.67		+0.5		0		-10.2
NH + SI => N + SIH									
MAYER-1968 J+P		2ND	-11.793		+0.68		+22.95		-19.71
NH2 + NH2 => NH + NH3									
TUNDER-1967 (2,14)		2ND	-11.8		+0.5		+1.5		-11.0
NH2 + O => NH + OH									
TUNDER-1967 OME (36)		2ND	-11.816		+0.5		0		-10.3
NH2 + O[-] => NH + OH[-]									
TUNDER-1967 OME		2ND	-12.8		+0.5		+2.5		-12.4
NH2 + OH => H2O + NH									
TUNDER-1967 J+P		2ND	-13.3		+0.7		+.5		-11.4
NH3 + O => NH2 + OH									
TUNDER-1967 OME (36)		2ND	-11.87		+0.5		0		-10.4
NH3 + OH => H2O + NH2									
TUNDER-1967 J+P		2ND	-13.2		+0.7		+.5		-11.3
NO + M => N + O + M (M= ANY)									
BAHN-1964 SEL (4)		2ND	-2.065		-1.5		+75.5		-39.3
TUNDER-1967 SEL (5)		2ND	-6.40		-0.5		+76.0		-40.9
NO + M => N + O + M (M= AR)									
BAHN-1964 SEL (4)		2ND	-3.179		-1.5		+75.5		-40.4
TUNDER-1967 (5,25)		2ND	-5.03		-1.0		+76.0		-41.0
NO + M => N + O + M (M= N2)									
BAHN-1964 SEL (4)		2ND	-3.179		-1.5		+75.5		-40.4
TUNDER-1967 (5,25)		2ND	-5.03		-1.0		+76.0		-41.0
NO + M => N + O + M (M= NO)									
BAHN-1964 SEL (4)		2ND	-3.179		-1.5		+75.5		-40.4
TUNDER-1967 (5,25)		2ND	-3.731		-1.0		+76.0		-39.7

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NO + M => N + O + M (M= N)										
BAHN-1964 SEL (4)		2ND	-1.878		-1.5		+75.5		-39.1	
TUNDER-1967 (5,25)		2ND	-3.731		-1.0		+76.0		-39.7	
NO + M => N + O + M (M= O2)										
BAHN-1964 SEL (4)		2ND	-3.179		-1.5		+75.5		-40.4	
TUNDER-1967 (5,25)		2ND	-5.03		-1.0		+76.0		-41.0	
NO + M => N + O + M (M= O)										
BAHN-1964 SEL (4)		2ND	-1.878		-1.5		+75.5		-39.1	
TUNDER-1967 (5,25)		2ND	-3.731		-1.0		+76.0		-39.7	
NO + M => NO[+] + E[-] + M (M= ANY)										
TUNDER-1967 SEL (5)		2ND	-19.0		+1.5		+107.7		-61.2	
NO + M => NO[+] + E[-] + M (M= E[-])										
TUNDER-1967 SEL (5)		2ND	-10.38		+0.5		+107.7		-55.6	
NO + NO => N + NO2										
TUNDER-1967 SEL (5)		2ND	-13.8		0		+44.3		-33.0	
NO + NO => N2 + O2										
CHERRY-1967 SEL (8)		2ND	-10.8	1.0	0		+40.		-28.2	1.1
NO + NO => N2O + O										
TUNDER-1967 (5,16)		2ND	-11.24		0		+32.2		-25.21	
NO + NO2 => N + NO3										
BAHN-1965 OME (1)		2ND	-9.0		-1.5		+48.26		-34.4	
NO + NO3 => NO2 + NO2										
BAHN-1965 SEL (3)		2ND	-11.0		0		0		-11.0	
NO + O => N + O2 SEE SUMMARY FOR REVERSE REACTION										
BAHN-1964 SEL (6)		2ND	-14.27		+1.0		+19.68		-19.8	
SCOFLD-1967 XP (10)	.4-5	2ND	-14.28		+1.0		+19.68		-19.8	
WILSON-1968 EVAL (1)	.3-5	2ND	-14.66	.30	+1.0		+19.2		-19.98	.34

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NO + O + M => NO2 + M (M= N2)										
SCOFLD-1967 XP (32)	.3-.5	3RD	-32.40		0		-.97		-31.98	
NO + O2 => N + O3										
BAHN-1964 SEL (12)		2ND	-9.35		-1.0		+63.11		-39.7	
NO + O2 => NO2 + O										
BAHN-1964 SEL (9)		2ND	-11.89		0		+22.85		-21.81	
NO + O3 => NO2(2A) + O2										
SCOFLD-1967 XP (16)	.2-.35	2ND	-11.77		0		+1.31		-12.34	
SCOFLD-1967 XP (16)	.2-.35	2ND	-11.55		0		+1.41		-12.16	
NO[+] + E[-] => N + O										
TUNDER-1967 SEL (44)		2ND	-3.33		-1.2		0		-6.9	
NO[+] + E[-] + M => NO + M										
TUNDER-1967 OME		3RD	-23.9		-1.5		0		-28.4	
NO[+] + O[-] => NO + O										
TUNDER-1967 SEL (44)		2ND	-4.22		-1.0		0		-7.2	
NO[+] + O2[-] => NO + O2										
TUNDER-1967 SEL (44)		2ND	-4.22		-1.0		0		-7.2	
NO2 + M => N + O2 + M										
BAHN-1964 SEL (12)		2ND	-9.0		-1.5		+52.59		-36.3	
NO2 + M => NO + O + M (M= ANY)										
BAHN-1964 SEL (10)		2ND	-1.95		-1.5		+36.19		-22.2	
NO2 + NO2 => NO + NO + O2										
BAHN-1964 SEL (18)		2ND	-10.38		0		+13.	3.	-16.0	1.3
SCOFLD-1967 XP (13)	.4-2.3	2ND	-10.46		0		+14.27		-16.65	
NO2 + O => N + O3										
BAHN-1964 SEL (15)		2ND	-9.21		-0.5		+40.3		-28.2	
NO2 + O => NO + O2										
SCOFLD-1967 SEL (9)	.3-.4	2ND	-10.49		0		+.53		-10.72	
TUNDER-1967 (32)		2ND	-10.5		0		+.55		-10.7	
NO2 + O2 => NO + O3										
BAHN-1964 SEL (16)		2ND	-11.738		0		+25.47		-22.792	

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\, T^{(B \pm B')}\, \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
NO2 + O2 => NO3 + O										
BAHN-1965 OME (1)		2ND	-9.0		-1.5		+32.2		-27.5	
NO2 + O3 => NO3 + O2										
BAHN-1965 SEL (4)		2ND	-12.63		0		+2.87		-13.88	
NO3 + M => NO + O2 + M (M= NO2)										
BAHN-1964 SEL (14)		2ND	-12.426		0		+2.2	.4	-13.38	.17
NO3 + M => NO2 + O + M (M= ANY)										
BAHN-1965 SEL (2)		2ND	+1.2		-2.		+24.96		-16.	
NO3 + NO3 => NO2 + NO2 + O2										
BAHN-1965 SEL (5)		2ND	-11.360		0		+3.9	.5	-13.05	.22
NO3 + O => NO + O3										
BAHN-1965 OME (1)		2ND	-9.0		-1.5		+8.00		-17.0	
O + E[-] => O[-] + PHOTON										
TUNDER-1967 SEL (5)		2ND	-14.92		0		0		-14.92	
O + E[-] + M => O[-] + M (M= ANY)										
JENSEN-1967 EST (35)	1-3.5	3RD	-29.5	1.5	0		0		-29.5	1.5
TUNDER-1967 (21)		3RD	-32.0		0		0		-32.0	
O + E[-] + M => O[-] + M (M= N2)										
TUNDER-1967 SEL (5)		3RD	-28.26		-0.5		0		-29.8	
O + E[-] + M => O[-] + M (M= O2)										
TUNDER-1967 SEL (5)		3RD	-32.0		0		0		-32.0	
O + O + M => O2 + M (M= ANY) SEE SUMMARY FOR REVERSE REACTION										
CHERRY-1967 XP (23)		3RD	-31.3	1.0	-0.5		0		-32.8	1.0
JENSEN-1967 XP (1)	1-3.5	3RD	-29.0	1.0	-1.0		0		-32.0	1.0
O + O + M => O2 + M (M= AR) SEE SUMMARY FOR REVERSE REACTION										
JONSTN-1968 EVAL (6)	.3-15	3RD	-30.5	.3	-1.0		0		-33.50	.34
KASKAN-1964 EVAL (7)		3RD	-34.22		0		0		-34.22	

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
O + O + M => O2 + M (M= N2)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (9)	.3-10	3RD	-32.9	.1	0		-.25	.13	-32.79	.11
O + O + M => O2 + M (M= O2)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (9)	.3-10	3RD	-32.9	.1	0		-.25	.13	-32.79	.11
JONSTN-1968 EVAL (6)	1-8	3RD	-29.4	.3	-1.0		0		-32.40	.34
KASKAN-1964 EVAL (7)		3RD	-33.26		0		0		-33.26	
O + O + M => O2 + M (M= O)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (9)	.3-10	3RD	-32.49	.01	0		-.25	.13	-32.381	.057
KASKAN-1964 EVAL (7)		3RD	-32.82		0		0		-32.82	
O + O[-] + M => O2[-] + M (M= ANY)										
TUNDER-1967 SEL (42)		3RD	-30.0		0		0		-30.0	
O + O2 => O + O2 (EXCHANGE)										
JONSTN-1968 (5)		2ND	-12.00		0		0		-12.00	
O + O2 + M => O3 + M (M= ANY)										
KASKAN-1964 XP (8)		3RD	-33.78		0		-.30		-33.65	
O + O2 + M => O3 + M (M= AR)										
SEE SUMMARY FOR REVERSE REACTION										
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.9	.2	0		-1.05		-34.44	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.85		0		-1.01		-34.41	
O + O2 + M => O3 + M (M= CO2)										
SEE SUMMARY FOR REVERSE REACTION										
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.4	.2	0		-1.05		-33.94	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.28		0		-1.01		-33.84	
O + O2 + M => O3 + M (M= HE)										
SEE SUMMARY FOR REVERSE REACTION										
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.8	.2	0		-1.05		-34.34	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.74		0		-1.01		-34.30	
O + O2 + M => O3 + M (M= N2)										
SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (7)	.3-3	3RD	-34.35	.15	0		-.5		-34.13	.16
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.7	.2	0		-1.05		-34.24	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.68		0		-1.01		-34.24	

RATE PARAMETERS FOR K = $10^{(A±A')}\ T^{(B±B')}\ \mathrm{EXP}(-1000(C±C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
O + O2 + M => O3 + M (M= O2) SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (7)	.3-3	3RD	-34.32	.14	0		-.5		-34.10	.15
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.7	.2	0		-1.05		-34.24	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.64		0		-1.01		-34.20	
O + O2 + M => O3 + M (M= O3) SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (7)	.3-3	3RD	-34.0	.2	0		-.5		-33.78	.20
JONSTN-1968 EVAL (2)	.2-1	3RD	-34.3	.2	0		-1.05		-33.84	.20
SCOFLD-1967 EVAL (29)	.2-.9	3RD	-34.28		0		-1.01		-33.84	
O + O2[-] => O2 + O[-]										
TUNDER-1967 SEL (42)		2ND	-11.2		0		0		-11.2	
O + O3 => O2 + O2 SEE REACTION SUMMARY FOR O3 + M => O + O2 + M										
BASCMB-1965 EVAL (8)	.3-3	2ND	-10.31	.04	0		+2.82		-11.534	.040
JONSTN-1968 EVAL (3)		2ND	-10.7	.2	0		+2.41		-11.75	.20
O + OH => H + O2 SEE SUMMARY FOR REVERSE REACTION										
BASCMB-1965 EVAL (2)	.3-3	2ND	-10.57	.24	0		+.1	.4	-10.61	.30
CHERRY-1967 XP,REV (11)		2ND	-12.3	.7	+0.4		+.05		-11.12	.72
KASKAN-1964 EVAL (2)		2ND	-12.27		+0.47		+.05		-10.88	
SCOFLD-1967 REV (2)	.3-.9	2ND	-10.686		0		0		-10.686	
O + OH => O + OH										
MAYER-1968 J+P		2ND	-13.09		+0.97		+.05		-10.20	
O + OH + M => H + O2 + M (M= H2O)										
TUNDER-1967 OME (19)		3RD	-28.86		-0.5		+3.0		-31.7	
O + PH => OH + P										
MAYER-1968 J+P		2ND	-12.793		+0.71		+5.13		-12.89	
O + SH => OH + S										
MAYER-1968 J+P		2ND	-12.42		+0.67		+.96		-10.83	

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN. LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')} T^{(B \pm B')}$ EXP(-1000(C±C')/T)

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
O + SIH => OH + SI										
MAYER-1968 J+P		2ND	-12.99		+0.68		+4.83		-13.05	
O2 + E[-] => O + O[-]										
TUNDER-1967 SEL (5)		2ND	-8.3		-1.0		+42.3		-29.7	
O2 + E[-] => O2[-] + PHOTON										
TUNDER-1967 SEL (43)		2ND	-18.8		0		0		-18.8	
O2 + E[-] + M => O2[-] + M (M= ANY)										
JENSEN-1967 SEL (36)	1-3.5	3RD	-29.5	1.0	0		0		-29.5	1.0
O2 + E[-] + M => O2[-] + M (M= N2)										
TUNDER-1967 SEL (43)		3RD	-31.1		0		0		-31.1	
O2 + E[-] + M => O2[-] + M (M= O2)										
TUNDER-1967 SEL (5)		3RD	-26.38		-1.0		0		-29.4	
O2 + M => O + O + M (M= ANY)										
SEE REACTION SUMMARY										
BAHN-1964 XP (1)		2ND	+1.277		-2.5		+59.4		-32.0	
TUNDER-1967 SEL (5)		2ND	-5.3		-1.0		+59.4		-34.1	
O2 + M => O + O + M (M= AR)										
SEE REACTION SUMMARY										
BAHN-1964 SEL (1)		2ND	-5.221		-1.		+59.4		-34.	
JONSTN-1968 EVAL (6)	.3-15	2ND	-5.4	.3	-1.0		+59.74		-34.33	.34
KASKAN-1964 EVAL (7)		2ND	-7.38		-0.5		+59.34		-34.6	
O2 + M => O + O + M (M= N2)										
SEE REACTION SUMMARY										
BAHN-1964 SEL (1)		2ND	-4.921		-1.		+59.4		-34.	
BASCMB-1965 EVAL (9)	.3-10	2ND	-7.84	.10	0		+59.68	.13	-33.74	.11
O2 + M => O + O + M (M= NO)										
BAHN-1964 SEL (1)		2ND	-5.221		-1.		+59.4		-34.	
O2 + M => O + O + M (M= N)										
BAHN-1964 SEL (1)		2ND	-5.221		-1.		+59.4		-34.	
O2 + M => O + O + M (M= O2)										
SEE REACTION SUMMARY										
BAHN-1964 SEL (1)		2ND	-4.267		-1.		+59.4		-33.	
BASCMB-1965 EVAL (9)	.3-10	2ND	-7.84	.10	0		+59.68	.13	-33.74	.11
JONSTN-1968 EVAL (6)	1-8	2ND	-4.3	.3	-1.0		+59.74		-33.23	.34
KASKAN-1964 EVAL (7)		2ND	-6.44		-0.5		+59.34		-33.7	

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \, T^{(B \pm B')} \, EXP(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±Δ
02 + M => 0 + 0 + M (M= 02)										
TUNDER-1967 SEL (5)		2ND	-4.5		-1.0		+59.4		-33.3	
02 + M => 0 + 0 + M (M= 0)										
SEE REACTION SUMMARY										
BAHN-1964 SEL (1)		2ND	-3.823		-1.		+59.4		-33.	
BASCMB-1965 EVAL (9)	.3-10	2ND	-7.46	.01	0		+59.68	.13	-33.361	.057
KASKAN-1964 EVAL (7)		2ND	-5.99		-0.5		+59.34		-33.2	
TUNDER-1967 (5,33)		2ND	-5.85		-1.0		+59.4		-34.6	
02 + 02 => 0 + 03										
SEE REACTION SUMMARY FOR 03 + M => 0 + 02 + M										
BAHN-1964 SEL (13)		2ND	-10.95		0		+49.92		-32.62	
BASCMB-1965 REV (8)	.3-3	2ND	-10.96	.04	0		+49.92		-32.625	.040
JONSTN-1968 REV (4)		2ND	-10.674		0		+50.63		-32.647	
TUNDER-1967 SEL (5)		2ND	-11.8		0		+48.8		-33.0	
02[-] + M => 02 + E[-] + M (M= ANY)										
TUNDER-1967 OMF		2ND	-10.1		0		+5.0		-12.3	
02[-] + OH => 02 + OH[-]										
TUNDER-1967 OME		2ND	-12.2		+0.5		0		-10.7	
03 + M => 0 + 02 + M										
BAHN-1964 SEL (13)		2ND	-8.12		0		+12.38		-13.49	
03 + M => 0 + 02 + M (M= ANY)										
SEE REACTION SUMMARY										
KASKAN-1964 XP (8)		2ND	-7.04		+0.44		+11.93		-10.90	
TUNDER-1967 (5,34)		2ND	-8.0		0		+12.6		-13.5	
03 + M => 0 + 02 + M (M= AR)										
SEE REACTION SUMMARY										
JONSTN-1968 EVAL (1)	.2-1	2ND	-9.4	.1	0		+11.43		-14.36	.10
03 + M => 0 + 02 + M (M= CO2)										
SEE REACTION SUMMARY										
JONSTN-1968 EVAL (1)	.2-1	2ND	-8.8	.1	0		+11.43		-13.76	.10

NOTE: RATE COEFFICIENTS ARE FOR CONCENTRATION IN MOLECULES PER CU.CM., TIME IN SECONDS AND TEMPERATURE IN KELVIN, LOG(BASE 10) K = A + B LOG T -434.3C/T. SUPERSCRIPTS SHOWN IN SQUARE BRACKETS. NOTES: BEBO= BOND ENERGY-BOND ORDER, CT= COLLISION THEORY, EST= ESTIMATE BY ANALOGY, EVAL= FULL SCALE EVALUATION, J+P= JOHNSTON + PARR CALC., REV= FROM THE REVERSE REACTION, SEL= SELECTED DATA, XP= BASED ON EXPERIMENTAL DATA. FOR NUMBERED NOTES, SEE CHAPTER 7

RATE PARAMETERS FOR $K = 10^{(A \pm A')} \; T^{(B \pm B')} \; \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A	±A'	B	±B'	C	±C'	LOG K AT T = 1000	±A
O3 + M => O + O2 + M (M= HE)										
SEE REACTION SUMMARY										
JONSTN-1968 EVAL (1)	.2-1	2ND	-9.3	.1	0		+11.43		-14.26	.10
O3 + M => O + O2 + M (M= N2)										
SEE REACTION SUMMARY										
BASCMB-1965 EVAL (7)	.3-3	2ND	-8.49	.03	0		+12.1		-13.741	.053
JONSTN-1968 EVAL (1)	.2-1	2ND	-9.2	.1	0		+11.43		-14.16	.10
O3 + M => O + O2 + M (M= O2)										
SEE REACTION SUMMARY										
BASCMB-1965 EVAL (7)	.3-3	2ND	-8.47	.03	0		+12.1		-13.721	.053
JONSTN-1968 EVAL (1)	.2-1	2ND	-9.1	.1	0		+11.43		-14.06	.10
O3 + M => O + O2 + M (M= O3)										
SEE REACTION SUMMARY										
BASCMB-1965 EVAL (7)	.3-3	2ND	-8.11	.02	0		+12.1		-13.361	.048
JONSTN-1968 EVAL (1)	.2-1	2ND	-8.8	.1	0		+11.43		-13.76	.10
OH + E[-] + M => OH[-] + M (M= ANY)										
JENSEN-1967 EST (35)	1-3.5	3RD	-29.5	1.5	0		0		-29.5	1.5
OH + M => H + O + M (M= ANY)										
KASKAN-1964 REV (6)		2ND	-9.63		+0.21		+50.98		-31.13	
OH + M => H + O + M (M= XE)										
BAHN-1965 SEL (11)		2ND	-2.8		-1.5		+50.8		-29.3	
OH + O[-] => O + OH[-]										
TUNDER-1967 OME		2ND	-12.1		+0.5		0		-10.6	
OH + OH => H2 + O2										
BASCMB-1965 SEL (11)	.3-3	2ND	-11.70		0		+13.23		-17.44	
CHERRY-1967 SEL (13)		2ND	-10.6	1.4	-0.02		+24.7		-21.4	1.4
OH + OH => H2O + O										
SEE REACTION SUMMARY										
BASCMB-1965 EVAL (10)	.3-3	2ND	-11.28	.21	0		+.5	.1	-11.50	.21
CHERRY-1967 SEL (12)		2ND	-10.7	1.0	-0.01		+.49		-10.9	1.0
JENSEN-1967 SEL (6)	1-3.5	2ND	-11.0	.7	0		+.5		-11.22	.70
KASKAN-1964 EVAL (4)		2ND	-10.90		0		+.5		-11.12	
SCOFLU-1967 XP (5)	.3	2ND	-10.860		0		+.5		-11.08	
WILSON-1968 EVAL (4)	.3		-11.59	.07	0		0			

RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±Δ AT T = 1000
OH + OH + M => H2O2 + M (M= H2O2) BASCMB-1965 REV (12)	.3-3	3RD	-32.74	0	-2.47	-31.67
OH + OH + M => H2O2 + M (M= H2O) BASCMB-1965 REV (12)	.3-3	3RD	-32.839	0	-2.47	-31.767
OH + OH + M => H2O2 + M (M= N2) BASCMB-1965 REV (12)	.3-3	3RD	-33.51	0	-2.47	-32.44
OH + OH + M => H2O2 + M (M= O2) BASCMB-1965 REV (12)	.3-3	3RD	-33.66	0	-2.47	-32.59
OH + OH[-] => H2O + O[-] TUNDER-1967 OMF		2ND	-12.8	+0.5	+4.5	-13.3
OH + P => O + PH MAYER-1968 J+P		2ND	-12.55	+0.73	+20.03	-19.05
OH + S => O + SH MAYER-1968 J+P		2ND	-12.14	+0.67	+8.76	-13.93
OH + SI => O + SIH MAYER-1968 J+P		2ND	-11.98	+0.71	+34.27	-24.72
OH[-] + M => OH + E[-] + M (M= ANY) TUNDER-1967 OMF		2ND	-10.1	0	+5.0	-12.3
P + PH => P + PH MAYER-1968 J+P		2ND	-14.0	+1.27	+.20	-10.3
P + SH => PH + S MAYER-1968 J+P		2ND	-12.22	+0.67	+7.95	-13.66
P + SIH => PH + SI MAYER-1968 BEBO		2ND	-11.95	+0.5	+.75	-10.8
PH + S => P + SH MAYER-1968 J+P		2ND	-12.25	+0.67	+.86	-10.61

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RATE PARAMETERS FOR $K = 10^{(A \pm A')}\ T^{(B \pm B')}\ \mathrm{EXP}(-1000(C \pm C')/T)$

REACTION SOURCE AND NOTES	RANGE T/1000	ORDER	A ±A'	B ±B'	C ±C'	LOG K ±A AT T = 1000
PH + SI => P + SIH MAYER-1968 BERO		2ND	-11.22	+0.5	+1.51	-10.4
S + SH => S + SH MAYER-1968 J+P		2ND	-12.17	+0.67	+.45	-10.36
S + SIH => SH + SI MAYER-1968 BERO		2ND	-11.97	+0.5	+.75	-10.8
SH + SI => S + SIH MAYER-1968 BERO		2ND	-11.27	+0.5	+22.40	-19.5
SI + SIH => SI + SIH MAYER-1968 J+P		2ND	-13.83	+1.25	+.40	-10.25

CHAPTER 5: RATE EVALUATIONS AND REACTION SUMMARIES

Two types of material are included in this chapter. The first is a set of rate coefficient evaluations for the reactions

$$CO + OH = CO_2 + H$$

$$H_2 + OH = H_2O + H$$

$$OH + OH = H_2O + O$$

$$CH_4 + OH = CO_2 + H$$

$$N + O_2 = NO + O$$

presented in that order.

The remainder of the chapter is a series of reaction summaries for reactions that have been studied widely and are reported on by several evaluators. These are for the reactions

$$H + O_2 = O + OH$$

$$H_2 + M = H + H + M$$

$$H_2 + O = H + OH$$

$$O_2 + M = O + O + M$$

$$O_3 + M = O + O_2 + M$$

$$O + O_3 = O_2 + O_2$$

Each summary is a collection of notes, one per evaluation, instead of a single descriptive statement. However, each summary has a common reference list covering all its notes. Usually the notes follow those given by the authors of the papers, but they have occasionally been rewritten. The sources, here identified by one author and a year, are identified in more detail in Chapter 7, Specific Notes.

KINETICS TABLES FOR THE REACTIONS OF HYDROXYL RADICALS[*]

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1. Introduction

Rate data for four gas phase reactions of hydroxyl radicals are reviewed. Recommendations, values for the rate constants, the applicable temperatures and uncertainties are:

$CO + OH \rightarrow CO_2 + H$

$k = 5.0 \times 10^{-13} \exp(-300/T)$, 300-2000 K, $\log k^{+0.7}_{-0.3}$

$H_2 + OH \rightarrow H + H_2O$

$k = 3.8 \times 10^{-11} \exp(-2600/T)$, 300-1500 K, $\log k^{+0.3}_{-0.7}$

$OH + OH \rightarrow H_2O + O$

$k = (2.57 \pm 0.50) \times 10^{-12}$, 300 K

$CH_4 + OH \rightarrow CH_3 + H_2O$

$k = 4.7 \times 10^{-11} \exp(-2.5 \times 10^3/T)$, 300-2000 K, $\log k \pm 0.7$

The concentration units for which these rates apply are molecules per cm^3. The hydroxyl disproportionation rate is one-half the rate for OH disappearance. Rates for the reverse reactions, calculated using equilibrium data are also given.

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[*] Work performed at The Applied Physics Laboratory under Contract NOw62-0604-c with the Bureau of Naval Weapons. An earlier version of this material was presented at the 1967 Spring Meeting of the Western States Section, The Combustion Institute, La Jolla, California 24-25 April 1967, Paper WSCI-67-16. Part of the material appeared in "Report on the Establishment of Chemical Kinetics Tables", Chemical Propulsion Information Agency, unnumbered report, April 1967, p. 20 and CPIA Publication No. 146, Vol. 1, p. 147 (May 1967).

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These rates are based upon an evaluation of the absolute rate for CO + OH and rate ratio data for the others. They are the same as those previously reported.[1,2*] The introduction of new data does not cause sufficient changes to warrant revisions at this time.

Each evaluation is presented in a separate section. The available data are tabulated and graphed. References and comments on them are given in each section.

2. Rate Constant for the Reaction $CO + OH = CO_2 + H$

The reaction of CO with OH is an important one for several reasons. This is the primary means of converting CO to CO_2. Much of the information of OH kinetics exists as ratios of the rate of CO + OH to that of other reactions. In particular the rates of $H_2 + OH$ and $CH_4 + OH$ are best determined from a value of the rate of CO + OH and measurements of the rate ratio. This reaction also provides a test for theoretical rate calculations.

This argument could, of course, be inverted and some other reaction chosen as the base for interpretation of rate ratio data. The only other choice at present is $H_2 + OH = H_2O + H$. Two reasons for rejecting this choice are advanced. (1) The available data on $H_2 + OH$ suitable for setting an absolute value for the rate constant, including its temperature dependence, are less reliable than those for CO + OH. This is discussed below and elaborated in the comments on the $H_2 + OH$ evaluation. (2) The activation energy of the CO + OH reaction is lower. Errors in its determination will have little effect on the rates of the other reactions.

There are only four experimental data points for $H_2 + OH$. Three different measurements at room temperature establish that point (and disprove Avramenko's measurements).[24] Kaufman[29] estimated an activation energy and frequency factor by using his room temperature point and an rate equation given by Fenimore and Jones.[27] Investigation of their equation indicates that it can give no better than order of magnitude estimates. Kaufman's expression was later used by Ripley and Gardiner[28]

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[*] See reference list in Section 2 for $CO + OH = CO_2 + H$.

to fit OH concentration data measured in a shock tube to a kinetic scheme. Although valuable data, this is not considered adequate to establish a rate equation because other mechanisms, or combinations of rate expressions might fit the data. In addition the calculated fit seemed to be less sensitive to k(H_2 + OH) than other parameters. A more reliable point is due to Dixon-Lewis[13] but he suggests that it may be only an upper limit. The conclusion then is that the rate of H_2 + OH is so poorly established that it can not be used with rate ratios to determine another rate. Because there is much more data on the CO + OH reaction it seems more logical to take it as a standard and use it with ratios to determine other rate constants.

The pertinent experimental data are presented in Table I and Figure 1. The suggested value was obtained by assuming the room temperature point of reference 1 to be correct and subjective weighing of the various high temperature points. The line was then adjusted to give only one significant figure in the activation energy. The quality and quantity of the data is not sufficient to justify more sophisticated fitting techniques. This 300 K point was chosen instead of the point due to Greiner because of the large scatter in Greiner's measurements.

The scatter of the points obtained in flames (over an order of magnitude) is perhaps not so bad as it looks at first glance. Some of the scatter can be explained. The analysis is complex. Figure 2 shows the data chain required for the reevaluation of the work of Fenimore and Jones.[5,8] The conclusion reached here is that their reported values are low because an incorrect value was used for the rate coefficient of $H + D_2 \rightarrow D + HD$. The high flame points, from the work of Westenberg and Fristrom[6] on hydrocarbon oxygen flames may be high because [OH], assumed to have its equilibrium value, may well exceed this in these flames.

Relation of this work to other evaluations. Bahn,[17] Cherry, et al,[18] Tunder, et al,[19] and Jensen and Kurzius[20] all select the rate expression of Dixon-Lewis, Wilson, and Westenberg[1] which is that suggested here. Fristrom and Westenberg[21] and also Kaskan and Browne[22] included the low temperature results of Avramenko[24] in their evaluations. These results are incorrect. They account for the higher activation energies in the two evaluations.

Schofield[23] gives $k = 1.1 \times 10^{-12} \exp(-515/T)$ as a least-square fit to the results of references 1, 4-6, 8, 13-16. His value falls within the error limits suggested here. Both analyses use the same low temperature tie point[1] and share the flame derived results of references 4, 6 and 8. Schofield includes explosion limit[15,16] and photolysis results[14] not used here. However, the two analyses differ in an important respect. The flame, photolysis and explosion limit work all determined rate ratios involving the two systems $CO + OH = CO_2 + H$ and $H_2 + OH = H + H_2O$. Schofield established the rates for the latter system first and then used them to calculate the CO + OH rate. His rate for $H_2 + OH$ is 50 percent higher at 1000 K than that presented in our evaluation of that reaction. This lead to higher values for the CO + OH high temperature data points, as recalculated by him, and to a higher recommended rate coefficient.

Baulch et al[31] recommend $k = (7.0 \pm 13.3) \times 10^{-13} \exp(-545 \pm 250/T)$. Their analysis uses the low temperature results of references 1 and 2, those of Ung and Back[14] and Baldwin and Cowe[15] in the middle region and the higher temperature results from references 3-7, 10-12. They note but do not use the recent report by Wong et al[30]. Their rate parallels Schofield's and uses a preassigned value for the rate of $H_2 + OH \rightarrow H_2O + O$ to interpret rate ratios.

The differences among these last two rate expressions and that given here are small, particularly when the scatter of the high temperature points is considered. More and better high temperature results are needed. A dashed line, $k = 8 \times 10^{-13} \exp(-450/T)$, is included in Figure 1 to show our estimate of the likely maximum temperature dependence of the reaction.

Both Baulch et al[31] and Kaskan and Browne[22] give rate constants for the reverse reaction. They are calculated from CO + OH and the equilibrium constant. Baulch also lists the single available value[32] for the reaction $CO + OD \rightarrow CO_2 + D$.

