NSRDS-NBS 73, Part 2

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

Compilation of Chemical Kinetic Data for Combustion Chemistry.

Part 2. Non-Aromatic C, H, O, N, and S Containing Compounds.

(1983)

The National Bureau of Standards[1] was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research to assure international competitiveness and leadership of U.S. industry, science and technology. NBS work involves development and transfer of measurements, standards and related science and technology, in support of continually improving U.S. productivity, product quality and reliability, innovation and underlying science and engineering. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Institute for Materials Science and Engineering.

The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; provides calibration services; and manages the National Standard Reference Data System. The Laboratory consists of the following centers:

- Basic Standards[2]
- Radiation Research
- Chemical Physics
- Analytical Chemistry

The National Engineering Laboratory

Provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

- Applied Mathematics
- Electronics and Electrical Engineering[2]
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering[3]

The Institute for Computer Sciences and Technology

Conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following divisions:

- Information Systems Engineering
- Systems and Software Technology
- Computer Security
- Systems and Network Architecture
- Advanced Computer Systems

The Institute for Materials Science and Engineering

Conducts research and provides measurements, data, standards, reference materials, quantitative understanding and other technical information fundamental to the processing, structure, properties and performance of materials; addresses the scientific basis for new advanced materials technologies; plans research around cross-cutting scientific themes such as nondestructive evaluation and phase diagram development; oversees Bureau-wide technical programs in nuclear reactor radiation research and nondestructive evaluation; and broadly disseminates generic technical information resulting from its programs. The Institute consists of the following Divisions:

- Ceramics
- Fracture and Deformation[3]
- Polymers
- Metallurgy
- Reactor Radiation

---

[1] Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.

[2] Some divisions within the center are located at Boulder, CO 80303.

[3] Located at Boulder, CO, with some elements at Gaithersburg, MD

Compilation of Chemical Kinetic Data for Combustion Chemistry.

Part 2. Non-Aromatic C, H, O, N, and S Containing Compounds. (1983)

Francis Westley, John T. Herron,
and R. J. Cvetanović

Chemical Kinetics Division
Center for Chemical Physics
National Bureau of Standards
Gaithersburg, MD 20899

NATIONAL STANDARD
NSRDS
REFERENCE DATA SYSTEM

U.S. DEPARTMENT OF COMMERCE, C. William Verity, Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued December 1987

Library of Congress Cataloging-in-Publication Data
(Revised for Vol. 2)

Westley, Francis.
Compilation of chemical kinetic data for combustion chemistry.

(NSRDS-NBS; 73, pt. 1–)
Includes bibliographies and index.
Contents: Pt. 1. Non-aromatic C, H, O, N, and S containing compounds (1971–1982)—pt. 2. Non-aromatic C, H, O, N, and S containing compounds (1983).

1. Combustion—Tables. 2. Chemical reaction, Rate of—
Tables. I. Herron, John Thomas, 1931–
II. Cvetanović, Ratimir J. III. Center for Chemical Physics (U.S.).
Chemical Kinetics Division. IV. Title.
V. Series: NSRDS–NBS ; 73, pt. 1, etc.
QC100.U573 no. 73 pt. 1, etc. 602'.18s 87–20244

[QD516] [541.3'61'0212]

NSRDS-NBS 73, Part 2

Natl. Stand. Ref. Data Ser., Natl. Bur. Stand. (U.S.), 73, Part 2, 142 pages (Dec. 1987)
CODEN: NSRDAP

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1987

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402

Foreword

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data. These tables are published in the *Journal of Physical and Chemical Reference Data*, in the NSRDS-NBS series of the National Bureau of Standards, and through other appropriate channels.

The task of critical evaluation is carried out in various data centers, each with a well-defined technical scope. A necessary preliminary step to the critical evaluation process is the retrieval from the world scientific literature of all papers falling within the scope of the center, followed by the extraction and organization of the numerical data contained in these papers. The present publication presents such a compilation of data prepared by the NBS Chemical Kinetics Data Center.

Further information on NSRDS and the publications which form the primary output of the program may be obtained by writing to the Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899.

DAVID R. LIDE, JR., *Director*
Office of Standard Reference Data

Contents

Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 2. Non-Aromatic C, H, O, N, and S Containing Compounds. (1983)

Francis Westley, John T. Herron, and R. J. Cvetanović

Chemical Kinetics Division, Center for Chemical Physics, National Bureau of Standards, Gaithersburg, MD. 20899

Chemical kinetic data for reactions of importance in combustion chemistry are compiled. Experimental, theoretical, evaluated, or estimated rate constants are given for reactions of O, O_3, H, H_2, OH, HO_2, H_2O, N, N_3, NO, NO_2, N_2O, NH, NH_2, SH, H_2S, SO, SO_2, and the aliphatic, alicyclic, and heterocyclic saturated and unsaturated C_1 to C_{15} hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides, and their free radicals. The data were taken from the literature published in 1983. Data omitted from Part 1 of this series, covering the period 1971 to 1982, are also included. The data are reported as rate constants or in terms of the parameters A, n, and B of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$, where $B = E/R$. Data are given for 434 reactions.

Key words: Arrhenius parameters; carbon; chemical kinetics; combustion; compilation; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

1. Introduction

1.1. Overview

This report provides a compilation of chemical kinetic data for use by modelers, experimentalists, and theoreticians interested in developing a detailed understanding of gas phase combustion processes involving fossil fuels. It is part of a larger effort to develop a comprehensive evaluated chemical kinetic data base, and is a necessary prelude to that effort. The present compilation covers the literature published in 1983. It supplements the recently issued compilation which covered the literature from 1971 to 1982[1].

1.2. Scope

Data are given for the reactions of aliphatic, alicyclic, and heterocyclic, saturated and unsaturated hydrocarbons and their derivatives, and for the reactions with inorganic species containing hydrogen, oxygen, nitrogen, and sulfur with themselves and with hydrocarbons and their derivatives. Not included are reactions involving aromatic species, halogens, halogen derivatives, ions, and, with few exceptions, excited states.

The data have been abstracted from the literature published in 1983. Data omitted from Part 1 of this series covering the period 1971 to 1982, are also included.

Only publications containing numerical data have been abstracted. The abstracted data are either rate constants at some given temperature or the parameters A, n, and B of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$. Additional data on temperature range, pressure, nature of the third body, and the type of data (i. e., experimental, theoretical, estimated, etc.) are also provided.

1.3. Guide to the Table

1.3.1. General

The compilation is divided into two parts — a table of rate constants and a bibliography, which contains the references to the cited literature. The following describes the arrangement of the table with respect to contents and the order in which reactions are listed.

1.3.2. Arrangement of the Table

The table is arranged in eight columns. These list the chemical reaction, the data type, the temperature, the rate constant or the Arrhenius A factor, the n factor, the B factor where $B = E/R$, a term indicating the appropriate units for the rate constants, and an error factor. Other necessary information such as the bibliographic citation, pressure and nature of bath gas, and notes on methodology or other factors is given in the same column as the chemical reaction. A detailed description follows:

(1) Column 1 gives the chemical reaction. The names of the reactants given are the Chemical Abstracts Standard Names. Synonyms, enclosed in parentheses, are in some cases also given. Product names are given only in those cases in which the product is a bridged compound.

The bibliographic citation is given in the form of a Reference Code, which consists of the last two digits of the year of publication, followed by the first three letters of the names of the first and second author (if present) separated by a slash. An integer index is attached at the end when it is necessary to differentiate between otherwise identical Codes.

This column may also include information on the experimental method, analytical procedures, nature of the third body, pressure, identity of reference reaction in the case of relative rate measurements, or other comments.

(2) Column 2 indicates the type of data. Data type codes are described in Sec. 2.

(3) Column 3 gives the temperature or temperature range.

(4) Column 4 lists the rate constant or the Arrhenius A factor, or the ratio of the rate constants.

(5) Column 5 gives the factor n for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$.

(6) Column 6 gives the parameter B for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$, where B is the Arrhenius activation energy divided by the gas constant, i.e., $B = E/R$. In the case of relative rate measurements the quantity reported is the difference $B - B(\text{ref})$, where $B(\text{ref})$ is the value of B for the reference reaction.

(7) Column 7 indicates the units of the rate constant or the Arrhenius A factor.

(8) Column 8 gives the error factor as reported in the original work.

1.3.3. Order of Reactions

The reactions are listed following the order of arrangement given in Table 1 of "The NBS Tables of Thermodynamic Properties".[2] In the present compilation the reactants contain any of the elements O, H, S, N, and C, and the order used is: O system, H-O system, S-O-H system, N-O-H-S system, and C-O-H-S-N system. Examples of the ordering of reactant species are given below:

(1) O system: O, O_2, O_3

(2) H-O system: H, H_2, OH, HO_2, H_2O, H_2O_2

(3) S-O-H system: S, S_2, SO, SO_2, SO_3, SH, H_2S

(4) N-O-H-S system: N, N_2, NO_2, NO_3, N_2O, N_2O_3, NH, etc.

(5) C-O-H-S-N system: C, CO, CO_2, CH, CH_2, CH_3, CH_4, etc.

Index of reactions given in Sec. 3 follows the same order of arrangement and can be used to find the page where a particular reaction is located in the Table of Chemical Kinetic Data for Combustion Chemistry. The reaction of ethylene with oxygen atoms, for example, is located at its proper place in the "O ATOM Reactions" at the beginning of the Index, since O atom (the O system) precedes ethylene (the C system).

1.3.4. Chemical Formulas and Nomenclature

Where possible, chemical formulas are written in semi-structural form. The following conventions are used:

(1) For C_1 through C_5 saturated hydrocarbons and their O, S, and N derivatives, semi-structural formulas are used, e.g., $(CH_3)_2CH_2CH_2ONO$. Beyond C_5 the condensed forms are used, e.g., $CH_3(CH_2)_8CH_2CN$.

(2) Unsaturated compounds are written to show the position of the double or triple bond, e.g., $CH_2=C=CH_2$.

(3) The structures of all alicyclic and heterocyclic compounds are specified with figures in the text.

1.4. Acknowledgments

This work was supported by the Department of Energy, Division of Basic Energy Sciences and the Office of Standard Reference Data of the National Bureau of Standards. The authors are especially indebted to Mrs. Geraldine Zumwalt and Ms. Rhoda Levin for their attention to many details in the keyboarding, editing and preparation of the manuscript.

1.5. References to the Introduction

[1] F. Westley, J. T. Herron, and R. J. Cvetanović "Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)", NSRDS-NBS 73, Part 1, U. S. Government Printing Office, Washington, D.C. 20402, (1987).

[2] D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, J. Phys. Chem. Ref. Data 11, Suppl. 2 (1982).

2. Summary of Symbols and Units

Data Type Codes:

EX	(experimentally measured absolute value)
RL	(experimentally measured relative value)
RN	(RL normalized to absolute value)
TH	(theoretical value)
DE	(derived indirectly, e.g. using reverse rate and equilibrium constant, or computer simulation of a complex mechanism)

CO (computed numerically)
ES (estimated, by analogy etc)
SE (selected in the literature as probable "best" value)

Type of excitation:
† (vibrationally excited)
* (electronically excited)

Decadic exponent notation: 1.2(11) (stands for 1.2×10^{11})

Temperature (T): in kelvins (K).

Arrhenius parameters are defined by
$k = A(T/298)^n \exp(-B/T)$.

Unit Codes for k, k/k(ref), A, A/A(ref):
1 ($\mathrm{s^{-1}}$)
2 ($\mathrm{cm^3\,mol^{-1}\,s^{-1}}$)
3 ($\mathrm{cm^6\,mol^{-2}\,s^{-1}}$)
1/1, 2/2 etc. (dimensionless)
2/1 ($\mathrm{cm^3\,mol^{-1}}$), etc.

($T/298$) and n [the exponent of ($T/298$)] are dimensionless.