TABLE I: $CO + OH \rightarrow CO_2 + H$ $\Delta H^\circ_{298}/R = -12.5$

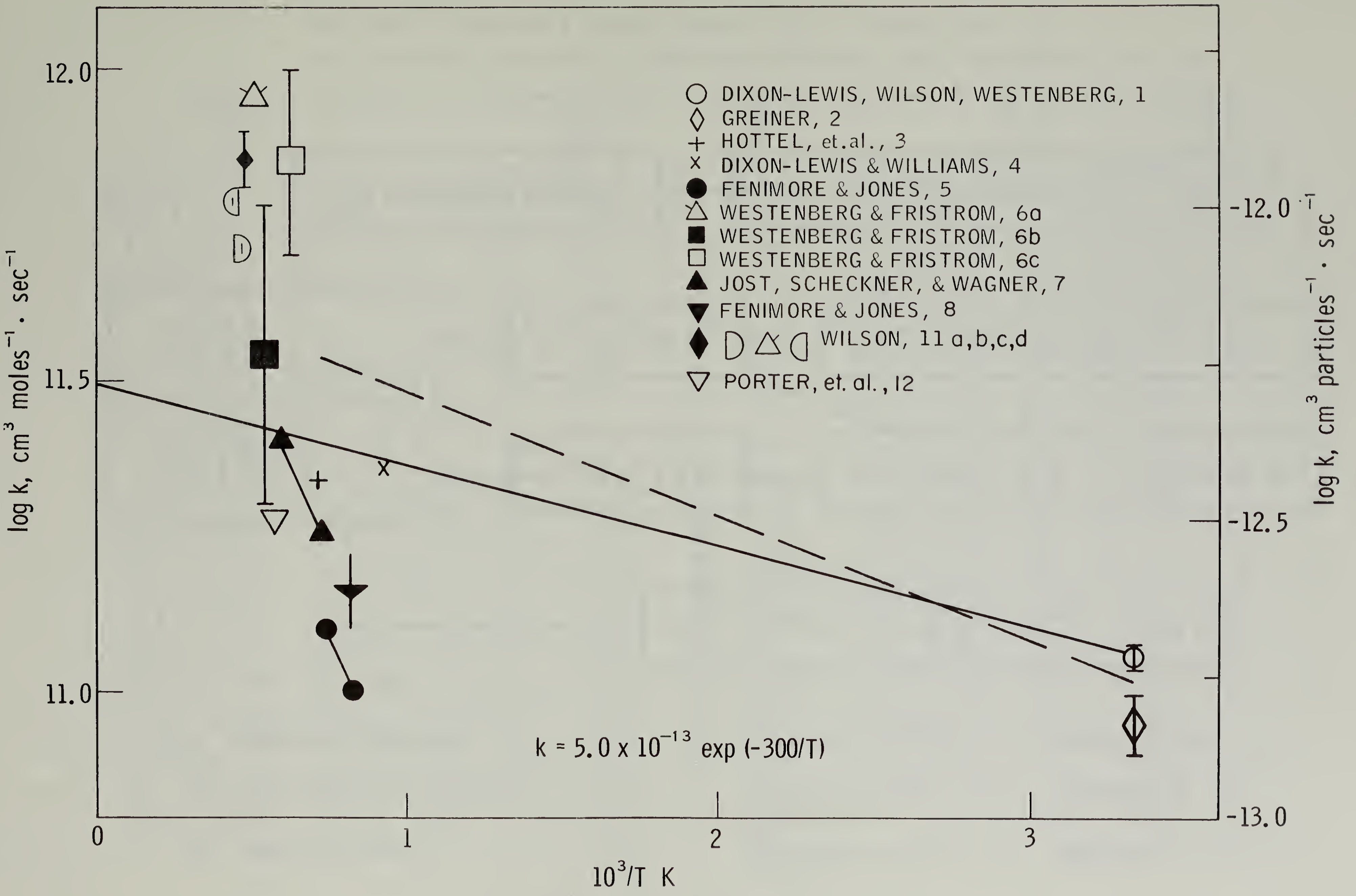
Equilibrium Constant, $K_p = 2.34 \times 10^{-3} \exp(12{,}400/T)$ 300-1000 K

$K_p = 8.26 \times 10^{-3} \exp(11{,}135/T)$ 1000-2500 K

Rate Constant 10^{13} k, cm^3 $molecule^{-1}$ s^{-1}	Temp. K	Ref.	Comment
1.91 ± .08	300	1	EST
1.48 ± .15	300	2	KS
3.67	1400	3	Well-stirred reactor
3.8	1072	4	Flame, reverse
1.66	1200	5	Flame, reverse
2.09	1350		
15	1950	6a	Flame
3-10	1850	6b	Flame
8-16	1650	6c	Flame
3.0	1380	7	CO reactor
4.2	1720		
2.5 ± 3	1200	9	Flame, reverse
11.5 ± 1.5	2000	9	CH_4 flame
8.3 ± .2	2150	9	$+CH_3Br$
15 ± .2	2000	9	+HCl
12.5 ± .5	2150	9	$+CH_3Cl$
.85 ± .3	300	10	Mass spec., production of CO_2
1.73 ± .02	300	11	
3.2	1600	12	Flame

Suggested Value 300-2000 K	k at 1000 K	Error Limits
$k = 5.0 \times 10^{-13} \exp(-300/T)$ cm^3 $molecule^{-1}$ s^{-1}	3.7×10^{-13}	$\log_{10} k^{+0.7}_{-0.3}$

For the reverse reaction, calculate $k_r = k/K_{eq}$ using K_{eq} appropriate to the temperature range of interest.



CO + OH → CO_2 + H

Figure 1: Rate data for CO + OH = CO_2 + H. Recommended value ——. Line with likely maximum slope — — — ($k = 8 \times 10^{-13} \exp(-450/T)$).

DATA CHAIN FOR k_5 DETERMINED FROM FLAME STRUCTURE

k = rate constant

K = equilibrium constant

* = experimental data

$CO + OH \rightarrow CO_2 + H$	Reaction 5
$H_2 + OH \rightarrow H_2O + H$	Reaction 4
$HD + OD \rightarrow D_2O + H$	Reaction 4D

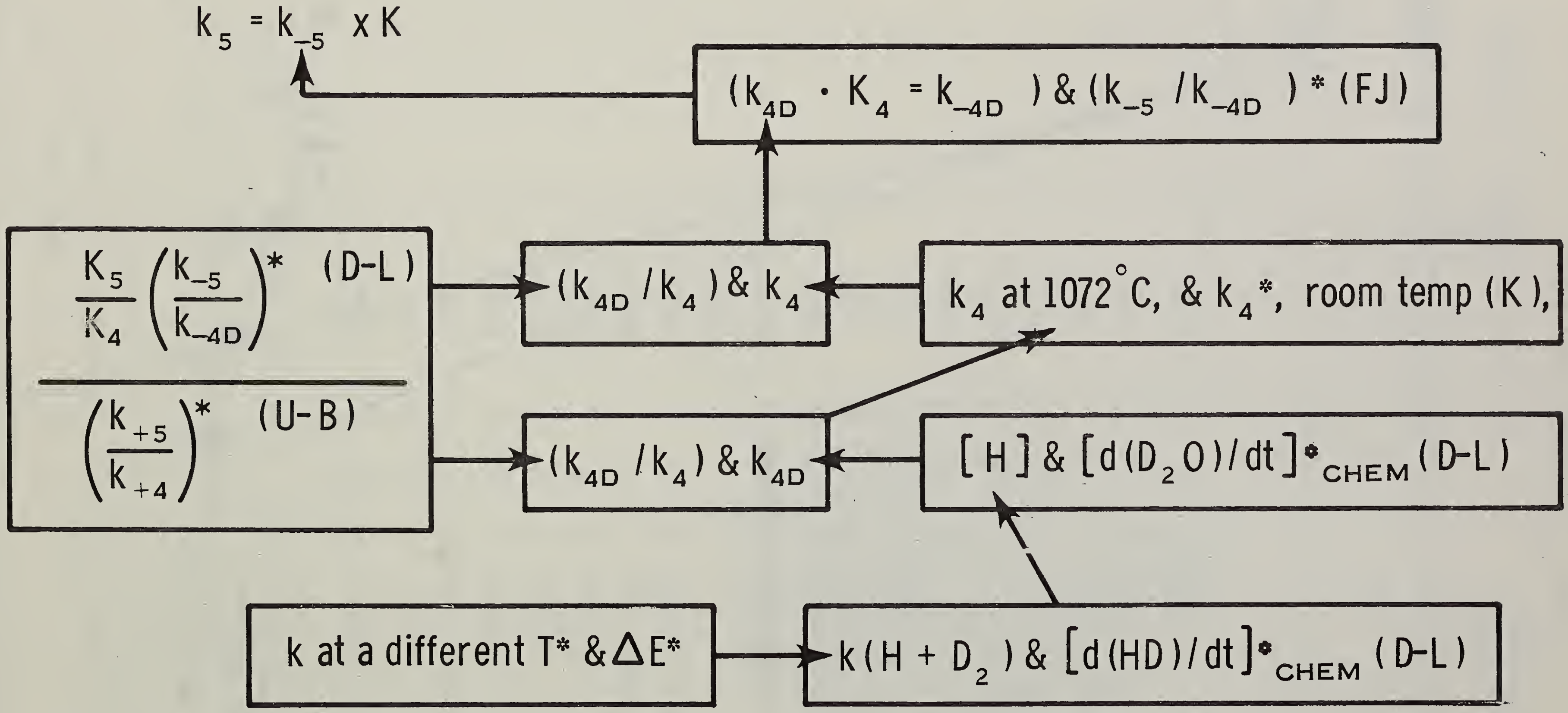


Figure 2: Initials in parentheses refer to authors of experimental papers: U-B = Ref. 14, D-L = Ref. 13, FJ = Ref. 5. The arrows indicate that information in one box was used to generate a number that was used in another box, etc.

References and Comments: $CO + OH = CO_2 + H$

1. Dixon-Lewis, G., Wilson, W. E., and Westenberg, A. A., "Studies of Hydroxyl Radical Kinetics by Quantitative ESR", J. Chem. Phys. <u>44</u>, 2877 (1966).
   The OH was generated by $H + NO_2 = NO + OH$. Quantitative electron spin resonance was used to determine the initial concentration and to follow the hydroxyl radical decay in a fast flow system at ~ 1mm pressure.

2. Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. I. Reactions with H_2, CO and CH_4 at 300°K", J. Chem. Phys. <u>46</u>, 2795 (1967).
   The OH was generated by flash photolysis of H_2O and the decay followed by kinetic spectroscopy (absorption, static system, pressure 20-200 mm.) Because of the short time of reaction ($< 200 \times 10^{-6}$ s) and the large ratio of reactant to OH the reaction could be treated as second order and wall and three-body reactions were not significant.

3. Hottel, H. C., Williams, G. C., Nerheim, N. M., and Schneider, G. R., "Kinetic Studies in Stirred Reactors: Combustion of Carbon Monoxide and Propane", Symp. Combust. 10th (The Combustion Institute, 1965) p. 111.
   k was calculated from a study of CO combustion rates in a well stirred reactor.

4. Dixon-Lewis, G., Sutton, M. M., and Williams, A., "Reactions Contributing to the Establishment of the Water Gas Equilibrium When Carbon Dioxide is Added to a Hydrogen-Oxygen Flame", Trans. Faraday Soc. <u>61</u>, 255 (1965).
   The ratio k $(H + D_2O \rightarrow HD + OD)$/k$(H + CO_2 \rightarrow CO + OH)$ = 4.3 was determined at 1072 K by the addition of small amounts of D_2O and CO to a previously studied $H_2 - O_2$ flame. k was calculated from the equilibrium constant and k$(H + D_2O) = 1.56 \times 10^{-10} \exp(-11,000/T)$ cm^3 $molecule^{-1}$ s^{-1} given in Dixon-Lewis, G., Sutton, M. M., and Williams, A. "The Reactions of Hydrogen Atoms with Nitrous Oxide." J. Chem. Soc. 5724 (1965). This value depends ultimately on k$(H + D_2 \rightarrow HD + D)$. The value used was probably high by a factor of 1.8; the resulting k may therefore be low by as much as a factor of 1.8.

5. Fenimore, C. P. and Jones, G. W., "The Reaction of Hydrogen Atoms with Carbon Dioxide at 1200-1350°K", J. Phys. Chem. <u>62</u>, 1578 (1958).
   The ratio k$(H + D_2O)$/k$(H + CO_2)$was determined in the post flame gases of several flames. The value 3 exp(-3900/T) for this work was reported in ref. 8. k may be slightly low because no corrections were made for diffusion. Comments under 4 apply here also.

6a. Westenberg, A. A. and Fristrom, D. M., "Methane-Oxygen Flame Structure. IV. Chemical Kinetics Considerations", J. Phys. Chem. <u>65,</u> 591 (1961).

6b,c. Westenberg, A. A. and Fristrom, R. M., "H and O Atom Profiles Measured by ESR in C_2 Hydrocarbon Flames", Symp. Combust. 10th (The Combustion Institute, 1965) p. 473.

k was determined in low pressure (1/10 atm) flames [(6a):$CH_4 + O_2$, (6b): $C_2H_6 + O_2$, (6c): $C_2H_4 + O_2$] from the measured [CO], [d CO/dt] chem, and assuming [OH] at hot boundary is given by chemical equilibrium conditions. Since [OH] may well exceed equilibrium values these rates may be too high.

7. Jost, W., Schecker, H. Gg., and Wagner, H. Gg., Z. Physik. Chem. (Frankfurt) <u>45,</u> 47 (1965).

OH was generated in a flame and the combustion gases allowed to come to equilibrium; additional CO was added and reaction rate measured.

8. Fenimore, C. P. and Jones, G. W., "Rate of Reaction in Hydrogen, Nitrous Oxide and in Some Other Flames", J. Phys. Chem. <u>63,</u> 1154 (1959).

The ratio $k(CO_2 + H)/k(D_2 + OH)$ was found to be 7-9 in the 1000-1200 K region of a flame. Diffusion corrections were made. See comments under 4.

9. Wilson, Wm. E., Jr., O'Donovan, J. T., and Fristrom, R. M., "Flame Inhibition by Halogen Compounds", Symp. Combust. 12th (Poitiers, France, 1968).

(a): $CH_4 + O_2$ uninhibited, (b): inhibited with CH_3Br, (c): inhibited with HCl, (d): inhibited with CH_3Cl. CH_3Br is the most effective inhibitor and Br is probably a good catalyst for recombination so 9a should have [OH] nearest the equilibrium value and does have the lowest rate. See comments under 8.

10. Herron, John T., "Mass-Spectrometric Study of the Rate of the Reaction of CO + OH", J. Chem. Phys. <u>45,</u> 1854 (1966).

The OH was generated by $H + NO_2 \rightarrow NO + OH$, with excess NO_2, the H generated by $CO + OH \rightarrow CO_2 + H$ regenerates a OH so that d(OH)/dt is not effected by the CO reaction. From a measurement of the initial [OH], the CO_2 formed as a function of [CO], and k for the OH decay it is possible to calculate k(CO + OH). Herron used k(OH + OH) = 0.75×10^{12} due to Kaufman. If k(OH + OH) = 1.55×10^{12} due to Dixon-Lewis, Wilson, Westenberg is used Herron's results give k(CO + OH) = $.45 - .92 \times 10^{11}$ (all in mole units). The low value and large scatter are the result of reaction of OH with NO_2 which was not recognized by Herron. This value was ignored in determining the suggested values.

11. Wilson, Wm. E., Jr. and O'Donovan, J. T., "Mass-Spectrometric Study of the Reaction Rate of OH with Itself and With CO", J. Chem. Phys. 47, 5455 (1967).

See 10 above. When Herron's experiment was repeated it was discovered that the value of k(CO + OH) obtained was a function of the $[NO_2]$. The reaction was studied as a function of $[NO_2]$ and $[NO_2]$ extrapolated to 0 to obtain the value shown.

12. Porter, R. P., Clark, A. H., Kaskan, W. E., and Browne, W. E., "A Study of Hydrocarbon Flames", Symp. Combust.11th (1967), p. 907.

The burnt gas region of a low pressure (18 Torr) acetylene-oxygen-nitrogen flame was analyzed. CO and CO_2 determined by gas chromatography. OH determined spectrophotometrically. The CO + OH reaction assumed (quite properly) to be the main producer of CO_2. This is a "preliminary analysis" of one flame.

13. Dixon-Lewis, G., Sutton, M. M., and Williams, A., Symp. Combust. 10th, (1965), p. 495.

14. Ung, A. Y-M. and Back, R. A., Can. J. Chem. 42, 753 (1964).

15. Baldwin, R. R., Jackson, D., Walker, R. W., and Webster, S. J., Symp. Combust. 10th (1965), p. 423.

16. Baldwin, R. R. and Cowe, D. W., Trans. Faraday Soc. 58, 1768 (1962).

17. Bahn, G. S., Pyrodynamics 6, 101 (1968).

18. Cherry, S. S., Gold, P. I., and Van Nice, L. J., TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.

19. Tunder, R., Mayer, S., Cook, E., and Schieler, L., Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1 (1967).

20. Jensen, D. E. and Kurzius, S. C., Aerochem Research Laboratories, Princeton, N. J., March 1967. Report TP-149.

21. Fristrom, R. M. and Westenberg, A. A., "Flame Structure" (McGraw-Hill Book Co., New York, p. 367 (1965)).

22. Kaskan, W. E. and Browne, W. G., General Electric Co. Space Sciences Laboratory Report R64SD37, July 1964.

23. Schofield, K., Planet. Space Sci. 15, 643 (1967).

Reaction 4, Table 1; Table 5; Figure 2c, Figure 5.

24. Avramenko, L. I. and Lorentso, R. V., Z. Fiz. Khim. 24, 207 (1950).

The objection to the use of results from this paper rests on an examination of the products of a discharge through water vapor. Hydroxyl concentrations are low and relatively constant. Rates based on measurement of [OH] will then be low and invalid. See references 25, 26.

25a. Kaufman, F. and Del Greco, F. P., "Formation, Lifetime and Decay of OH Radicals in Discharge-Flow Systems", J. Chem. Phys. 35, 1895 (1961).

25b. Del Greco, F. P. and Kaufman, F., "Lifetime and Reactions of OH Radicals in Discharge Flow Systems", Dis. Faraday Soc. 33, 128 (1962).

Measurements of the concentration of OH downstream of an electric discharge through water vapor (optical absorption) showed that the discharge is an inefficient source of OH (but is efficient in producing H) and that the concentration of OH exhibited an abnormal variation, often S-shaped, instead of the expected monotonic decrease with distance. O_2 increases the [OH] slightly. It is suggested that reactions of H with O_2 regenerate OH and that OH is readily dissociated by the discharge. The chemical production of OH by $H + NO_2 = NO + OH$ does not exhibit this behavior. A graph comparing the two OH sources is included in the second paper.

26. Westenberg, A. A. and De Haas, N., "Quantitative ESR Measurements of Gas Phase H and OH Concentrations in the $H-NO_2$ Reaction", J. Chem. Phys. 43, 1550 (1965).

A study of the H and OH concentrations from $H + NO_2 = NO + OH$ showed that this method is a reliable producer of OH and that the [OH] is directly related to the NO_2 flow at low [OH]. At higher levels, the concentration reaches a plateau due to the reactions $OH + OH = H_2O + O$, $O + OH = H + O_2$ competing with OH production. See ref. 11.

27. Fenimore, C. P. and Jones, G. W., J. Phys. Chem. 65, 993 (1961).

28. Ripley, D. L. and Gardiner, Wm. C., Jr., J. Chem. Phys. 44, 2285 (1966).

29. Kaufman, F. and Del Greco, F. P., Symp. Combust. 9th, p. 659 (1963).

30. Wong, E. L., Potter, A. E., and Belles, F. E., NASA TN D-4162 (1967).

31. Baulch, D. L., Drysdale, D. D., and Lloyd, A. C., High Temperature Reaction Rate Data, Report No. 1, May 1968, Dept. of Physical Chemistry, The University, Leeds, England.

The value cited here is taken from page 4 of the report. That on page 1 appears to be a misprint. The estimated precision on page 1 has been interpreted as logk ± 0.3.

32. Westenberg, A. A. and Wilson, Wm. E., Jr., J. Chem. Phys. 45, 338 (1966).

3. Rate Constant for the Reaction $H_2 + OH = H + H_2O$

This reaction has received much attention since it figures large in the interpretation of the hydrogen-oxygen system. It has been studied directly at room temperature using three analytical techniques, estimated from competitive experiments in studies on water photolysis, explosion limits in various flames, and determined in shock wave studies of the H_2-O_2 reaction.

This reaction is the alternative to $CO + OH = CO_2 + H$ as the basic reaction against which rates of other OH reactions are to be scaled. There are direct measures of the rate of the $H_2 + OH$ reaction. They are not considered to be sufficiently accurate to be used to establish a value for the rate. Consequently, rate ratio data are relied upon here. The choice of the base reaction is discussed in the introductory material for this set of evaluations. The limitations of the individual numbers are discussed in the notes following each reference.

Analytical problems concerning the determination of [OH] are discussed in the evaluation of $OH + OH = H_2O + H$. They are not so important here because this reaction has been studied in the presence of a high concentration of H_2, that is, under pseudo-first order conditions. In contrast to the OH disproportionation the room temperature rates for this reaction are in good agreement.

The data are listed in Table II. The rate ratio $k(H_2 + OH = H_2O + H)/k(CO + OH = CO_2 + H)$ is shown in Figure 3 (from reference 2). This is used to determine the temperature coefficient, the rate constant for CO + OH being taken from a separate evaluation. The ratios at 300 K are not from competitive studies, but were calculated from direct measurements on the two reactions. The lower 300 K ratio is used as a tie-point on the graph. Adjustment to include the work of Greiner would raise the pre-exponential factor to 0.038 but would not affect the activation energy. In view of the spread of the high temperature values, introduction of this small change is not warranted at present. Figure 4 shows the recommended rate constant as a function of temperature.

Relation to Other Evaluations

For the reaction $H_2 + OH = H + H_2O$ both Tunder, et al[14] and Cherry, et al[15] adopt the rate of Dixon-Lewis, Wilson, and Westenberg.[2] By considering the range of other reported data (mostly higher) the latter assigns an uncertainty factor of 10 to cover the probable value. Tunder, et al recast the rate to include a $T^{+0.5}$ term. They also give a rate for $H + H_2O = H_2 + OH$ calculated by a modified Johnston and Parr technique. The ratio of this rate and that in reference 1 do not yield the equilibrium constant.

Bahn[16] and also Kaskan and Browne[17] chose rates recommended by Kaufman and Del Greco.[3b]

Bascombe[18] used the data of Del Greco and Kaufman[3a] and Dixon-Lewis, Sutton and Williams[6b] to construct the rate for $H_2 + OH = H + H_2O$ and then used equilibrium data to get that for the reverse.

Schofield[19] bases his value on the measurements of reference 2 (300 K) and the shock tube study (1500-2500 K) of Ripley and Gardiner.[5] His rate and that given here agree at 300 K. His is 40% higher at 1000 K.

Fristrom and Westenberg[20] developed a rate constant for $H + H_2O = H_2 + OH$, $k = 8.3 \times 10^{-11} \exp(-1.0 \times 10^{4}/T)$ from the results of references 3b, 6a, 7a.

Jensen and Kurzius[21] suggest that the higher temperature work indicates higher activation energies for both the forward and reverse reaction than by Fristrom and Westenberg. Their rate is 40% lower at 300 K than that given here and agrees with it around 1000 K.

TABLE II: $H_2 + OH \rightarrow H_2O + H$ $\Delta H°_{298}/R = -7.56$

Equilibrium Constant, $K = 0.211 \exp(7640/T)$

Rate Constant k, cm^3 $molecule^{-1}$ s^{-1}	Temp. K	Ref.	Comment
$3.65 \times 10^{-13} T^{0.56} \exp(-2200/T)$	$1\text{-}4 \times 10^3$	1	Calc.
$6.5 \pm 0.3 \times 10^{-15}$	300	2	ESR
$7 \pm 2 \times 10^{-15}$	300	3	Abs. Spec.
$6.6 \pm 0.3 \times 10^{-15}$	301	4	RS
$6.5 \times 10^{-11} \exp(-2850/T)$	$1.4\text{-}2.5 \times 10^3$	5	Shock wave Computer fit
2.9×10^{-12}	1072	6	Flame
$4.2 \times 10^{-13} \exp(-5000/T)$	1285-1700	7	Flame

Rate ratio: $k(H_2 + OH \rightarrow H_2O + H)/k(CO + OH \rightarrow CO_2 + H)$

$0.034 \pm .003$	300	2	Direct studies
0.045 ± 0.006	301	4	both k's
0.429	473	8	H_2O photolysis
0.615	523		
0.875	573		
1.221	623		
4.5 ± 0.5	773	9	Explosion limits
8.4	1072 K	10	Flame
22.3	1275	11	Flame

Suggested Values 300-1500 K	k at 1000 K	Error Limits
$R = k_{H_2}/k_{CO} = 0.034 \pm 0.003$ $\exp\{[2300 \pm 150]/[1/300 - 1/T]\}$	7.3	$\log R^{+0.3}_{-0.17}$
Using $k\ (CO + OH) =$ $5.0 \times 10^{-13} \exp(-300/T)$		$\log R\ -0.17$
$k(H_2 + OH) =$ $3.8 \times 10^{-11} \exp(-2600/T)$	2.8×10^{-12}	$\log k^{+0.3}_{-0.7}$
For the reverse reaction $k(H + H_2O) =$ $1.8 \times 10^{-10} \exp(-1.0 \times 10^4/T)$	8.2×10^{-15}	

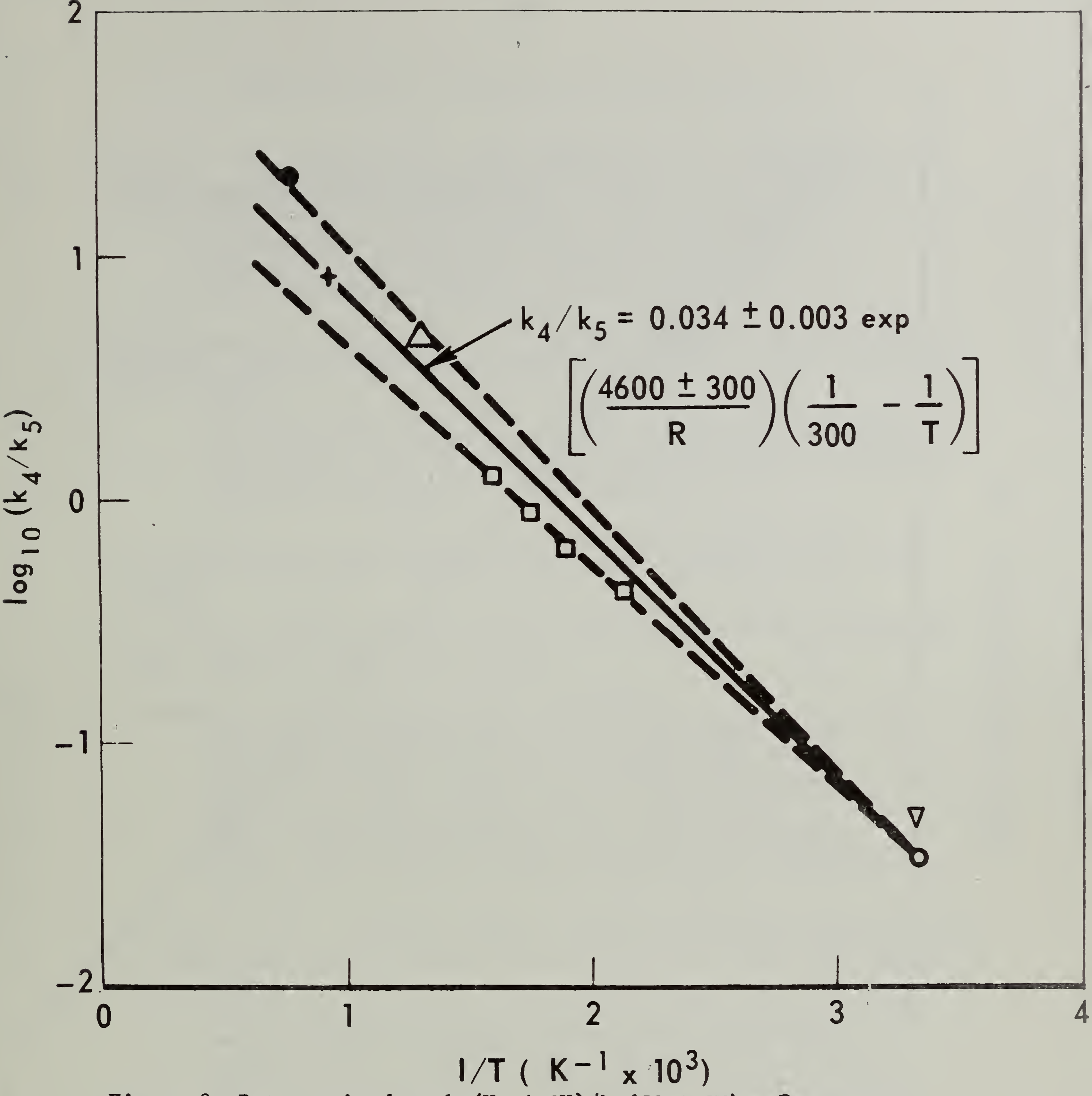


Figure 3: Rate ratio data $k_4(H_2 + OH)/k_5(CO + OH)$. ● Fenimore and Jones, ref. 11, + Dixon-Lewis et al, ref. 10, △ Baldwin, ref. 9, □ Ung and Back, ref. 8, ○ Dixon-Lewis et al, ref. 2, ▽ Greiner, ref. 4. Figure reproduced from J. Chem. Phys. 44, 2883 (1966) with the permission of the American Institute of Physics. Point from ref. 4 added.

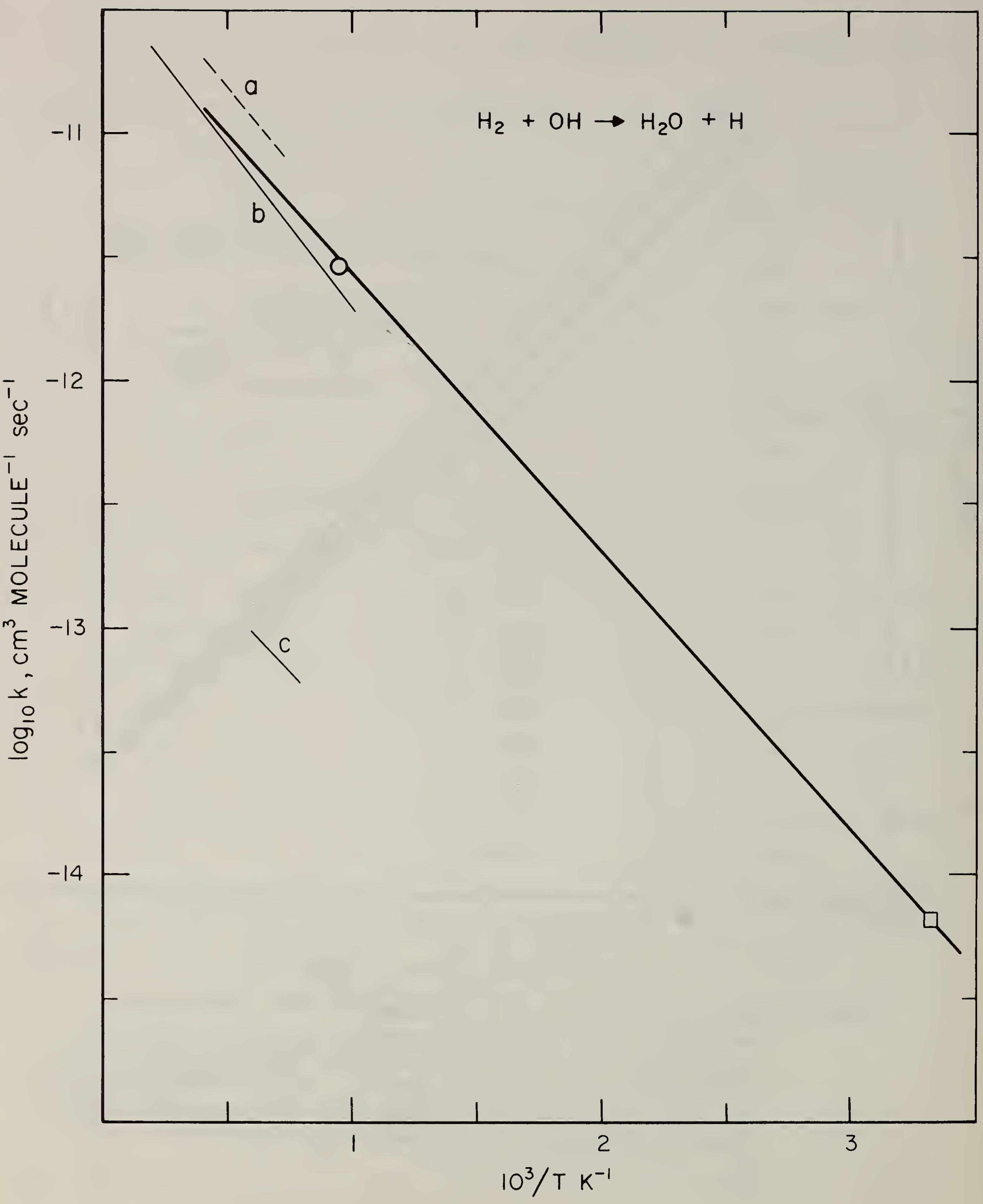


Figure 4: Rate data for H_2 + OH → H_2O + H —— recommended value, $k = 3.8 \times 10^{-11}$ exp(2600/T). □ refs 2, 3,4. O–ref. 6, a–ref. 1, b–ref. 1, c–ref. 5

References and Comments: $H_2 + OH = H_2O + H$

1. Mayer, S. W., Schieler, L., and Johnston, H. S., "Computation of High-Temperature Rate Constants for Bimolecular Reactions of Combustion Products", Symp. Combust. 11th, p. 837 (1967).
   Equation fits calculated rates from 1000-4000 K. This equation agrees well, within a factor of 2, with the suggested value from 300-2500 K.