Units for B, $B - B$(ref): kelvins (K). (Activation energy $E = R \times B$).

k(ref), A(ref) and B(ref) are the values for the "reference reaction" in relative rate determinations.

k err. factor: Estimated overall Uncertainty Factor. It multiplies and divides k or A to indicate approximate error limits. It does not imply that errors in k are necessarily lognormally distributed.

3. Index of Reactions

O ATOM Reactions:

O_3 Reactions:

H ATOM Reactions:

H_2 Reactions:

OH RADICAL Reactions:

HO_2 RADICAL Reactions:

H_2O Reactions:

SO_x-COMPOUND Reactions:

SH_x-COMPOUND Reactions:

N_x-COMPOUND Reactions:

N_xO_y-COMPOUND Reactions:

N_xH_y-COMPOUND Reactions:

C ATOM Reactions:

CO_x-COMPOUND Reactions:

CH RADICAL Reactions:

CH_2 Reactions:

CH_3 RADICAL Reactions:

CH_4 Reactions:

CH_xO_y-COMPOUND Reactions:

CS_x-COMPOUND Reactions:

CH_xS_y-COMPOUND Reactions:

CN RADICAL Reactions:

CH_xN_y-COMPOUND Reactions:

C_2H_x-COMPOUND Reactions:

$C_2H_xO_y$-COMPOUND Reactions:

$C_2H_xS_y$-COMPOUND Reactions:

$C_2H_xO_yS_z$-COMPOUND Reactions:

C_2N_x-COMPOUND Reactions:

$C_2H_xN_y$-COMPOUND Reactions:

$C_2H_xO_yN_z$-COMPOUND Reactions:

C_3 (Carbon trimer) Reactions:

C_3H_x-COMPOUND Reactions:

$C_3H_xO_y$-COMPOUND Reactions:

$C_3H_xN_y$-COMPOUND Reactions:

$C_3H_xO_yN_z$-COMPOUND Reactions:

C_4H_x-COMPOUND Reactions:

$C_4H_xO_y$-COMPOUND Reactions:

$C_4H_xO_yS_z$-COMPOUND Reactions:

$C_4H_xN_y$-COMPOUND Reactions:

$C_4H_xO_yN_z$-COMPOUND Reactions:

C_5H_x-COMPOUND Reactions:

$C_5H_xO_y$-COMPOUND Reactions:

$C_5H_xO_yN_z$-COMPOUND Reactions:

C$_6$H$_x$-COMPOUND Reactions:

C$_6$H$_x$O$_y$-COMPOUND Reactions:

C$_6$H$_x$S$_y$-COMPOUND Reactions:

C$_6$H$_x$N$_y$-COMPOUND Reactions:

$C_6H_xO_yN_z$-COMPOUND Reactions:

C_7H_x-COMPOUND Reactions:

$C_7H_xO_y$-COMPOUND Reactions:

$C_7H_xO_yN_z$-COMPOUND Reactions:

C_8H_x-COMPOUND Reactions:

C$_8$H$_x$O$_y$-COMPOUND Reactions:

$C_8H_xS_y$-COMPOUND Reactions:

C_9-COMPOUND Reactions:

C_{10} to C_{14}-COMPOUND Reactions:

4. Table of Chemical Kinetic Data for Combustion Chemistry

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + O_3 \rightarrow O_2 + O_2$							
Oxygen atom + Ozone							
83 WIN/NIC	EX	237-377	(3.37±1.26)(12)	0	1950±110	2	
Reaction of O atoms with Ozone in a flow system. O atoms generated by pulsed Laser Photolysis of O_3 at 532 nm. Time-resolved Resonance-fluorescence. P = (15-150) torr. $[O_3]/[O]_o$ = 1940-21700							
$O + H_2 \rightarrow OH + H$							
Oxygen atom + Hydrogen molecule							
78 CAM/HAN	EX	350-490	(3.1±0.5)(13)	0	4950±300	2	
Reaction of O atom with H_2 in a discharge-flow stirred reactor. O atoms generated by reacting N with NO.							
$O + OH \rightarrow O_2 + H$							
Oxygen atom + Hydroxyl							
83 BRU/SCH2	EX	298	(1.87±0.30)(13)			2	
Reaction of O atom with OH in a fast-flow reactor. Laser-magnetic resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)							
83 TEM	EX	296	(4.0±1.2)(13)			2	
Reaction of O atoms with OH by Far-IR Laser-Magnetic-Resonance Spectrometry.							
$O + HO_2 \rightarrow OH + O_2$							
Oxygen atom + Hydroperoxo							
79 TEM	EX	298	(2.0±0.6)(13)			2	
Reaction of O atoms with HO_2 in an isothermal flow-reactor. ESR-spectrometry. LMR-spectrometry. O atoms generated by dissociation of O_2 in a microwave discharge. HO_2 generated by reacting F with H_2O_2.							
83 BRU/SCH2	EX	298	(3.13±0.48)(13)			2	
Reaction of O atom with HO_2 in a fast-flow reactor. Laser-Magnetic Resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
83 KEY Reaction of O atom with HO_2 in a fast discharge-flow system. HO_2 generated by reacting H with O_2 in excess. H atom generated by a microwave discharge of H_2 in He. Resonance-fluorescence. k_{ref}: $O + OH \rightarrow O_2 + H$. P(Total) = 2 torr.	RL	299	1.7±0.2			2/2	
83 RAV/WIN Reaction of O atoms with HO_2 by Pulsed-Laser-Photolysis/Resonance-fluorescence. O atoms and HO_2 generated by Photolysis of O_3 and H_2O_2 in N_2, at 248.5 nm., by using a KrF excimer laser. $P(N_2)$ = (10-500) torr. $[HO_2] > [O^3P]$. $[H_2O_2] = (0.30\text{-}1.71)\times10^{16}$ molec.cm^{-3}. k isindependent of N_2 pressure.	EX	298	(3.73±0.66)(13)			2	
$O + H_2O_2 \rightarrow OH + HO_2$ (a) **$\rightarrow O_2 + H_2O$ (b)** Oxygen atom + Hydrogen peroxide							
83 WIN/NIC Reaction of O atoms with H_2O_2 in a flow-system equipped with a Pyrex reactor and a Brass reactor. O atoms generated by pulsed Laser Photolysis of O_3 at 532 nm. Time-resolved Resonance-fluorescence. $[O]_o = (0.4\text{-}57)\times10^{11}$ molec.cm^{-3}. P = (15-150) torr.	EX	298-386	(6.81±3.25)(11)	0	2000±160	2	
$O + NO (+ M) \rightarrow O_2 + N (+ M)$ (a) **$\rightarrow NO_2 (+ M)$ (b)** Oxygen atom + Nitrogen oxide (NO)							
83 SCH/KOH (k_b. M = He)	EX	200-370	(8.27±0.58)(15)	0	-290±17	3	
(k_b. M = He)	EX	300	2.25(16)			3	
(k_b. M = NO)	EX	200-370	(1.36±0.05)(16)	0	-355±11	3	
(k_b. M = NO)	EX	300	4.57(16)	0	0	3	
(k_b. M = N_2)	EX	200-370	(8.85±0.83)(15)	0	-380±25	3	
(k_b. M = N_2)	EX	300	3.19(16)			3	
(k_b. M = CH_4)	EX	200-370	(1.02±0.18)(16)	0	-414±40	3	
(k_b. M = CH_4)	EX	300	4.17(16)			3	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
Reaction of O atoms with NO in a reactive chamber with a VUV-Laser emitting light at about 160 nm. Small amounts of O atoms generated in the H_2-Laser photolysis of NO. Chemiluminesxcence emission. $P(He, or N_2, or CH_4) = (10-55)$ torr. $P(NO) = (0.04-1.11)$ torr.							
O + NH → NO + H (a) (main channel) **→ OH + N (b)**							
Oxygen atom + Imidogen							
83 TEM	EX	296	(5.0±2.0)(13)			2	
$k_a + k_b$. Far-IR Magnetic-Resonance Spectrometry.							
O + NH_2 → OH + NH (a) **→ HNO + H (b)**							
Oxygen atom + Amidogen							
83 TEM (k_a)	EX	296	(7.0±3.0)(12)			2	
(k_b)	EX	296	(4.6±1.2)(13)			2	
Reaction of O atoms with NH_2 by Far-IR Laser-Magnetic-Resonance Spectrometry.							
O + HNO → OH + NO							
Oxygen atom + Nitrosyl hydride							
83 TEM	EX	296	5.0(12)			2	
Reaction of O atoms with HNO by Far-IR Laser-Magnetic-Resonance Spectrometry.							
O + CHO → OH + CO (a) **→ H + CO_2 (b)**							
Oxygen atom + Methyl, oxo- (Formyl)							
78 CAM/HAN	RL	425	(4.0±2.0)(-1)			2/2	
k_a/k_b. Estimated rate ratio. Reaction of O CHO in a discharge-flow stirred reactor. O atoms generated by reacting N with NO. CHO generated by reacting H with CO.							
O + HCHO → OH + CHO							
Oxygen atom + Formaldehyde							
83 GUE/VAN	EX	~1400	4.0(13)	0	1807	2	
Reaction of O atoms with HCHO in premixed flames. Molecular-beam sampling. Mass-spectrometry. Unspecified T-range. P = (22.5-40) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_3ONO_2 \rightarrow OH + CH_2ONO_2$ Oxygen atom + Nitric acid methyl ester							
77 SAL/THR Reaction of O atoms with Methyl nitrate in a fast-flow system. O atoms generated by dissociation of O_2 (1% in Ar) through a microwave-discharge. P(Total) = (0.75-15) torr.	EX	294-473	1.5(13)	0	2646±120	2	
$O + CH\equiv CH \rightarrow CO + CH_2$ (a) $O + CH\equiv CH \rightarrow H + CH{=}C{=}O \rightarrow CH_2{=}C{=}O$ (b) $\rightarrow C{=}C{=}O + H_2$ (c) $\rightarrow OH + CH\equiv C$ (d) Oxygen atom + Ethyne							
83 HOM/WEL1 $k_b + k_d$. Reaction of O atoms with Ethyne in a discharge-flow reactor. O atoms generated by the reaction: $N + NO \rightarrow N_2 + O$, or by decomposition of O_2 in a microwave discharge. Mass-spectrometry. Channel (b) occurs at lower temperatures, while channel (d) occurs at high temperatures. P(Total) = 2 torr.	EX	295-1330	(1.6±0.5)(13)	0	1550	2	
83 HOM/WEL2 k_b. Reaction of O atoms with $CH\equiv CH$, studied in a flow-reactor, with or without added H atoms. P(Total) = 2 Torr.	EX	1000	2(12)			2	
$O + CH_2{=}CH_2 \rightarrow HCHO + CH_2$ (a) $\rightarrow CHO + CH_3$ (b) $\rightarrow CH_2{=}C{=}O + H_2$ (c) $\rightarrow$  (d) $\rightarrow H + CH_2CHO$ (e) Oxygen atom + Ethene							
83 FON/MAE (k$_b$ + k$_e$. P(He) = 0.5 torr.)	EX	298	(4.10±0.48)(11)			2	
(k$_b$ + k$_e$. P(He) = 2 torr.)	EX	298	(4.04±0.60)(11)			2	
(k$_b$ + k$_e$. P(He) = 5 torr.)	EX	298	(3.79±0.18)(11)			2	
(k$_b$ + k$_e$. P(He) = 0.5 torr.)	EX	552	(1.57±0.06)(12)			2	
(k$_b$ + k$_e$. P(He) = 2 torr.)	EX	552	(1.45±0.08)(12)			2	
(k$_b$ + k$_e$. P(He) = 5 torr.)	EX	552	(1.45±0.04)(12)			2	
(k$_b$ + k$_e$. P(He) = 0.5 torr.)	EX	736	(2.95±0.20)(12)			2	
(k$_b$ + k$_e$. P(He) = 2 torr.)	EX	736	(2.77±0.22)(12)			2	
(k$_b$ + k$_e$. P(He) = 5 torr.)	EX	736	(2.77±0.24)(12)			2	

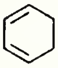
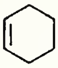
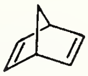
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
Reaction in He diluent, by discharge-flow. Molecular-beam sampling. Mass-spectrometry.							
83 SRI/KAU	EX	298	(4.76±0.60)(11)	0	0	2	
k_e. Channel (e) is major path. Discharge-flow reactor. O atoms generated by dissociation of O_2 in a microwave-discharge, in He diluent. Resonance-fluorescence. P-independent k. [Ethene] = $(0.5-6.0)x10^{14}$ molec.cm^{-3}. $[O]_o$ = $(0.2-1.2)x10^{11}$atom.cm^{-3}. P(Total) = (0.42-6) torr.							
83 TEM	RL	296	0.44±0.15	0	0	2/2	
$k_b/k_{overall}$. Far-IR Laser-Magnetic-Resonance Spectrometry.							
O + CH_2=C=O → products							
Oxygen atom + Ethenone (Ketene)							
83 WAS/HAT	EX	230-449	(1.76±0.47)(12)	0	679±78	2	
Fast-flow. Pulse-Radiolysis. Resonance-absorption. Photoionization Mass-spectrometry. O atoms generated by dissociation of CO_2 in Ar. Measurements at 298 made by using an O atoms source generated by dissociation of either a O_2/He mixture, or a NO/N_2/He mixture in a microwave-discharge. P(Ketene) = (18-62) mtorr. P(CO_2) = (2.37-3.39) torr. P(Ar) = (417-526) torr.							
O + $CH_3CH_2ONO_2$ → OH + CH_3CHNO_2							
Oxygen atom + Nitric acid ethyl ester							
77 SAL/THR	EX	294-473	2.6(13)	0	2598±313	2	
Low-pressure fast-flow system, with a Pyrex reactor. O atoms generated by dissociation of O_2 (1% in Ar) through a microwave-discharge. P(Total) = (0.75-15) torr.							
O + CH_3C≡CH → CO + CH_3CH (a)							
→ H + [C_3H_3O] (b)							
Oxygen atom + 1-Propyne							
83 HOM/WEL1	EX	295-1330	(1.5±0.4)(13)	0	1060	2	
$k_{overall}$. Discharge-flow. O atoms generated by the reaction: N + NO → N_2 or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							

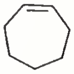
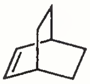
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_3CH{=}C{=}O \rightarrow$ products Oxygen atom + 1-Propen-1-one (Methylketene)							
83 WAS/HAT	EX	230-449	(2.89±0.79)(12)	0	249±82	2	
Fast-flow reactor. Pulse-Radiolysis. Resonance-absorption. Photoionization Mass-spectrometry. O atoms generated by dissociation of CO_2 in Ar. Measurements at 298 K made by using an O atom source generated by dissociation of either a O_2/He mixture, or a NO/N_2/He mixture in a microwave-discharge. P(Methylketene) = (2.0-8.8) mtorr. P(CO_2) = (2.5-3.9) torr. P(Ar) = (450-540) torr.							
$O + CH{\equiv}CC{\equiv}CH \rightarrow$ products Oxygen atom + 1,3-Butadiyne							
83 HOM/WEL1	EX	300-1000	(2,8±0.6)(13)	0	870	2	
Discharge-flow reactor. O atoms generated by the reaction: $N + NO \rightarrow N_2 + O$, or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							
$O + CH{\equiv}CCH{=}CH_2 \rightarrow$ products Oxygen atom + 1-Buten-3-yne							
83 HOM/WEL1	EX	295-500	(3.0±1.1)(13)	0	910	2	
Discharge-flow reactor. O atoms generated by the reaction: $N + NO \rightarrow N_2 + O$, or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							
$O + CH_3CH_2C{\equiv}CH \rightarrow CO + CH_3CH{=}CH_2$ (a) **→ any other products (b)** Oxygen atom + 1-Butyne							
83 HOM/WEL1	EX	290-1000	(2.3±0.7)(13)	0	870	2	
$k_{overall}$. Low-pressure discharge-flow reactor. O atoms generated by the reaction: $N + NO \rightarrow N_2 + O$, or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$O + CH_3CH_2CH{=}C{=}O \rightarrow$ products							
Oxygen atom + 1-Buten-1-one (Ethylketene)							
83 WAS/HAT	EX	230-449	(3.23±0.50)(12)	0	224±47	2	
Fast-flow reactor. Pulse-Radiolysis. Resonance-absorption. Photoionization Mass-spectrometry. O atoms generated by dissociation of CO_2 in Ar. Measurements at 298 K made by using an O atoms source generated by dissociation of either a O_2/He mixture, or a NO/N_2/He mixture in a microwave-discharge. P(Ethylketene) = (1.8-7.2) mtorr. P(CO_2) = (2.5-3.5) torr. P(Ar) = (450-550) torr.							
$O + (CH_3)_2C{=}C{=}O \rightarrow$ products							
Oxygen atom + 1-Propen-1-one, 2-methyl- (Dimethylketene)							
83 WAS/HAT	EX	230-449	(3.57±0.57)(12)	0	569±43	2	
Fast-flow reactor. Pulse-Radiolysis. Resonance-absorption. Photoionization Mass-spectrometry. O atoms generated by dissociation of CO_2 in Ar. For experiments at 298 K the measurements were made by using an O atoms source generated by dissociation of either a O_2/He mixture, or a NO/N_2/He mixture in a microwave-discharge. P(Dimethylketene) = (2.3-8.5) mtorr. P(CO_2) = (2.6-3.5) torr. P(Ar) = (450-540) torr.							
$O + CH_3CH_2CH_2CH_2OH \rightarrow OH + CH_3CH_2CH_2CHOH$ (a) **$\rightarrow OH + [C_4H_8OH]$ (b)**							
Oxygen atom + 1-Butanol							
83 ROS 1) (k_a)	EX	298-606	(1.35±0.39)(13)	0	1756+505	2	
The O atom abstracts an H atom only from a CH bond in position α to OH.							
($k_{overall}$)	EX	298-606	2.99(13)	0	1780±190	2	1.17
The O atom abstracts an H atom from any CH bond.							
1) Flow-system. O atoms generated by reacting N with NO. N atoms generated by dissociation of N_2 in a microwave-discharge. Gas-chromatography.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + $CH_3CH_2CH(OH)CH_3 \rightarrow OH + CH_3CH_2C(OH)CH_3$ (a) $\rightarrow OH + [C_4H_8OH]$ (b) Oxygen atom + 2-Butanol							
83 ROS 1) (k_a) The O atom abstracts an H atom only from a CH bond in position α to OH.	EX	298-606	(3.06±0.49)(12)	0	1083±289	2	
($k_{overall}$) The O atom abstracts an H atom from any CH bond.	EX	298-606	4.47(12)	0	1190±190	2	1.17
1) Flow-system. O atoms generated by reacting N with NO. N atoms generated by dissociation N_2 in a microwave-discharge. Gas-chromatography.							
O + $(CH_3)_2CHCH_2OH \rightarrow OH + (CH_3)_2CHCHOH$ (a) $\rightarrow OH + [C_4H_8OH]$ (b) Oxygen atom + 1-Propanol, 2-methyl-							
(k_a) The O atom abstracts an H atom only from the CH bond in position α to OH.	EX	298-606	(1.39±0.18)(12)	0	1010±289	2	
($k_{overall}$) The O atom abstracts an H atom from any CH bond.	EX	298-606	3.66(12)	0	1100±150	2	1.14
1) Flow-system. O atoms generated by reacting N with NO. N atoms generated by dissociation of N_2 in a microwave-discharge. Gas-chromatography.							
O + $(CH_3)_3COH \rightarrow OH + [C_4H_8OH]$ Oxygen atom + 2-Propanol, 2-methyl-							
83 ROS Flow-system. O atoms generated by reacting N with NO. N atoms generated by dissociation of N_2 in a microwave-discharge Gas-chromatography. The O atom abstracts an H atom from any CH bond.	EX	298-606	4.99(12)	0	2190±270	2	1.22
$O_3 + SO \rightarrow O_2 + SO_2$ Ozone + Sulfur monoxide							
83 BLA/SHA SO generated by ArF Laser-photodissociation of SO_2 at 193 nm. $P(SO_2)$ = 30 mtorr. $P(O_2)$ < 0.4 torr.	EX	230-420	2.89(12)	0	1170±120	2	1.33

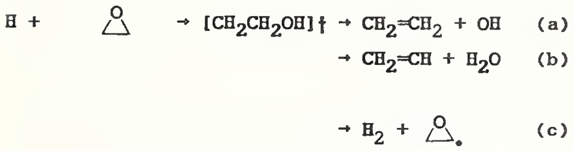
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O_3 + OCHCHO → products							
Ozone + Ethanedial (Glyoxal, or Diformyl)							
83 PLU/SAN	EX	298	<1.81(3)	0	0	2	
Reaction in a Teflon bag.							
[OCHCHO] ~3.0×10^{15} molec.cm^{-3}.							
O_3 + $CH_3C(O)ONO_2$ → products							
Ozone + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	3.24(4)			2	
Reaction in a Teflon-lined aluminum tank.							
Gas-chromatography. Mass-spectrometry.							
IR-Absorption spectrometry.							
[Peroxide] = (2.9-9.6) ppm.							
[O_3] = (13-660) ppm.							
O_3 + $CH_3C(O)CHO$ → products							
Ozone + Propanal, 2-oxo- (Methylglyoxal)							
83 PLU/SAN	EX	298	<3.61(3)			2	
Reaction in a Teflon bag.							
[$CH_3C(O)CHO$]] ~3.0×10^{15} molec.cm^{-3}.							
O_3 + cis-$CH_3CH{=}CHCH_3$ → products							
Ozone + 2-Butene, (Z)-							
83 ATK/ASC4	EX	297	(8.31±0.96)(7)			2	
Irradiation in a Teflon reaction bag.							
Gas-chromatography.							
[Ozone]$_o$ = $(0.12-1.2)\times10^{13}$ molec.cm^{-3}.							
O_3 +  → products							
Ozone + Furan							
83 ATK/ASC2	EX	298	(1.46±0.17)(6)			2	
Irradiation in a Teflon reaction bag.							
Gas-chromatography.							
P(Total) = 735 torr.							
[Ozone]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
O_3 +  → products							
Ozone + Thiophene							
83 ATK/ASC2	EX	298	<3.61(4)			2	
Irradiation in a Teflon reaction bag.							
Gas-chromatography. P(Total) = 735 torr.							
[Ozone]$_o$ = 2.38×10^{13} molec.cm^{-3}.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O_3 +  → products							
Ozone + Cyclopentene							
83 ATK/ASC4	EX	297	(1.66±0.20)(8)			2	
Irradiation in a Teflon bag.							
Gas-chromatography.							
$[\text{Ozone}]_o = (0.12\text{-}1.2)\times10^{13}$ molec.cm^{-3}.							
O_3 +  → products							
Ozone + 1,3-Cyclohexadiene							
83 ATK/ASC4	EX	297	(1.19±0.17)(9)			2	
Irradiation in a Teflon bag.							
Gas-chromatography.							
$[\text{Ozone}]_o = (0.12\text{-}1.2)\times10^{13}$ molec.cm^{-3}.							
O_3 +  → products							
Ozone + 1,4-Cyclohexadiene							
83 ATK/ASC4	EX	297	(3.85±0.45)(7)			2	
Irradiation in a Teflon bag.							
Gas-chromatography.							
$[\text{Ozone}]_o = (0.12\text{-}1.2)\times10^{13}$ molec.cm^{-3}.							
O_3 +  → products							
Ozone + Cyclohexene							
83 ATK/ASC4	EX	297	(6.26±0.84)(7)			2	
Irradiation in a Teflon bag.							
Gas-chromatography.							
$[\text{Ozone}]_o = (0.12\text{-}1.2)\times10^{13}$ molec.cm^{-3}.							
O_3 +  → products							
Ozone + Bicyclo[2.2.1]hepta-2,5-diene (2,5-Norbornadiene)							
83 ATK/ASC4	EX	297	(2.81±0.78)(9)			2	
Irradiation in a Teflon bag.							
Gas-chromatography.							
$[\text{Ozone}]_o = (0.12\text{-}1.2)\times10^{13}$ molec.cm^{-3}.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O_3 +  → products							
Ozone + Bicyclo[2.2.1]hept-2-ene (2-Norbornene)							
83 ATK/ASC4	EX	297	(1.29±0.21)(9)			2	
Irradiation in a Teflon bag. Gas-chromatography. $[Ozone]_o$ = (0.12-1.2)x10^{13} molec.cm^{-3}.							
O_3 +  → products							
Ozone + Cycloheptene							
83 ATK/ASC4	EX	297	(1.92±0.22)(8)			2	
Irradiation in a Teflon bag. Gas-chromatography. $[Ozone]_o$ = (0.12-1.2)x10^{13} molec.cm^{-3}.							
O_3 +  → products							
Ozone + Bicyclo[2.2.2]oct-2-ene							
83 ATK/ASC4	EX	297	(4.38±0.54)(7)			2	
Irradiation in a Teflon bag. Gas-chromatography. $[Ozone]_o$ = (0.12-1.2)x10^{13} molec.cm^{-3}.							
H + O_2 (+ M) → OH + O (+ M) (a) **→ HO_2 (+ M) (b)**							
Hydrogen atom + Oxygen molecule							
83 PRA/WOO	EX	231-512	(2.85±1.27)(14)	0	-796±159	3	
k_b. Fast-flow discharge. P = (2-10) torr. Mass-spectrometry. Gas-chromatography. M = Ar. [H] = (2.6-6.0)x10^{15} molec.cm^{-3}. $[O_2]$ = (0-6.0)x10^{15} molec.cm^{-3}.							
H + HO_2 → H_2 + O_2 (a) **→ OH + OH (b)** **→ H_2O + O (c)**							
Hydrogen atom + Hydroperoxo							
83 PRA/WOO (k_b/k_a)	RL	231-464	2.75	0	320±120	2/2	2.45
(k_b/k_a)	RL	298	2.3±0.5			2/2	
(k_b/k_a)	RL	550	7.2±3.1			2/2	
(k_a)	SE	231-464	1.02(12)	0	-200±170	2	3.39
(k_b)	SE	231-464	2.82(13)	0	120±120	2	2.29
Fast-flow discharge. P = (2-10) torr. M = Ar. HO_2 generated by the reaction: H + O_2 + M → HO_2 + M.							