2. Dixon-Lewis, G., Wilson, W. E., and Westenberg, A. A., "Studies of Hydroxyl Radical Kinetics by Quantitative ESR", J. Chem. Phys. <u>44</u>, 2877 (1966).
   The OH was generated by $H + NO_2 = NO + OH$. Quantitative electron spin resonance was used to determine the initial concentration and to follow the hydroxyl radical decay in a fast flow system at ~ 1 mm pressure.

3a. Del Greco, F. P. and Kaufman, F., "Lifetime and Reactions of OH Radicals in Discharge Flow Systems", Dis. Faraday Soc. <u>33</u>, 128 (1962).

b. Kaufman, F. and Del Greco, F. P., "Fast Reactions of OH Radicals", Symp. Combust. 9th, p. 659 (1963).

c. Kaufman, F., Ann. Geophys. <u>20</u>, 106 (1964).
   The OH was generated by $H + NO_2 = NO + OH$. Adsorption spectrometry was used to determine the initial concentration and to follow the OH decay in a fast flow los pressure system. In the experiments $H_2 + OH$ and $OH + OH$ are competitive, the former being the faster. The first two papers describe the experimental work. The value is quoted from the last.

4. Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. I. Reactions with H_2, CO and CH_4 at 300°K", J. Chem. Phys. <u>46</u>, 2795 (1967).
   The OH was generated by flash photolysis of H_2O and the decay followed by kinetic spectroscopy (absorption). (static system, pressure 20-200 mm.) Because of the short time of reaction ($< 200 \times 10^{-6}$ s) and the large ratio of reactant to OH the reaction could be treated as second order and wall and three-body reactions were not significant.

5. Ripley, D. L. and Gardiner, W. C., Jr., "Shock-Tube Study of the Hydrogen-Oxygen Reaction. II. Role of Exchange Initiation", J. Chem. Phys. <u>44</u>, 2285 (1966).
   Induction time measurements on the H_2-O_2 reaction (~ 1400-2500 K) were interpreted in terms of hydrogen

and oxygen dissociation, $H + O_2 = OH + O$, $O + H_2 = OH + H$ and $OH + H_2 = H_2O + H$. The analytical solution for this set of reactions yielded the best fit rate parameters. The results suggest that the behavior of the system is not very sensitive to the rate of $OH + H_2$. Because of this and because some modified mechanism might fit the data equally well this rate constant is not considered adequate for use in establishing a recommended rate.

6a. Dixon-Lewis, G. and Williams, A., "Some Observations on the Structure of a Slow Burning Flame Supported by the Reaction between Hydrogen and Oxygen at Atmospheric Pressure", Symp. Combust 9th, p. 576 (1963).

6b. Dixon-Lewis, G., Sutton, M. M., and Williams, A., "Some Reactions of Hydrogen Atoms and Simple Radicals at High Temperatures", Symp. Combust. 10th, p. 495 (1965).

Potentially, this work provides a rate estimate independent of rate ratios involving other hydroxyl reactions. The first paper reported $k(H + D_2O = HD + OH) = 5.0 \times 10^9 cm^3 mol^{-1} s^{-1}$ at 1072 K from $(d[D_2O]/dt)_{chem}$ and [H]. [H] established by D_2 tracer technique $H + D_2 = HD + D$ in early part of flame, chemiluminescence in central portion, and D_2O tracer in burned gas portion of flame, The D_2 tracer gives absolute [H], the others relative. D_2 trace results are then used to scale [H] in other regions. The k then depends on a number of assumptions. The authors state "this may be an upper limit". The k also depends on the value of $k(H + D_2)$ used. Recent studies of $H + D_2$ indicates a rate of $k(H + D_2)$ only about one-half of that used.[19] This value is therefore, not considered reliable enough to use in establishing a value of k.

The second paper includes a value for $k(H + D_2O \rightarrow HD + OH = 3.6 \times 10^9 cm^3 mol^{-1} s^{-1}$ at 1072 K based on new experiments on H_2-O_2 flames and a revised estimate for $k(H + H_2O \rightarrow H_2 + OH) = 6.7 \times 10^9$ based on references 6a, 3b. The value in the table was calculated from the latter and the equilibrium constant.

7a. Fenimore C. P. and Jones, G. W., "Determination of Hydrogen Atoms in Rich, Flat, Premixed Flames by Reaction with Heavy Water", J. Phys. Chem. 62, 693 (1958).

7b. Fenimore, C. P. and Jones, G. W., "Rate of Reaction, $O + H_2 \rightarrow OH + H$, in Flames", J. Phys. Chem. 65, 993 (1961).

Potentially this work would provide a measurement of the rate that is independent of rates of other hydroxyl radical reactions.

D_2O was added to a rich H_2 and H_2 + CO Flames and $(d\ HD/dt)_{chem}$ from $H + D_2O \rightarrow HD + OD$ determined. The temperature range was 1285-1500 K in H_2 flames and 1345-1700 K in hydrocarbon flames. The Avramenko and Lorentso[12] value for $k(OH + H_2)$ and the equilibrium constant were used to obtain $k(H + H_2O)$. This value was then increased by a factor of two in the flame temperature range. This value of $k(H + H_2O)$ was then used to determine [H]. (All isotopic rates were assumed to be the same.) The [H] found was said to be consistent with that of Bulewicz, James and Sugden measured by a different method at a higher temperature. The consistency was based on log $[H]/[H]_{eq}$. being linear with 1/T for both sets of flames. Considering the number and extent of assumptions made and that Avramenko and Lorentso's rate value is low by 100 to 1000 in the temperature in which they measured it, the agreement between the [H] of Bulewicz, et al and that reported here is more accidental than meaningful.

The rate $(d[D_2O]/dt)_{chem}$ was also measured in rich hydrocarbon flames. The $k(H + D_2O)$ used earlier gave [H] equal to the equilibrium concentration. This is better evidence for $k(H_2 + OH)$ but still can hardly be considered to be of better than order of magnitude accuracy.

In the second paper, the rate equation $k(H_2 + OH) = 2.5 \times 10^{11} \exp(-5 \times 10^3/T)\ cm^3 mol^{-1} s^{-1}$ was stated for these experiments. This retains the Avramenko and Lorentso temperature dependence. Kaufman[3b] used his room temperature value and a value for 1500 K calculated from this equation to give $k = 10^{10.8} \pm .7 \exp(-2.95 \pm 1.0/T)$. This value has been widely quoted in the literature, usually without the large uncertainty given by Kaufman. Considering how the high temperature point was obtained an uncertainty of only 1 kcal was decidedly optimistic. In all fairness it should be pointed out that in 1960 order of magnitude values of reaction rates in flame were of interest. To attempt to use them today to provide rate constants reliable to a factor of two or better is not justified.

8. Ung, A. Y. M. and Back, R. A., "The Photolysis of Water Vapor and Reactions of Hydroxyl Radicals", Can. J. Chem. 42, 753 (1964).
   The OH was generated by photolysis of water, CO_2 was formed when CO was present. The rate ratio was determined from the decrease in CO_2 formed when H_2 was added. Evidently the three body recombination to form H_2O_2 was sufficiently fast to interfere at lower temperatures.

The H present would react with H_2O_2 to give HO_2 which might react with CO. If this reaction sequence contributed above 473 K it would cause the measured k's to be low.

9. Baldwin, R. R., private communication. A revision of the value, 3, reported earlier by Baldwin, R. R. and Cowe, D. W., "The Inhibition of the Hydrogen and Oxygen Reaction by Formaldehyde", Trans. Faraday Soc. <u>58</u>, 1768 (1962). Quoted from reference 2.

10. Dixon-Lewis, G., Sutton, M. M., and Williams, A., "Reactions Contributing to the Establishment of the Water Gas Equilibrium When Carbon Dioxide is Added to a Hydrogen-Oxygen Flame", Trans. Faraday Soc. <u>61</u>, 255 (1965).
    The ratio of $k(H + CO_2)$ to $k(H + D_2O) = 4.3 \pm 0.5$ was measured in a H_2-O_2 flame. Assuming $k(H + H_2O)$ to be larger than $k(H + D_2O)$ by a factor determined by the zero-point energy difference between single O-H and O-D bonds ($5.4\ kJ\ mol^{-1}$), $k(H + H_2O)/k(H + CO_2) = 7.9 \pm 1.0$, k is then obtained via the water-gas reaction, $CO_2 + H_2 = CO + H_2O$, equilibrium constant. Their article, Symp. Combust. 10th, p. 495 (1965) also reports on this work.

11. Fenimore, C. P. and Jones, G. W., "The Reaction of Hydrogen Atoms with Carbon Dioxide at 1200-1350 K", J. Phys. Chem. <u>62</u>, 1578 (1958), Idem, Ibid <u>63</u>, 1154 (1959).
    Measured $k(H + D_2O)/k(H + CO_2) = 7.0$. The second paper states the ratio as 3 exp(-3925/T). The value in the table calculated from this. For conversion method see comment on reference 10.

12. Avramenko, L. I. and Lorentso, R. V., Z. Fiz. Khim. <u>24</u>, 207 (1950).
    Discharge through water vapor used as OH source. Rejected.
13. Bulewicz, E. M., James, C. G., and Sugden, T. M., Proc. Roy. Soc. <u>A235</u>, 89 (1956).

14. Tunder, R., Mayer, S., Cook, E., and Schieler, L., Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1 (1967).

15. Cherry, S. S., Gold, P. I., and Van Nice, L. J., TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.

16. Bahn, G. S., Pyrodynamics <u>3</u>, 245 (1965).

17. Kaskan, W. E. and Browne, W. G., General Electric Co. Space Sciences Laboratory Report R64SD37, July 1964.

18. Bascombe, K. N., "Reaction Rate Data: The Hydrogen/Oxygen System", Ministry of Aviation, Explosives Research and Development Establishment, Waltham Abbey, Essex, England, E.R.D.E. 1/S/65

19. Schofield, K., Planet. Space Sci. 15, 643 (1967).

20. Fristrom, R. M. and Westenberg, A. A., "Flame Structure" (McGraw-Hill Book Co., New York, p. 367 (1965)).

21. Jensen, D. E. and Kurzius, S. C., Aerochem Research Laboratories, Princeton, N. J., March 1967. Report TP-149.

4. Rate Constant for the Reaction $OH + OH = H_2O + O$

Studies on the disproportionation of hydroxyl radicals at 300 K have been made using several techniques. Higher temperature values are not available. There is one estimate[8] for the activation energy of the reverse reaction, $E^* = 19$ kcal mol^{-1}, slightly greater than the endothermicity of the reaction. Kaufman has suggested, on the basis of the magnitude of the rate constant that the forward reaction cannot have an activation energy of more than 1.5 kcal mol^{-1}. This is reasonable but as yet not supported by measurements.

Here the procedure is to establish only a value at 300 K. That chosen is the higher value. This is consistent with modern work on the CO + OH reaction. The rate constant for the latter is developed in a separate evaluation.

An accurate estimate of the absolute concentration of OH is needed for rate measurements on this reaction. The need is acute, the reaction being second order on OH and a value for the concentration appearing in the rate expression. This is in contrast to the other OH reactions which can be run in the presence of an excess of the other reagent, that is, under pseudo-first order conditions. Most of the discrepancy between the two measurements on this reaction is undoubtedly due to uncertainty in the analytical calibrations.

Relation to Other Evaluations

The work of Kaufman and Del Greco[2] is the basis for several evaluations. They used their 300 K measurements and an assumed 1000 kcal $mole^{-1}$ activation energy. The alternative energy item, $E^* = 18$ kcal/mole for the reverse reaction[8] is also used. These are equivalent. Kaskan and Browne,[9] Bascombe,[10] Bahn,[11] and Tunder, et al[12] all report numbers traceable to Kaufman. Cherry, et al[13] selected a value calculated by Bahn based on Langen and Creswell's[14] equivalent expression for the reverse reaction. Schofield[15] adopts the 1000 cal mol^{-1} activation energy and the room temperature value from reference 1. For his definition of k, this value should be doubled. His rate for the reverse reaction uses equilibrium data and the 18 kcal mol^{-1} value.

TABLE III

$OH + OH = H_2O + O$ $\Delta H^o_{298}/R = 8.49 \times 10^3$

Equilibrium Constant, $K = 5.88 \times 10^{-2} \exp(8580/T)$

Rate Constant* cm^3 $molecule^{-1} s^{-1}$	Temp. K	Ref.	Comment
$2.57 \pm 0.25 \times 10^{-12}$	300	1	ESR
1.4 ± 0.25	300	2	Abs. Spec.
$2.2 \pm 0.6 \times 10^{-12}$	300	3	ESR
$\geq 1.7 \times 10^{-13}$	300	4	Surface combination of H atoms
Several mass-spectrometric studies support the higher value of k if $k(CO + OH \rightarrow CO_2 + H) = 1.9 \pm 0.4 \times 10^{-13}$ cm^3 $molecule^{-1}$ s^{-1} is accepted		5 6 7	

*Definition of k: $d[OH]/dt = -2k[OH]^2$

Suggested Values	k at 300 K	
$OH + OH = H_2O + O$	$2.57 \pm 0.50 \times 10^{-12}$ cm^3 $molecule^{-1} s^{-1}$	
$H_2O + O = OH + OH$	3.4×10^{-24}	

References and Comments: OH + OH = H_2O + O

1. Dixon-Lewis, G., Wilson, W. E., and Westenberg, A. A., "Studies of Hydroxyl Radical Kinetics by Quantitative ESR", J. Chem. Phys. 44, 2877 (1966).

   The OH was generated by H + NO_2 → NO + OH. Quantitative electron spin resonance was used to determine the initial concentration and to follow the second order OH decay in a fast flow system at ~ 1mm pressure.

2. Del Greco, F. P. and Kaufman, F., "Lifetime and Reactions of OH Radicals in Discharge Flow Systems", Disc. Faraday Soc. 33, 128 (1962); Kaufman, F. and Del Greco, F. P., "Fast Reactions of OH Radicals", Symp. Combust. 9th, p. 659 (1963); Kaufman, F., "Aeronomic Reactions Involving Hydrogen. A Review of Recent Laboratory Studies", Ann. Geophys. 20, 106 (1964).

   The OH was generated by H + NO_2 → NO + OH and the second order decay measured by absorption spectroscopy near 3000 A. The initial OH concentration [OH] was determined by assuming 1) that there was a region where H + NO_2 → NO + OH had gone to completion and OH + OH → H_2O + O had not yet begun and 2) that [OH] in this region was given by the NO_2 flow rate. The light absorption path integrated 1/3 msec of reaction time and mixing required 1 msec. It appears that the initial OH concentration was overestimated because both the finite mixing time and the overlapping of the formation and decay reactions would lead to a lower actual [OH] than given by the NO_2 flow rate. If the actual [OH] were ½ of the anticipated [OH] the derived k would agree with that from Ref. 1. The calibration, [OH] vs absorption, may also require revision. This depends upon the f number for OH. A recent study (reference 16) reports an f number higher by a factor of 2 than that used by Kaufman.[17] Use of a higher f number would reduce [OH] and increase the rate.

   Experimental procedures and results are described in the first two papers. The value quoted here is based on the last. (The definition of k in these papers is $d[OH]/dt = -k[OH]^2$. That used here is $d[OH]/dt = -2k[OH]^2$.)

3. Westenberg, A. A. and De Haas, N., "Quantitative ESR Measurements of Gas Phase H and OH Concentrations in the H-NO_2 Reaction", J. Chem. Phys. 43, 1550 (1965).

   A study of H and OH concentrations as a function of H and NO flow rates showed the occurance of $OH + OH \rightarrow H_2O + O$ and $O + OH \rightarrow H + O_2$. The value quoted in the table is the revised one given in reference 1. Considered by the authors to be an estimate, and to be superseded by the later study (reference 1).

4. Wise, H., Ablow, C. M., and Sancier, K. M., "Diffusion and Heterogeneous Reaction. VI. Surface Recombination in the Presence of Distributed Atom Sources", J. Chem. Phys. 41, 3569 (1964).

   Only a lower limit for the rate coefficient was obtained.

5. Reference 1 also reports a mass-spectrometric study of the CO-OH reaction in which the ratio O_2/CO_2 (O_2 formed via $OH + OH = H_2O + O$, $O + OH = O_2 + H$ and CO_2 formed via $CO + OH = CO_2 + H$) supports the higher value of k.

6. Herron, J. T., "Mass Spectrometric Study of the Rate of Reaction of CO with OH", J. Chem. Phys. 45, 1845 (1966).

   If the rate of CO + OH is assumed to have the value indicated in the table, Herron's measurements, corrected for the effect of NO_2 on the rate, support the suggested value. See reference 7.

7. Wilson, Wm. E., Jr. and O'Donovan, J. T., "Mass Spectrometric Study of the Reaction Rate of OH with Itself and with CO", J. Chem. Phys. 47, 5455 (1967).

   A repetition of the experiments of reference 6 showing that the CO + OH rate depends upon the NO_2 concentration. (The reaction $NO_2 + H = NO + OH$ used to produce hydroxyl.) The suggested value for OH + OH given in the table is shown to be consistent with the recommended CO + OH rate.

8. Voevodsky, V. V. and Kondratiev, V. N., Progr. Reaction Kinetics 1, 41 (1961).

   Citing preliminary work of Azatyan.

9. Kaskan, W. E. and Browne, W. G., General Electric Co. Space Sciences Laboratory Report R64SD37, July 1964.

10. Bascombe, K. H., "Reaction Rate Data: The Hydrogen/Oxygen System", Ministry of Aviation, Explosives Research and Development Establishment, Waltham Abbey, Essex, England, E.R.D.E. 1/S/65

11. Bahn, G. S., "Chemical Kinetics. Reactions Among H_2O, HO_2, H_2O_2, and O_3, also Involving H_2, O_2, OH, H and O", Pyrodynamics 3, 245 (1965).

12. Tunder, R., Mayer, S., Cook, E., and Schieler, L., Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1 (1967).

    Quoting from Fristrom, R. M. and Westenberg, A. A., "Flame Structure" (McGraw-Hill Book Co., New York, p. 367 (1965))

13. Cherry, S. S., Gold, F. I., and Van Nice, L. J., TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.

14. Langen, W. T., Creswell, J. D., and Browne, W. G., "Effects of Ablation Products on Ionization in Hypersonic Wakes", J. Am. Inst. Aeron. Astronaut. 3, 2211 (1965).

    A secondary source for rate data. The report of these authors, General Electric Technical Information Series 65SD208 (January 1965), same title, is stated to contain the detailed analysis. (Not examined)

15. Schofield, K., Planet. Space Sci. 15, 643 (1967).

16. Anketell, J. and Pery-Thorne, A., "Oscillator Strength in the Band System of OH by the Hook Method", Proc. Roy. Soc. A301, 343 (1967).

    The value, $f_{oo} = 14.8 \times 10^{-4}$ is the highest of those that need to be considered. Based on assumed equilibrium [OH] produced from an $O_2 + H_2O$ mixture in a flow system 1550-1675°C. The product [OH] x f is always measured. In f number determination, understatement of [OH] produces a high f. At comparable temperatures in flames, [OH] can exceed the equilibrium value. In analysis, a low f causes overstatement of [OH]. Other recent f number determinations reviewed.

17. Golden, D. M., Del Greco, F. P., and Kaufman, F., "Experimental Oscillator Strength of OH, ${}^2\Sigma^+ \rightarrow {}^2\Pi$, by a Chemical Method", J. Chem. Phys. 39, 3034 (1963).

    Hydroxyl production and initial concentrations based on $H + NO_2 = NO + OH$ in a flow system. The value, $f_{oo} = 7.1 \times 10^{-4}$, is considered by the authors to be more likely low than high.

5. Rate Constant for the Reaction $CH_4 + OH = CH_3 + H_2O$

The reaction of methane with hydroxyl radical has been studied directly over the temperature range 300-1200 K using three different methods of analysis, in the "slow combustion" of CH_4 by O_2 (700-900 K) and in flames. In the last two, rate ratios are determined, the rates of CH_4 and CO with OH usually being compared.

The data are presented in Table IV. Remarks on individual papers are included in the reference list. Most of the intermediate temperature range data must be discarded because of the likely importance of other reactions, notably that of HO_2 with CH_4, which may compete that of hydroxyl. These studies, which are marked in the table, give lower rates than those accepted.

The rate constant for the CH_4 + OH reaction has been set here by first establishing the temperature variation of the ratio k(CH_4 + OH)/ k(CO + OH) and then using the value of the rate for the latter, $k = 5.0 \times 10^{-13} \exp(-300/T)$ cm^3 $molecule^{-1}s^{-1}$, discussed in a separate evaluation and based on reference 16. The ratio data are plotted in Figure 5. The 300 K points are combinations of direct measurements. That based on references 5 and 16 is used as a pivot on the plot.

The recommended value is shown in Figure 6 together with several data items not used in determining the rate ratio and two high temperature rate expressions. The 300 K fit is, of course, not independent of Figure 5. If the pre-exponential factor were lowered by only 20% the line would run through the points of Greiner and Dixon-Lewis and Williams. When the spread of the high temperature data is considered, it is not appropriate to introduce this change at present.

The suggested rate for $CH_3 + H_2O$ was obtained using the equilibrium constant.

Schofield has also presented an analysis of this reaction. His value $k = 1.2 \times 10^{-10} \exp(-2980/T)$, is a least squares fit to the data of references 2,5,6,9-12,14. The data of the last two have been rejected here. Apart from the influence of these points, his rate has a stronger temperature dependence because of the stronger dependence adopted by him for the CO + OH rate coefficient, $k = 1.1 \times 10^{-12} \exp(-519/T)$.

TABLE IV: $CH_4 + OH \rightarrow CH_3 + H_2O$ $\Delta H^\circ_{298}/R = -8.1$

Equilibrium Constant, K = 5.87 exp(8600/T), 300-2500 K

Rate Constant, $k = AT^B \exp(C/T)$ cm^3 molecule^{-1} s^{-1}			Temp. K	Ref.	Comment
A	B	C			
1.83×10^{-13}	0.675	1100	1000-5000	1	Calc
1.8×10^{-10}	0	3270	1350-1850	2	Flame
4×10^{-10}	0	4250	300-600	3	NG*
k, cm^3 molecule^{-1} s^{-1}					
$8.8 \pm 0.3 \times 10^{-15}$			301	4	KS
$10.8 \pm 2.5 \times 10^{-15}$			300	5	ESR
$5 \pm 2 \times 10^{-12}$			1285	6	Flame

Rate ratio: $k(CH_4 + OH \rightarrow CH_3 + H_2O)/k(CO + OH \rightarrow CO_2 + H)$

0.056 ± 0.013 at 300 K	5,16	
0.060 ± 0.006 at 301 K	4	
3.2 - 6.0 at 773 K	7	Exp lim
20 - 25 at 1750-3000 K	8	Flame
17 at 1748, 24 at 1789 K	9	Flame
38 at 1709, 27 at 1743, 33 at 1797 K	10	Flame
15.2 exp (650/T) at 1200-1800 K	11	Flame
1.8 ± 0.9 at 773 K	12	NG* Slow
1.0 at 673 K, 1.5 at 773 K	13	NG* Comb.
0.83 at 673 K, 1.10 at 723 K, 2.1 at 798 K	14	NG*, H_2O_2
3-5 at 1200 K	15	NG*

*NG: Not considered reliable. Not used in determining the suggested value.

TABLE IV (Cont'd)

Suggested Values 300-2000 K	k at 1000 K	Error Limits
$R = k_{CH_4}/k_{CO} = (5.6 \pm 1.3) \times 10^{-2} \times$ $\exp\{[2200 \pm 150]/[1/300 - 1/T]\}$	9.5	log R ± 0.3
$k_{(CH_4 + OH)} = 4.7 \times 10^{-11} \exp(-2.5 \times 10^3/T)$	3.86×10^{-12}	$\log k^{+0.7}_{-0.3}$
using $k(CO + OH) = 5.0 \times 10^{-13} \exp(-300/T)$		
$k_{(CH_3 + H_2O)} = 8.0 \times 10^{-12} \exp(-11.1 \times 10^3/T)$	1.2×10^{-16}	

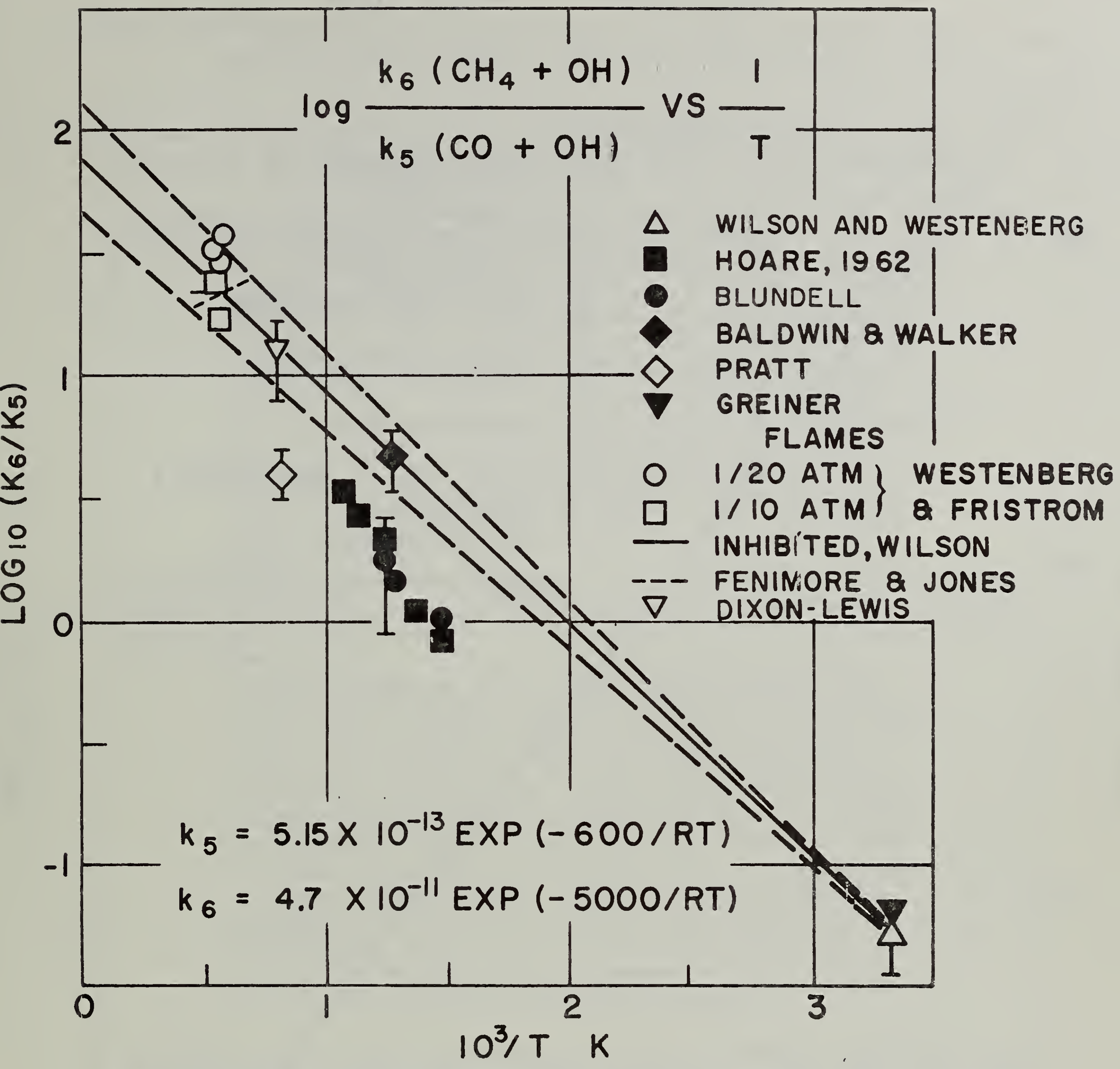


Figure 5: Rate ratio data for $k(CH_4 + OH)/k(CO + OH)$. △-ref. 5,16, ■-ref. 14, ●-ref. 12, ◆-ref. 7, ◇-ref. 15, ▽-ref. 4, O-ref. 9, □-ref. 10, — ref. 8, --- ref. 11, ▽-ref. 6. Reproduced from Symp. Combust. 11th, p. 1148 (1967) by permission of the Combustion Institute. Point from reference 4 added.

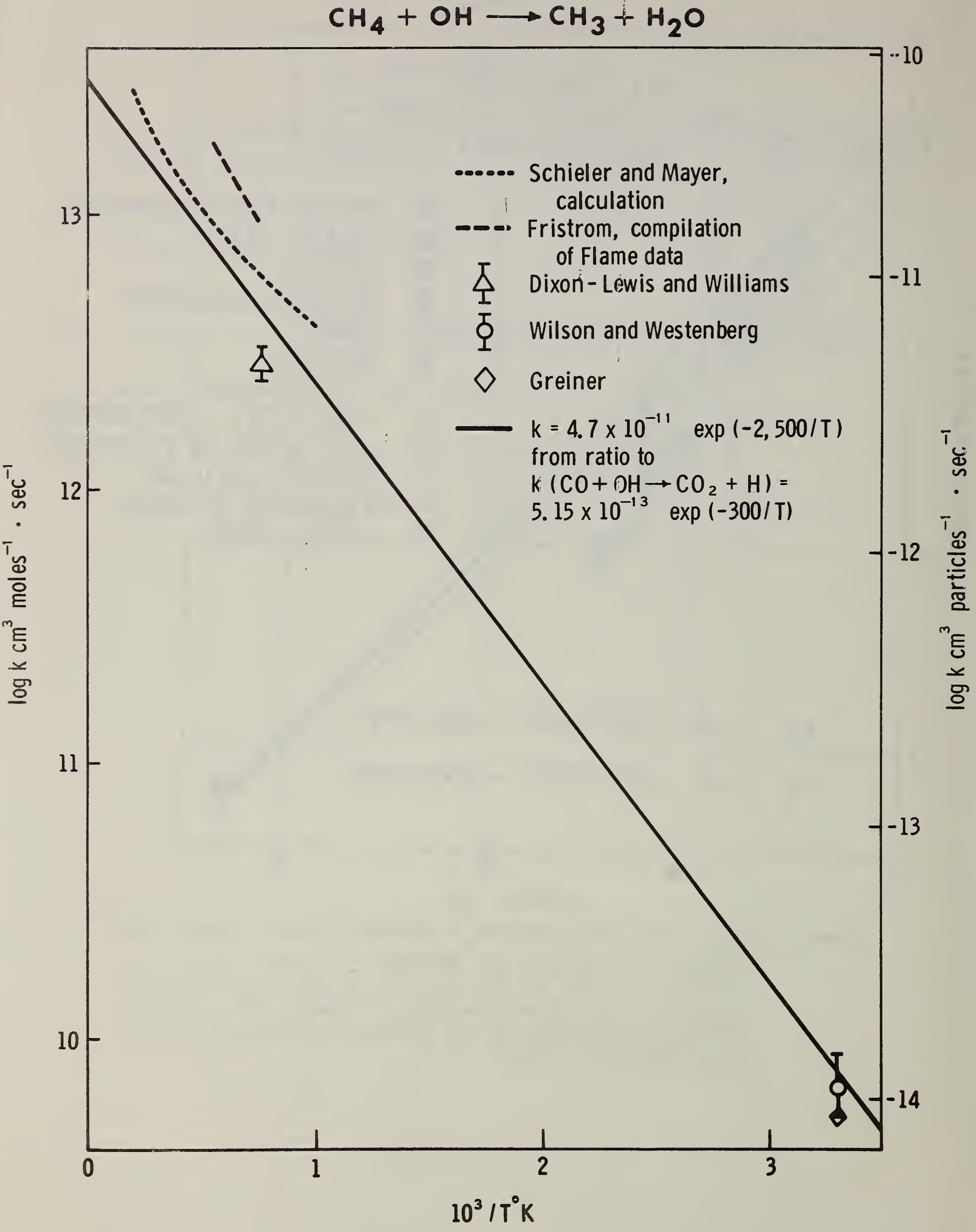


Figure 6: Rate constants determined directly, calculations and recommended values for $CH_4 + OH = CH_3 + H_2O$.