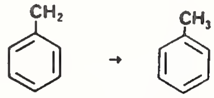
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$H + SH \rightarrow H_2 + S$							
Hydrogen atom + Mercapto							
81 TIE/WAM	EX	298	≤1.02(13)			2	
Laser-induced Fluorescence in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. P(H_2S] = (30-100) mtorr. P(Ar) = (5-10) torr.							
$H + HN_3 \rightarrow NH_2 + N_2$ (a) **$\rightarrow H_2 + N_3$ (b)**							
Hydrogen atom + Hydrazoic acid							
83 KOD1	RL	303	1.15			2/2	
k_a/k_b. Photolysis of Hydrazoic acid in Xe, at 313 nm. Rate constant ratio estimated on the basis of a proposed mechanism. Gas-chromatography. IR-spectrometry. P(Xe) = (0-600) torr. P(HN_3) = 50 torr.							
$H + CO (+ M) \rightarrow CHO (+ M)$							
Hydrogen atom + Carbon monoxide							
78 CAM/HAN (M = N_2)	EX	425	(1.44±0.12)(14)			3	
(M = Ar)	EX	425	(9.7±0.9)(13)			3	
Discharge-flow stirred reactor. H atoms generated by dissociation of H_2.							
$H + CH_2 \rightarrow H_2 + CH$							
Hydrogen atom + Methylene							
83 HOM/WEL2	ES	295	5.0(13)			2	
	ES	500	5.5(13)			2	
	ES	1000	6.0(13)			2	
Estimations based on a suggested mechanism for the reaction of Ethyne with O atoms, studied in a high-temperature flow-reactor, with or without added H atoms. P = 2 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$H + CHO \rightarrow H_2 + CO$ (a)							
$\rightarrow HCHO$ (b)							
$\rightarrow O + CH^2$ (c)							
Hydrogen atom + Methyl, oxo-							
78 CAM/HAN	RL	425	2.1±0.3			2/2	
k_a/k_{ref}. Discharge-flow stirred reactor.							
H atoms generated by dissociation of H_2.							
CHO generated by reacting H with CO.							
k_{ref}: O + CHO → products.							
$H + HCHO \rightarrow H_2 + CHO$ (a)							
$\rightarrow CH_2OH$ (b)							
Hydrogen atom + Formaldehyde							
83 GUE/VAN	EX	~1400	2.0(14)	0	2607	2	
k_a. Premixed flames. Molecular-beam sampling.							
Unspecified T-range. P = (22.5-40) torr.							
$H + CH_3SH \rightarrow H_2S + CH_3$ (a)							
$\rightarrow H_2 + CH_3S$ (b)							
Hydrogen atom + Methanethiol (Methyl mercaptan)							
83 AMA/YAM (k_a)	DE	312-454	6.9(12)	0	841	2	
(k_b)	DE	312-454	2.9(13)	0	1311	2	
Discharge-flow reactor. P = (2.7-2.9) torr.							
$H + CH_3NH_2 \rightarrow H_2 + CH_2NH_2$ (a)							
$\rightarrow H_2 + CH_3NH$ (b)							
Hydrogen atom + Methanamine (Methylamine)							
73 BLU/WAG	EX	473-683	(1.8±0.3)(13)	0	2667±151	2	
$k_a + k_b$. Fast-flow reactor. H atoms generated.							
by decomposition of H_2 in a microwave dis-							
charge. ESR-, and Mass-spectrometry.							
$[CH_3NH_2]_o = 6.0x10^{17}$ molec.cm^{-3}.							
P = 5.4 torr.							
$H + C_2O \rightarrow CH + CO$							
Hydrogen atom + Carbon oxide (C_2O)							
83 HOR/BAU	EX	298	(2.23±0.60)(13)			2	
Flow-reactor. M = Ar. C_2O generated in the							
C_3O_2 photolysis by KrF excimer Laser pulses							
at 248 nm. and detected by Laser-induced							
fluorescence. H atoms generated in a micro-							
wave discharge mixture. $[C_3O_2]$ = 0.4 mtorr.							
[H] = (0.8-6.5) mtorr. $[H_2]$ = (1.5-70) mtorr.							
P(Total) = 1.1 torr. (Ar)							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
83 SCH/MEU	EX	298	(1.93±0.72)(13)			2	
Flow-reactor. C_2O generated by the photolysis of O=C=C=C=O with a KrF excimer laser pulse at 248 nm. H atoms generated by dissociation of H_2 in Ar by a microwave-discharge. Laser-induced Fluorescence. [H] = (0.8-8.0) mtorr. $[C_3O_2]$ = 0.4 torr.							
$H + CH_2{=}CH_2$ (+ M) → $H_2 + CH_2{=}CH$ (+ M) (a) **→ CH_3CH_2 (+ M) (b)** Hydrogen atom + Ethene							
83 SRI/KAU (P(Total) = 0.42 torr.)	EX	298	7.47(10)			2	
(P(Total) = 6.0 torr.)	EX	298	2.02(11)			2	
$k_a + k_b$. Discharge-flow reactor. H atoms generated by dissociation of H_2 in a microwave-discharge. Resonance-fluorescence. M = He. P(Total) = (0.42-6) torr. [Ethene] = $(0.5\text{-}6.0)\times10^{14}$ molec.cm^{-3}. $[H]_o \sim 8\times10^{10}$ atom.cm^{-3}. Other rate constants tabulated for various pressures within the given P-range. The rate constant increases with the pressure.							
$H + CH_3CH_3 \rightarrow CH_3 + CH_4$ Hydrogen atom + Ethane							
83 BAC	ES	823	≤4.4(1)			2	
	ES	983	≤1.4(2)			2	
Thermolysis of Ethane. P = 300 torr.							
							