References and Comments: $CH_4 + OH = CH_3 + H_2O$

1. Mayer, S. W. and Schieler, L., "Computed High-Temperature Rate Constants for Polyatomic Combustion Products", to be published.

2. Fristrom, R. M., "Radical Concentrations and Reactions in a Methane-Oxygen Flame", Symp. Combust. 9th, p. 560 (1963).

   A compilation of results from several flame studies. Actually, based on the experimental determination of $k(CH_4 + OH)/k(CO + OH)$ and the use of a value of k, now known to be incorrect, for $k(CO + OH)$. However, the value of [OH] does not change much in the temperature range covered so an experimental value of [OH] determined in a flame similar to the one studied here was used to correct this value, i.e. the rate constant in the reference was multiplied by 0.8 to account for the difference between the experimental value of [OH] and that calculated using $k(CO + OH)$.

3. Avramenko, L. I. and Kolensnikova, R. V., "Mechanisms and Rate Constants of Elementary Gas Phase Reactions Involving Hydroxyl Radicals and Oxygen Atoms", Advances in Photochemistry, Vol. 2, Interscience, N. Y., 1964, p. 25.

   Citing Avramenko, L. I., Ph.D. Thesis Moscow 1952. This article reviews the Russian work. In the cited study OH was generated by an electric discharge in water, the decay in a flow tube was measured by absorption spectroscopy. Since this is not a satisfactory source of OH for kinetic studies this value is ignored. This was for many years the only value at lower than flame temperatures and is responsible for many erroneous rate equations with activation energies of ~ 10 kcal which are still found in the literature. This value should be ignored. The production of OH in electric discharges is discussed in the CO + OH rate evaluation, Section 2.

4. Greiner, N. R., "Hydroxyl Radical Kinetics by Kinetic Spectroscopy. I. Reactions with H_2, CO, and CH_4 at 300 K", J. Chem. Phys. 46, 2795 (1967).

   The OH was generated by flash photolysis of H_2O and the decay was followed by kinetic spectroscopy. (static system, pressure range 20-200 mm) Because of the short time of reaction ($< 200 \times 10^{-6}$ s) and the large ratio of reactant to OH the reaction could be treated as first order in OH and wall reactions could not be significant.

5. Wilson, W. E. and Westenberg, A. A., "Study of the Reaction of Hydroxyl Radical with Methane", Symp. Combust. 11th, p. 1143 (1967).

   The OH was generated by H + $NO_2 \rightarrow NO + OH$. Quantitative electron spin resonance was used to determine the initial concentration and to follow the hydroxyl decay in a fast flow system at ~ 1 mm pressure. The large error limits give the limits set by several possible reaction mechanisms involving OH reactions subsequent to the initial reaction.

6. Dixon-Lewis, G. and Williams, A., "Some Observations on the Combustion of Methane in Premixed Flames", Symp. Combust. 11th, p. 951 (1967).

   $[CH_4]$ and $d[CH_4]/dt_{chem}$ were measured in a flame by flame structure techniques; [OH] was determined by absorption spectroscopy and $k(CH_4 + OH)$ calculated at the point of maximum rate of disappearance of CH_4.

7. Baldwin, R. R., Norris, A. C., and Walker, R. W., "Reactions of Methane in Slowly Reacting Hydrogen-Oxygen Mixtures", Symp. Combust. 11th, p. 889 (1967).

   Computer treatment of explosion limits of H_2-O_2 with small additions of methane to give $k(CH_4 + OH)/k(H_2 + OH)$ and CO to give $k(CO + OH)/k(H_2 + OH)$; these ratios then give $k(CH_4 + OH)/k(CO + OH)$.

8. Wilson, Wm. E. Jr., O'Donovan, J. T., and Fristrom, R. M., "Flame Inhibition by Halogen Compounds", Symp. Combust. 12th, Potiers, France, July 1968, paper 93.

9,10. Westenberg, A. A. and Fristrom, R. M., "Methane-Oxygen Flame Structure. IV. Chemical Kinetic Considerations", J. Phys. Chem. <u>65</u>, 591 (1961).

   Flame structure studies of (9) 1/10 and (10) 1/20 atm CH_4 - O_2 flames.

11. Fenimore, C. P. and Jones, G. W., "Rate of Reaction of Methane with H Atoms and OH Radicals", J. Chem. Phys. <u>65</u>, 2200 (1961).

   Flame structure studies of several flames. Ratio quoted in Table IV calculated (Reference 5) from the rate constants given by Fenimore and Jones. Note that the activation energy has the opposite sign from the suggested equation, but that absolute values agree within the range of experimental measurements.

12. Blundell, R. V., Cook, W. G. A., Hoare, D. E., and Milne, G. S., "Rates of Radical Reactions in Methane Oxidation", Symp. Combust. 10th, p. 445 (1965).

Slow combustion of CH_4 with analysis of CO, CO_2 and H_2CO at times up to 750 sec., pressure 60-450 mm, temp. 773-998 K. Catalytic oxidation of CO on the surface and reaction with HO_2 probably cause this value to be low. Because of expected errors this number is ignored.

13. Slow combustion studies by a variety of workers. Discussion and references given in Ref. 12 above. These numbers are ignored because of the reasons given under Ref. 12.

14. Hoare, D. E., "Reactions of Gaseous Hydroxyl Radicals", Nature <u>194</u>, 283 (1962). Hoare, D. E., "Studies of the Reactions of Hydroxyl Radicals. I", Proc. Roy. Soc. <u>A291</u>, 73 (1966). Hoare, D. E. and Peacock, G. B., "Studies of the Reactions of Hydroxyl Radicals. II", Proc. Roy. Soc. <u>A291</u>, 85 (1966).

The thermal decomposition of H_2O_2 was used as a source of OH. The OH formed reacts rapidly with H_2O_2 to form HO_2 which complicates the reaction mechanism. Because of the presence of HO_2 which also reacts with CO and possibly with CH_4 these numbers are ignored.

15. Pratt, N. H., Symp. Combust. 11th, p. 1150 (1967) and Ph.D. Thesis, University of London, 1962.

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KINETICS TABLES FOR THE REACTIONS

$N + O_2 = NO + O \ (k_+)$

$NO + O = N + O_2 \ (k_-)$

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The rates of both reactions in this system have been studied, the forward rate in the temperature range 300-900 K and the reverse rate in the ranges 1500-1900 and near 5000 K. Data points (which usually are averages) and rate expressions are listed in Tables I and II. Remarks on the papers are included in the reference list.

The O + NO reaction catalyzes the homogeneous decomposition of NO, the oxygen atoms being formed by dissociation of O_2 or possibly by $NO + NO \rightarrow N_2O + O$. Oxygen molecules also promote the recombination of N atoms, the simplest sequence being $N + O_2 = NO + O$, $N + NO = N_2 + O$. The second reaction is much faster, having a rate near the collision frequency. The net effect is the replacement of N atoms by O atoms with the release of 445 kJ/mol of O_2 consumed.

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*Work performed at The Applied Physics Laboratory under Contract NOw62-0604-c with the Bureau of Naval Weapons. An earlier version (by W.E.W.) appeared in "Report on the Establishment of Chemical Kinetics Tables", Chemical Propulsion Information Agency, unnumbered report, April 1967, p. 20 and CPIA Publication No. 146, Vol. 1, p. 147 (May 1967).

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The preferred rate coefficient given in Table III cannot be obtained by averaging the rate parameters. Nor is it easy to visualize from them the relationship between the various expressions or their agreement or disagreement. A plot of the points is necessary (Figure 1). Here, the data for k_- has been converted to k_+ using the equilibrium constant values listed in Table I (which have been calculated from the JANAF Tables).[5] All of the measurements agree well in the temperature range in which they overlap except for that of Kretschmer and Petersen.[9] The range of log k at any temperature is only 0.3. It is reasonable to treat all of the data as samples drawn from the same set. The suggested rate expression is a least squares fit to $\log k - \log T = A + C/T$. Only the $N + O_2$ data have been used. The O + NO data has been used only to dictate the inclusion of a log T term. The listed rate for O + NO has been calculated from that for $N + O_2$ and the equilibrium constant (300-900 K).

The kinetic data for this reaction are extensive and good. It is unusual to find agreement of better than a factor of two over a temperature range as large as 300-5000 K. When there is such good agreement among a variety of different types of studies the rate equation may be considered reliable.

Relation to other evaluations. Wray and Teare[17] combined their 5000 K value for the rate of $O + NO = N + O_2$ with 'mid-range' values taken from references 4,6,8 and 10b. Tunder, et al[13] estimated k_+ from Wray and Teare. Schofield[12] also lists Wray's k_- value and remarks that it fits well, as indeed it does. He presents two least squares fits for $N + O_2 = NO + O$

$$k = 2.46 \times 10^{-16} T^{1.5} \exp(-2860/T) \qquad 400\text{-}5000\ \mathrm{K}$$

and

$$k = 2.52 \times 10^{-11} \exp(-3922/T) \qquad 400\text{-}1700\ \mathrm{K}$$

The former uses data from references 4,6,8,10b and 17. The latter excludes the 5000 K point. A figure is given which shows points representing the ends of the experimental temperature ranges for each study.

The fits are good. The present evaluation extends the coverage to include references 10a and 15, which were not available to Schofield. Cherry[3] quotes the value of Bortner[2] and assigns an uncertainty factor (maximum range?) of log k ± 0.7. Bortner cites references 4, 6-8, 10b, 11, 14, 16. Bahn,[1] in 1964, recommended k_- calculated from the work of Kistiakowsky and Volpi.[8] Kaufman[18] adopts the value of Clyne and Thrush[4] for $N + O_2$ (see Table I) and then calculates a value for $O + NO$, $k = (3.1 \pm 0.6 \times 10^{-12} \exp[-(19.8 \pm 0.2) \times 10^3/T]$, using equilibrium data for the 1000-5000 K range.

TABLE I

(k_+) $N + O_2 = NO + O$ $\Delta H^\circ_{298}/R = -16,03_2$

Rate Constant $cm^3 molecule^{-1} s^{-1}$	Temp. K	Ref.	Comment
$k = 3 \times 10^{-12} \exp(-3100/T)$	394-517	8	Mass spec. analysis
$10^{14}\ k = 0.13$	394		
0.33	437		
0.45	471		
0.89	517		
$k = (1.4 \pm 0.2) \times 10^{-12} \exp(-3550 \pm 200/T)$	412-755	4	NO titration of N
$10^{14}\ k = 0.25 \pm 0.02$	412		
0.42 ± 0.02	435		
0.83 ± 0.03	476		
1.5 ± 0.1	538		
4.2 ± 0.3	610		
6.6 ± 0.8	665		
15 ± 0.5	775		
$k = 6.3 \times 10^{-12} \exp(-3500/T)$	453-603	10a	NO titration of N. NO_2 reaction for O
$10^{14}\ k = 0.18$	453		
0.93	538		
2.1	603		
$k = (2.34 \pm 0.12) \times 10^{-11} \exp(-3975 \pm 100/T)$	300-910	15	ESR
$5.0 \times 10^{-13} T^{0.5} \exp(-3590/T)$			
$1.44 \times 10^{-14} T \exp(-3390/T)$			
$10^{14}\ k = 0.008 \pm 0.001$	300		
0.0360 ± 0.0008	353		
0.050 ± 0.003	360		
0.14 ± 0.02	408		
0.48 ± 0.02	470		
2.71 ± 0.08	586		
29.4 ± 1.3	910		
$10^{14}\ k = 0.008$	350	9	Emission from $N + O + M \rightarrow NO + M$

TABLE II

(k_-) $O + NO = N + O_2$ $\Delta H°_{298}/R = +16{,}03_2$

Rate Constant $cm^3 molecule^{-1} s^{-1}$	Temp. K	Ref.	Comment
$k = 6.0 \times 10^{-12} \exp(-19.8_7 \times 10^3/T)$	1575-1663	6	NO decomp. in presence of O_2. Optical absorption
log k = -16.72	1575		
-16.59	1606		
-16.52	1637		
-16.42	1663		
$k = 2.3 \times 10^{-11} \exp(-21._0 \times 10^3/T)$	1525-1912	14,7,6	NO decomp. in presence of O_2. Chemical analysis
log k = -16.57 ± 0.01	1525		
-15.99 ± 0.06	1690		
-15.61 ± 0.04	1840		
-15.38 ± 0.05	1912		
$k = 5.3 \times 10^{-15} T \exp(-19.6_5 \times 10^3/T)$	400-5000	17	Evaluation Shock heating $NO + O_2$ Optical absorption of NO
log k = -12.30	5000		

Equilibrium Constant, $K = k_+/k_-$			
log K = 2.03	5000	5	Calculated, ideal gas functions
log K = 0.678 + 7003/T	1500-1900		
log K = 0.673 + 6963/T	300-900		

TABLE III

Suggested Values 300-5000 K

Rate Constant $cm^3 molecule^{-1} s^{-1}$	k at 1000 K	Error Limits
$k(N + O~) = 1.00 \times 10^{-14}~T \exp(-3.2 \times 10^3/T)$	25×10^{-13}	$\log_{10} k \pm 0.3$
$k(O + NO) = 2.2 \times 10^{-15}~T \exp(-19.2 \times 10^3/T)$	1.0×10^{-20}	

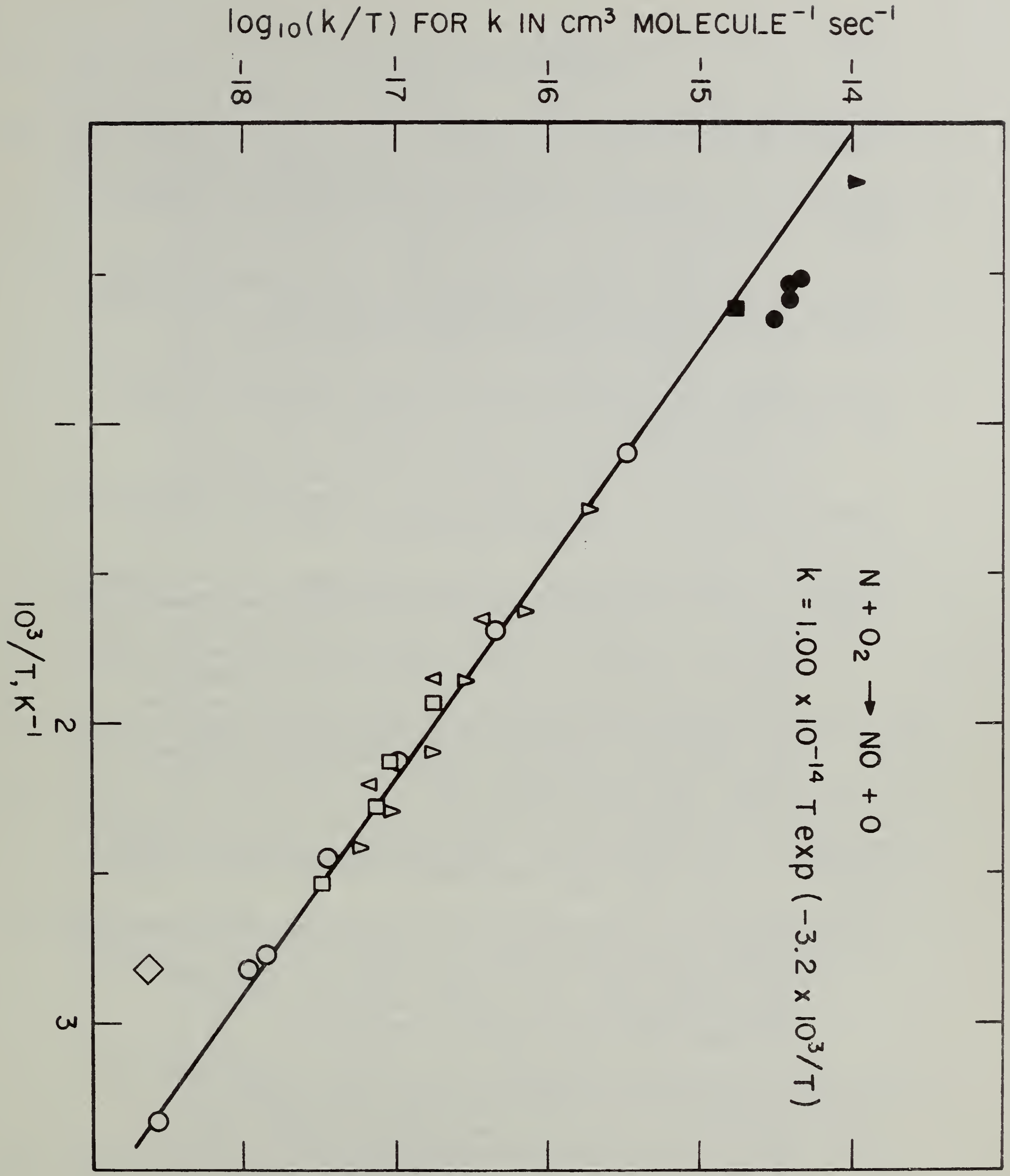

Figure 1: Rate data for $N + O_2 \rightarrow NO + O$. Points above 1000 K and that from ref. 9 not used in setting the recommended value. ○–Wilson (15), ◇ –Kretchmer and Petersen (9), □ –Kistiakowsky and Volpi (8), △ –Clyne and Thrush (4), ▽ –Vlastaras and Winkler (10a), ■ –Kaufman and Decker (6), ● –Vetter (14,7,6), △ –Wray and Teare (17).

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   Effect of oxygen on thermal decomposition of NO in furnace. Interpretation requires a value of the rate coefficient for NO decomposition and assumption of O-atoms in equilibrium with O_2. Both of these have stronger temperature dependences than does the O + NO reaction. Points scaled from figure showing k as a function of temperature.

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   Low pressure (~ 1 mm) stirred reactor, N determined by mass spectroscopy. Points scaled from figure showing k as a function of temperature.

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   N + N, N + O and H + H combination studied. The $N + O_2 = NO + O$ rate determined in the N + O study. A mixture of N_2 and O_2 passed through a microwave discharge. The intensity of NO emission (blue afterglow) studied. The rate quoted in Table I is lower than others by a factor of 5. The N atom recombination rate in this paper is also low. The reason for the discrepancy is unknown to us. Point is not used in developing the suggested rate.

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10a supersedes results reported in 10b where a faulty analytical method was used. In the later study N and O_2 at roughly equal concentrations but in a vast excess of N_2 were reacted in a flow reactor at 3 torr. N-atoms analyzed by NO titration and O-atoms from NO production in the $O + NO_2$ reaction (chemical analysis). The O formed is less than the N reacted, contrary to the mechanism used. This would have only a slight effect on the reported rates. Atom combination and wall losses (not considered in the analysis) would reduce the rates. Reported rates are lower by a factor of two than others in the same temperature range. Overstatement of the pressure could cause this.

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Study of thermal decomposition of NO from 1500-1900 K including work with added oxygen. NO_2 used as source of NO. Values given in Table I are from the reinterpretation by Kaufman and Kelso[7] who used their NO decomposition rate in the fit of Vetter's data. The expression is quoted from Kaufman and Decker.[6]

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Fast flow (~ 1 mm), N determined by quantitative electron spin resonance.

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Thermal decomposition of NO in the presence of O_2. Optical absorption of NO used for analysis. Several reactions occur, the $O + NO = N + O_2$ being relatively minor. A value for the rate was developed from studies of a 0.5% NO, 0.25% O_2, 99.25% Ar mixture in the 3900-600 K range. The expression is based on a fit to this work and references 4,6,8,10b. The 5000 K value in Table I was calculated from the expression. Since this work provides the high temperature tie point, more information on the spread of the experimental values is desirable.

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REACTION SUMMARY[†]

$H + O_2 = O + OH$

CHERRY-1967

Bahn[6] has calculated the rate reported here for the reverse reaction on the basis of that for the forward (endothermic) reaction estimated by Langen et al.[28] The rate is in good agreement with those determined from experimental data. An uncertainty factor of 5 was assessed.

JENSEN-1967

This reaction has been studied over a very wide range of temperatures. Fristrom and Westenberg[18] recommend a rate constant of $3.7 \times 10^{-10}e^{-16500/RT}$. Kurzius[26] finds $k = 2.8 \times 10^{-10}e^{-16200/RT}$. It is difficult to see how this rate constant can be greatly in error in the temperature range of interest.

SCHOFIELD-1967

Least squares fit for the forward reaction combining room temperature flow system,[13-14,25] flame,[16,17] explosion limit[1,3,5,7,22,27] and high temperature shock tube[29,30] data. Rate for the reverse reaction calculated using equilibrium data. Data and recommended value presented in both graphical and tabular forms.

TUNDER-1967

Rate quoted from Kaskan and Browne.[23]*

BAHN-1965

The preferred expressions for the forward reaction are from Kaufman and Del Greco.[25] Two values are provided for different temperature ranges

$k = 1.2 \times 10^{15}\exp(-17{,}800/RT)$ cm^3/mol-s 300-600 K

$k = 7.2 \times 10^{14}\exp(-16{,}900/RT)$ cm^3/mol-s 1500-1700 K

For general utility the latter expression is preferred. Equilibrium constant expression also given.

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[*] Listed separately in this reaction summary.

[†] Quoted activation energies are in cal mol^{-1}. R = 1.987 cal mol^{-1} K^{-1}.

BASCOMBE-1965

The value of the forward reaction is that suggested by Baldwin.[8*] The rate for the reverse reaction was developed using equilibrium data. This rate coefficient is cited as being consistent with other contemporary evaluations.[10a,13,14,34]

The available data are abundant. Sources recorded are references 2,7,9,10,12,15-17,19-22,24,30-33. The rate parameters of Karmilova, et al[22,32] and of Azatyan, et al[2] were considered to be low and those of Fenimore and Jones[17] to be high. Schott and Kinsey's results[30] were recalculated.

KASKAN-1964

The reaction has previously been reviewed by Kaufman and Del Greco[25] and by Voevodskii and Kondratiev.[33] The estimates for the rate coefficients listed combine data on the forward reaction from references 4,7, 11,17,22,30,33 and from references 12,25 for the reverse reaction. Strehlow and Cohen's[32a] activation energy for the forward reaction is consistent with the other data.

The experimental data and recommended values are graphed.

BALDWIN-1963

Selected data for $H + O_2 = O + OH$ were used to determine the rate coefficient applicable to the temperature range 293-1500 K. These data are taken from references 10,12,17,25,30,31, the studies of Kaufman and Del Greco[25] and Clyne[12] being on the reverse reaction. Reference 10 summarizes earlier work.

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REACTION SUMMARY

$H_2 + M = H + H + M$

CHERRY-1967

Hydrogen atom recombination is perhaps more thoroughly studied than any other. The identity of the third body, however, materially affects the rate constant. The rate (based on references 3,4,18,28) chosen was selected to provide an effective check on the upper limit with an uncertainty of a factor of 10.

JENSEN-1967

Values given only for the combination reaction. Work reported by Fristrom and Westenberg[11] suggests, for various third bodies,

$$k = 3 \times 10^{-29} T^{-1} \qquad (M \equiv H)$$

$$k = 1 \times 10^{-29} T^{-1} \qquad (M \equiv H_2)$$

$$k = 4 \times 10^{-30} T^{-1} \qquad (M \equiv \text{rare gas atom})$$

$$k \sim 4 \times 10^{-29} T^{-1} \qquad (M \equiv H_2O)$$

The direct measurements of H atom combination, however, are in consider able disagreement, and shock tube measurements on the dissociation are also difficult to interpret.[11] The value given is in reasonable agreement with the most convincing experiments.[16,22] It implies a pre-exponential factor in the rate constant for the dissociation of several hundred times the collision frequency. Our practice of listing rate constants for "average" third bodies is open to considerable doubt in this case; H_2O appears to be very much more efficient than H_2, for example.

SCHOFIELD-1967

Values for the combination rate coefficient are tabulated from references 5a,8,12,12a,15-17,17a,17b,18,18a,19-20,22 and 26. No synthesis is made nor rate coefficient recommended.

TUNDER-1967

Values given only for the combination rate. For M = H_2, H, H_2O and the general case these are the rates given by Kaskan and Browne.[142] The value for M = OH is from Wilde.[28]

BAHN-1965

Values given for the dissociation rate. An equilibrium constant expression is included for use in calculating the combination rate. For the generalized third body, the preferred expression is that of Duff,[9] which has been cited in many collections. The rates for M = Xe, H_2 and H are from Gardiner and Kistiakowsky.[12] Those for M = Ar and H_2O are from Skinner, et al.[23]

BASCOMBE-1965

Recombination data from studies near room temperature[15,16] and shock wave dissociation data (2800 K and above)[12,18,19,26] were used to set the recombination rates for M = H and M = H_2. Interpolation to 1400 K and comparison with flame data[8,13,20] was used to set rates for M = H and M = H_2O. These results lead to small negative activation energies for recombination. They are reflected in the reported activation energies for dissociation. Other references cited: 1,2,10,5, 21,24,25,27,29.

KASKAN-1964

$H + H + M = H_2 + M$

Evaluation of this rate is made in connection with that for $H + OH + M = H_2O + M$, since they occur together in flames where H and OH appear to be present in their equilibrium ratio.

The rates for H_2 dissociation and H atom combination are based on room temperature combination data[17] and high temperature shock tube[6,18,18,26] and flame[5,7,13] studies of the dissociation.

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REACTION SUMMARY†

$H_2 + O = H + OH$

MAYER-1968

Rate coefficients for both directions calculated by a modified Johnston and Parr technique. (See J+P in General Notes).

CHERRY-1967

The rate reported for the reverse reaction has been calculated by Bahn[5] on the basis of estimates[20] for the forward (endothermic) reaction. This rate is in good agreement with those determined from experimental data.[16] An uncertainty factor of 5 was assessed.

JENSEN-1967

Fristrom and Westenberg[14] suggest $k = 2 \times 10^{-11} e^{-9400/RT}$, but their estimate is perhaps rather too heavily weighted in favor of the results of Clyne and Thrush,[10] and the results in Fig. XIV-20 of Ref. 14 themselves suggest a somewhat lower activation energy. The rate constant given above is in fair agreement with the results of Wong and Potter[25] and of Kurzius[19] and seems a fair compromise.

SCHOFIELD-1967

Data from low temperature flow experiments[8,10] and high temperature shock tube work[22] were combined to give the recommended value for the forward reaction. These and other data[6,13,24,25] are presented in tabular and graphical form. The rate coefficient for the reverse reaction was calculated using equilibrium data. Other references noted: Nos. 1,3, but not used on the basis of Baldwin's[7] discussion.

TUNDER-1967

Value cited by A. A. Westenberg in 'Report on the Establishment of Chemical Kinetics Tables', CPIA unnumbered report April 1967, p. 48.

BAHN-1965

The preferred rate coefficient is that of Kaufman and Del Greco[17] who have examined this and related reactions in detail.

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† Quoted activation energies are in cal mol^{-1}. $R = 1.987$ cal mol^{-1} K^{-1}.

BASCOMBE-1965

The value selected for the forward reaction is that of Clyne[8,9] and Clyne and Thrush.[10,11] The rate coefficient of the reverse reaction was derived using equilibrium data. Other work discussed: references 4,6,13,15,18,21,23,24. Of these, the early work of Harteck and Kopsch[15] was rejected. Azatyan's[3] value was rejected on the basis of Baldwin's discussion.[7] [He states that he could not find evidence in their papers for a surface reaction destroying O atoms (as assumed) and that the comparison with $CO + O = CO_2$ required in interpreting their data may not be valid, since this combination is likely to be termolecular.] Baldwin's experimental value[6] for the activation energy was accepted, but his preexponential factor rejected. The value finally selected is representative of the modern work.

KASKAN-1964

Data from the work of Clyne,[8] Fenimore and Jones,[12] and Azatyan, et al[2] (cited in reference 16) were combined in this estimate. Reference 12 includes Baldwin's estimate[6] which was previously considered as the coefficient for $H_2 + OH = H + H_2O$. The data and recommended value for the rate of the forward reaction are graphed. The reverse rate was calculated using equilibrium data.

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REACTION SUMMARY

$O_2 + M = O + O + M$
$O + O + M = O_2 + M$

JOHNSTON-1968

Data points for the dissociation of O_2[1-6] and for recombination of O in Ar and O_2[7-13] were analyzed separately then combined (using equilibrium data) to permit calculation of the rate of dissociation over a wide range of temperature. From this analysis, the individual recommended rate coefficients $k_D(Ar)$, $k_D(O_2)$, $k_R(Ar)$, and $k_R(O_2)$ were developed, assuming the same temperature dependence for O_2 and Ar as third bodies. Rate coefficients for Ar as the third body are for the temperature range 300-15,000 K. Those for O_2 as the third body are for 1000-8000 K.

Reports considered but not used in the analysis (usually because data points were not available: references 14-17.

BASCOMBE-1965

Combination of O atoms has been studied below 700 K[6-9,11,12,18] and in shocks above 1500 K.[5,9,13] Dissociation experiments (3000 K and above)[1,2,5,14,16,17] also lead to combination rates, via the equilibrium constant. The temperature dependence derived from the dissociation experiments scatter (and are at times assumed). The rates do not extrapolate to the room temperature values. There are earlier reviews by Kaufman[18] and Wray.[4]

The recommended rates are based on the choice of a value (for combination) at 3500 K, the lower end of the temperature range for the shock tube work, of $(1.4 \pm 0.3) \times 10^{-33} cm^6 molecule^{-2} s^{-1}$, and a value at room temperature of $(3.0 \pm 0.5) \times 10^{-33}$. Nitrogen is taken as equally efficient as O_2 and O atoms as 2.5 times more efficient. The dissociation rate was recalculated from the combination results.

Other references cited: Nos. 3, 19-22.

JENSEN-1967

Fristrom and Westenberg[23] recommend the results of Morgan and Schiff[11] as the only unambiguous ones for direct recombination. For

$$O_2 + M = O + O + M$$

$$O + O + M = O_2 + M$$

$M = N_2$ they give $k = 3 \times 10^{-33}$ cm^6 $molecule^{-2}$ s^{-1} at room temperature, which suggests $k = 10^{-30}T^{-1}$. Shock tube studies[4,14,16,17] on dissociation would imply that k should be much larger, and suggest that the T^{-1} temperature dependence is reasonable in the range 1500-3500 K range. Note that dissociation rate constants[14,16,17] agree quite well with each other and have pre-exponential factors some 100 times larger than the collision frequency. The recombination rate coefficient selected implies pre-exponential factor in the dissociation rate coefficient of only 10 times the collision frequency. Discrepancies could perhaps be explained in terms of deviations from the macroscopic rate quotient law. The value of k given seems a reasonable compromise for an 'average' third body.

KASKAN-1964

The recommended values for $M = O_2$ are based on Wray's results[5,6] for the dissociation reaction. The available information on this system both at low and high temperatures is graphed (as combination rates). The data scatter badly. [Wray's rate coefficients are the lowest of those reported for the combination reaction.]

Critical reviews of the dissociation and combination reactions have been made by Harteck and Reeves,[24] Kaufman and Kelso[9] and Kaufman.[18] The low temperature work surveyed[7,9,11,12,19,25-28] is all for the combination reaction. Kaufman and Kelso suggest a combination rate of about $(1 \pm 0.3) \times 10^{15}$ cm^6 $molecule^{-2}$ s^{-1} for low temperatures and $M = O_2$. High temperature data are available both for the dissociation (2500-18,000 K)[1,2,5,6,14,16,17] and combination (1300-3000 K)[5,6,30] in shock tubes. The third body efficiencies measured in the various experiments conflict. Those recommended reflect the general trend of the high temperature data.