Hydrogen atom + Oxirane (Ethylene oxide)							
83 LIF/BEN (k_a)	ES	830-1200	9.5(10)	0	2516	2	
(k_b)	ES	830-1200	5.0(9)	0	2516	2	
(k_c)	ES	830-1200	2.0(13)	0	4177	2	
Pyrolysis of Ethylene oxide diluted in Ar, behind reflected shock-waves, in a single-pulse shock-tube. Gas-chromatography. P = (1.5-10) atm. Rate constants estimated on the basis of a suggested mechanism.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$H + O{=}C{=}C{=}C{=}O \rightarrow$ products							
Hydrogen atom + 1,2-Propadiene-1,3-dione							
76 HAC/PIL	EX	296-481	(1.7±0.6)(13)	0	1480±180	2	
Isothermal discharge-flow. ESR-spectrometry. P = (2-4) torr.							
$H + C_3H_3 \rightarrow CH_2{=}C{=}CH_2$ (a) **$\rightarrow CH_3C{\equiv}CH$ (b)**							
Hydrogen atom + 1-Propynyl, or 2 Propynyl, or 1,2-Propadienyl							
83 HOM/WEL2 $(k_a + k_b)$	ES	295	2.7(13)			2	
$(k_a + k_b)$	ES	500	4.3(13)			2	
$(k_a + k_b)$	ES	1000	6.3(13)			2	
Estimations based on a suggested mechanism for the reaction of Ethyne with O atoms in a high-temperature flow-reactor, with or without added H atoms. P = 2 torr.							
$H + CH{\equiv}CC{\equiv}CH \rightarrow$ products							
Hydrogen atom + 1,3-Butadyine							
83 HOM/WEL2	ES	295	1.3(12)			2	
	ES	500	3.5(12)			2	
	ES	1000	7.5(12)			2	
Estimations based on a suggested mechanism for the reaction of Ethyne with O atoms in in a high-temperature flow-reactor, with or without added H atoms. P = 2 torr.							
$H + CH_3CH_2CH{=}CH_2 \rightarrow CH_3CH_2CH_2CH_2$ (b)							
Hydrogen atom + 1-Butene							
83 KYO/WAT	EX	200-500	(1.49±0.26)(13)	0	751±47	2	
k_b. Pulse-Radiolysis. Resonance-Absorption. H atoms generated by pulse-irradiation of H_2 with high-energy electrons. $P(H_2)$ = 600 torr. P(1-Butene) = (0.01-0.1) torr.							
$D + CH_3CH_2CH{=}CH_2 \rightarrow CH_3CH_2CHDCH_2$ (a) **$\rightarrow CH_3CH_2CHCH_2D$ (b)**							
Deuterium atom + 1-Butene							
83 KYO/WAT	EX	200-500	(1.46±0.43)(13)	0	826±85	2	
k_a. Pulse-Radiolysis. Resonance-absorption. D atoms generated by pulse-irradiation of D_2 with high-energy electrons. $P(D_2)$ = 600 torr. P(1-Butene) = (0.01-0.1) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\mathrm{H + cis\text{-}CH_3CH{=}CHCH_3 \rightarrow H_2 + CH_3CH{=}CHCH_2}$ (a) $\mathrm{\rightarrow H_2 + CH_3CHCH{=}CH_2}$ (b) $\mathrm{\rightarrow CH_3CH_2CHCH_3}$ (c) Hydrogen atom + 2-Butene, (Z)-							
83 KYO/WAT k_c. Pulse-Radiolysis. Resonance-Absorption. H atoms generated by pulse-irrediation of H_2 with high-energy electrons. P(1-Butene) = (0.01-0.1) torr. P(H_2) = 600 torr.	EX	200-500	(1.61±0.23)(13)	0	965±42	2	
$\mathrm{D + cis\text{-}CH_3CH{=}CHCH_3 \rightarrow CH_3CHDCHCH_3}$ Deuterium atom + 2-Butene, (Z)-							
83 KYO/WAT Pulse-Radiolysis. Resonance-Absorption. D atoms generated by pulse-irradiation of D_2 with high-energy electrons. P(D_2) = 600 torr. P(1-Butene) = (0.01-0.1) torr.	EX	200-500	(1.36±0.11)(13)	0	1048±24	2	
$\mathrm{H + trans\text{-}CH_3CH{=}CHCH_3 \rightarrow H_2 + CH_3CH{=}CHCH_2}$ (a) $\mathrm{\rightarrow H_2 + CH_3CHCH{=}CH_2}$ (b) $\mathrm{\rightarrow CH_3CH_2CHCH_3}$ (c) Hydrogen etom + 2-Butene, (E)-							
83 KYO/WAT k_c. Pulse-Radiolysis. Resonance-Absorption. H atoms generated by pulse-irradiation of H_2 with high-energy electrons. P(H_2) = 600 torr. P(1-Butene) = (0.01-0.1) torr.	EX	200-500	(2.39±0.16)(13)	0	1055±19	2	
$\mathrm{D + trans\text{-}CH_3CH{=}CHCH_3 \rightarrow CH_3CHDCHCH_3}$ Deuterium etom + 2-Butene, (E)-							
83 KYO/WAT Pulse-Rediolysis. Resonance-Absorption. D atoms genereted by pulse-irradietion of D_2 with high-energy electrons. P(D_2) = 600 torr. P(1-Butene) = (0.01-0.1) torr.	EX	200-500	(1.40±0.14)(13)	0	1025±27	2	
$\mathrm{H + (CH_3)_2C{=}CH_2\ (+ M) \rightarrow (CH_3)_3C\ (+ M)}$ (a) Hydrogen atom + 1-Propene, 2-methyl- (Isobutene)							
83 KYO/WAT k_a. Pulse-Radiolysis Resonance-Absorption. H atoms generated by pulse-irradiation of H_2 with high-energy electrons. P(H_2) = 600 torr. P(1-Butene) = (0.01-0.1) torr.	EX	200-500	(1.25±0.10)(13)	0	433±25	2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$D + (CH_3)_2C{=}CH_2 \rightarrow (CH_3)_2CDCH_2$ (a) $\rightarrow (CH_3)_2CCH_2D$ (b) Deuterium atom + 1-Propene, 2-methyl- (Isobutene)							
83 KYO/WAT k_b. Pulse-Radiolysis. Resonance-Absorption. D atoms generated by pulse-irradiation of D_2 with high-energy electrons. P(1-Butene) = (0.01-0.1) torr. $P(D_2)$ = 600 torr.	EX	200-500	(9.28±0.11)(12)	0	442±41	2	
H +  Hydrogen atom + Methyl, phenyl- (Benzyl) → Benzene, methyl- (Toluene)							
75 LUU/GLA Benzyl generated by Flash-photolysis of ~0.06 torr. 1,3,5-Cycloheptatriene, in Ar or N_2.	ES	298	(5.95±4.05)(13)			2	
$H_2 + C_2O \rightarrow$ products Hydrogen momecule + Carbon oxide (C_2O)							
83 HOR/BAU Flow-reactor. M = Ar. C_2O generated in the C_3O_2 photolysis by KrF excimer Laser pulses at 248 nm. and detected by laser-induced Fluorescence. P(Total) = 1.6 torr. (Ar). $[H_2]$ = (1.5-70) mtorr. [O] = 2.1 mtorr. $[C_3O_2]$ = 7 mtorr.	EX	298	(4.22±1.81)(11)			2	
$OH + HO_2 \rightarrow H_2O + O_2$ Hydroxyl + Hydroperoxo							
83 SCH Reaction of OH with HO_2 in a fast-flow reactor. Laser-magnetic resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)	EX	298	(4.46±0.12)(13)			2	
83 TEM Reaction of OH with HO_2 by Far-Infrared Laser-Magnetic-Resonance Spectrometry.	EX	296	(4.0±1.2(13)			2	
$OH + H_2O_2 \rightarrow HO_2 + H_2O$ Hydroxyl + Hydrogen peroxide							
83 LAM/MOL	EX	241-413	(6.47±1.84)(10)	2.5	-838±86	2	
	EX	294	(1.08±0.18)(12)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
The preexponential factor expressed as: $(T/298)^{2.5}$. Reaction in a Pyrex cell. Resonance-fluorescence. OH generated by Flash-photolysis of H_2O_2, or $HONO_2$. $P(HONO_2) = (5-10)$ torr. $P(He) = 760$ torr. $P(H_2O_2) = (0.7-1.2)$ torr.							
83 TEM	EX	296	(1.0±0.2(12)			2	
Reaction by Far-IR Laser-Magnetic-Resonance Spectrometry.							
$OH + SO_2$ (+ M) $\rightarrow$ HSO_3 (+ M) Hydroxyl + Sulfur dioxide							
83 PAR/SIN (M = N_2. P = 55 torr.)	EX	297	(1.4±0.4)(11)			2	
(M = N_2. P 760 torr.)	EX	297	(5.7±0.8)(11)			2	
(M = SF_6. P = 100 torr.)	EX	297	(3.0±0.4)(11)			2	
(Limiting low-pressure k.) Extrapolation of experimental data to low P's.	ES	297	5.7(16)			3	
(Limiting high-pressure k.) Fit of experimental data to Lindeman mechanism.	ES	297	(7.4±0.4)(11)			2	
Reaction of OH with SO_2 in excess N_2 by Flash-photolysis/Resonance-absorption. OH generated by Flash-Photolysis of N_2O/H_2 mixtures, or by Photolysis of H_2O. $P(N_2) = (55-760)$ torr. $P(H_2) = 50$ torr. $[OH] = (1.81-3.01)x10^{12}$ molec.cm^{-3}. $[SO_2]$ ~$2.1x10^{16}$ molec.cm^{-3}. Pressure-dependent reaction. Other k's at different pressures in the (55-760) torr. range are given. The pressure dependence is given by the expression: $k = (7.4x10^{11})/(1+237/P)$ where P is in torr. and k is in cm^{3}mol^{-1}s^{-1}.							
OH + NO (+ M) $\rightarrow$ HONO (+ M) Hydroxyl + Nitrogen oxide (NO)							
83 BUR/WAL	EX	295	(3.99±0.36)(17)			3	
M = N_2. M-efficiencies relative to N_2 are: 1.00(N_2), 0.55(He), 0.67(Ar). Discharge-flow system. OH generated by reacting H with NO_2. Resonance-fluorescence. P(Total) = (1-5) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + NO_2 (+ M) \rightarrow HO_2 + NO (+ M)$ (a)							
$\rightarrow HONO_2 (+ M)$ (b)							
Hydroxyl + Nitrogen oxide (NO_2)							
83 BUR/WAL	EX	295	(9.79±0.73)(17)			3	
$M = N_2$. M-efficiencies relative to N_2 are:							
1.00(N_2), 0.59(Ar), 0.59(He), 0.96(O_2),							
1.67(CO_2). Discharge-flow system.							
OH generated by reacting H with NO_2.							
Resonance-fluorescence.							
P(Total) = (1-5) torr.							
$OH + CO \rightarrow H + CO_2$ (a)							
$\rightarrow$ any other products (b)							
Hydroxyl + Carbon monoxide							
83 RAV/THO (k_a)	EX	250-350	(1.33±0.55)(11)	0	145±100	2	
(k_a)	EX	298	(8.67±0.72)(10)			2	
Resonance-fluorescence. Flash-photolysis.							
OH generated by pulse-radiolysis of H_2O,							
at 165 nm. [OH] = $(1-10)x10^{11}$ molec.cm^{-3}.							
[CO] = $(0.1-6.0)x10^{15}$ molec.cm^{-3}.							
Experimental rate constants at various							
temperatures within the (251-1040) K range							
are tabulated, giving a strongly curved							
Arrhenius plot. A non-linear least-squares							
fit gives the expression:							
$k = 6.02x10^{23}exp(-30.03 \pm 1.22x10^{-3}T)$							
$cm^3mol^{-1}s^{-1}$.							
$OH + CH_4 \rightarrow H_2O + CH_3$							
Hydroxyl + Methane							
83 BAU/CRA	RN	403-696	2.87(11)	2.13	1233	2/2	
(Alternate eqn.)	RN	403-696	1.65(11)	2.4	1060	2/2	
The preexponential factors expresed as:							
$(T/298)^n$. Reaction in a conventional							
"mercury free" vacuum line. OH generated							
by photolysis of H_2O at 184.9 nm.							
Gas-chromatography. [CO] = (5.7-75) torr.							
$[H_2O]$ = (12.3-28.1) torr.							
P(Total) < 97.5 torr.							
k_{ref}: $OH + CO \rightarrow H + CO_2$							
$OH + CHO \rightarrow H_2O + CO$							
Hydroxyl + Methyl, oxo-							
83 TEM	EX	296	(1.1±0.3)(14)			2	
Far-IR Laser-Magnetic-Resonance Spectrometry.							

Reaction, Reference Code, Notes		Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + HCHO \rightarrow H_2O + CHO$ (a)								
$\rightarrow H_2O + CHO^\dagger$ (b)								
$\rightarrow HCOOH + H$ (c)								
Hydroxyl + Formaldehyde								
83 GUE/VAN		EX	~1400	4.1(13)	0	710	2	
k_a. Premixed flames.								
Molecular-beam sampling.								
Mass-spectrometry.								
Unspecified T-range.								
P = (22.5-40) torr.								
83 TEM		EX	296	(5.0±1.0)(12)			2	
k_a. Far-IR Laser-Magnetic-Resonance Spectrometry.								
$OH + CH_3OH \rightarrow H_2O + CH_2OH$ (a)								
$\rightarrow H_2O + CH_3O$ (b)								
Hydroxyl + Methanol								
83 HAG/LOR	$(k_a + k_b)$	EX	295-420	(7.23±1.81)(12)	0	810±50	2	
	$(k_a/(k_a + k_b))$	RL	298	(1.1±0.3)(-1)			2/2	
	$(k_a/(k_a + k_b))$	RL	393	(2.2±0.7)(-1)			2/2	
Laser-photolysis/Resonance-fluorescence.								
OH generated by Laser-photolysis of $HONO_2$ at 248 nm.								
$P(HONO_2)$ <75 mtorr.								
$[OH] = 4.0\times10^{11}$ $molec.cm^{-3}$.								
83 TUA/CAR1		RL	300	0.314±0.024			2/2	
$k_a + k_b$. Teflon rectangular vessel.								
FTIR-Spectrometry.								
OH generated by reacting O_3 with $NH_2=NH_2$.								
k_{ref}: $OH + (CH_3)_2O \rightarrow$ products.								
P = 735 torr.								
$OH + CH_3OOH \rightarrow H_2O + CH_2OOH$ (a)								
$\rightarrow H_2O + CH_3O_2$ (b)								
Hydroxyl + Hydroperoxide, methyl-								
83 NIK/MAK	(k_a/k_b)	RL	298	0.77±0.15			2/2	
	$(k_a + k_b)$	RN	298	6.02(12)			2	
FTIR-technique. OH generated by photolysis of CH_3ONO, or CH_3CH_2ONO.								
$k_a + k_b$ derived from the ratios $(k_a + k_b)/k_{ref1}$ and $(k_a + k_b)/k_{ref2}$,								
where k_{ref1}: $OH + CH_2=CH_2$, and								
k_{ref2}: $OH + CH_3CHO$.								

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + CS_2 \rightarrow SH + COS$ (a) $\rightarrow SOH + CS$ (b) $\rightarrow$ any other products (c) Hydroxyl + Carbon disulfide							
83 BAR/BEC $k_{overall}$. FTIR-Spectroscopy using photolytic and nonphotolytic competitive techniques. The effective k is dependent on T,P, and O_2 concentrations. P(Total) = 760 torr.	EX	293	(1.63±0.36)(12)			2	
$OH + CH_3SH \rightarrow$ products Hydroxyl + Methanethiol (Methyl mercaptan)							
83 LEE/TAN Discharge-flow. OH generated by the reaction: $H + NO_2 \rightarrow OH + NO$. H atoms generated by decomposition of H_2 in He, by a microwave-discharge. Resonance-fluorescence. $[OH] = 7x10^{10}$ molec.cm^{-3}. $[CH_3SH] = (1.3-9.7)x10^{12}$ molec.cm^{-3}.	EX	296	(1.54±0.27)(13)			2	
83 MAC/POU Discharge-flow. EPR-spectrometry.	EX	293	(1.26±0.60)(12)			2	
$OH + CH_3ONO \rightarrow$ products Hydroxyl + Nitrous acid methyl ester							
83 TUA/CAR1 1) k_{ref}: $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products	RL	300	0.038±0.007			2/2	
83 TUA/CAR1 1) Put on absolute basis by using the literature value of the rate constant for the reaction: $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products.	RN	300	(1.33±0.24(11)			2	
83 TUA/CAR1 1) k_{ref}: $OH + (CH_3)_2O \rightarrow$ products.	RL	300	0.041±0.009			2/2	
83 TUA/CAR1 1) Put on absolute basis by using the literature value of the rate constant for the reaction: $OH + (CH_3)_2O \rightarrow$ products.	RN	300	(8.43±2.40(10)			2	
83 TUA/CAR1 1) Average of the two normalized rate constants given above.	SE	300	1.08(11)			2	

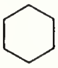
1) Teflon vessel. FTIR-Spectrometry. OH generated by reacting O_3 with NH_2=NH_2.
P = 735 torr.

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + CH{\equiv}CH \rightarrow H + CH_2{=}C{=}O$ (a) $\rightarrow H_2 + CH{=}C{=}O$ (b) $\rightarrow CO + CH_3$ (c) $\rightarrow H + CH{\equiv}COH$ (d) $\rightarrow [HO.CH{\equiv}CH]^*$ (e) Hydroxyl + Ethyne							
83 TEM $k_{overall}$. Reaction of OH with CH≡CH by Far-IR Laser-Magnetic-Resonance Spectrometry.	EX	296	(9.4±2.0)(10)			2	
$OH + CH_2{=}CH_2 \rightarrow CH_2CH_2OH \rightarrow$ products (a) $\rightarrow H_2O + CH_2{+}CH$ (b) Hydroxyl + Ethene							
83 TUL k_a. Reaction in a flow-reactor, in He diluent. OH generated by the 193 nm. photolysis of N_2O to O(${}_1$D) and N_2 and subsequent reaction of O(^{1}D) with H_2O. Tunable dye Laser Fluorescence. P(He) = (50-600) torr.	EX	291-591	(1.05±0.32)(12)	0	-462±108	2	
$OH + CH_3CH_3 \rightarrow H_2O + CH_3CH_2$ Hydroxyl + Ethane							
83 BAU/CRA ^{1}) OH generated by the photolysis of H_2O at 184.9 nm. Gas-chromatography. P(Total) < 97.5 torr. [CO] = (5.7-75) torr. $[H_2O]$ = (12.3-28.1) torr. k_{ref}: $OH + CO \rightarrow H + CO_2$	RN	300-2000	1.11(12)	1.9	570	2/2	
83 TUL/RAV ^{1}) Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H_2O. ^{1}) The preexponential factors expressed as: $(T/298)^n$.	EX	297-800	3.41(12)	1.05	911	2	
OH + OCHCHO → products Hydroxyl + Ethanedial (Glyoxal, or Diformyl)							
83 PLU/SAN Reaction of OH with Glyoxal by a competitive technique, in an environmental chamber. OH generated by photolysis of a CH_3ONO/Air mixture. k_{ref}: OH +  → products.	RN	298	(6.93±0.24)(12)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + CH_3CH_2SH \rightarrow$ products							
Hydroxyl + Ethanethiol (Ethyl mercaptan)							
83 LEE/TAN	EX	296	(2,21±0.11)(13)			2	
Discharge-flow. OH generated by the reaction:							
$H + NO_2 \rightarrow OH + NO$.							
H atoms generated by decomposition of H_2 in a microwave-discharge.							
Resonance-fluorescence.							
$[OH] = 7x10^{10}$ molec.cm^{-3}.							
$[CH_3SH] = (1.3\text{-}9.7)x10^{12}$ molec.cm^{-3}.							
83 MAC/POU	EX	293	(1.63±0.12)(13)			2	
Discharge-flow. EPR-spectrometry.							
$OH + (CH_3)_2S \rightarrow$ products							
Hydroxyl + Methane, thiobis- (Dimethyl sulfide)							
83 MAC/POU	EX	373	(5.54±0.36)(12)			2	
	EX	573	(4.70±0.60)(12)			2	
Discharge-flow. EPR-Spectrometry.							
$OH + O{=}C{=}C{=}C{=}O \rightarrow CO_2 + CH{=}C{=}O$ (a)							
$\rightarrow$ any other products (b)							
Hydroxyl + 1,2-Propadiene-1,3-dione							
76 HAC/PIL	EX	296-481	(5.0±2.0)(12)	0	1560±130	2	
$k_{overall}$. Discharge-flow.							
ESR-Spectrometry.							
P = (2-4) torr.							
$OH + CH_2{=}C{=}CH_2 \rightarrow$ products							
Hydroxyl + 1,2-Propadiene (Allene)							
83 OHT	RN	297	(6.20±0.66)(12)			2	
Reaction in O_2/N_2 gas, in a quartz reaction cell. OH generated by H_2O_2 photolysis.							
$P(H_2O_2) = 1$ torr. $P(O_2) = 10$ torr.							
P(Total) ~ 760 torr. (mostly N_2).							
P(Allene) ~ 1 mtorr.							
k determined relative to the reaction:							
$OH + CH_2{=}CHCH{=}CH_2 \rightarrow$ products.							
$OH + CH_3CH{=}CH_2 \rightarrow$ products							
Hydroxyl + 1-Propene							
83 ATK/ASC2 $^{1})$	RL	298	4.74±0.17			2/2	
k_{ref}: $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products.							
83 ATK/ASC2 $^{1})$	RN	298	(1.63±0.07)(13)			2	
Placed on an absolute basis by using the k for the reaction of OH with Hexane.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
1) Irradiation in a Teflon bag. OH generated by Photolysis of CH_3ONO in Air. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite] = $2.38x10^{14}$ molec.cm^{-3}.							
83 OHT	RN	297	(1.76±0.06)(13)			2	
Reaction of OH with 1-Propene in O_2/N_2 gas, in a quartz reaction cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ = 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(1-Propene) ~ 1 mtorr. k determined relative to the reaction: OH + CH_2=CHCH=CH_2 → products.							
83 SMI	EX	255-458	9.58(10)	0	-1470±130	2	1.18
	EX	298	(1.14±0.18)(13)			2	
Discharge-flow. Resonance-fluorescence. OH generated by the reaction: H + NO_2 → OH + NO_2. [1-Propene] = $(0.07-8.51)x10^{13}$ molec.cm^{-3}.							
OH + $CH_3CH_2CH_3$ → H_2O + $(CH_3)_2CH$ (a) **→ H_2O + $CH_3CH_2CH_2$ (b)** Hydroxyl + Propane							
83 BAU/CRA 1) (k_a + k_b)	RN	300-2000	1.03(11)	3.4	590	2/2	
"Mercury free" vacuum system. OH generated by Photolysis of H_2O at 184.9 nm. Gas-chromatography. [CO] = (5.7-75) torr. k_{ref}: OH + CO → H + CO_2. P(Total) < 97.5 torr. $[H_2O]$ = (12.3-28.1) torr.							
83 TUL/RAV 1) (k_a + k_b)	EX	297-800	2.79(12)	1.40	428	2	
Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H_2O. 1) The preexponential factors expressed as: $(T/298)^n$.							
OH + CH_2=CHCHO → H_2O + CH_2=CHCO (a) **→ any other products (b)** Hydroxyl + 2-Propenal (Acrolein) (Acrylaldehyde)							
83 ATK/ASC3 ($k_{overall}/k_{ref}$)	RL	299	0.727±0.050			2/2	
k_{ref}: OH + CH_3CH=CH_2 → products.							
($k_{overall}$)	RN	299	(1.10±0.08)(13)			2	
Irradiation of Acrolein/Methyl nitrite/Air mixtures in a Teflon reaction bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography. P = 735 torr. $[Methyl nitrite]_o$ = $2.38x10^{13}$ molec.cm^{-3}.							