CHERRY-1967

The value selected for the combination reaction was determined for the third bodies O_2[31,39] H[31,32,39] and H_2O.[16,27,31,32,39] An assigned uncertainty of a factor of 10 ensures coverage of the full range of probable values reported.[5,31,33-38]

TUNDER-1967

The values reported for the dissociation rates ($M = O$, O_2, and in general) are those selected by Bortner[31] and reported by Wray.[6]

$O_2 + M = O + O + M$

$O + O + M = O_2 + M$

BAHN-1964

Dissociation rates are given, and an equilibrium expression for use in calculating the combination rate. Where the third body is identified, the values are those of Wray.[39] The generalized third body rate coefficient is based on the data of Matthews[16] for which $M + O_2$.

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$O_2 + M = O + O + M$

$O + O + M = O_2 + M$

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REACTION SUMMARY

$O_3 + M = O + O_2 + M$ (1,2)
$O + O_3 = O_2 + O_2$ (3,4)

JOHNSTON-1968

The evaluation of rate coefficients for these four reactions was combined. They are interrelated, 1, 2 and 3 being steps in the thermal decomposition of ozone. Only two values may be extracted from the ozone decomposition rate. The ratio k_2/k_3 is also available from photolyses of ozone. Reactions 2 and 3 have been studied directly. Reaction 4 has not been studied. Its rate is deduced from 3 and equilibrium data.

Recommended rate coefficients for reactions 1, 2 and 3 were developed from photolysis[6] and thermal decomposition data.[1,7,11,12,15,17,22,26-8,31,32] Other earlier work (reviewed in reference 1) that shows large scatter of points was rejected. The recommended third body efficiencies of O_3, O_2, He, Ar, N_2, and CO_2 were estimated from the papers cited above and reference 2.

The values for the rate coefficients for reactions 1 and 2 (developed solely from kinetic data) were shown to be consistent with the equilibrium constant.[16] Then the equilibrium data was used to extend the range of applicability of measurements on reactions 1, 2 and 3 in developing the reported recommended values.

The rate coefficients are applicable from 200 to 1000 K. The data used are tabulated and graphed.

SCHOFIELD-1967

Least squares fit for $O + O_2 + M = O_3 + M$. Ozone decomposition rates[2,3,17,32] and flow reactor studies of the $O + O_2$ reaction[7,21,22] used. Results of reference 32 recalculated. Results presented in tabular and graphical form. The data fit the Arrhenius form $k = A \exp(-E/RT)$ well, but fit the form $k = AT^{-n}$ poorly. [Not listed as a recommended value.]

TUNDER-1967

The value for the rate coefficient for decomposition of ozone (reaction 1) is based on those recommended by Bortner[4] and by Benson and Axworthy.[2,3]

$$O_3 + M = O + O_2 + M \quad (1,2)$$
$$O + O_3 = O_2 + O_2 \quad (3,4)$$

BASCOMBE-1965

A value was set for the rate coefficient $O + O_2 + M = O_3 + M$ at room temperature; $k = (2.5 \pm 0.8) \times 10^{-34}$ cm^6 $molecule^{-2}$ s^{-1}, $M = O_2$ and E taken as -1000 calories. Both the rate and E emphasize Benson and Axworthy's[2] 1957 reinterpretation of most of the earlier ozone pyrolysis work, particularly that of Glissman and Schumacher.[12] A later revision of the O_2 dissociation energy[5] was used in setting E. Other work is included in the analysis, both ozone pyrolysis[17,24], and direct combination studies.[9,10,13,18-21,25] Rates for $M = O_3$ and $M = N_2$ are scaled approximately as set by Benson and Axworthy.[2] The pyrolysis rate (reaction 1) was reevaluated using equilibrium data after establishment of the values for the combination.

The value for reaction 3 is that of Benson and Axworthy[2] with a revised activation energy, E = 5600 cal/mol (because of the revision of the dissociation energy of oxygen).[5] This leads to a rate coefficient at room temperature of $(8.3 \pm 0.6) \times 10^{-15}$ $cm^3 molecule^{-1} sec^{-1}$. Shock wave ozone pyrolysis data[17] are in good agreement. However, other ozone pyrolyses[20] and direct studies of reaction 3 (mass spec. analysis and O formed by an electric discharge)[30] give room temperature values of 3.5×10^{-14} and 2.5×10^{-14}, respectively. The activation energy is considered to be uncertain. The rate for reaction 4 was calculated using the equilibrium constant.

KASKAN-1964

The recommended expression for reaction 2 is that of Benson and Axworthy,[2] and that for reaction 1 is consistent with it and equilibrium data. Results from references 2,9,10,14,17,18,23,24,29,32 are considered. With the exception of a shock wave decomposition study[17] the experiments are for low temperatures. Certain results from references 9,10,14 were rejected because of likely wall effects, impurities and incorrect assumptions. See reference 23 for discussion. Earlier reviews are to be found in references 14,20, and 23.

BAHN-1964

On an "engineering selection" basis the preferred expressions are those of Davidson.[8] Rate coefficients are stated for reactions 1 and 4 Equilibrium constant equations are provided for calculation of the other rates.

CHAPTER 6: GENERAL NOTE CODES

BEBO	Bond energy-bond order calculation of activation energy. See description in this chapter.
CT	Collision theory estimate.
EST	The rate has been estimated by analogy to similar specific reactions. Usually no experimental data are available.
EVAL	A detailed analysis of the available data is presented. The basis for (or method used in deriving) the recommended rate is made evident.
J+P	Johnston and Parr linear transition state calculation of rate coefficient, including BEBO determined activation energy. See description in this chapter.
OME	Order of Magnitude Estimate used for reactions of similar formal type (bimolecular, termolecular, ion-molecule, etc.). See description in this chapter.
REV	From data (usually experimental) on the reverse reaction.
SEL	The rate reported is a value selected from the available data. It may be the only available datum.
XP	Rate developed from available experimental data. May include acceptance of an earlier evaluation .

BEBO Bond-energy-bond order calculation of activation energies

This technique is a component of the Johnston and Parr method described in a separate general note. References are given there. The notation BEBO in the table means that the activation energy was calculated by this technique, but that collision theory was used for the pre-exponential term (because of the appearance of unreasonable geometric factors in the transition state calculation).

The bond energy-bond order technique calculates an activation energy from a potential energy surface that represents the interaction of the (linear) reacting system. The problem solved is how to calculate the surface, or at least the energies along the reaction coordinate. An empirical surface is used that is based on atom-pair interactions and includes repulsive interaction of the type introduced by Sato. The atom-pair interactions are needed at distances other than equilibrium (where they are given by molecular constants). These interactions are set by correlating equilibrium bond-energies of similar bonds with inter-atom distances and then using the functional relationship to establish energies at other distances. This permits calculation of the surface.

The reaction coordinate is specified by another postulate: that the total bond order remains constant along the reaction coordinate. That is, as one bond is formed, its order increases while the order of the bond being broken decreases a corresponding amount. A definition of bond order as a function of distance is needed. This is established by correlating equilibrium bond orders with distance for related bonds, as for example, the carbon-carbon triple, double and single bonds, using inert gas interaction distances for zero bond order. In effect, the technique applies the chemist's concept of bond order, as developed by Pauling, to the calculation of activation energies.

This method has been applied extensively in the computation of reaction rates by Tunder, Mayer, Cook and Schieler and by Mayer and Schieler that are included in this compendium.

J+P Johnston and Parr technique for the calculation of rate coefficients

This is an empirical (or semiempirical) method for calculating rate of reaction.[3,7] It is a development that uses the formalism of absolute rate theory and a special approximation (bond energy-bond order) for estimating the activation energy.[1,2]

The application of the technique to elementary reactions in this table is primarily to hydrogen atom transfers:[4,6,9]

$$A + BH \rightarrow AH + B$$

(although some application has been made to other transfers[5]) and is limited to the estimation of their rates at high temperatures. This last restriction deemphasizes any errors in the activation energy calculation.

In the Johnston and Parr technique for hydrogen transfer reactions, a linear transition state is assumed. The partition function ratio between this state and the reagents is calculated from molecular parameters for the reagents and the structure of the transition state as determined by the bond energy-bond order approximation to the potential surface. The BEBO also gives the activation energy. In effect there are no parameters derived from kinetics introduced into the calculation.

In recent work certain atom transfer reactions have been excluded from the Johnston and Parr treatments. The exclusion is based on the appearance in the partition function of unreasonable geometric factors for the angle of approach of the atom to the diatomic molecule.[4,6]

The technique has been used extensively in the compilations of Tunder, Mayer, Cook and Schieler[8] and of Mayer and Schieler[6] included here.

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ORDER OF MAGNITUDE ESTIMATES FOR RATE COEFFICIENTS

When no experimental data nor theoretical calculations are available for a reaction, estimates are often made. These usually fall into two categories: argument by analogy to specific reactions similar to the one in question, and formal estimates based on reaction types.

It is the latter class that is described here. For these formal estimates one does not enquire about what atoms or molecules react, but merely is the reaction one between two atoms, between an atom and a molecule, how many atoms there are in the molecule, whether the mechanism is an atom (or group) transfer or a four center exchange. At times the size of the molecule is considered. A number of these estimates are tabulated at the end of this section.

DISCUSSION

All order of magnitude estimates should be taken with a grain of salt. They may be good or very bad. Chemistry is not that simple. Also, estimates do not always match the tabulated rules. The evaluator tends to shift the value to fit the specific case. It is common to find lower estimates as the molecular complexity increases.

These estimates are invariably estimates of the rate <u>parameters</u>: pre-exponential factor, coefficient of a temperature term and activation energy as opposed to a direct estimate of the rate coefficient. They are not precise. They are intended to serve either until more specific information becomes available on the reaction or to set a limit on the likely value of the rate.

Collision theory provides an upper limit for bimolecular reaction rate pre-exponential factors although a rough one. The term $10^A T^B$ may be estimated from

$$k = \left(\frac{8\pi kT}{\mu}\right)^{\frac{1}{2}} \frac{d^2}{\sigma} P \alpha$$

where μ is the reduced mass in g/mole, d, the collision diameter in Å, σ the symmetry number (1 for unlike reactants, 2 for like), P, the steric factor and α is a count of equivalent reaction paths.

The path count as used by Tunder, et al[3] for hydrogen atom transfers in the reaction AH + B = A + BH is

$$\alpha = r_s \left(g_{BH}\, g_A / g_{AH}\, g_B\right)^{\frac{1}{2}}$$

where r_s is the number of equivalent hydrogens and the g's are electronic multiplicities.

The estimation of activation energies is an art. The simple rules are empirical or semi-empirical. Hirschfelder's two rules, for atom transfer and exchange reactions are listed in the tables. The Johnston and Parr Technique calculations (which also rest on linear transition state theory) do not give results that agree with these rules.

Another widely cited rule for atom transfer reactions is based on the suggestion of Evans and Polanyi.[8] This calls for a proportionality between the heat of an exothermic reaction and the activation energies in a set of homologous reactions. As developed and displayed by Semenov[9]

$$E^* = 11.5 + 0.25\ \Delta H \quad \text{kcal mol}^{-1}$$

where ΔH has its normal sign (- for exothermic reactions). Benson and DeMore[6] have discussed this and other rules. They point out exceptions and suggest that the rules have limited use since 90% of measured exothermic radical abstraction reactions have activation energies of 8 ± 3 kcal mol^{-1} and the rules rarely predict this well.

The same article summarizes the work on the development of a model for estimating activation energies of four center molecule-molecule reactions.[10,11] This model assumes polarization of the bonds involved ("semi-ion pair"). Activation energies for a number of exothermic reactions have been calculated to ±1 kcal mol^{-1} with a maximum deviation of ±3 kcal mol^{-1}.

One may hope that the simple order of magnitude estimates will fade away, will be replaced by more powerful calculation techniques. But the history of kinetics suggests that the refinement of theories does not often lead to improved precision. Empirical correlations will continue to be useful. It appears desirable to develop more of these and to develop ones that are restricted to sets of closely similar reactions.

Order of Magnitude Estimates $k = 10^A T^B \exp(-1000C/T)$

	A^a	B^b	$1000 \cdot C^c$	Notes
Termolecular combination, of neutrals, exothermic[d]				
$X + Y + M = XY + M$	~ -31.1 ~ -31.6	-0.5 -0.5	0 0	e,f g
Bimolecular, neutral, exothermic	~ -11.1 log P	+0.5	any rule	h
Atom transfer, atom and diatomic molecule				
$X + YZ = XY + Z$	~ -12.1	+0.5	$a\Delta E(Y-Z)/R$	e,f,i
Atom (group) transfer, four or more atoms in collision complex				
$\left.\begin{array}{l} W + XYZ = WX + YZ \\ WZ + XY = WZX + Y \end{array}\right\}$	~ -12.8	+0.5	$a\Delta E(Y-Z)/R$	e,f,i
$R_1H + R_2 = R_1 + R_2H$	collision theory	+0.5	0	f,j
Atom transfer from polyatomic molecule to atom				
$X + RY = XR + Y$	~ -(9.8 ± 0.5)	0	$(2.0 \pm 1.5) \times 10^3$	g
Atom transfer from diatomic molecule to polyatomic radical				
$R + XY = RX + Y$	~ -(10.8 ± 0.5)	0	$(4.0 \pm 1.5) \times 10^3$	g
Atom (group) transfer from polyatomic molecule to polyatomic radical				
$R_1 + XR_2 = R_1X + R_2$	~ -(12.3 ± 0.5)	0	$(4.0 \pm 1.5) \times 10^3$	g
Exchange (four center)				
$XY + WZ = XW + YZ$	~ -13.8	+0.5	$b(\Delta E(XY) + \Delta E(WZ))/R$	e,k

Order of Magnitude Estimates (Cont'd)

	A^a	B^b	$1000 \cdot C^c$	Notes
Bimolecular, neutral, exothermic (cont'd)				
Radical-radical combination				
$R_1 + R_2 = R_1R_2$	~ -10.3	0	0	g
Addition of atom to unsaturated molecule				
$X + {>}C{=}C{<} = {>}CX{-}C{<}$	~ -10.8	0	$(0.75 \pm 0.25) \times 10^3$	g
Addition of radical to unsaturated molecule				
$R + {>}C{=}C{<} = {>}CR{-}C{<}$	~ -12.3	0	$(4.0 \pm 1.5) \times 10^3$	g
Unimolecular reactions of neutrals				
Expulsion of atom from molecule				
$R_1X = R_1 + X$	~ 14 to 15	0	$> \Delta E(R_1X)/R$	1
Expulsion of stable molecule producing unsaturation (four center)				
${>}CX{-}CY{<} = {>}C{=}C{<} + XY$	~ 13.5 ± 0.5	0	$> \Delta E/R$	1
Decomposition with internal ring formation	~ 11.5 ± 0.5	0	$> \Delta E/R$	1

Order of Magnitude Estimates (Cont'd)

	A^a	B^b	$1000 \cdot C^c$	Notes
<u>Reactions involving charged particles</u>				
Charge Transfer				
$\left.\begin{array}{l} X^+ + Y = X + Y^+ \\ X^- + Y = X + Y^- \end{array}\right\}$	~ -12.2	+0.5	0	f,m
Ion-electron combination				
$X^+ + e^- + M = X + M$	~ -23.9	-1.5	0	f,m
Electron attachment				
$X + e^- + M = X^- + M$	~ -27.6	-1.0	0	f,m
Ion combination-neutralization				
$X^+ + Y^- + M = XY + M$	~ -29.2	-0.5	0	f,m
Ion neutral combination				
$X + Y^- + M = XY^- + M$	~ -29.2	-0.5	0	f,m
Associative detachment				
$X^- + Y = XY + e^-$	~ -12.1	+0.5	0	f,m

NOTES

a. Units: time in seconds, temperature in Kelvin, concentration in molecules/cm^3. The order of the reaction is equal to the number of reactants shown.

b. Coefficients of the temperature term are invariably based on theory, when they are non zero.

c. 1000·C is the activation energy, E^*, divided by the gas constant, R. The factor of 1000 is introduced to maintain consistency with the main table where C is scaled. To convert C to kilojoules/mole, multiply by 8.315.

An activation energy for an exothermic reaction represents the dynamic energy barrier. That for the reverse, endothermic reaction should be the endothermicity plus the same barrier. However, for highly endothermic decompositions the experimental activation energy is often very close to the energy of the reaction.

d. These estimates are, essentially, for reaction on every triple collision. Schofield[1] tabulates measured combination rates for atoms and atoms plus diatomic molecules. These k's show small negative temperature coefficients and fall in the range 10^{-34} to 10^{-29} $cm^6 molecule^{-2} s^{-1}$.

e. Reference 2.

f. Reference 3.

g. Benson's estimates for bimolecular reactions based on examination of rates of reaction of organic molecules.[4] The decomposition rates apply in the high pressure region.

h. Collision theory value for unlike reactants ($\sigma = 1$), collision diameter, d = 0.2 nm, reduced mass 4 g/mol^{-1}(M = 8) and one reaction path ($\alpha = 1$),see discussion. P is the steric factor < 1.

i. Activation energy set according to Hirschfelder's rule.[5] Cherry, et al use a = 0.055. Tunder, et al use a = 0.06. ΔE is the energy of the dissociation reaction: $YZ + M = Y + Z + M$ $\Delta E = \Delta H - RT$ Also see discussion.

j. A modified collision theory equation is used by Tunder, et al[3] for hydrogen transfer reactions in which there is more than one equivalent hydrogen, e.g. for $NH_3 + F = NH_2 + HF$. The modification consists of counting the reaction paths in terms of the number of equivalent hydrogens and the electronic multiplicities. P (steric factor) = 0.1. This method gives slightly higher value than do other formal estimates.

k. Activation energy set according to Hirschfelder's rule for exchange. reactions.[5] Cherry, et al use b = 0.2. Also see discussion.

l. Estimated by Benson and DeMore.[6] A comprehensive review of unimolecular reactions by S. W. Benson and H. O'Neil that provides evaluated rates for several hundred reactions is in press (NSRDS Series).

m. Estimates developed by Tunder, et al[3] based on rates compiled by Bortner.[7]

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2. Cherry, S. S., Gold, P. I., and Van Nice, L. J. TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.
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4. Benson, S. W., Ind. Eng. Chem. 56, 18 (1964).
5. Hirschfelder, J. O., J. Chem. Phys. 9, 645 (1941).
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7. Bortner, M., General Electric Missile and Space Division, Report No. R63SD34 (1964).
8. Evans, M. G. and Polanyi, M., Trans. Faraday Soc. 34, 11 (1938).
9. Semenov, N. N., "Some Problems in Chemical Reactivity", trans. by M. M. Boudart (Princeton 1958), Vol. 1, Ch. 1, p. 29.
10. Benson, S. W. and Bose, A. N., J. Chem. Phys. 39, 3463 (1963).
11. Benson, S. W., Bose, A. N., and Nangia, P., J. Am. Chem. Soc. 85, 1388 (1963).

CHAPTER 7: SPECIFIC NUMBERED NOTES FOR THE TABLE OF RATE COEFFICIENTS

A set of notes for each evaluation source cited in the table is included here. These refer to the numbers in parentheses after the source identification. Each source has a separate set. These sets are arranged alphabetically by author.

If the paper or report was written as a table with notes, those given here follow the original material. However, they have been rewritten to make them fit into this larger collection. Internal cross references have been spelled out and references included. Occasionally an obvious error has been rectified or an ambiguity noted. If the paper was in the form of an extended discussion, only the briefest summary has been extracted. This shows the data considered and, occasionally, the basis of the evaluation.

The sources for which notes are provided here follow.

BAHN-1964, 1965, 1968
Bahn, G. S., Pyrodynamics 1, 147, 271, 335 (1964); 2, 91, 197, 315 (1965); 3, 245 (1965); 6, 101 (1968).

BALDWN-1963
Baldwin, R. R., Ninth Symposium (International) on Combustion, p. 667 (1963), Academic Press, N. Y.

BASCMB-1965
Bascombe, K. N., "Reaction Rate Data" The Hydrogen/Oxygen System", Ministry of Aviation, Explosives Research and Development Establishment, Waltham Abbey, Essex, England, E.R.D.E. 1/S/65

BAULCH-1968
Baulch, D. L., Drysdale, D. D., and Lloyd, A. C., "Critical Evaluation of Rate Data for Homogeneous, Gas-Phase Reactions of Interest in High-Temperature Systems", Dept. of Physical Chemistry, The University, Leeds, England, High Temperature Reaction Rate Data, Report No. 1, May 1968.

CHERRY-1967
Cherry, S. S., Gold, P. I., and Van Nice, L. J., Phase I Final Report, "Screening of Reaction Rates" 22 May 1967. TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.

JENSEN-1967
Jensen, D. E. and Kurzius, S. C., "Rate Constants for Calculations on Nozzle and Rocket Exhaust Flow Fields", AeroChem Research Laboratories, Princeton, New Jersey, March 1967. Report TP-149.

JONSTN-1968
Johnston, H. S., "Gas Phase Reaction Kinetics of Neutral Oxygen Species", NSRDS-NBS Monograph Series (in press, 1968).

KASKAN-1964
Kaskan, W. E. and Browne, W. G., "Kinetics of the $H_2/CO/O_2$ System", General Electric Company Space Sciences Laboratory Report R64SD37, July 1964.

MAYER-1968
Mayer, S. W. and Schieler, L., "Computed Activation Energies and Rate Constants for Forward and Reverse Transfers of Hydrogen Atoms", J. Phys. Chem. 72, 236 (1968). Also appeared in Chemical Propulsion Information Agency publication No. 146, Vol. I, p. 121, (1967).

SCOFLD-1967
Schofield, K., "An Evaluation of Kinetic Rate Data for Reactions of Neutrals of Atmospheric Interest", Planet. Space Sci. 15, 643 (1967).

TUNDER-1967
Tunder, R., Mayer, S., Cook, E., and Schieler, L., "Compilation of Reaction Rate Data for Nonequilibrium Performance and Reentry Calculation Programs", Aerospace Corp., Thermochemistry Research Dept., Aerospace Report No. TR-1001(9210-02)-1 (1967).

WILSON-1968
Wilson, Wm. E., Jr., "Kinetics Tables for the Reactions of Hydroxyl Radicals", see Chapter V of this report.

Wilson, Wm. E., Jr. and Garvin, David, "Kinetics Tables for the Reactions $N + O_2 = NO + O$ (k_+), $NO + O = N + O_2$ (k_-)", see Chapter V of this report.

BAHN, G. S., Pyrodynamics 1 (1964); 2 (1965); 3 (1965); 6 (1968)

CHEMICAL KINETICS

Introduction

The Chemical Kinetics Section of Pyrodynamics has featured compilations of rate data and lists of selected, "preferred" values for rate coefficients.

Selected values for the O, N, H, O-N, and H-O are presented in Vols. 1, 2 and 3. Two reactions, $CO + OH = CO_2 + H$ and $CO + O + M = CO_2 + M$ are covered in the first issue of Vol. 6. It is these sections that are summarized in this compendium. The other Chemical Kinetics Sections are compilations without selection. Of particular interest is the extensive compilation (with rate expressions and bibliographic family trees for them) that has also appeared in Pyrodynamics.[1] This bibliography is very good in its coverage of the report literature (as well as published material). It cites secondary as well as primary sources and thus carries a heavy burden of simple quotations.

The selection of rate constants has been described as having an "engineering" as opposed to a "scientific" basis.[2-4] "Engineering selection" is examination of the available material of the most representative (or widely accepted) value. Simple tests are made for reasonableness, i.e. bimolecular rates not exceeding the collision number. "Scientific" selection, on the other hand, includes examination of the method and possible errors.

This compendium includes most of the reactions listed in Vol. 1 (1964) and Vols. 2 and 3 (1965). Some of the HO_2 radical and some for which temperature dependences are not available have been omitted. Items that may have been outdated by later work have not been removed.

Rates are tabulated by Bahn for one direction and, in most cases, equilibrium data are provided for use in calculating the rate in the other. The equilibrium data are not listed here (nor indicated repeatedly in the notes). Only reactions explicitly tabulated in the original appear in this compendium.

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1. Pyrodynamics 5, 49, 75, 221, 375 (1967).
2. Bahn, Western States Section, The Combustion Institute, Paper 67-11, April 1967.
3. Ellis and Bahn, Western States Section, The Combustion Institute, Paper 62-27, November 1962, Part 1.
4. Bahn, Western States Section, The Combustion Institute, Paper 62-27, November 1962, Part 2.

Pyrodynamics 1, 147 (1964).
"Chemical Kinetics. Reactions Involving N_2, O_2, NO, N and O"

Pyrodynamics 1, 271 (1964).
"Chemical Kinetics. Reactions Involving N_2O, NO_2 and O_3, but Only One of these Species, with N_2, O_2, NO, N and O"

Pyrodynamics 1, 335 (1964).
"Chemical Kinetics. Reactions Among N_2O, NO_2, and O_3, Also Involving N_2, O_2, NO, N and O"

1. $O_2 + M = O + O + M$

See Reaction Summary.

2. $N_2 + M = N + N + M$

For the generalized third body, the value is that of Eschenroeder, Boyer and Hall for which $M = N_2$. The preferred rates when M is to be identified are those of Wray.

Eschenroeder, et al, Cornell Aeron. Lab. Report AF-1413-A-1 (May 1961).

Wray, "Hypersonic Flow Research" p. 181 (1962), Academic Press, N.Y.

3. $N_2 + O_2 = NO + NO$

Freedman and Daiber, J. Chem. Phys. 34, 1271 (1961).

4. $NO + M = N + O + M$

The rate expression for the generalized third body is that of Eschenroeder. That for identified third bodies is from Wray's summary.

Eschenroeder, et al, Cornell Aeron. Lab. Report AF-1413-A-1 (May 1961).

Eschenroeder, et al, Phys. Fluids 5, 615 (1962).

Wray, "Hypersonic Flow Research" p. 181 (1962), Academic Press, N.Y.

5. $N_2 + O = NO + O$

Marrone, Anti-Missile Res. Advisory Council Proc. 4, 353 (1961).

6. $NO + O = N + O_2$

Kistiakowsky and Volpi, J. Chem. Phys. 27, 1141 (1957).

Also see Reaction Summary for $N + O_2 = N + NO$.

7. $O + N_2O = NO + NO$

Fenimore and jones, Symp. Combust. 8th, p. 127 (1962).

8. $N_2 + O_2 = N_2O + O$

9. $NO + O_2 = NO_2 + O$

Davidson, AVCO Mfg. Corp. Research Report 32 (June 1958).

10. $NO_2 + M = NO + O + M$

Expression from Levitt, based on data of Huffman and Davidson.

Levitt, Trans. Faraday Soc. 59, 59 (1963).

Huffman and Davidson, J. Am. Chem. Soc. 81, 2311 (1959).

11. $N_2O + O = N + NO_2$

$N_2 + O_2 = N + NO_2$

Nawrocki and Papa, "Atmospheric Processes" (1963), Prentice-Hall, N.J.

12. Estimate (no data) made by Ludwig and Sulzmann. No other expression is available.

Ludwig and Sulzmann, Convair Division, General Dynamics Corp. Report ZPh-082 (February 1961).

13. $O_2 + O_2 = O + O_3$

$O_3 + M = O + O_2 + M$

See Reaction Summary for $O_3 + M = O + O_2 + M$.

14. $NO_3 + M = NO + O_2 + M$

Schott and Davidson, J. Am. Chem. Soc. 80, 1841 (1958).

15. $NO_2 + O = N + O_3$

This expression, fabricated by Ludwig and Sulzmann is the only one available for the forward reaction that incorporates a temperature dependence.

Ludwig and Sulzmann, General Dynamics Corp. Report ZPh-082 (Feb. 1961).

16. $NO_2 + O_2 = NO + O_3$

The preferred expression is that of Davidson, which was derived from the data of Johnston and Crosby [on the reverse reaction].

Davidson, AVCO Mfg. Corp. Research Report 32 (June 1958).

Johnston and Crosby, J. Chem. Phys. 22, 689 (1954).

17. $N_2 + NO_2 = NO + N_2O$

From the compilation of Davidson derived from data of Kaufman and Kelso.

Davidson, AVCO Mfg. Corp. Research Report 32 (June 1958).

Kaufman and Kelso, J. Chem. Phys. 23, 1702 (1955).

18. $NO_2 + NO_2 = NO + NO + O_2$

Huffman and Davidson, J. Am. Chem. Soc. 81, 2311 (1959).

BAHN-1964, 1965

19. $N + NO_2 = N_2 + O + O$

Harteck and Dondes, J. Phys. Chem. 63, 956 (1959).

20. $N_2O + NO_2 = N_2 + NO + O_2$

Bortner, GE Missile & Space Vehicle Dept. Rept. R61SD122 (June 1961).

Only available rate constant - determined at 199°K.

BAHN-1965

Pyrodynamics 2, 91 (1965).
"Chemical Kinetics. Reactions Involving NO_3 with N_2O, NO_2, O_3, O_2, NO, N and O. Reactions Involving N_2O_4 and N_2O_5 with NO_2 and NO_3"

Pyrodynamics 2, 197 (1965).
"Chemical Kinetics. Reactions Involving H_2, O_2, OH, H and O"

Pyrodynamics 2, 315 (1965).
"Chemical Kinetics. Reactions Involving H_2O, HO_2, and O_3 but Only One of these Species with H_2, O_2, OH, H and O"

Pyrodynamics 3, 245 (1965).
"Chemical Kinetics. Reactions Among H_2O, HO_2, H_2O_2, and O_3, also Involving H_2, O_2, OH, H and O"

1. Ludwig and Sulzmann, General Dynamics Corp. Rept. ZPh-082 (Feb. 1961).

   Only expression available. Estimated. No data.

2. $NO_3 + M = NO_2 + O + M$

   The preferred expression is that documented by Huffman and Davidson. It is the only one available containing a T^{-s} term.

   Huffman and Davidson, J. Am. Chem. Soc. 81, 2311 (1959).

3. $NO + NO_3 = NO_2 + NO_2$

The preferred expression is that of Davidson and Schott, indicating that the rate is essentially independent of temperature.

Davidson and Schott, J. Chem. Phys. 27, 317 (1957).

4. $NO_2 + O_3 = NO_3 + O_2$

The preferred expression, given by Ford, is the only one available containing a temperature dependence.

Ford, Symp. Combust. 8th, p 119 (1962).

5. $NO_3 + NO_3 = NO_2 + NO_2 + O_2$

This preferred expression is that documented by Schott and Davidson, including a stated tolerance on the activation energy.

Schott and Davidson, J. Am. Chem. Soc. 80, 1841 (1958).

6. $N_2O_4 + M = NO_2 + NO_2 + M$
$N_2O_4 = NO_2 + NO_2$

The preferred expressions for N_2O_4 decomposition are the only ones available containing temperature dependencies. The bimolecular reaction applies at low pressure, and the monomolecular at high pressure.

Carrington and Davidson, J. Phys. Chem. 57, 418 (1953).

7. $N_2O_5 + M = NO_3 + NO_2 + M$

The preferred expression, given by Schott and Davidson is the only one available for the forward direction. It applies at high pressure.

Schott and Davidson, J. Am. Chem. Soc. 80, 1841 (1958).

8. $N_2O_5 = NO_2 + NO_3$

These expressions are the only ones available for N_2O_5 decomposition that contain temperature dependencies.

Histasune, et al, J. Am. Chem. Soc. 79, 4648 (1957).

9. $H_2 + M = H + H + M$

See Reaction Summary.

10. The preferred expression is that reported by Skinner, et al based on their research.

Skinner, et al, U.S.A.F. Systems Command Report ASD-TDR-62-1042 (Dec. 1962)

11. $OH + M = O + H + M$

The preferred expression is that of Duff, because of its general citation and use. Other expressions are not markedly different.

Duff, J. Chem. Phys. 28, 1193 (1958).

12. $H + H_2O = H_2 + OH$
$H_2O + O = OH + OH$
$H_2 + O = H + OH$

In each case the preferred expression is that of Kaufman and Del Greco. These authors examined these reactions in very careful detail. Also see Reaction Summaries.

Kaufman and Del Greco, Symp. Combust. 9th, p 659 (1963).

13. $H + O_2 = O + OH$

See Reaction Summary.

14. $H_2O + M = H + OH + M$

The four available expressions are from Duff for M = Xe, He, and from Skinner, et al. for M = Ar, H_2O. If the third body is not to be identified, the value for M = Xe is preferred as more widely known.

Duff, J. Chem. Phys. 28, 1193 (1958).

Skinner, et al, U.S.A.F. Systems Command Report ASD-TDR-62-1042 (Dec. 1962)

15. $H_2O_2 + M = OH + OH + M$

The only available expressions for peroxide decomposition are those of Baldwin and Brattan. These authors report an activation energy of 46.3 kcal mol^{-1}. They demonstrate that this value is consistent with the heat of reaction (50.3 kcal by their citation, 51.19 kcal by the JANAF Thermochemical Tables) if the Rice-Ramsperger Theory is applied with S = 4 in the equation

$$k = Z \exp(-E/RT) \cdot (E/RT)^{S-1}/(S-1)!$$

This implies zero activation energy for the recombination reaction and leads to the alternative expression

$$k = 7.5 \times 10^{26} T^{-3} \exp(-50,100/RT) cm^3 \; mol^{-1} s.$$

which is also listed.

Baldwin and Brattan, Symp. Combust. 8th, p 110 (1962).

16. $HO_2 + M = H + O_2 + M$

The only available expression.

Skinner, et al, U.S.A.F. Systems Command Report ASD-TDR-62-1042 (Dec. 1962)

17. $HO_2 + H_2O = H_2O_2 + OH$

Voevodsky, Symp. Combust. 7th, p 34 (1959).

Pyrodynamics 6, 101 (1968).
"Chemical Kinetics. The Reactions $H + CO_2 = OH + CO$ and $CO_2 + M = O + CO + M$"

1. $CO + OH = CO_2 + H$

See Reaction Summary.

2. $CO_2 + M = CO + O + M$

The value cited is an empirical curve fit to the data of Olschewski, et al (1967) making the activation energy equal to the dissociation energy and the rate coefficient for the reverse reaction not exceed the collision frequency at low temperature. "The expression reproduces the experimental work in the 2000-5000°K range and precludes ridiculous recombination rates around 500-1000°K. Clearly, however, this reaction urgently needs a detailed scientific review and evaluation of available data, and probably needs extensive additional experimentation after that." Data compiled from the following references.

Brabbs, et al, J. Chem. Phys. 38, 1939 (1963).

Michel, et al, Z. Phys. Chem. 39, 129 (1963).

Michel, et al, Z. Phys. Chem. Neue Folge 44, 160 (1965).

Olschewski, et al, Symp. Combust. 11th, p 155 (1967).

Howe, et al, Nat. Aeron. Space Admin. Tech. Note D-1885 (June 1963).

Howe and Sheaffer, Nat. Aeron. Space Admin. Tech. Note D-2131 (Feb. 1964).

Davies, J. Chem. Phys. 41, 1846 (1964).

Davies, Ibid 43, 2809 (1965).

Steinberg, Nat. Aeron Space Admin. Contractor Rept. CR-166 (Feb. 1965).

Fishburne, et al, J. Chem. Phys. 45, 160 (1966).

Myers and Sulzmann, General Dynamics/Astro. Rept. GDA-DBE-64-001(June 1964).

Heicklen, AIAA J. 5, 4 (1967).

BALDWIN, R. R., Ninth Symposium (International) on Combustion, p. 667
(1963), Academic Press, N. Y.

1. H + O_2 = O + OH

Selected data for H + O_2 = OH + O are used to determine the rate coefficient for the range 293-1500 K. Data used are from

Schott and Kinsey, J. Chem. Phys. 29, 1177 (1958)

Fenimore and Jones, J. Phys. Chem. 63, 1154 (1959)

Baldwin and Cowe, Trans. Faraday Soc. 58, 1768 (1962)

who summarize earlier work

Semenov, Acta Physicochim. URSS 20, 291 (1945)

Clyne, Symp. Combust. 9th, p. 211 (1962)

Kaufman and Del Greco, Symp. Combust. 9th, p. 659 (1962)

the last two being studies of the reverse reaction

Also see Reaction Summary.

BASCOMBE, K. N., "Reaction Rate Data: The Hydrogen/Oxygen System", Ministry of Aviation, Explosives Research and Development Establishment, Waltham Abbey, Essex, England, E.R.D.E. 1/S/65

Introduction

This report summarizes and evaluates the experimental rate data available for twenty reactions (counting forward and reverse as one) in the hydrogen-oxygen system. "Best values" are given for most of these. One hundred thirty-seven references are cited.

The species in the reactions are H, H_2, H_2O, H_2O_2, HO_2, O, O_2, O_3 and OH. Rate coefficients are stated in the Arrhenius form: $k = A \exp(-E/RT)$, no use being made of a T^B term. Where possible uncertainty limits are given for the rate parameters, these being assessments of reliability of the numbers, not all-inclusive ranges.

Each reaction system (forward and reverse) is discussed separately. The available data are summarized, commented upon and selected for use in establishing the best value. Data for both the forward and reverse reaction are employed (using equilibrium data) to set the rate in one direction. The other rate is then recalculated.

The "best values" are included in this compendium. The other reactions discussed in the report are:

$HO_2 + M = H + O_2 + M$

$H + O_3 = OH + O_2$

$OH + O_3 = HO_2 + O_2$

$H + HO_2 = OH + OH$

$H + HO_2 = H_2 + O_2$

$H + HO_2 = H_2O + O$

$HO_2 + O = OH + O_2$

$H_2 + HO_2 = H + H_2O_2$

$HO_2 + HO_2 = H_2O_2 + O_2$

$HO_2 + H_2O = H_2O_2 + OH$

$H + H_2O_2 = H_2O + OH$

$H_2O_2 + O = HO_2 + OH$

$H_2O_2 + HO_2 = H_2O + OH + O_2$

The applicable temperature range for the best values is stated as follows: "The [derived rates] should be applicable not only to hydrogen/oxygen at all temperatures but also to hydrogen/air systems at temperatures up to 3000°K". Arbitrarily, for this compendium the range is stated as 300°K to 3000°K except where the reported experimental data include higher temperatures.

The notes given here are drastic abridgments of Bascombe's discussions.

1. $H_2 + OH = H + H_2O$

See Reaction Summary for $H + H_2O = H_2 + OH$

2. $H + O_2 = O + OH$

See Reaction Summary.

3. $H_2 + O = H + OH$

See Reaction Summary

4. $H + O_2 + M = HO_2 + M$

Only the forward reaction has been studied. Evaluation consisted of setting the rate for one third body (H_2O) and then scaling the rates for others (H_2, O_2, and N_2) on the basis of relative efficiency data.

For the rate in the presence of water, high temperature data from several sources[1-7] were combined with the room temperature results of Clyne and Thrush.[8,9] Relative efficiencies of H_2 and H_2O are derived from the comparison of H_2 and Ar by Lewis and Von Elbe.[10] The efficiency of O_2 relative to H_2 was set using data from references 5, 12, and that for N_2 on the basis of references 6, 11.

The sources combined in the evaluation and others discussed cover work on flames, flow studies of the H_2/O_2 reaction and the combination reaction and the mercury photosensitized oxidation of hydrogen.

1. Baldwin and Brooks, Trans. Faraday Soc. 58, 1782 (1962).
2. Baldwin and Precious, Nature 169, 290 (1952); and unpublished work.
3. Nalbandyan, Zhur. fiz. Khim. 19, 210 (1945).
4. Broida and Oldenberg, J. Chem. Phys. 19, 196 (1951).
5. Ashmore and Tyler, Trans. Faraday Soc. 58, 1108 (1962).
6. Willbourn and Hinshelwood, Proc. Roy. Soc. A185, 353 (1946).
7. Voevodskii and Tal'rose, Zhur. fiz. Khim. 22, 1192 (1948).
8. Clyne and Thrush, Proc. Roy. Soc. A275, 544 (1963).

9. Clyne and Thrush, Proc. Roy. Soc. A275, 559 (1963).

10. Von Elbe and Lewis, J. Chem. Phys. 10, 366 (1942).

11. Lewis and Von Elbe, "Combustion, Flames and Explosions in Gases" Chapter II (1961).

12. Voevodsky and Kondratiev, "Progress in Reaction Kinetics", Vol. 1 (1961), p. 43.

13. Hoare and Walsh, Chem. Soc. Spec. Pub. No. 9, p. 17 (1957).

14. Baldwin and Walsh, Disc. Faraday Soc. 17, 96 (1954).

15. Robertson, Disc. Faraday Soc. 17, 98, 99 (1954).

16. Patrick and Robb, Disc. Faraday Soc. 17, 98 (1954).

17. Warren, Proc. Roy. Soc. A211, 96 (1952).

18. Avramenko and Kolesnikova, Izvest. Akad. Nauk SSSR, Otdel Khim. Nauk, 1971 (1961).

19. Callear and Pereira, Trans. Faraday Soc. 59, 2774 (1963), quoting Clyne and Thrush for $H + O_2 + H_2 \rightarrow HO_2 + H_2$, $k = 2.0 \times 10^{16}$ $cm^3 mol^{-1} s^{-1}$ at 293 K.

20. Baldwin and Doran, Trans. Faraday Soc. 57, 1578 (1961).

5. $H_2 + M = H + H + M$

See Reaction Summary.

6. $H + OH + M = H_2O + M$

The combination rate was set at $k = (4 \pm 1) \times 10^{-31} cm^6 s^{-1}$ at 2000°K for $M = H_2O$, based on the flame studies of Padley and Sugden[1] and McAndrew and Wheeler.[2] A negative activation energy E = -1850 cal/mol was selected by analogy to the combination of H atoms. The relative efficiencies of third bodies was set at $H_2O:N_2 = 5:1$ based on the work of Rosenfeld and Sugden.[3] Room temperature data combination studies involving water photolysis,[4] and discharge production of radicals[5] give much lower rates than the extrapolation from higher temperatures (and were not used). Other references cited: 6,7.

1. Padley and Sugden, Proc. Roy. Soc. A248, 248 (1958).

2. McAndrew and Wheeler, J. Phys. Chem. 66, 229 (1962).

3. Rosenfeld and Sugden, Combustion and Flame 8, 44 (1964).

4. Black and Porter, Proc. Roy. Soc. A266, 185 (1962).
5. Oldenberg and Rieke, J. Chem. Phys. 7, 485 (1939).
6. Bulewicz and Sugden, Trans. Faraday Soc. 54, 1855 (1958).
7. Dixon-Lewis, et al, Symp. Combust. 10th, p 495 (1965).

7. $O + O_2 + M = O_3 + M$

See Reaction Summary for $O_3 + M = O + O_2 + M$.

8. $O + O_3 = O_2 + O_2$

See Reaction Summary for $O_3 + M = O + O_2$.

9. $O_2 + M = O + O + M$

See Reaction Summary.

10. $OH + OH = H_2O + O$

See Reaction Summary.

11. $H_2 + O_2 = OH + OH$

"Semenov, quoted by Singer and Williams [Ann. Rept. Chem. Soc. 45, 77 (1958)] gives $A = 2.46 \times 10^{-12}\ T^{0.5}$, $E = 45{,}000$ cal/mol for the forward reaction." Using these data the Arrhenius equation pre-exponential factor was set at 7×10^{-11}. This gives $k = 2 \times 10^{-12}$, $\exp(-26{,}330/RT)$ cm^3 molecule^{-1} sec^{-1} for $OH + OH = H_2 + O_2$.

12. $H_2O_2 + M = OH + OH + M$

The rate for peroxide dissociation ($M = H_2O_2$) is that of Baldwin and Brattan.[1] Rates with other partners are averages that include the relative efficiencies reported by Forst[2] and Hoare, Protheroe and Walsh.[3] Both references 2 and 3 provide evaluations of this system and discuss earlier work.[4-6] Direct studies of the OH combination (flash photolysis of water vapor[7]) are discounted. The rates are high. The combination rate is calculated using equilibrium data.

1. Baldwin and Brattan, Symp. Combust. 8th, p 110 (1962).
2. Forst, Can. J. Chem. 36, 1308 (1958).
3. Hoare, et al, Trans. Faraday Soc. 55, 548 (1959).
4. McLane, J. Chem. Phys. 17, 379 (1949).
5. Giguere and Liu, Can. J. Chem. 35, 283 (1957).
6. Satterfield and Stein, J. Phys. Chem. 61, 537 (1957).
7. Black and Porter, Proc. Roy. Soc. A266, 185 (1962).

13. $HO_2 + HO_2 = H_2O_2 + O_2$

Dixon-Lewis and Williams room temperature value used to set the pre-exponential factor. Activation energy taken as zero. Burgess and Robb's value, 30 times greater is close to the collision frequency and is considered surprising.

Dixon-Lewis and Williams, Nature 196, 1309 (1962).

Burgess and Robb, Chem. Soc. Spec. Pub. No. 9, p. 167 (1957).

BAULCH, D. L., DRYSDALE, D. D., and LLOYD, A. C., "Critical Evaluation of Rate Data for Homogeneous, Gas-Phase Reactions of Interest in High-Temperature Systems", Dept. of Physical Chemistry. The University, Leeds, England, High Temperature Reaction Rate Data, Report No. 1, May 1968.

Data sheets on each reaction include thermodynamic data, a table and a figure showing the available experimental results, a discussion and a bibliography. The authors do not hesitate to state that no reliable estimate can be made for a reaction. The general format is excellent.

1(a). $CO + OH = CO_2 + H$
(b). $CO + OD = CO_2 + D$

See reaction summary for $CO + OH = CO_2 + H$.

2(a). $CO + O = CO_2 + h\nu$
(b). $CO + O = CO_2$
(c). $CO + O + M = CO_2 + M$

These three reactions are discussed in the same report. A recommended rate is given for (a), a value stated for the 400-550 K range for (b), and only an activation energy estimate, 2.5 kcal mole^{-1} given for (c). This reflects the limited pool of conflicting data.

The mechanism for CO combination with O can be written as a combination of steps (a), (b) and (c). In all three steps, reaction of ground state CO and O must lead to an electronically excited CO_2.

The recommended rate for (a) is based on analysis of chemiluminescence. It combines the data of Clyne and Thrush,[4] Hartunian et al[9], Myers and Bartle[14] and Kaskan.[10] The work of Mahan and Solo[12] which leads to a high activation energy is rejected. The authors accompany their rate estimate with a warning that the reaction may not be a simple bimolecular process.

The tentative recommendation for (b) is based on the results in the 400-500 K region[1,11] and shock wave dissociation studies.[16] Both stirred flow reactor studies are rejected.[12,15] Their rate coefficients are lower by one or two orders of magnitude. The authors note that (b) is unlikely to yield a product stable for any length of time without participation of a third body.

No rate is given for either the forward or reverse reactions of (c) because of the great scatter of the data. Recent studies by Wong et al[18] that show a strong impurity effect are cited to explain this. Data tabulated from references 1a, 2-6, 8, 10a, 13, 17, 19 and graphed.

1. Avramenko and Kolesnikova, Izvest. Akad. Nauk. S.S.S.R., Otdel. Khim. Nauk (1959), 1562. (Same as 1a)

1a. Idem, Bull. Acad. Sci. USSR 9, 1506 (1959). Quoted in ref. 4.

2. Brabbs and Belles, Symp. Combust. 11th, p. 125 (1967).

3. Brabbs, et al, J. Chem. Phys. 38, 1939 (1963).

4. Clyne and Thrush, Proc. Roy. Soc. A269, 404 (1962).

5. Davies, J. Chem. Phys. 41, 1846 (1964); 43, 2809 (1965).

6. Fishburne, et al, J. Chem. Phys. 45, 160 (1966).

7. Generalov and Losev, J. Quant. Spectry. Radiative Transfer 6, 101 (1966).

8. Harteck and Dondes, J. Chem. Phys. 23, 902 (1955).

9. Hartunian, et al, J. Chem. Phys. 44, 1765 (1966).

10. Kaskan, Combust. Flame 3, 39 (1959).

10a. Kaufman, Proc. Roy. Soc. A247, 123 (1958).

11. Kondratiev and Ptichkin, Kinetika i Kataliz 2, 492 (1961).

12. Mahan and Solo, J. Chem. Phys. 37, 2669 (1962).

13. Michel, et al, Z. Phys. Chem. Neue Folge 39, 129 (1963).

14. Myers and Bartle, J. Chem. Phys. 47, 1783 (1967).

15. Mulcahy and Williams, Trans. Faraday Soc. 64, 59 (1958).

16. Olschewski, et al, Symp. Combust. 11th, p. 155 (1967).

17. Steinberg, NASA, CR 68229, February 1965.

18. Wong, et al, NASA, TN D-4162 (1967); CA 68, 72748b (1968).

19. Zeegers, Ph.D. Thesis, University of Utrecht, Holland (1966).

3. $CO_2 + O = CO + O_2$

The value for the forward reaction cited is an average of the rate calculated by Schofield from the data of Sulzmann et al on the reverse and the rate developed by Brokaw reinterpreting the same data. Authors recommend use of this value with caution. Data tabulated and graphed.

1. Schofield, Planet. Space Sci. 15, 643 (1967).

2. Sulzmann, et al, J. Chem. Phys. 42, 3969 (1965).

3. Brokaw, Symp. Combust. 11th, p. 1063 (1967).

CHERRY, S. S., GOLD, P. I., and VAN NICE, L. J., Phase I Final Report, "Screening of Reaction Rates" 22 May 1967. TRW Systems, Redondo Beach, California, Report 08832-6001-T0000.

Introduction

This report is part of a study performed by TRW Systems for the Theoretical Methods Committee of the Interagency Chemical Rocket Propulsion Group. Phase I of the study was concerned with identifying the chemical reactions that significantly affect performance calculations for important liquid propellant systems. One objective of developing such a list was the establishment of criteria for the minimum set of reactions with which future non-equilibrium performance calculations should be made. This was the concern of Phase II of the project.[1] Another objective was to indicate to reaction kineticists those reactions for which precisely determined rate constants are needed.

Both the Phase I and Phase II reports list the reactions cited here as CHERRY-1967. Only the Phase I report lists the notes and references pertinent to specific reactions.

A prime objective of the Phase I study was the establishment of uncertainties for the rate coefficients. These are given for each reaction. They are not measures of the precision of the data so much as they are ranges within which the rate coefficients must lie. Thus they are pertinent to the boundary conditions for the design of propulsion systems. The authors state:

> "Selected rates were divided into two categories: those obtained from the literature which are based on experimental evidence, and those which were analytically determined on the basis of theoretical treatments or otherwise estimated. The limits of reliability of those based on experiment were assigned on a somewhat qualitative evaluation of the experimental techniques utilized in their determination as well as their reported accuracy. Theoretically determined or estimated rate constants were in most cases assigned uncertainty limits based on collision frequency considerations.
>
> "In several instances, a choice was made from widely differing rates. In these cases, rates and uncertainty limits were selected to insure coverage of the range of probable values [when the rates were used in] the perturbation study."

The uncertainties given are multiplicative: $1/a < k/k_o < a$. These convert, in the notation used in the present compilation, to uncertainties in A: A ± log a.

The authors have made use of other evaluations and compilations in developing their list. Over 150 references are cited. There are quotations from compilations that are also included in this compendium. Usually these are not repeated. Instead, a notation appears in the descriptive material provided for the quoted source.

A substantial number of the reactions also carry notes indicating the participation of G. S. Bahn in the development of the recommended rates and the uncertainties. These are all summarized in the notes here as "private communications". (The notes that appear in the Phase I report are reproduced below.[2]) The details of these evaluations and calculations are not available. However, Bahn has also published evaluations and selections of preferred rates (see BAHN-1964, 1965, 1968 in this compendium and reference 3). There is some overlap. Bahn has indicated that the published values adequately reflect his approach to the problem of selecting and calculating rate coefficients.

Some rate parameters in CHERRY-1967 are stated to a number of significant figures exceeding the assigned uncertainties. Usually these numbers were the results of curve fitting procedures or theoretical calculations. Most of them were rounded prior to being processed for this compendium. The notes provided here follow those in CHERRY-1967 closely. The units used in the report and for quotations in these notes are: time in seconds, temperature in Kelvin, concentration in moles/cm^3 and activation energies in cal/mole. The reactions in the report run from <u>right</u> to <u>left</u>. For some reactions the activation energy, E^*, is given, and for some E^*/R.

1. Cherry, S. S. and Van Nice, L. J., "Screening of Reaction Rates," Phase II Final Report, Vol. I Technical Analysis, TRW Systems Group, Redondo Beach, California, 6 December 1967, No. 08832-6002-T0000.

2. "Private Communication from Bahn (Marquardt Corp.) to L. J. Van Nice and RFP SN-82-102 (ICRPG)."

   "Unpublished Report on Reactions in the F-Cl-H-O-N System by G. S. Bahn, Marquardt Corporation, February 1967."

   "Private Communication with G. S. Bahn, April 27, 1967"

3. Bahn, G. S., Pyrodynamics <u>1</u>, 147, 271, 335 (1964); Ibid <u>2</u>, 91, 197, 315 (1965); Ibid <u>3</u> 245 (1965); Ibid <u>4</u>, 63, 211, 305, 371 (1966); Ibid <u>5</u>, 49, 75, 221, 375 (1967); Ibid <u>6</u>, 101 (1968).

1. $F_2 + H = F + HF$

Collision theory value, i.e. A set at the collision frequency recommended by various authors. This is a factor of 10 higher than the formal order of magnitude estimate for this type of reaction. The value given is probably somewhat high. Uncertainty assessed at collision frequency limit.

Bahn, Private communication.

Tunder, et al, Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1, January 1967.

Sarli, et al, United Aircraft Res. Lab. Report UAR-E72, May 1966.

Burwell, et al, United Aircraft Corp. preprint for Third Conference on Performance of High Temperature Systems (December 1964).

Klein and Wolfsberg, J. Chem. Phys. 34, 1494 (1961). [Not directly applicable to $H + F_2$. Paper deals with $H + Cl_2$.]

2. $F + H_2 = H + HF$

Determined by analogy to $OH + H = H_2 + O$ for which consult references 1-6. The value given here agrees to within a factor of 10 with rates derived from experimental data[2,3,7,8] $k = 1 \times 10^{12} \exp(-E/RT)$, E = 5000 or 7000 cal/mol . Compared to the rate estimated by the Johnston and Parr method[2,3,9,10] there is a discrepancy of a factor of 70. The uncertainty was assessed at a factor of 50.

1. Patch, J. Chem. Phys. 36, 1919 (1962).
2. Bahn, Private communication.
3. Bittker, NASA TN D-3607, August 1966.
4. Mayer, et al, Aerospace Corp. Report No. TDR-269(4210-10)-6, 18 September 1964.
5. Gold and Weekley, TRW Systems, Redondo Beach, California, Report 02874-6001-R000, 6 December 1966.
6. Cook and Schieler, Aerospace Corp. Report TDR-269(9210-02)-1, October 1964.
7. Jacobs, et al, J. Chem. Phys. 43, 3688 (1965).
8. Levy and Copeland, J. Phys. Chem. 69, 408 (1965).
9. Tunder, et al, Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1, January 1967.
10. Mayer, et al, J. Chem. Phys. 45, 385 (1966).

3. $H + Cl_2 = Cl + HCl$

A number of estimated rates are available.[1-7] These values agree to within an order of magnitude. In view of the lack of experimental data, the selected value[1,5-7] was assessed at an uncertainty equal to the collision frequency limit.

1. Bahn, Private communication.
2. Mayer, et al, Aerospace Corp. Report TDR-269(4210-10)-6, 18 September 1964.
3. Mayer and Schieler, Aerospace Corp. Report TDR-669(9210-02)-2, May 1966.
4. Schieler and Mayer, CPIA Publication 108, p. 131 (June 1966).
5. Ashmore and Chanmugam, Trans. Faraday Soc. 49, 254 (1953).
6. Thrush, "Progress in Reaction Kinetics", Vol. 3, p. 63 (Pergamon Press, Oxford, 1965).
7. Klein and Wolfsberg, J. Chem. Phys. 34, 1494 (1961).

4. $H + HCl = Cl + H_2$

A number of experimentally based rate constants are available.[1-5] Although these are based on low temperature data, they agree with each other to within a factor of 4. Furthermore, when compared to several well based estimated rates, the agreement is still better than a factor of 5. The value selected, $6.2 \times 10^{11}T^{0.5} \exp(-3100/RT)$ was assessed with an uncertainty of one order of magnitude.

1. Bahn, Private communication.
2. Clyne and Stedman, Trans. Faraday Soc. 62, 2164 (1966).
3. Fettis and Knox, "Progress in Reaction Kinetics", Vol. 2, p. 1 (Pergamon Press, New York, 1964).
4. Fishburne, J. Chem. Phys. 45, 4053 (1966).
5. Steiner and Rideal, Proc. Roy. Soc. A173, 503 (1939).

5. $ClF + H = Cl + HF$
$ClF + H = F + HCl$

Several estimates are available for rates of these reactions.[1-5] The spread is over one order of magnitude. That from the Johnston and Parr technique was selected [see General Notes]. There are no experimental data. The uncertainty was assessed at the collision limit.

1. Bahn, Private communication.
2. Tunder, et al, Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1, January 1967. [Order of magnitude estimate]
3. Mayer, et al, J. Chem. Phys. 45, 385 (1966).
4. Mayer and Schieler, Aerospace Corp. Report TDR-669(9210-02)-2 May 1966.
5. Schieler and Mayer, CPIA Publication 108, p. 131 (June 1966).

6. $CO + O_2 = CO_2 + O$

This is the only literature value found. The rate compares rather poorly [is higher] with formal order of magnitude estimates.

Tunder, et al, Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1, January 1967. [quoting Sulzmann, et al, below]

Sulzmann, et al, J. Chem. Phys. 42, 3969 (1965).

7. $N + NO = N_2 + O$

Bortner[1] reviews a considerable body of experimental data regarding this reaction[2-9] and concludes that the rate chosen should have an uncertainty of about a factor of 2. This might be somewhat optimistic. A factor of 5 was chosen.

1. Bortner, GE Missile and Space Division Report No. R63SD63, August 1963.
2. Wray and Teare, J. Chem. Phys. 36, 2582 (1962).
3. Kaufman and Decker, Symp. Combust. 7th, p. 57 (1959).
4. Glick, et al, J. Chem. Phys. 27, 850 (1957).

5. Kistiakowsky and Volpi, J. Chem. Phys. 27, 1141 (1957).
6. Verkeke and Winkler, J. Phys. Chem. 64, 319 (1960).
7. Herron, J. Chem. Phys. 35, 1138 (1961).
8. Clyne and Thrush, Proc. Roy. Soc. A261, 259 (1961).
9. Duff and Davidson, J. Chem. Phys. 31, 1018 (1959).

8. $NO + NO = N_2 + O_2$

Bortner[1] reviews a considerable body of experimental data regarding this reaction.[2-4] Because of uncertainties in the mechanism, it was concluded that the rate has a factor of 10 uncertainty.

1. Bortner, GE Missile and Space Division Report No. R63SD63, August 1963.
2. Freedman and Daiber, J. Chem. Phys. 34, 1271 (1961).
3. Kistiakowsky and Volpi, J. Chem. Phys. 27, 1141 (1957).
4. Wise and Frech, J. Chem. Phys. 20, 22 (1952).

9. $N + O_2 = NO + O$

See Reaction Summary.

10. $H_2 + OH = H + H_2O$

See Reaction Summary for $H + H_2O = H_2 + OH$.

11. $O + OH = H + O_2$
$H + OH = H_2 + O$

See Reaction Summaries for each of the reverse reactions.

12. $OH + OH = H_2O + O$

See Reaction Summary.

13. $OH + OH = H_2 + O_2$

The selected value was calculated[1] based on data[2] for the reverse (endothermic) reaction. It is agreed[1,3] that this reaction must be very slow with respect to other possible mechanism. The collision frequency limit was assigned as the uncertainty.

1. Bahn, Private communication.
2. Langen, et al, AIAA J. 3, 2211 (1965).
3. Kaskan and Browne, General Electric Report No. R64SD37, February 1964.

14. $CO + O + M = CO_2 + M$

Kaskan and Browne evaluate the available data and recommend this value as do Gurney, et al. Some uncertainty must, however, be attached to this value. In fact, in the presence of hydrogen, H-O recombination dominates and this reaction may well be ignored. Because of uncertainties regarding third body efficiency, a factor of $10^{2.5}$ was assigned.

Kaskan and Browne, General Electric Report No. R64SD27, February 1964.

Gurney, et al, in "Aerospace Chemical Engineering", (Chem. Eng. Progr. Symp. Series, No. 61, Vol. 62, 1966), p. 142.

15. $N + N + M = N_2 + M$

$N + O + M = NO + M$

Bortner has made a relatively thorough study of the available experimentally based rates. Because of uncertainties in the arbitrary third body assumption, a factor of 10 was assigned.

Bortner, GE Missile and Space Division Report No. R63SD63, August 1963.

16. $H + Cl + M = HCl + M$

No experimental data are available. The selected rate, an order of magnitude estimate, agrees to within a factor of two with that calculated by cascade deactivation theory.[1] Other estimated rates[2,3] differ by as much as $10^{2.5}$. Thus, the uncertainty was assessed at the collision frequency limit.

1. Crowe, et al, United Technology Center Report UTC 2128-FR (15 June 1966).
2. Jensen and Kurzius, Aerochem Research Laboratories, Princeton, N. J., March 1967. Report TP-149.
3. Cook and Schieler, Aerospace Corp. Report TDR-269(9210-02)-1, October 1964.

19. $\underline{H + F + M = HF + M}$

As has been done by others[1-3] the rate for this reaction is assumed to be equal to that for $H + H + M = H_2 + M$. Other theoretical estimates are given in references 4-7. The only data measured are for M = Ar with assumed third body efficiencies.[8,9] The value given here lies in about the middle of the range of reported values. Assignment of an uncertainty factor of $10^{1.5}$ assures that the maximum reported rate will be included.

1. Bahn, Private communication.
2. Bittker, NASA TN D-3607, August 1966.
3. Wilde, AIAA J. 2, 374 (1964).
4. Burwell, et al, United Aircraft Corp. preprint for Third Conference on Performance of High Temperature Systems (December 1964).
5. Cole and Roquemore, Boeing Co. Document D5-12210 (29 March 1965).
6. Jacobs, et al, Aerospace Corp. Report TR-669(6240-201)-11 (June 1966).
7. Crowe, et al, United Technology Center Report UTC 2128-FR (15 June 1966).
8. Weber, Rocketdyne Memo No. RM 12/4-358 (March 1, 1966).
9. Jacobs, et al, Aerospace Corp. Report No. TDR-469(5240-20)-10 (June 1965). Published as J. Chem. Phys. 43, 3688 (1965).

20. $\underline{H + OH + M = H_2O + M}$

The value given here is based on evaluation of a series of rate estimates cited below. There is considerable uncertainty regarding the effects of third bodies. A factor of 10^3 uncertainty must be assessed to assure coverage of the upper limit of the probable range in the case of arbitrary third bodies.

Lezberg, et al, NASA TN D-2883, June 1965.

Bahn, Private communication.

Weber, Rocketdyne Memo No. RM 12/4-358, March 1, 1966.

Mayer, et al, Aerospace Corp. Report No. TDR-269(4210-10)-6, 18 September 1964.

Lezberg and Franciscus, AIAA J. 1, 2071 (1963).

Langen, et al, AIAA J. 3, 2211 (1965).

Rosenfeld and Sugden, Combust. Flame 8, 44 (1964).

Dixon-Lewis, et al, Symp. Combust. 10th, p. 495 (1965).

Bulewicz and Sugden, Trans. Faraday Soc. 54, 1855 (1958).

Westenberg and Favin, Symp. Combust. 9th, p. 785 (1963).

21. $H + H + M = H_2 + M$

See Reaction Summary for $H_2 + M = H + H + M$.

22. $H + O + M = OH + M$

The value selected[1,2] [is an estimate that equates this reaction to $H + H + M = H_2 + M$]. It adequately covers the data found[3,4] to within an uncertainty factor of five.

1. Tunder, et al, Aerospace Corp., Thermochemistry Research Dept., Report No. TR-1001(9210-02)-1, January 1967.
2. Westenberg and Favin, Symp. Combust. 9th, p. 785 (1963).
3. Bahn, Private communication.
4. Langen, et al, AIAA J. 3, 2211 (1965).

23. $O + O + M = O_2 + M$

See Reaction Summary for $O_2 + M = O + O + M$.

24. $CO + OH = CO_2 + H$

See Reaction Summary.

25. $CO_2 + N = CO + NO$

This reaction is a so-called "spin-forbidden" reaction and cannot occur with all species in their ground states. The reaction can, however, occur with atomic nitrogen in its first excited electronic state, that is,

$$CO_2 + N^* = CO + NO \quad k_1$$

An "effective" rate constant for $CO_2 + N = CO + NO$ k_2 can be obtained as follows: Suppose the populations of N atoms in the various electronic states are related by a Boltzmann distribution

$$\frac{(N^*)}{(N)} = e^{-\Delta E/RT}$$

where $\Delta E = 55000$ cal is the energy difference between the ground and first excited state of N. Then,

$$r = -k_1 (CO_2)(N^*) = -k_1 e^{-\Delta E/RT} (CO_2)(N)$$

or,

$$k_2 = k_1 e^{-\Delta E/RT}$$

The constant k_1 is an order of magnitude estimate. The uncertainty was assessed at the collision frequency limit.