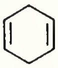
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$k_{overall}$ placed on an absolute basis by using the k for OH + 1-Propene.							
$OH + CH_3C(O)CHO \rightarrow$ products							
Hydroxyl + Propanal, 2-oxo- (Methylglyoxal)							
83 PLU/SAN	RN	298	(1.04±0.08)(13)			2	
Competitive technique, in an environmental chamber. OH generated by photolysis of a CH_3ONO/Air mixture. The rate constant put on an absolute basis by using k for the reaction: OH +  → products. [Methylglyoxal] ~2.4×10^{14} molec.cm^{-3}. [CH_3ONO] ~$(3-20)\times10^{13}$ molec.cm^{-3}.							
$OH + (CH_3)_2CO \rightarrow H_2O + CH_2C(O)CH_3$ (a) **→ any other products (b)**							
Hydroxyl + 2-Propanone (Acetone)							
83 CHI/BIG ($k_{overall}$)	RN	298	(3.98±0.54)(11)			2	
Reaction in a 20 l. Pyrex chamber. OH generated by HONO vapors in synthetic air. Gas-chromatography. IR-spectrometry. k determined relative to the reaction: $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products.							
$OH + CH_2{=}CHCH{=}CH_2 \rightarrow$ products							
Hydroxyl + 1,3-Butadiene							
83 OHT	RN	297	(1.62±0.13)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ = 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(1,3-Butadiene) ~ 1 mtorr.							
$OH +$ trans-$CH_3CH{=}CHCH_3 \rightarrow$ products							
Hydroxyl + 2-Butene, (E)-							
83 OHT	RN	297	(3.67±0.19)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ = 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(trans-2-Butene) ~ 1 mtorr. k determined relative to the reaction: $OH +$ cis-$CH_2{=}CHCH{=}CHCH_3 \rightarrow$ products.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + CH_3CH_2CH_2CH_3 \rightarrow H_2O + CH_3CH_2CH_2CH_2$ (a)							
$\rightarrow H_2O + CH_3CH_2CHCH_3$ (b)							
Hydroxyl + Butane							
83 TUA/CAR1 $(k_a + k_b)$	RL	300	0.347±0.005			2/2	
Reaction in a Teflon vessel. FTIR-Spectrometry.							
OH generated by reacting O_3 with NH_2=NH_2.							
P(Total) = 735 torr.							
k_{ref}: OH +  → products.							
OH +  → products							
Hydroxyl + Furan							
83 ATK/ASC2 [1])	RL	298	7.04±0.50			2/2	
k_{ref}: $OH + CH_3(CH_2)_4CH_3 \rightarrow$ products.							
83 ATK/ASC2 [1])	RN	298	(2.41±0.18)(13)			2	
Placed on an absolute basis by using the k for the reaction of OH with Hexane.							
[1]) Irradiation of CH_3ONO/Furan/Air mixtures in a Teflon reaction bag. OH generated by Photolysis of CH_3ONO in Air. Gas-chromatography.							
P(Total) = 735 torr.							
[Methyl nitrite] = 2.38×10^{14} molec.cm^{-3}.							
$OH + CH_3CH$=$CHCHO \rightarrow$ products							
Hydroxyl + 2-Butenal (Crotonaldehyde)							
83 ATK/ASC3 [1])	RL	299	1.39±0.16			2/2	
k_{ref}: $OH + CH_3CH$=$CH_2 \rightarrow$ products.							
83 ATK/ASC3 [1])	RN	299	(2.19±0.24)(13)			2	
Placed on an absolute basis by using the k for the reaction of OH with CH_3CH=CH_2.							
[1]) Irradiation of Crotonaldehyde/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography.							
P(Total) = 735 torr.							
[Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
$OH + CH_2$=$C(CH_3)CHO \rightarrow$ products							
Hydroxyl + 2-Propenal, 2-methyl- (Methacrolein)							
83 ATK/ASC3 [1])	RL	299	1.13±0.09			2/2	
k_{ref}: $OH + CH_3CH$=$CH_2 \rightarrow$ products.							
83 ATK/ASC3 [1])	RN	299	(1.72±0.14)(13)			2	
Placed on an absolute basis by using the k for $OH + CH_3CH$=CH_2.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
[1]) Irradiation of Methacrolein/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = $2.38x10^{13}$ molec.cm^{-3}.							
OH + $CH_3C(O)CH{=}CH_2$ → products Hydroxyl + 3-Buten-2-one (Methyl vinyl ketone)							
83 ATK/ASC3 [1]) k_{ref}: OH + $CH_3CH{=}CH_2$ → products.	RL	299	0.747±0.055			2/2	
83 ATK/ASC3 [1]) Placed on an absolute basis by using the k for OH + $CH_3CH{=}CH_2$.	RN	299	(1.13±0.08)(13)			2	
[1]) Irradiation of Methyl vinyl ketone/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in air. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = $2.38x10^{13}$ molec.cm^{-3}.							
OH +  **→ products** Hydroxyl + Thiophene							
83 ATK/ASC2 [1]) k_{ref}: OH + $CH_3(CH_2)_4CH_3$ → products.	RL	298	1.68±0.06			2/2	
83 ATK/ASC2 [1]) Placed on an absolute basis by using the k for OH + Hexane.	RN	298	(5.77±0.23)(12)			2	
[1]) Irradiation of Methyl nitrite/Thiophene/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography. P(Total) 735 torr. [Methyl nitrite] = $2.38x10^{14}$ molec.cm^{-3}.							
83 MAC/JOU Discharge-flow reactor. OH generated by the reaction: H + NO → OH + N. OH atoms gene- rated by dissociation of H_2 traces in He by a microwave-discharge. EPR-spectrometry. $[OH]_o$ = $(0.5\text{-}1.9)x10^{11}$atoms.cm^{-3}. $[Thiophene]_o$ = $(0.23\text{-}4.87)x10^{13}$ molec.cm^{-1}. P = (0.47-0.60) torr.	EX	293-473	(7.83±4.82)(10)	0	-1750±200	2	

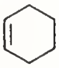
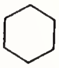
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH + CH_2=C=$CHCH_2CH_3$ → products Hydroxyl + 1,2-Pentadiene							
83 OHT Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(H_2O_2) = 1 torr. P(O_2) 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(1,2-Pentadiene) ~ 1 mtorr. k determined relative to the reaction: OH + CH_2=CHCH=CH_2 → products.	RN	297	(2.19±0.08)(13)			2	
OH + cis-CH_2=CHCH=$CHCH_3$ → products Hydroxyl + 1,3-Pentadiene, (Z)-							
83 OHT Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(H_2O_2) = 1 torr. P(O_2) 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(cis-1,3-Pentadiene) ~ 1 mtorr. k determined relative to the reaction: OH + CH_2=CHCH=CH_2 → products.	RN	297	(6.20±0.18)(13)			2	
OH + CH_2=$CHCH_2CH$=CH_2 → products Hydroxyl + 1,4-Pentadiene							
83 OHT Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(H_2O_2) = 1 torr. P(O_2) = 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(1,4-Pentadiene) ~ 1 mtorr. k determined relative to the reaction: OH + CH_3CH=CH_2 → products.	RN	297	(3.05±0.08)(13)			2	
OH + CH_2=C=$C(CH_3)_2$ → products Hydroxyl + 1,2-Butadiene, 3-methyl-							
83 OHT Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(3-Methyl-1,2-Butadiene) ~ 1 mtorr. P(Total) ~ 760 torr. (mostly N_2). P(O_2) = 10 torr. P(H_2O_2) 1 torr. k determined relative to the reaction: OH + CH_2=CHCH=CH_2 → products.	RN	297	(3.49±0.11)(13)			2	

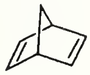
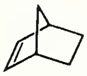
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$OH + CH_2{=}C(CH_3)CH{=}CH_2 \rightarrow$ products							
Hydroxyl + 1,3-Butadiene, 2-methyl-							
83 OHT	RN	297	(6.08±0.18)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ = 10 torr. P(2-Methyl-1,3-Butadiene) ~ 1 mtorr. P(Total) ~ 760 torr. (mostly N_2). k determined relative to the reaction: $OH + CH_2{=}CHCH{=}CH_2 \rightarrow$ products.							
OH +  **→ products**							
Hydroxyl + Cyclopentene							
83 ATK/ASC5 (1)	RL	298	0.666±0.024			2/2	
k_{ref}: $OH + CH_2{=}C(CH_3)CH{=}CH_2 \rightarrow$ products.							
83 ATK/ASC5 (1)	RN	298	(3.85±0.14)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene). (1) Irradiation of Cyclopentene/CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. P(Total) = 735 torr. $[\text{Methyl nitrite}]_o = 2.38 \times 10^{13}$ molec.cm^{-3}							
OH + trans-$CH_3CH{=}CHCH_2CH_3 \rightarrow$ products							
Hydroxyl + 2-Pentene, (E)-							
83 OHT	RN	297	(4.13±0.13)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(trans-2-Pentene) ~1 mtorr. k determined relative to the reaction: $OH + CH_2{=}CHCH{=}CH_2 \rightarrow$ products.							
$OH + (CH_3)_2C{=}CHCH_3 \rightarrow$ products							
Hydroxyl + 2-Butene, 2-methyl-							
83 OHT	RN	297	(5.25±0.16)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. $P(H_2O_2)$ = 1 torr. $P(O_2)$ = 10 torr. P(Total) ~ 760 torr. (mostly N_2). P(2-Methyl-2-Butene) ~1 mtorr. k determined relative to the reaction: $OH + CH_2{=}CHCH{=}CH_2 \rightarrow$ products.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  **→ products**							
Hydroxyl + 1,3-Cyclohexadiene							
83 ATK/ASC5 [1]	RL	298	1.62±0.05			2/2	
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1]	RN	298	(9.40±0.33)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
[1] Irradiation of 1,3-Cyclohexadiene/CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = 2.38x10^{13} molec.cm^{-3}.							
OH +  **→ products**							
Hydroxyl + 1,4-Cyclohexadiene							
83 ATK/ASC5 [1]	RL	298	0.988±0.040			2/2	
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1]	RN	298	(5.70±0.23)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
[1] Irradiation of 1,4-Cyclohexadiene/CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = 2.38x10^{13} molec.cm^{-3}.							
83 OHT	RN	297	(5.94±0.19)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. P(H_2O_2) = 1 torr. P(O_2) = 10 torr. OH generated by photolysis of H_2O_2. P(1,4-Cyclohexadiene) ~ 1 mtorr. P(Total) ~760 torr. (mostly N_2). k determined relative to the reaction: OH + CH_2=CH$CH_2$$CH_2$CH=$CH_2$ → products.							
OH + trans-CH_2=CHCH=CH$CH_2$$CH_3$ → products							
Hydroxyl + 1,3-Hexadiene, (E)-							
83 OHT	RN	297	(6.92±0.18)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(H_2O_2) = 1 torr. P(O_2) = 10 torr. P(trans-1,3-Hexadiene) ~ 1 mtorr. P(Total) ~ 760 torr. (mostly N_2). k determined relative to the reaction: OH + CH_2=CHCH=CH_2 → products.							

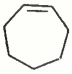
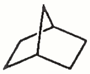
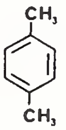
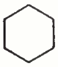
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH + trans-CH_2=$CHCH_2CH$=$CHCH_3$ → products							
Hydroxyl + 1,4-Hexadiene, (E)-							
83 OHT [1]	RN	297	(5.19±0.24)(13)			2	
k determined relative to the reaction:							
OH + CH_3CH=CH_2 → products.							
83 OHT [1]	RN	297	(5.57±0.33)(13)			2	
k determined relative to the reaction:							
OH + CH_2=CHCH=CH_2 → products.							
[1] Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(H_2O_2) = 1 torr. P(O_2) = 10 torr.							
P(trans-1,4-Hexadiene) ~ 1 mtorr.							
P(Total) ~ 760 torr. (mostly N_2).							
OH + CH_2=$CHCH_2CH_2CH$=CH_2 → products							
Hydroxyl + 1,5-Hexadiene							
83 OHT [1]	RN	297	(3.52±0.20)(13)			2	
k determined relative to the reaction:							
OH + CH_3CH=CH_2 → products.							
83 OHT [1]	RN	297	(3.82±0.08)(13)			2	
k determined relative to the reaction:							
OH + CH_2=CHCH=CH_2 → products.							
[1] Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(H_2O_2) = 1 torr. P(O_2) = 10 torr.							
P(Total) ~ 760 torr. (mostly N_2).							
P(1,5-Hexadiene) ~ 1 mtorr.							
OH + CH_3CH=CHCH=$CHCH_3$ → products							
Hydroxyl + 2,4-Hexadiene (mixture of cis,cis- and trans,trans- forms)							
83 OHT	RN	297	(8.31±0.30)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(H_2O_2) = 1 torr. P(O_2) = 10 torr.							
P(Total) ~ 760 torr. (mostly N_2).							
P(2,4-Hexadiene) ~ 1 mtorr.							
k determined relative to the reaction:							
OH + CH_2=CHCH=CH_2 → products.							
OH + CH_2=$CHC(CH_3)$=$CHCH_3$ → products							
Hydroxyl + 1,3-Pentadiene, 3-methyl-							
83 OHT	RN	297	(8.37±0.48)(13)			2	

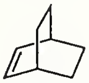
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(3-Methyl-1,3-Pentadiene) ~ 1 mtorr.							
P(Total) ~760 torr. (mostly N_2).							
$P(H_2O_2)$ = 1 torr.							
$P(O_2)$ = 10 torr.							
k determined relative to the reaction:							
OH + cis-CH_2=CHCH=$CHCH_3$ → products.							
OH + CH_2=CHC=$CH(CH_3)_2$ → products							
Hydroxyl + 1,3-Pentadiene, 4-methyl-							
83 OHT	RN	297	(8.07±0.24)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(4-Methyl-1,3-Pentadiene) ~ 1 mtorr.							
$P(O_2)$ = 10 torr. $P(H_2O_2)$ = 1 torr.							
P(Total) ~760 torr. (mostly N_2).							
k determined relative to the reaction:							
OH + cis-CH_2=CHCH=$CHCH_3$ → products.							
OH + CH_2=$C(CH_3)CH_2CH$=CH_2 → products							
Hydroxyl + 1,4-Pentadiene, 2-methyl-							
83 OHT	RN	297	(4.81±0.49)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(2-Methyl-1,4-Pentadiene) ~ 1 mtorr.							
$P(O_2)$ = 10 torr. $P(H_2O_2)$ = 1 torr.							
P(Total) ~760 torr. (mostly N_2).							
k determined relative to the reaction:							
OH + cis-CH_2=CHCH=$CHCH_3$ → products.							
OH + CH_2=$C(CH_3)C(CH_3)$=CH_2 → products							
Hydroxyl + 1,3-Butadiene, 2,3-dimethyl-							
83 OHT	RN	297	(4.81±0.49)(13)			2	
Reaction in O_2/N_2 gas, in aquartz cell.							
OH generated by photolysis of H_2O_2.							
P(2,3-Dimethyl-1,3-butadiene) ~ 1 mtorr.							
$P(O_2)$ = 10 torr. $P(H_2O_2)$ = 1 torr.							
P(Total) ~760 torr. (mostly N_2).							
k determined relative to the reaction:							
OH + CH_2=CHCH=CH_2 → products.							