26. Bahn, Private communication.

JENSEN, D. E. and KURZIUS, S. C., "Rate Constants for Calculations on Nozzle and Rocket Exhaust Flow Fields," AeroChem Research Laboratories, Princeton, New Jersey, March 1967. Report TP-149.

Introduction

This report is an annotated tabulation of rate coefficients for 111 reactions (single direction - forward and reverse rates for the same system are given rarely.) The H-O system, reactions of halogens and halogen oxides, reactions of alkali metals, CO, CHO and CH_2O are considered. Some ionization reactions are included. The coefficients are intended for use in calculations for systems at temperatures between 1000 and 3500 K.

The rate coefficients are the result of an evaluation of experimental data (where they exist) and estimates based on analogy to similar reactions. The basis for the value reported is explained. Uncertainty ranges are given for each case. They are presented as multiplicative factors: k x 1/a, k x a which, in the notation used in this compilation, convert to A ± log a (or log k ± log a). These uncertainties are explained by the authors as follows.

> "The upper possible error factor is defined as the ratio of our estimate of the probable upper limit of the rate constant to our estimated rate constant k itself at the temperature at which the rate constant is least accurately known. The lower possible error factor is the ratio of k to our estimate of the probable lower limiting value of the rate constant at this temperature. These error factors are the result of reasonable semi-quantitative appraisal rather than detailed statistical analysis of the available data and are intended principally to give the engineer a feeling for the uncertainty in each rate constant. The factors are usually considerably larger than the uncertainties attached to their results by the original experimenters; this is almost always because we have had to extrapolate available results into temperature ranges considerably different from those of the experiments themselves."

Where Jensen and Kurzius give unequal upper and lower uncertainty limits, the larger has been used for the uncertainty in <u>A</u>. Each of these cases is identified in the notes.

Combination and dissociation reactions involving a "third body" energy transfer agent are assigned rates applicable to a generalized third body. This is a molecule as opposed to an atom. These rates, as are all the others, are thermal rates. The authors find it impractical at present to take into account excited states in an explicit manner.

The rate quotient law, $K_{eq} = k_f/k_r$ is assumed to hold for all reactions.

The values given are "considered to be the best that can be gleaned from the literature published up to December 1966." Sixty-nine references are cited.

The notes in this compendium are based on those of the authors and are often abbreviated quotations. Some have been rewritten to make them more understandable in the context and format of the present compilation.*

1. $O + O + M = O_2 + M$

See Reaction Summary for $O_2 + M = O + O + M$.

2. $O + H + M = OH + M$

It appears that no experimental work has been done on this reaction. [The rate constant was set equal to that for $O + O + M = O_2 + M$ and $H + H + M = H_2 + M$.]

3. $H + H + M = H_2 + M$

See Reaction Summary for $H_2 + M = H + H + M$.

4. $H + OH + M = H_2O + M$

Little reliable data are available for this reaction. The agreement between independent values of k obtained by Bulewicz and Sugden and by McAndrew and Wheeler, for example, is fortuitous in view of the lack of distinction between contributions from

$$H + H + H_2O = H_2O + H_2$$

and

$$H + OH + H_2 = H_2O + H_2$$

---

*The units used in the report and in the quoted values in these notes are: time in seconds, temperature in Kelvin, concentration in molecules/cm^3, and activation energy in calories/mole.

in the former work. Schott and Bird appear to have obtained a reasonably reliable value, however, and the wide error limits suggested here reflect uncertainties in third-body efficiencies. The rate constant given corresponds to a very large ($\sim 3 \times 10^{-7}$) pre-exponential factor for the dissociation reaction.

Bulewicz and Sugden, Trans. Faraday Soc. 54, 1855 (1958).

McAndrew and Wheeler, J. Phys. Chem. 66, 229 (1962).

Schott and Bird, J. Chem. Phys. 41, 2869 (1964).

5. $CO + O + M = CO_2 + M$

The surprising exponential term is suggested by the work of Clyne and Thrush at temperatures lower than those encountered in rocket exhausts. At 2000 K, the exponential term does not carry a great deal of weight by comparison with the uncertainties in the rate constant as a whole. Zeegers' work suggests that O_2 has a very high third-body efficiency in this reaction ($k \sim 2.4 \times 10^{-33}$ for $M \equiv O_2$ at 2350 K) but that CO_2 is inefficient ($k \sim 2.4 \times 10^{-33}$ for $M \equiv CO_2$ at 2350 K). The value of k listed is probably an upper-limit value. Unequal error limits given: $0.033 < k/k_o < 3$.

Clyne and Thrush, Symp. Combust. 9th, p. 57 (1963).

Zeegers, Ph.D. Thesis, University of Utrecht, Holland (1966).

6. $OH + OH = H_2O + O$

See Reaction Summary.

7. $H_2 + OH = H + H_2O$

See Reaction Summary for $H + H_2O = H_2 + OH$.

8. $H_2 + O = H + OH$

See Reaction Summary.

9. $H + O_2 = O + OH$

See Reaction Summary.

10. $CO + OH = CO_2 + H$

See Reaction Summary.

11. $H + Cl_2 = Cl + HCl$

The rate constant given was estimated by Fristrom and Westenberg on the basis of results obtained by Klein and Wolfsberg.

Fristrom and Westenberg, "Flame Structure" (McGraw-Hill Book Co., New York, 1965).

Klein and Wolfsberg, J. Chem. Phys. 34, 1494 (1961).

12. $H_2 + Cl = H + HCl$

The estimates of this rate constant given by Fristrom and Westenberg and by Fettis and Knox are in good agreement with one another. The rate constant given here is based on these two estimates.

Fristrom and Westenberg, "Flame Structure" (McGraw-Hill Book Co., New York, 1965).

Fettis and Knox, "Progress in Reaction Kinetics", Vol. 2, p. 1 (Pergamon Press, New York, 1964).

13. $Cl + H_2O = HCl + OH$

Estimated by comparison with $Cl + HCl = Cl_2 + H$, due allowance being made for a steric hindrance factor and for an activation energy 4000 cals/mole greater than the endothermicity.

14. $Cl + OH = HCl + OH$

Estimated by comparison with that for $OH + H = H_2 + O$ ($k = 1.3 \times 10^{-11} e^{-6300/RT}$). Each of these reactions is spin allowed and approximately thermoneutral.

15. $H + HF = F + H_2$

This rate constant is the result of an experimental study of the kinetics of decomposition of HF by Jacobs, Giedt, and Cohen. Note that the pre-exponential factor in the rate constant for similar reaction $H + HCl = H_2 + Cl$, given by Fristrom and Westenberg, 1.0×10^{-10}, is 5 times larger.

Jacobs, et al, AIAA Second Propulsion Joint Specialist Conference, Colorado Springs, June 1966, Paper 66-637.

Fristrom and Westenberg, "Flame Structure" (McGraw-Hill Book Co., New York, 1965).

16. $F_2 + H = F + HF$

This rate constant is set equal to that for $H + Cl_2 = HCl + Cl$. The pre-exponential factor is approximately equal to the collision frequency. Both reactions are strongly exothermic.

17. $HCl + Li = H + LiCl$
$HCl + Cs = CsCl + H$

Estimated by comparison with those for $Na + HCl = NaCl + H$ and $K + HCl = KCl + H$, the bond energy of the metal halide used being that listed by Gaydon. [Unequal error limits given: $0.033 < k/k_o < 10$.]

Gaydon, "Dissociation Energies" (Chapman and Hall, London, 1953).

18. $HCl + Na = H + NaCl$

This estimate is based on measurements made by M. Polanyi in 1932; no recent measurements appear to be available. However, Kondratiev reports results of Taylor and Datz which suggest that the rate constant of the reaction

$$K + HBr = KBr + H; \quad \Delta H = -4000 \text{ cals/mol}$$

is given by

$$k = 3.0 \times 10^{-12} T^{0.5} e^{-3400/RT}, \quad 500 < T < 800 \text{ K}$$

or, at 1600 K, by

$$k = 1.2 \times 10^{-10} e^{-3400/RT}.$$

These results and others cited by Kondratiev suggest that the pre-exponential factors of rate constants of reactions like this one are close to the collision frequencies. The rate constant given here stems from adoption of this suggestion. Taylor and Datz used a molecular beam technique; Polanyi's early work suffers from uncertainties concerning the possible effects of solid particles. [Unequal error limits given: $0.033 < k/k_o < 10.$]

Polanyi, "Atomic Reactions" (Williams and Norgate, London, 1932).

Kondratiev, "Chemical Kinetics of Gas Reactions"(Pergamon Press, New York, 1964) p. 90.

Taylor and Datz, J. Chem. Phys. 23, 1711 (1955).

19. $HCl + K = H + KCl$

This rate constant is based on the work of Polanyi and the discussion given by Kondratiev. [Unequal error limits given: $0.033 < k/k_o < 10.$]

Polanyi, "Atomic Reactions" (Williams and Norgate, London, 1932).

Kondratiev, "Chemical Kinetics of Gas Reactions" (Pergamon Press, New York, 1964) p. 90.

20. $Me + H_2O = MeOH + H$ (Me = Li, Na, K, Cs)

The rate constant for $Li + H_2O = LiOH + H$ was estimated on the basis of arguments given by Sugden[1] and experimental evidence obtained by Jensen[2] and Jensen and Padley.[3] The activation energy is estimated through reference to the work of Jensen and Padley;[4] 3000 cals/mol are arbitrarily added to the known endothermicity. The reactions of Na, K and Cs with H_2O were estimated in a similar manner.

1. Sugden, Trans. Faraday Soc. 52, 1465 (1956).
2. Jensen, Ph.D. Dissertation, University of Cambridge, 1965.
3. Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966).
4. Jensen and Padley, Trans. Faraday Soc. 62, 2132 (1966).

21. $H + Cl + M = HCl + M$

No experimental data appear to be available for this reaction. The value given is estimated through comparison with rate constants for other ternary reactions, including $H + F + M = HF + M$. [Unequal error limits given: $0.033 < k/k_o < 10$.]

22. $Cl + Cl + M = Cl_2 + M$

The work of Jacobs and Giedt[1] suggests a rate constant smaller by a factor of 10. Hiraoka and Hardwick,[2] on the other hand, find that $k = 7 \times 10^{-33}$ at 1600 K for argon as a third body. This would correspond to our value for molecular third bodies, assumed to be three times as efficient as Ar. [The reported pre-exponential is derived from $3 \times 7 \times 10^{-33} = A \times (1600)^{-1}$.] Fristrom and Westenberg[3] suggest [that] the results of Hiraoka and Hardwick are to be preferred to those of Jacobs and Giedt [because the former check results on Br atom combination[4]].

1. Jacobs and Giedt, J. Chem. Phys. <u>39</u>, 749 (1963).
2. Hiraoka and Hardwick, J. Chem. Phys. <u>36</u>, 1715 (1962).
3. Fristrom and Westenberg, "Flame Structure" (McGraw-Hill Book Co., New York, 1965).
4. Palmer and Hornig, J. Chem. Phys. <u>26</u>, 98 (1957).

23. $F + H + M = HF + M$

This rate constant has been measured[1] with Ar as third body in the temperature range $4000 < T < 5300$ K. The results obtained could be described in terms of $k_{Ar} = 5 \times 10^{-29} T^{-1}$, but the scatter of results was rather large. Multiplication of k_{Ar} by 5 to allow for greater efficiency of molecular third bodies would give $k = 2.5 \times 10^{-28} T^{-1}$. This seems rather high. The value stated is preferred as a compromise until further work is done. Note that the experimental rate constant[1] is of the same order of magnitude as that predicted by Benson and Fueno.[2]

1. Jacobs, et al, AIAA Second Propulsion Joint Specialist Conference, Colorado Springs, June 1966, Paper 66-637.
2. Benson and Fueno, J. Chem. Phys. <u>36</u>, 1597 (1962).

24. $F + F + M = F_2 + M$

The rate constant for this reaction is based on the work of Johnson and Britton[1] and Diesen,[2] who studied the dissociation of F_2 by Ar in shock tubes. The temperature-dependence given corresponds approximately to that found for the reserve reaction by Johnson and Britton; that suggested by Diesen's work appears improbably high. Allowance is made for molecules in rocket exhausts being more efficient in producing dissociation than Ar atoms. Note that the pre-exponential factor in the rate constant for the reverse reaction is considerably smaller than those for the corresponding reactions for the other halogens.[2] [This value and its uncertainty also cited by Cherry.[3]]

1. Johnson and Britton, J. Phys. Chem. 68, 3032 (1964).
2. Diesen, J. Chem. Phys. 44, 3662 (1966).
3. Cherry, et al, TRW Systems, Redondo Beach, Calif., Report 08832-6001-T0000 (1967).

25. $Me + OH + M = MeOH + M$ (Me = Li, Na, K, Cs)

The value for $Li + OH + M = LiOH + M$ is a very high rate constant, although certainly not the highest ever suggested for a ternary recombination reaction - see, for example, McAndrew and Wheeler. Combination of theoretical arguments of Sugden and experimental results of Jensen and Padley and Bulewicz and Sugden shows that the rate constant for the reverse reaction cannot be much smaller than $6 \times 10^{-4}T^{-1}e^{-101000/RT}$, and that <u>k</u> therefore cannot be much smaller than $10^{-27}T^{-1}$. (The equilibrium constant for formation of LiOH is approximately $1.6 \times 10^{-24}e^{10100/RT}$.) The value of <u>k</u> recommended above seems a reasonable compromise: it is not much smaller than $10^{-27}T^{-1}$ and not much greater than the rather high rate constant for the formally similar reaction $H + OH + M = H_2O + M$. The ternary combinations of Na, K and Cs with OH were estimated on the same basis. [Unequal error limits given: $0.033 < k/k_o < 10$.]

McAndrew and Wheeler, J. Phys. Chem. 66, 229 (1962).

Sugden, Trans. Faraday Soc. 52, 1465 (1956).

Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966); Ibid 62, 2132 (1966).

Bulewicz and Sugden, Trans. Faraday Soc. 52, 1481 (1956).

26. $Me + Cl + M = MeCl + M$ (M = Li, Na, K, Cs)

No experimental data are available for these reactions. The rate constant k is perhaps likely to be somewhat smaller than that for reaction $Li + OH + M = LiOH + M$ (the collision is less "sticky"- note that the rate coefficient of $H + Cl + M = HCl + M$ is less than that of $H + OH + M = H_2O + M$.) The value given for Li + OH is (for no particularly good reason) the geometric mean of those for $Cl + Cl + M = Cl_2 + M$ and $Li + OH + M = LiOH + M$. The rates for Na, K and Cs combining with Cl in a ternary collision were estimated in a similar manner. [Unequal error limits given: $0.01 < k/k_o < 30$.]

27. $Li^+ + e^- + M = Li + M$

This rate constant was calculated from measurements on the reverse reaction by Jensen and Padley at 2475 K. The temperature dependence is assumed to be the same as that of $Na^+ + e^- + M = Na + M$. All molecular third bodies are assumed to have equal third-body efficiencies. Hollander indicates that atomic third bodies are less efficient.

Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966).

Jensen and Padley, Symp. Combust. 11th, p. 351 (1967).

Hollander, Ph.D. Thesis, University of Utrecht, Holland (1964).

28. $Na^+ + e^- + M = Na + M$

Jensen and Padley measured the rate constant of the reverse reaction at 2020 to 2450 K at atmospheric pressure in $H_2/N_2/O_2$ flames and calculated $k = 1.4 \times 10^{-20}T^{-2}$. Hollander, Alkemade, and Kalff, using $CO/N_2/O_2$ flames in a similar (but narrower) range of temperature, find $k = 1.6 \times 10^{-20}T^{-2}$. Molecular third bodies tend to have approximately equal efficiencies in this reaction, but atomic third bodies are much less efficient (Hollander).

Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966).

Jensen and Padley, Symp. Combust. 11th, p. 351 (1967).

Hollander, et al, J. Chem. Phys. 39, 2558 (1963).

Hollander, Ph.D. Thesis, University of Utrecht, Holland (1964).

29. $K^+ + e^- + M = K + M$

This rate constant was calculated from measurements on the reverse reaction by Jensen and Padley. The corresponding value for atmospheric-pressure $CO/N_2/O_2$ flames is $1.5 \times 10^{-22} T^{-1.5}$.

Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966).

Jensen and Padley, Symp. Combust. 11th, p. 351 (1967).

30. $Cs^+ + e^- + M = Cs + M$

Calculated from measurements on the reverse reaction by Jensen and Padley.[1,2] Hollander, Alkemade and Kalff[3] find a much smaller rate constant ($2 \times 10^{-23} T^{-1.5}$) in $CO/N_2/O_2$ flames. Jensen and Padley's results are preferred (a) because two independent analytical techniques (optical emission spectroscopy and microwave cavity resonance) gave the same rate constant--within the limits of experimental error--in their work, and (b) because the order of magnitude of their results is consistent with equilibrium ionization of cesium being closely approached under conditions employed by other workers,[4-6] whereas that of Hollander, Alkemade, and Kalff's results is not.

1. Jensen and Padley, Trans. Faraday Soc. 62, 2140 (1966).
2. Jensen and Padley, Symp. Combust. 11th, p. 351 (1967).
3. Hollander, et al, J. Chem. Phys. 39, 2558 (1963).
4. Knewstubb, Ph.D. Dissertation, University of Cambridge (1956).
5. Hayhurst, Ph.D. Dissertation, University of Cambridge (1964).
6. Padley and Sugden, Symp. Combust. 8th, p. 164 (1962).

31. $Li^+ + Cl^- = Li + Cl$
$Cs^+ + Cl^- = Cs + Cl$

Estimated by comparison with the rates for $Na^+ + Cl^- = Na + Cl$ and $K^+ + Cl = K + Cl$. It may be noted that the value of k for $Li^+ + Cl^- = Li + Cl$ corresponds to a rate constant for the reverse reaction of $4 \times 10^{-10} e^{-34000/RT}$ at 2000 K: the pre-exponential factor of the reverse reaction rate constant is thus close to the collision frequency. It should also be borne in mind that uncertainties in crossings of potential energy curves cause one to doubt the validity of this simplified approach to the determination of mutual neutralization rate constants. It is implicitly assumed, for example, that for this reaction the potential energy curves involved are favorably placed with respect to one another. [Unequal error limits given for $Li^+ + Cl$: $0.01 < k/k_o < 10$.]

32. $Na^+ + Cl^- = Na + Cl$

An approximate value for this rate constant was measured by Hayhurst and is discussed by Hayhurst and Sugden. Baulknight and Bortner estimate the following theoretical rate constants:

$$O^+ + O^- = O + O \qquad k = 5.5 \times 10^{-7} T^{-0.5}$$

$$N^+ + O^- = N + O \qquad k = 8.4 \times 10^{-7} T^{-0.5}$$

Comparison with these estimates is the basis for the $T^{-0.5}$ temperature dependence in k; Sugden reports that the measured temperature dependence is slight.

Hayhurst, Ph.D. Dissertation, University of Cambridge, 1964.

Hayhurst and Sugden, "The Ionization Processes Associated with Metallic Additives in Flame Gases," presented at IUPAC Meeting on Plasmas, Moscow, 1965 (to be published).

Hayhurst and Sugden, Proc. Roy. Soc. A293, 36 (1966).

Baulknight and Bortner, General Electric Corp. Report R64SD12 (1964).

Sugden, AGARD Combustion and Propulsion Panel Meeting, Pisa, Italy, September 1965 (to be published).

33. $K^+ + Cl^- = K + Cl$

Measured by Hayhurst and reported by Hayhurst and Sugden. The temperature dependence of k is based on the theoretical estimate for $O^+ + O^- = O + O$ and $N^+ + O^- = N + O$ made by Baulknight and Bortner. [Unequal error limits given: $0.01 < k/k_o < 10$.]

Hayhurst, Ph.D. Dissertation, University of Cambridge, 1964.

Hayhurst and Sugden, "The Ionization Processes Associated with Metallic Additives in Flame Gases," presented at IUPAC Meeting on Plasmas, Moscow, 1965 (to be published).

Baulknight and Bortner, General Electric Corp. Report R64SD12 (1964).

34. $Me^+ + OH^- = Me + OH$ (Me = Li, Na, K, Cs)

This rate constant is estimated by comparison with $Li^+ + Cl^- = Li + Cl$ and the rate constants[1] suggested for the reactions

$$O^+ + O^- = O + O \qquad k = 5.5 \times 10^{-7} T^{-0.5}$$

$$N^+ + O^- = N + O \qquad k = 8.4 \times 10^{-7} T^{-0.5}$$

The estimate implies that the pre-exponential factor of the reverse reaction rate constant is close to the collision frequency. [Unequal error limits given: $0.01 < k/k_o < 10.$]

1. Baulknight and Bortner, General Electric Corp. Report R64SD12 (1964).

35. $O + e^- + M = O^- + M$

$OH + e^- + M = OH^- + M$

$Cl + e^- + M = Cl^- + M$

This rate constant for each of these reactions is taken to be the same as that for $O_2 + e^- + M = O_2^- + M$. It is difficult to justify this assumption, but equally difficult to suggest a better means of estimating k on the basis of present knowledge.

36. $O_2 + e^- + M = O_2^- + M$

The value of k given is based on measurements made at about 500 K by Pack and Phelps. These authors found that k increased slightly with increasing temperature, which is perhaps contrary to what one might expect. A temperature independent value has been adopted for $1000 < T < 3500$ K. The data on third-body relative efficiencies are meager; Pack and Phelps find that H_2O is about four times as efficient as O_2 in this reaction. For a review of attachment of electrons to O_2 see McDaniel's book.

Pack and Phelps, Symp. Combust. 10th, p. 569 (1965).

Pack and Phelps, J. Chem. Phys. 44, 1870 (1966).

McDaniel, "Collision Phenomena in Ionized Gases" (Wiley and Sons Inc., New York, 1964).

37. $HCl + e^- = H + Cl^-$

This rate constant was estimated by Calcote and Jensen on the basis of collision cross-section data obtained by Buchel'nikova. Note, however, that recent results of Fehsenfeld, Ferguson, and Schmeltekopf suggest that the reaction may be considerably faster. [Unequal error limits given: $0.1 < k/k_o < 300.$]

Calcote and Jensen, Advances in Chemistry Series 58, p. 291 (1966).

Buchel'nikova, J. Exp. Theoret. Phys. (USSR) 35, 1119 (1958).

Fehsenfeld, et al, J. Chem. Phys. 45, 1844 (1966).

38. $LiH_2O^+ + M = Li^+ + H_2O + M$

This rate constant was estimated by Calcote and Jensen on the basis of results obtained by Hayhurst and Hayhurst and Sugden.

Calcote and Jensen, Advances in Chemistry Series 58, p. 291 (1966).

Hayhurst, Ph.D. Dissertation, University of Cambridge, 1964.

Hayhurst, Symp. Combust. 10th, p. 602 (1965) in general discussion of Schofield and Sugden, Symp. Combust. 10th, p. 589 (1965).

Hayhurst and Sugden, Proc. Roy. Soc. A293, 36 (1966).

39. $NaH_2O^+ + M = Na^+ + H_2O + M$
$KH_2O^+ + M = K^+ + H_2O + M$

Estimated in a manner similar to that used by Calcote and Jensen for $LiH_2O^+ + M = Li^+ + H_2O + M$.

Calcote and Jensen, Advances in Chemistry Series 58, p. 291 (1966).

40. $MeH_2O^+ + e^- = Me + H_2O$ (Me = Li, Na, K)

This rate constant is estimated by comparison with the known rate constant of $H_3O^+ + e^- = H + H + OH$. [Unequal error limits given: $0.033 < k/k_o < 10$.]

Calcote, et al, Symp. Combust. 10th, p. 605 (1965).

41. $MeH_2O^+ + Cl^- = Me + Cl + H_2O$ (Me = Li, Na, K)
$MeH_2O^+ + OH^- = Me + OH + H_2O$

Estimated by comparison with preliminary values for the rate constants of the reactions

$$H_3O^+ + OH^- = \text{neutral products},$$

$$H_3O^+ + Cl^- = \text{neutral products}$$

measured by Kurzius and Calcote. [Unequal error limits given: $0.01 < k/k_o < 10$.]

Kurzius and Calcote, AeroChem Research Lab., Princeton, N. J., TP-92, DDC AD 351 824, July 1964. (Confidential)

42. $Cl + O + M = ClO + M$

This rate constant is estimated by comparison with the values for $O + O + M = O_2 + M$ and $Cl + Cl + M = Cl_2 + M$.[q.v.]

43. $Me + ClO = MeCl + O$ (Me = Li, Na, K)

The pre-exponential factor is thought likely to be close to the collision frequency. An arbitrary activation energy of 3000 cals/mol has been inserted as a result of comparison with other bimolecular reactions. ($Li + ClO = LiCl + O$ is 52 kcal/mol exothermic) [Unequal error limits given: $0.01 < k/k_o < 10$.]

44. $ClO + H = HCl + O$

Estimated by comparison with $O + H_2 = OH + H$ and $OH + Cl = HCl + O$. [q.v.]

45. $ClO + O = Cl + O_2$

This reaction is thought by Kaufman to be rapid at room temperature, which would imply that the activation energy is small. Arbitrarily, the activation energy has been set equal to 3000 cals/mol . Comparison of this reaction with $OH + O = O_2 + H$ would suggest a pre-exponential factor of about 2×10^{-11}.

Kaufman, Progress in Reaction Kinetics, Vol. 1, p. 1 (1961).

46. $ClO + OH = Cl + HO_2$

The rate constant for the reverse reaction is estimated by comparison with the rate constant of $H + HO_2 = OH + OH$; both these reactions proceed with essentially zero activation energy. Note that the ratio of the rate constant for $Cl + HO_2 = ClO + OH$ to that for $Cl + HO_2 = HCl + O_2$ has been set equal to 3:1, which is also the ratio of the rate constants of $H + HO_2 = OH + OH$ or $H_2O + O$ and $H + HO_2 = H_2 + O_2$ according to Clyne and Thrush. [Unequal error limits given: $0.01 < k/k_o < 2$.]

Clyne and Thrush, Proc. Roy. Soc. A275, 559 (1963).

47. $Li + O_2 + M = LiO_2 + M$

$K + O_2 + M = KO_2 + M$

Set equal to the rate of $Na + O_2 + M = NaO_2 + M$.

48. $Na + O_2 + M = NaO_2 + M$

This rate constant is estimated from the work of Kaskan and Carabetta, who found values of k ranging from 6.0×10^{-34} to 8.2×10^{-34} over the temperature range $1540 < T < 1730$. This work was done on clean H_2/CO/air flames at 100 Torr.

Kaskan and Carabetta, "Kinetic Studies of Sodium in Flames" in "Effect of Contaminants on Observables in Re-Entry", (General Electric Corp., Final Report, Sept. 1965, AD 470984) p. 9.

49. $Cl + MeO_2 = MeCl + O_2$ (Me = Li, Na, K)

Estimated by comparison with $H + HO_2 = H_2 + O_2$. [Unequal error limits given: $0.033 < k/k_o < 50$.]

50. $H_2 + MeO_2 = MeOH + OH$ (Me = Li, Na, K)

Estimated by comparison with $H_2 + HO_2 = H_2O + OH$.

51. $HO_2 + OH = H_2O + O_2$

$OH + MeO_2 = MeOH + O_2$ (Me = Li, Na, K)

$Cl + HO_2 = HCl + O_2$

$HO_2 + O = O_2 + OH$

Estimated by comparison with $H + HO_2 = H_2 + O$. [Unequal error limits given: $0.033 </k_o < 50$ for the first three and $0.1 < k/k_o < 100$ for $HO_2 + O = O_2 + OH$.]

52. $H + O_2 + M = HO_2 + M$

This reaction has been quite widely studied. Getzinger and Schott found $k = 3.9 \times 10^{-33}$ for M = Ar at 1500 K in a shock tube. Clyne and Thrush, using a fast flow discharge system, found $k = 35 \times 10^{-33}$ at 225 K, $k = 30 \times 10^{-33}$ at 244 K and $k = 22 \times 10^{-33}$ at 293 K for M = Ar. Baldwin gives values obtained from second explosion limit studies; for M = Ar, $k = 4.7 \times 10^{-33}$ at 813 K, and for M = H_2, k = 23 x 10^{-33} at 813 K. Kurzius found k = 30 x 10^{-33} at 800 K for M = H_2 in his first explosion limit studies. The value given for a "general" third body thus seems fairly reliable.

Getzinger and Schott, J. Chem. Phys. 43, 3237 (1965).

Clyne and Thrush, Proc. Roy. Soc. A275, 559 (1963).

Baldwin, Symp. Combust. 9th, p. 218 (1963).

Kurzius, Ph.D. Dissertation, Princeton University, 1964. AD 635 159.

53. $H + HO_2 = OH + OH$

This rate constant was estimated by Dixon-Lewis and Williams to be 1.1 x 10^{-10} at 500 K, on the basis of data from several sources. One might note that the species H and HO_2 are thought to produce H_2O and O at a small proportion of collisions.

Dixon-Lewis and Williams, Nature 196, 1309 (1962).

54. $H + HO_2 = H_2 + O_2$

This rate constant is estimated by comparison with $H + HO_2 = OH + OH$; Clyne and Thrush obtained a value of 3 ± 1 for the ratio of the rate of chain propagation to the rate of chain breaking in the reaction between H and HO_2.

Clyne and Thrush, Proc. Roy. Soc. A275, 559 (1963).

55. $H_2 + HO_2 = H_2O + OH$ (overall)

The rate constant of the reaction between H_2 and HO_2 was estimated by Dixon-Lewis and Williams[1] to be 2.2 x 10^{-18} at 500 K. These authors made use of data from several sources. This estimate is some 50 times greater than that made earlier by Voevodsky and Tal'rose,[2] who suggested k = 2 x $10^{-13}e^{-24000/RT}$. It is important to note that the reaction is thought[1] to lead to H_2O_2 + H rather than to H_2O + OH, as written above. We have elected to eliminate H_2O_2 from our programs as a result of its relative unimportance as a reaction intermediate in high-temperature environments. The overall reaction, as written here, is satisfactory for the purposes of our programs.

1. Dixon-Lewis and Williams, Nature 196, 1309 (1962).
2. Voevodsky and Tal'rose, Zh. Fiz. Khim. 22, 1192 (1948).

56. $CO + HO_2 = CO_2 + OH$

Estimated by comparison with $CO + OH = CO_2 + H$ and $H_2 + HO_2 = H_2O + OH$. Reaction of CO with HO_2 is thought by Baldwin, Jackson, Walker and Webster to be important at temperatures as low as 500°C, which in itself argues against an activation energy much higher than 10,000 cals/mol .

Baldwin, et al, Symp. Combust. 10th, p. 423 (1965).

57. $CHO + O = CO + OH$ $ClOH + H = ClO + H_2$
$CHO + OH = CO + H_2O$ $ClOH + OH = ClO + H_2O$
$CHO + H = CO + H_2$ $ClOH + O = ClO + OH$

No quantitative data are available for these reactions. The rate constant given for $CHO + OH = CO + H_2O$ was estimated by comparison with $CO + OH = CO_2 + H$, $OH + HO_2 = H_2O + O$ [which was estimated by comparison with $H + HO_2 = O_2$] and the rate constant for the reaction $CHO + H_2O = CH_2O + OH$. [Avramenko and Lorentso[1] cited here and by Fristrom and Westenberg[2] for the reverse reaction. Probably reference 3 is intended. Trotman-Dickenson and Milne[4] give $1 \times 10^{14}\exp(-900/RT)$ from reference 3 and $5 \times 10^{15}\exp(-13000/RT)$ from reference 5, both for the reverse reaction.]

The others were estimated in a similar manner. [Unequal error limits given for CHO + OH and CHO + H, $0.01 < k/k_o < 30$.]

1. Avramenko and Lorentso, Doklady Akad. Nauk SSSR 67, 867 (1949).
2. Fristrom and Westenberg, "Flame Structure" (McGraw-Hill Book Co., New York, 1965).
3. Avramenko and Lorentso, Doklady Akad. Nauk SSSR 69, 205 (1949).
4. Trotman-Dickenson and Milne, NSRDS-NBS 9, U.S. Dept. Commerce, Natl. Bur. Stands. (1967)
5. Westenberg and Fristrom, Symp. Combust. 10th, p. 473 (1965).

58. $CO + H + M = CHO + M$

No quantitative data are available for this reaction. The rate constant given is estimated by comparison with $H + OH + M = H_2O + M$ and $CO + O + M = CO_2 + M$. [Unequal error limits given: $0.033 < k/k_o < 10$.]

59. $CH_4 + OH = CO + H_2O$ (overall)

This "rate constant" is based upon the recommendation of Wilson and Westenberg for the rate constant of the reaction between CH_4 and OH and on the arguments presented by Pergament and Calcote for the use of an artificial overall reaction for the oxidation of methane.

Wilson and Westenberg, Symp. Combust. 11th, p. 1143 (1967).

Pergament and Calcote, Symp. Combust. 11th, p. 597 (1967).

60. $CH_4 + OH = H_3O^+ + e^- + CO_2$ (overall)

The artificial overall "rate constant" was estimated by Pergament and Calcote.

Pergament and Calcote, Symp. Combust. 11th, p. 597 (1967).

61. $CH + O = CHO^+ + e$

The value given for k is a compromise between theoretical values of 3×10^{-12} and 1×10^{-11} reported by Green and Sugden and by Calcote, respectively.

Green and Sugden, Symp. Combust. 9th, p. 607 (1963).

Calcote, AeroChem Research Lab., Princeton, N. J., TP-119 (1965).

62. $CHO^+ + H_2O = CO + H_3O^+$

This rate constant is based on arguments put forward by Calcote.

Calcote, AeroChem Research Lab., Princeton, N.J., TP-119 (1965).

63. $H_3O^+ + Me = H + H_2O + Me^+$ (Me = Li, K, Cs)

These rate constants estimated by comparison with $H_3O^+ + Na = Na^+ + H_2O + H$.

64. $H_3O^+ + Na = H + H_2O + Na^+$

Hayhurst and Telford measured this rate constant in the range $1800 < T < 2500$ K. They observed little significant dependence of k on temperature.

Hayhurst and Telford, Nature 212, 813 (1966).

65. $H_3O^+ + e^- = H + H + OH$

This rate constant has been measured by several workers; the most up-to-date value is given by Calcote, Kurzius and Miller.

Calcote, et al, Symp. Combust. 10th, p. 605 (1965).

66. $Cl^- + H_3O^+ = H + HCl + OH$
$H_3O^+ + OH^- = H + H_2O + OH$

These preliminary values were measured by Kurzius and Calcote.

Kurzius and Calcote, AeroChem Research Lab., Princeton, N. J., TP-92, DDC AD 351 824, July 1964. (Confidential)

67. $Cl + OH + M = ClOH + M$

Estimated by comparison with $O + Cl + M = ClO + M$ [which was estimated by comparison with $O + O + M = O_2 + M$ and $Cl + Cl + M = Cl_2 + M$.]

JOHNSTON, H. S., "Gas Phase Reaction Kinetics of Neutral Oxygen Species", NSRDS-NBS Monograph Series (in press, 1968).

This review examines the available experimental data on reactions among O, O_2 and O_3: atom transfer (including exchange), combination and dissociation. For the latter two types the effect of various third bodies is considered. Recommended values of rate coefficients are given. These are based on a reanalysis of the individual data points reported in the papers considered. Reports giving only rate coefficient expressions are excluded from the analysis. The data used are tabulated, and displayed in extenso in figures.

The notes are limited to simple descriptions of the approach and citation of references. They do not adequately display the scope of the monograph.

1. $O_2 + M = O + O + M$

   See Reaction Summary.

2. $O_3 + M = O + O_2 + M$
   $O + O_3 = O_2 + O_2$

   See Reaction Summary for $O_3 + M = O + O_2 + M$.

3. $O + O_2 = O + O_2$ (Exchange)

   Oxygen atom exchange, using ^{18}O as a tracer, has been studied only near room temperature. The recommended value is for 273°K. Data used were taken from the following sources.

   1. Brennen and Niki, J. Chem. Phys. 42, 3725 (1965).
   2. Herron and Klein, J. Chem. Phys. 40, 2731 (1964).
   3. Jaffe and Klein, Trans. Faraday Soc. 62, 3135 (1966).
   4. Ogg and Sutphen, J. Chem. Phys. 21, 2078 (1953).
   5. Ogg and Sutphen, Disc. Faraday Soc. 17, 47 (1954).

KASKAN, W. E. and BROWNE, W. G., "Kinetics of the $H_2/CO/O_2$ System", General Electric Company Space Sciences Laboratory Report R64SD37, July 1964.

Introduction

This report is an evaluation of rates of elementary reactions of importance in the H-O, C-O and H-C-O combustion systems. It is widely quoted. It is an example of well organized treatment of rate data on a reaction by reaction basis.

The experimental results are listed in each discussion and the data are graphed for most reactions. The forward and reverse reactions are considered together. The estimate for one direction is made then equilibrium data are used to set the rate for the reverse.

Twenty-one reactions (counting forward and reverse as one) are considered. Recommended values are given for eleven of these. The others discussed are:

$OH + OH = H_2 + O_2$

$O + OH + M = HO_2 + M$

$OH + OH + M = H_2O_2 + M$

$CO + O = CO_2$

$CO + O + M = CO_2$

$H_2 + O_2 = H_2O + O$

$OH + OH =$ products

$H + O_3 = O_2 + OH$

$O + O_3 = O_2 + O_2$

$CO + O = CO_2 + h\nu$

The discussion of reactions involving the HO_2 radical and that for CO + O combination are especially extensive and informative.

1. $H_2 + OH = H + H_2O$

See Reaction Summary.

2. $H + O_2 = O + OH$

See Reaction Summary.

3. $H_2 + O = H + OH$

See Reaction Summary.

4. $H_2O + O = OH + OH$

See Reaction Summary for $OH + OH = H_2O + O$.

5. $H + H + M = H_2 + M$
$H + OH + M = H_2O + M$

The analyses of these two reactions are interrelated. While the combination of H atoms has been studied separately, the combination of H and OH has been studied only under conditions where H-H combination occurs.

The rates for the combination of H atoms and dissociation of H_2 are based on room temperature combination data,[1] high temperature shock tube studies of the dissociation,[2-5] and flame studies.[6-8] See also Reaction Summary for $H_2 + M = H + H + M$.

The rate for the H + OH combination (water dissociation rates have not been studied) is based on flame studies.[6-9] Early direct studies using radicals produced from discharged water vapor[10] have been criticized[11] and are not used. The interpretation of flame data is discussed in detail. The temperature dependence adopted is from Ref. 7. The value for $M = H_2O$ is recommended only for mixtures containing about 20% H_2O.

Data and recommendations for both systems are graphed.

1. Marshall, Phys. Fluids 5, 743 (1962).
2. Chesick and Kistiakowsky, J. Chem. Phys. 28, 956 (1958).
3. Rink, J. Chem. Phys. 36, 262 (1962).
4. Patch, J. Chem. Phys. 36, 1919 (1962).
5. Sutton, J. Chem. Phys. 36, 2923 (1962).
6. Kaskan, Combustion and Flame 2, 229 (1958).
7. Bulewicz and Sugden, Trans. Faraday Soc. 54, 1855 (1958).
8. Dixon-Lewis, et al, Disc. Faraday Soc. 33, 205 (1962).
9. Bulewicz, et al, Proc. Roy. Soc. A235, 89 (1956).
10. Oldenberg and Rieke, J. Chem. Phys. 7, 485 (1939).
11. Kaufman and Del Greco, Symp. Combust. 9th, p. 659 (1963).

6. $H + O + M = OH + M$

No data found. Forward reaction rate estimated as an average of the rates for $H + H + M = H_2 + M$ and $O + O + M = O_2 + M$. Reverse reaction rate calculated using equilibrium data.

7. $O_2 + M = O + O + M$

See Reaction Summary.

8. $O + O_2 + M = O_3 + M$

See Reaction Summary for $O_3 + M = O + O_2 + M$.

9. $H + O_2 + M = HO_2 + M$

This reaction is discussed in extenso along with $O + OH + M = HO_2 + M$, $OH + OH =$ products, and $OH + OH + M = H_2O_2 + M$ all of which are interrelated in flames.

Apart from flame data,[1,2] the results considered for $H + O_2$ combination are from direct studies at room temperature and explosion limit experiments.[3-6] The value given for the combination is an estimate, and may be a weighted average of $H + O_2 + M = HO_2 + M$ and $O + OH + M = HO_2 + M$. Recent data are graphed.

1. Kaskan, Combustion and Flame 2, 286 (1958).
2. Dixon-Lewis and Williams, Symp. Combust. 9th, p. 576 (1963).
3. Baldwin and Walsh, Disc. Faraday Soc. 17, 96 (1954).
4. Hoare and Walsh, Trans. Faraday Soc. 53, 1102 (1957).
5. Clyne, Symp. Combust. 9th, p. 211 (1963).
6. Voevodsky and Kondratiev, "Progress in Reaction Kinetics", Vol. 1 (1961), p. 41.

10. $CO + OH = CO_2 + H$

See Reaction Summary.

MAYER, S. W. and SCHIELER, L., "Computed Activation Energies and Rate Constants for Forward and Reverse Transfers of Hydrogen Atoms", J. Phys. Chem. 72, 236 (1968). Also appeared in Chemical Propulsion Information Agency publication No. 146, Vol. I, p. 121, (1967).

Activation energies were computed for 324 gas phase hydrogen-atom transfers

$$X + YH \rightarrow XH + Y$$

where X and Y each run through all members of the set: Al, B, Be, Br, C, Cl, F, H, I, K, Li, Mg, N, Na, O, P, S, and Si.

The 324 reactions include the 18 exchange reactions ($X = Y$) and both the exothermic and endothermic reactions for $X \neq Y$.

A modification of the Johnston and Parr method that considers the temperature region in which the activated complex can be expected to obey small vibration theory was used to calculate rate constants for 234 reactions at temperatures from 298 to 2500°K. The criterion used for applicability of this method is that the average vibrational amplitude of the activated complex be less than $(2\pi)^{0.5}$ at 1000°K. Rate parameters for these reactions were calculated by fitting the rate constants to $k = AT^B \exp(-E/RT)$. These values are marked J + P in this compendium. See general notes under this heading.

Rate parameters for the other 90 reactions were calculated using a collision theory treatment for A, B = 0.5 and the bond energy-bond order method for E. These are marked BEBO in this compendium. See general notes.

For $H_2 + O = H + OH$ also see the Reaction Summary.

Comparisons with experimental data are presented for five cases.

Some values in this paper apply to reactions for which the authors have previously reported similar calculations.[1,2] Those reported here supersede the earlier ones.[3]

1. Mayer, et al, J. Chem. Phys. 45, 385 (1966).
2. Tunder, et al, Aerospace Corp. Rpt. No. TR-1001(9210-02)-1 (1967).
3. Private communication, L. Schieler (March 26, 1968).

SCHOFIELD, K., "An Evaluation of Kinetic Rate Data for Reactions of Neutrals of Atmospheric Interest", Planet. Space Sci. 15, 643 (1967).[†]

Introduction

This is a tabulation and analysis of bimolecular and termolecular rate coefficients for reactions involving H_2, O_2, N , H_2O, H, O, N, OH, HO , O , the oxides of nitrogen, CO, CO_2, SO_2 low molecular weight hydrocarbons, aldehydes, alkyl and alkoxy radicals.

It is an important paper for modern rate coefficient evaluation. Approximately 100 reaction systems are included, with rates given for both directions (where data are available). Rate coefficient expressions are tabulated for each source, data are recalculated when necessary to allow for revisions in thermodynamic and rate data. The tables indicate the possible presence of excited products, the temperature range for each expression, an identification of method and Schofield's remarks on the results.

Plots of the rate data for eleven reactions are included. These show the analyses to be based on data points, as opposed to rate expressions. Least squares fits are used to develop best values based on selected data.

The paper covers the published literature up to October 1966 and lists 280 references.

This compendium lists only a fraction of the material in the paper. All those rates designated as "recommended values" are included here. In addition there are listed those cases where a data fit is reported, the available data are shown in a graph, or a reverse rate is calculated from a recommended value although not marked recommended. These items are identified in the notes.

The notes written for this compendium record references, experimental methods, some of the author's remarks and the method used for setting the recommended value of the rate coefficient.

1. $H + H_2 = H + H_2$ (exchange) and the Deuterium Reactions

Experimental data (low temperature)[1,6-8] are combined with potential energy surface calculations[2,5] in least squares fits. The apparently reliable experimental values reported[1,6,8] recently

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[†] Activation energies quoted from this paper are in cal mol^{-1}
$R = 1.987$ cal $mol^{-1}K^{-1}$

cover only a small temperature range. Consequently an uncertainty of the order of a factor of two still exists for these rates. The data and recommended values are presented both in tabular and graphical form.

Recommended values for more limited temperature ranges are:

$H + p\text{-}H_2 = o\text{-}H_2 + H$

$\log_{10}k = -8.326 - 3490/T + 3.836 \times 10^5/T^2$ for $300 < T < 444$ K (Ref. 1)

$D + H_2 = H + OH$

$\log_{10}k = -7.539 - 3753/T + 4.154 \times 10^5/T^2$ for $274 < T < 468$ K (Ref. 6)

$H + D_2 = D + HD$

$k = 7.2 \times 10^{-12} \exp(-7300/RT)$ for $368 < T < 468$ K (Ref. 8)

1. Schulz and LeRoy, J. Chem. Phys. 42, 3869 (1965).
2. Weston, J. Chem. Phys. 31, 892 (1959).
3. Rapp and Weston, J. Chem. Phys. 36, 2807 (1962).
4. Karplus, et al, J. Chem. Phys. 40, 2033 (1964); 43, 3259 (1965).
5. Shavitt, J. Chem. Phys. 31, 1359 (1959).
6. Ridley, et al, J. Chem. Phys. 44, 3344 (1966).
7a. Boato, et al, J. Chem. Phys. 24, 783 (1956).
7b. Cimino, et al, J. Chem. Phys. 33, 616 (1960).
8. Schulz and LeRoy, Can. J. Chem. 42, 2480 (1964).

2. $H + O_2 = O + OH$

See Reaction Summary.

3. $H_2 + O = H + OH$

See Reaction Summary.

4. $H_2 + OH = H + H_2O$

See Reaction Summary for $H + H_2O = H_2 + OH$.

5. $OH + OH = H_2O + O$

See Reaction Summary

6. $H + N_2O = N_2 + OH$

Mean value of rates reported in atmospheric pressure flame studies[1,2] and (recalculated) low pressure flame data.[3] The recommended rate, based on 900-1780 K measurements has a value six times that measured in flow experiments[4] when extrapolated down to their temperature (423 K).

1. Dixon-Lewis, et al, Symp. Combust. 10th, p. 495 (1965).
2. Dixon-Lewis, et al, J. Chem. Soc. 5724 (1965).
3. Fenimore and Jones, J. Phys. Chem. 63, 1154 (1959).
4. Schiavello and Volpi, J. Chem. Phys. 37, 1510 (1962).

7. $N_2O + O = NO + NO$

This is the best fit to low pressure flame data,[1,2] shock tube luminescence studies[3] and equilibrium measurements on NO decomposition.[4,5] [Not listed as a recommended value by the author.] Other data tabulated: references 6,7.

1. Fenimore and Jones, J. Phys. Chem. 62, 178 (1958).
2. Fenimore and Jones, Symp. Combust. 8th, p. 127 (1962).
3. Fishburne and Edse, J.Chem. Phys. 44, 515 (1966).
4. Kaufman and Kelso, J. Chem. Phys. 23, 1702 (1955).
5. Kaufman and Decker, Symp. Combust. 7th, p. 57 (1959).
6. Kaufman, et al, J. Chem. Phys. 25, 106 (1956).
7. Bradley and Kistiakowsky, J. Chem. Phys. 35, 256 (1961).

8. $H + NO_2 = NO + OH$

Based on flow reactor[1] (mass spectrometry analysis) and static[2] (pressure analysis) studies, the rate for the latter being recalculated. Another static measurement[3] is listed, but the rate (10 times the collision frequency) is rejected.

1. Phillips and Schiff, J. Chem. Phys. 37, 1233 (1962).
2. Ashmore and Tyler, Trans. Faraday Soc. 58, 1108 (1962).
3. Rosser and Wise, J. Phys. Chem. 65, 532 (1961).

9. $NO_2 + O = NO + O_2$

Rate determined in a flow reactor study[1] (mass spectrometric analysis) adopted. Other results tabulated: references 2,3 the former being recalculated.

1. Klein and Herron, J. Chem. Phys. 41, 1285 (1964); 44, 3645 (1966).
2. Ford and Endow, J. Chem. Phys. 27, 1156 (1957).
3. Phillips and Schiff, J. Chem. Phys. 36, 1509 (1962).

10. $NO + O = N + O_2$

See Reaction Summary for $N + O_2 = NO + O$.

12. $H + HNO = H_2 + NO$

Atmospheric pressure flame (1600-2000 K)[1] and flow reactor (226 K)[2] data, both using spectrometric analysis were combined in this estimate.

1. Bulewicz and Sugden, Proc. Roy. Soc. A277, 143 (1964).
2. Clyne and Thrush, Disc. Faraday Soc. 33, 139 (1962).

13. $NO_2 + NO_2 = NO + NO + O_2$

Least squares fit to rates determined from thermal (static) measurements,[1,2] shock tube studies (1400-2300 K)[3,4] and from NO oxidation rates[5-9] plus the equilibrium constant. Scatter of points is small. Activation energy, 28,630 cal/mol , "a little too large", i.e. 500 to 1000 cal/mol more than the endothermicity of the reaction. [Not listed as a recommended value.]

1. Rosser and Wise, J. Chem. Phys. 24, 493 (1956).
2. Ashmore and Burnett, Trans. Faraday Soc. 58, 253 (1962).
3. Huffman and Davidson, J. Am. Chem. Soc. 81, 2311 (1959).
4. Fishburne, et al, J. Chem. Phys. 43, 1847 (1965).
5. Glasson and Tuesday, J. Am. Chem. Soc. 85, 2901 (1963).
6. Bufalini and Stephens, Intern. J. Air Water Pollution 9, 123 (1965).
7. Greig and Hall, Trans. Faraday Soc. 62, 652 (1966).
8. Hall and Greig, Chem. Comm. 326 (1966).
9. Ashmore, et al, Trans. Faraday Soc. 58, 685 (1962).

14. $H + O_3 = O_2 + OH$

Flow reactor (titration and mass spectrometric analysis) value[1] was selected. Data from ref. 2 also listed.

1. Phillips and Schiff, J. Chem. Phys. 37, 1233 (1962).
2. Garvin and McKinley, J. Chem. Phys. 24, 1256 (1956).

15. $N + O_3 = NO + O_2$

Flow reactor (mass spectrometric analysis) value[1] selected. Data from ref. 2 listed, but considered questionable.

1. Phillips and Schiff, J. Chem. Phys. 36, 1509 (1962).
2. Chen and Taylor, J. Chem. Phys. 34, 1344 (1961).

16. $NO + O_3 = NO_2\ (^2A) + O_2$

Two values developed from experiments using flow reactors[1-3] "stopped flow",[4] photolysis[5] and supersonic nozzles.[6]

The value $k = 2.8 \times 10^{-12} \exp(-2820/RT)$ is a least squares fit to all these data. The value $k = 1.7 \times 10^{-12} \exp(-2620/RT)$ excludes ref. 5.

1. Phillips and Schiff, J. Chem. Phys. 36, 1509 (1962).
2. Clyne, et al, Trans. Faraday Soc. 60, 359 (1964).
3. Clough and Thrush, Chem. Comm. 783 (1966).
4. Johnston and Crosby, J. Chem. Phys. 19, 799 (1951); 22, 689 (1954).
5. Ford, et al, Adv. Chem. Series 21, 410 (1959); J. Chem. Phys. 26, 1337 (1957).
6. Marte, et al, J. Chem. Phys. 39, 3277 (1963).

17. $CH_4 + H = CH_3 + H_2$

Least squares fit to flame,[1,2] photolysis,[3,4] flow reactor[5] and explosion limit data.[6,7] Results from references 1 and 4 recalculated. Data presented both in tabular and graphical form.

1. Fenimore and Jones, J. Phys. Chem. 65, 2200 (1961).
2. Dixon-Lewis and Williams, Symp. Combust. 11th, p. 951 (1966).
3. Majury and Steacie, Disc. Faraday Soc. 14, 45 (1953).
4. Klein , et al, J. Chem. Phys. 30, 58 (1959).
5. Jamieson and Brown, Can. J. Chem. 42, 1638 (1964).
6. Gorban and Nalbandyan, Russ. J. Phys. Chem. 36, 946 (1962).
7. Azatyan, et al, Kinetics and Catalysis USSR 5, 177 (1964).

18. $C_2H_6 + H = C_2H_5 + H_2$

Least squares fit to flame,[1] photolysis[2] and explosion limit data.[3,4,7,8] Results of references 2 and 3 recalculated. Flow reactor (probe detection) results[5] rejected per discussions in references 6 and 8. "Quite well defined fit."

1. Fenimore and Jones, Symp. Combust. 9th, p. 597 (1963).
2. Darwent and Roberts, Disc. Faraday Soc. 14, 55 (1953).
3. Baldwin, et al, Symp. Combust. 10th, p. 423 (1965).
4. Gorban and Nalbandyan, Russ. J. Phys. Chem. 36, 946 (1962).
5. Berlie and LeRoy, Disc. Faraday Soc. 14, 50 (1953).
6. Schulz and LeRoy, Can. J. Chem. 40, 2413 (1962).
7. Baldwin, Symp. Combust. 9th, p. 604 (1963).
8. Voevodskii and Kondrat'ev, Progress in Reaction Kinetics, Vol. 1, p. 41 (1961).

19. $C_3H_8 + H = C_3H_7 + H_2$

Least squares fit to flame,[1,8] photolysis[2] (recalculated), flow (probe detection)[3] and explosion limit data.[4-7] "Well defined fit."

1. Fristrom, et al, Rev. Inst. Fr. Petrole 13, 544 (1958).
2. Darwent and Roberts, Disc. Faraday Soc. 14, 55 (1953).
3. Kazmi, et al, Can. J. Chem. 41, 690 (1963).
4. Gorban and Nalbandyan, Russ. J. Phys. Chem. 36, 946 (1962).
5. Voevodskii and Kondrat'ev, Progress in Reaction Kinetics, Vol. 1, p. 41 (1961).

6. Baldwin, et al, Symp. Combust. 10th, p. 423 (1964).
7. Baldwin, Trans. Faraday Soc. 60, 527 (1964).
8. Fristrom and Westenberg,"Flame Structure," p. 366, 1965.

20. $n\text{-}C_4H_{10} + H = n\text{-}C_4H_9 + H_2$

Least squares fit to photolysis[1] (recalculated), explosion limit[2,3] and flow (probe detection plus gas chromatography)[4] results. "Confirmatory data required."

1. Darwent and Roberts, Disc. Faraday Soc. 14, 55 (1953).
2. Baldwin, et al, Symp. Combust. 10th, p. 423 (1965).
3. Baldwin and Walker, Trans. Faraday Soc. 60, 1236 (1964).
4. Kazmi and LeRoy, Can. J. Chem. 42, 1145 (1964).

21. $iso\text{-}C_4H_{10} + H = iso\text{-}C_4H_9 + H_2$

Least squares fit to photolysis[1] (recalculated), and explosion limit data.[2-5] "More data required outside 600-900 K range."

1. Darwent and Roberts, Disc. Faraday Soc. 14, 55 (1953).
2. Baldwin, et al, Symp. Combust. 10th, p. 423 (1965).
3. Gorban and Nalbandyan, Russ. J. Phys. Chem. 36, 946 (1962).
4. Voevodskii and Kondrat'ev, Progress in Reaction Kinetics, Vol. 1, p. 41 (1961).
5. Baldwin and Walker, Trans. Faraday Soc. 60, 1236 (1954).

22. $C_2H_4 + H = C_2H_3 + H_2$

Based on explosion limit data[1] taking E = 6900. (Reasonable agreement with data of references 2,3.)

1. Baldwin, et al, Trans. Faraday Soc. 62, 2476, 2486 (1966).
2. Voevodskii and Kondrat'ev, Progress in Reaction Kinetics, Vol. 1, p. 41 (1961).
3. Azatyan, et al, Proc. Acad. Sci. USSR Phys. Chem. Sec. 149, 312 (1963).

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23. $C_2H_4 + H = C_2H_5^*$

Least squares fit to photolysis,[1,2] radiolysis[3] (recalculated) explosion limit[4] and flow reactor experiments.[5] Photolysis results (reference 6) not used. "Reasonable agreement between data."

1. Allen, et al, Proc. Roy. Soc. A218, 311 (1953).
2. Jennings and Cvetanovic, J. Chem. Phys. 35, 1233 (1961).
3. Yang, J. Am. Chem. Soc. 84, 719 (1962).
4. Baldwin, et al, Trans. Faraday Soc. 62, 2476, 2486 (1966).
5. Brown, et al, Chem. Comm. 843 (1966).
6. Darwent and Roberts, Disc. Faraday Soc. 14, 55 (1953).

24. $CH_4 + OH = CH_3 + H_2O$

Flow[1], thermal[2,4] and flame[5-8] data combined in a least square fit. Data from reference 2 recalculated. Results presented in tabular and graphical form. Flow experiments in which water was passed through an electric discharge to form OH,[9] were rejected.

1. Wilson and Westenberg, Symp. Combust. 11th, p. 1143 (1966).
2. Blundell, et al, Symp. Combust. 10th, p. 445 (1965).
3. Hoare, Nature 194, 293 (1962); Proc. Roy. Soc. A291, 73 (1966).
4. Hoare and Peacock, Proc. Roy. Soc. A291, 85 (1966).
5. Fenimore and Jones, J. Phys. Chem. 65, 2200 (1961).
6. Westenberg and Fristrom, J. Phys. Chem. 65, 591 (1961).
7. Fristrom, Symp. Combust. 9th, p. 560 (1963).
8. Dixon-Lewis and Williams, Symp. Combust. 11th, p. 951 (1966).
9. Avramenko and Kolesnikova, Advances in Photochemistry, Vol. 2 p. 25 (1964).

25. $CH_4 + O = CH_3 + OH$

Stirred reactor[1] flow,[2,3] low pressure flame[4] and explosion limit data[5] combined in a least squares fit. Results given in tabular and graphical form.

1. Wong and Potter, J. Chem. Phys. 39, 2211 (1963); 43, 3371 (1965).
2. Avramenko, et al, Bull. Acad. Sci. USSR Div. Chem. Sci. 557 (1963).
3. Cadle and Allen, J. Phys. Chem. 69, 1611 (1965).
4. Fenimore and Jones, J. Phys. Chem. 65, 2200 (1961).
5. Azatyan, et al, Kinetics and Catalysis 5, 177 (1964).

26. $C_2H_6 + O = C_2H_5 + OH$

Least squares fit to explosion limit,[1] flow reactor[2] and photolysis data.[3] "Reasonable agreement between data but more needed."

1. Azatyan, et al, Proc. Acad. Sci. USSR Chem. Sect. 147, 973 (1962).
2. Avramenko, et al, Bull. Acad. Sci. USSR Div. Chem. Sci. 557 (1963).
3. Saunders and Heicklen, J. Phys. Chem. 70, 1950 (1966).

27. $CH_3CHO + O = CH_3CO + OH$

Value selected is that of R. D. Cadle and J. W. Powers (private communication). Method used: flow reactor with oxygen atoms produced in an electric discharge and gas chromatographic analysis of trapped products.

28. $CO + OH = CO_2 + H$

See Reaction Summary.

29. $O + O_2 + M = O_3 + M$

See Reaction Summary for $O_3 + M = O + O_2 + M$.

30. $H + O_2 + M = HO_2 + M$

Least squares fit to flow reactor,[1,2] explosion limit[3-7] and shock tube data.[8] Data from references 4 and 5 recalculated. Flame data of reference 9 not used. Results presented graphically and in tabular form. Both the Arrhenius equation and the $k = AT^{-en}$ form are presented (and are included in this compendium). [Not listed as recommended values.]

1. Clyne and Thrush, Proc. Roy. Soc. A275, 559 (1963).
2. Larkin and Thrush, Disc. Faraday Soc. 37, 112 (1964).
3. Ashmore and Tyler, Trans. Faraday Soc. 58, 1108 (1962).
4. Webster and Walsh, Symp. Combust. 10th, p. 463 (1965).
5. Baldwin, et al, Trans. Faraday Soc. 56, 93 (1960).
6. Baldwin and Brooks, Trans. Faraday Soc. 58, 1782 (1962).
7. Lewis and Von Elbe, Combustion, Flames and Explosions of Gases, p. 29 (Academic Press, N. Y., 1961).
8. Getzinger and Schott, J. Chem. Phys. 43, 3237 (1965).
9. Fenimore and Jones, Symp. Combust. 10th, p. 489 (1965).

31. $N + N + M = N_2 + M$

This is a mean value for 300 K based on flow and static experiments in which the nitrogen afterglow[1-5] was monitored, atom concentrations were measured by titration[1,3-8] ESR[9], probes[2] and Wrede gauges.[3] When combined with shock tube measurements at 6400 K,[9-11] this room temperature value suggests a $T^{-0.7}$ dependence.

1. Harteck, et al, J. Chem. Phys. 29, 608 (1958).
2. Wentink, et al, J. Chem. Phys. 29, 231 (1958).
3. Kretschmer and Petersen, J. Chem. Phys. 39, 1772 (1963).
4. Barth, Ann. Geophys. 20, 182 (1964).
5. Campbell and Thrush, Chem. Comm. 250 (1965).
6. Herron, et al, J. Chem. Phys. 30, 879 (1959).
7. Mavroyannis and Winkler, Can. J. Chem. 39, 1601 (1961).
8. Avramenko and Krasenen'kov, Bull. Acad. Sci. USSR Div. Chem. Sci. 1095 (1963).

9. Evenson and Burch, J. Chem. Phys. 45, 2450 (1966).
10. Allen, et al, Phys. Fluids 5, 284 (1962).
11. Byron, J. Chem. Phys. 44, 1378 (1966).

32. $NO + O + M = NO_2 + M\ (M = N_2)$

This value, with an apparent negative activation energy (-1930 cal/mol) is that determined by Klein and Herron[1] in a flow system, using discharge production of atoms and mass spectrometric analysis. Other data tabulated: references 2-8.

1. Klein and Herron, J. Chem. Phys. 41, 1285 (1964); 44, 3645 (1966).
2. Ford and Endow, J. Chem. Phys. 27, 1156 (1957).
3. Clyne and Thrush, Proc. Roy. Soc. A269, 404 (1962).
4. Clyne, et al, Trans. Faraday Soc. 61, 2701 (1965).
5. Ogryzlo and Schiff, Can. J. Chem. 37, 1690 (1959).
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Introduction

This report lists rate parameters for over 1000 reactions of atoms and small molecules. The molecules are compounds (or ions) of the following elements: Al, Be, B, C, Li, N, K, Na, Cl, F, O and H. The report is arranged in 13 tables, the first containing reactions of Al and its compounds with all others, the second is for Be and its compounds and all other species except those of Al. Succeeding tables follow this rule, the last containing only reactions of H, H^+, H^-, H_2 with each other.

Many of the reactions listed have never been studied experimentally. Order of magnitude estimates are given for many of these. Such estimates are keyed to the "General Notes" section by the code OME, and are not keyed to a specific note in the list below. The next largest class of rates in this report are those calculated by the Johnston and Parr linear transition state, bond energy-bond order method. These are keyed to the "General Notes" section by J+P or BEBO depending upon whether the full method was used or only the activation energy was estimated by this technique.

In the text of the report those items now identified by OME were identified by notes 2, 21 and 36 and were explained in its introduction. The items keyed J+P or BEBO were keyed to their note 22.

Schieler has indicated[1] that the group at Aerospace consider that the "order of magnitude estimate" represents a particularly antiquated state-of-the-art. This type of estimate was made by them before they decided to explore the possibilities for computing rate constants. Their later work emphasizes the calculational approach, the details of which continue to be developed.[2,3,4] Rates reported in the later papers are to be preferred, calculated rates are to replace estimates ones. At least in principle large parts of the compilation (TR-1001(9210-02)-1) have been superseded.

In keeping with this view we have deleted estimated rates that have also been calculated by them. The newer values are listed in the main table and are taken from reference 2.

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