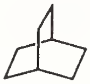
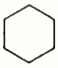
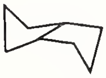
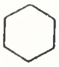
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + Cyclohexene							
83 ATK/ASC5 [1])	RL	298	(6.7±0.17)(-1)			2/2	
k_{ref}: OH + $CH_2=C(CH_3)CH=CH_2$ → products.							
83 ATK/ASC5 [1])	RN	298	(3.87±0.10)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
[1]) Irradiation of Cyclohexene/CH_3ONO/Air mixtures in a Teflon bag.							
Gas-chromatography. P(Total) = 735 torr.							
[Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
83 OHT	RN	297	(3.86±0.15)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell.							
OH generated by photolysis of H_2O_2.							
P(H_2O_2) = 1 torr. P(O_2) = 10 torr.							
P(Total) ~760 torr. (mostly N_2).							
P(Cyclohexene) ~ 1 mtorr.							
k determined relative to the reaction:							
OH + $CH_2=CHCH_2CH_2CH=CH_2$ → products							
OH + $(CH_3)_2C=C(CH_3)_2$ → products							
Hydroxyl + 2-Butene, 2,3-dimethyl-							
83 ATK/ASC5 [1])	RL	298	1.14±0.04			2/2	
k_{ref}: OH + $CH_2=C(CH_3)CH=CH_2$ → products.							
83 ATK/ASC5 [1])	RN	298	(6.57±0.24)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
[1]) Irradiation of 2,3-Dimethyl-2-Butene/CH_3ONO/ Air mixtures in a Teflon bag.							
Gas-chromatography. P(Total) = 735 torr.							
[Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
OH +  → products							
Hydroxyl + Cyclohexane							
83 ATK/ASC3 [1])	RL	299	0.270±0.016			2/2	
k_{ref}: OH + $CH_3CH=CH_2$ → products.							
83 ATK/ASC3 [1])	RN	299	(4.10±0.25)(12)			2	
Placed on an absolute basis by using the k for OH + $CH_3CH=CH_2$.							

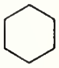
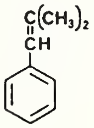
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
1) Irradiation of Cyclohexane/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography. P = 735 torr. [Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
OH +  **→ products**							
Hydroxyl + Bicyclo[2.2.1]hepta-2,5-diene (2,5-Norbornadiene)							
83 ATK/ASC5 1)	RL	298	1.19±0.10			2/2	
k_{ref}: OH + $CH_2=C(CH_3)CH=CH_2$ → products.							
83 ATK/ASC5 1)	RN	298	(6.87±0.60)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
1) Irradiation of 2,5-Norbornadiene/CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
OH +  **→ products**							
Hydroxyl + Bicyclo[2.2.1]hept-2-ene (2-Norbornene)							
83 ATK/ASC5 1)	RL	298	0.488±0.040			2/2	
k_{ref}: OH + $CH_2=C(CH_3)CH=CH_2$ → products.							
83 ATK/ASC5 1)	RN	298	(2.81±0.23)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
1) Irradiation of 2-Norbornene/CH_3ONO/Air mixtures in a Teflon cylindrical bag. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
OH + $CH_2=C(CH_3)CH_2CH_2CH=CH_2$ → products							
Hydroxyl + 1,5-Hexadiene, 2-methyl-							
83 OHT	RN	297	(5.75±0.26)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cylindrical cell. OH generated by photolysis of H_2O_2. P(2-Methyl-1,5-Hexadiene) ~ 1 mtorr. P(H_2O_2) = 1 torr. P(O_2) = 10 torr. P(Total) ~760 torr. (mostly N_2). k determined relative to the reaction: OH + $CH_2=CHCH_2CH_2CH=CH_2$ → products.							

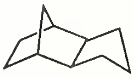
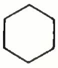
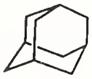
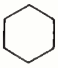
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

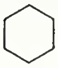
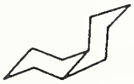
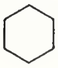
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + Cycloheptene							
83 ATK/ASC5 [1])	RL	298	0.737±0.023			2/2	
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1])	RN	298	(4.26±0.13)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
[1]) Irradiation of Cycloheptene/CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. [Methyl nitrite]$_o$ = 2.38x10^{13} molec.cm^{-3}. P(Total) = 735 torr.							
OH +  → products							
Hydroxyl + Bicyclo[2.2.1]heptane (Norbornane)							
83 ATK/ASC1 [1])	RL	299	0.731±0.018			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 [1])	RN	299	(3.33±0.09)(12)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane.							
[1]) Irradiation of Norbornane/CH_3ONO/Air mixtures in a Teflon bag. H generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.							
OH +  → products							
Hydroxyl + Benzene, 1,3-dimethyl- (m-Xylene)							
83 ATK/ASC1 [1])	RL	299	2.85±0.18			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 [1])	RN	299	(1.30±0.08)(13)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
1) Irradiation of m-Xylene/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 235 torr. Gas-chromatography.							
OH +  **→ products**							
Hydroxyl + Bicyclo[2.2.2]oct-2-ene							
83 ATK/ASC5 [1])	RL	298	0.404±0.019			2/2	
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1])	RN	298	(2.34±0.11)(13)			2	
Placed on an absolute basis by using the k for OH + 2-Methyl-1,3-Butadiene (Isoprene).							
1) Irradiation of Bicyclo[2.2.2]oct-2-ene/ CH_3ONO/Air mixtures in a Teflon bag. Gas-chromatography. P(Total) = 735 torr. [Methyl nitrite]$_o$ = 2.38x10^{13} molec.cm^{-3}.							
OH + CH_2=C(CH_3)CH_2CH_2C(CH_3)=CH_2 → products							
Hydroxyl + 1,5-Hexadiene, 2,5-dimethyl-							
83 OHT	RN	297	(7.23±0.11)(13)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(2,5-Dimethyl-1,5-Hexadiene) ~ 1 mtorr. P(Total) ~760 torr. (mostly N_2). P(H_2O_2) = 1 torr. P(O_2) = 10 torr. k determined relative to the reaction: OH + CH_2=$CHCH_2CH_2$CH=CH_2 → products.							
OH + $(CH_3)_2$C=CHCH=C$(CH_3)_2$ → products							
Hydroxyl + 2,4-Hexadiene, 2,5-dimethyl-							
83 OHT	RN	297	(1.26±0.06)(14)			2	
Reaction in O_2/N_2 gas, in a quartz cell. OH generated by photolysis of H_2O_2. P(2,5-Dimethyl-2,4-Hexadiene) ~ 1 mtorr. P(H_2O_2) = 1 torr. P(O_2) = 10 torr. P(Total) ~760 torr. (mostly N_2). k determined relative to the reaction: OH + CH_2=C(CH_3)CH_2CH_2CH=CH_2 → products.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + Bicyclo[2.2.2]octane							
83 ATK/ASC1 1)	RL	299	1.96±0.13			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1)	RN	299	(8.91±0.60)(12)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane.							
1) Irradiation of Bicyclo[2.2.2]octane/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.							
OH +  → products							
Hydroxyl + Pentalene, octahydro- (Bicyclo[3.3.0]octane)							
83 ATK/ASC1 1)	RL	299	1.47±0.07			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1)	RN	299	(6.69±0.36)(12)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane.							
1) Irradiation of Bicyclo[3.3.0]octane/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.							
OH +  → products							
Hydroxyl + 1H-Indene, octahydro-, cis- (cis-Bicyclo[4.3.0]nonane)							
83 ATK/ASK1 1)	RL	299	2.29±0.16			2/2	
k_{ref}: OH +  → products.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
83 ATK/ASC1 1) Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of cis-Bicyclo[4.3.0]nonane/ CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.	RN	299	(1.04±0.08)(13)			2	
OH +  → products							
Hydroxyl + 1H-Indene, octahydro-, trans- (trans-Bicyclo[4.3.0]nonane)							
83 ATK/ASC1 1)	RL	299	2.35±0.17			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1) Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of trans-Bicyclo[4.3.0]nonane/ CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.	RN	299	(1.07±0.08)(13)			2	
OH +  → products							
Hydroxyl + Benzene, (2-methyl-)-propenyl- (β-Dimethylstyrene)							
83 CHI/BIG Photooxidation of β-Dimethylstyrene in a Polymethylmetacrylate smog-chamber. OH generated by HONO vapors in synthetic air. Gas-chromatography. k determined relative to the reaction: OH + $(CH_3)_3CCH_2CH(CH_3)_2$ → products.	RN	298	(1.99±0.30)(13)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + 4,7-Methano-1H-Indene, octahydro-, (3aα,4β,7β,7aα)- (Tricyclo[5.2.1.$0^{2,6}$]decane) (exo-Tetrahydrodicyclopentadiene)							
83 ATK/ASC1 1)	RL	299	1.51±0.05			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1) Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of exo-Tetrahydrodicyclopentadiene/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.	RN	299	(6.87±0.24)(12)			2	
OH +  → products							
Hydroxyl + Tricyclo[3.3.1.$1^{3,7}$]decane (Adamantane)							
83 ATK/ASC1 1)	RL	299	3.07±0.27			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1) Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of Adamantane/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.	RN	299	(1.39±0.13)(13)			2	
OH +  → products							
Hydroxyl + Naphthalene, decahydro-, cis- (cis-Decalin) (cis-Bicyclo[4.4.0]decane)							
83 ATK/ASC1 1)	RL	299	2.65±0.18			2/2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
k_{ref}: OH +  → products.							
83 ATK/ASC1 1)	RN	299	(1.21±0.08)(13)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of cis-Decalin/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.							
OH +  → products							
Hydroxyl + Naphthalene, decahydro-, trans- (trans-Bicyclo[4.4.0]decane) (trans-Decalin)							
83 ATK/ASK1 1)	RL	299	2.72±0.16			2/2	
k_{ref}: OH +  → products.							
83 ATK/ASC1 1)	RN	299	(1.24±0.07)(13)			2	
Placed on an absolute basis by using the k for OH + Cyclohexane. 1) Irradiation of trans-Decalin/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO/Air mixtures at 290 nm. and 735 torr. Gas-chromatography.							
$HO_2 + HO_2 (+ M) \rightarrow H_2O_2 + O_2 (+ M)$							
Hydroperoxo							
79 TSU/NAK	EX	298	(2.8±0.3)(12)			2	
Disproportionation of HO_2 in a quartz flow- reactor. HO_2 generated by reacting H with O_2. H atoms generated by Hg-photosensitized decomposition of H_2. P = 760 torr.							
$HO_2 + NO (+ M) \rightarrow O_2 + HNO (+ M)$ (a) $\rightarrow OH + NO_2 (+ M)$ (b) $\rightarrow HONO_2 (+ M)$ (c)							
Hydroperoxo + Nitrogen oxide (NO)							
78 HAC/KAU	EX	296	(3.5±1.0)(12)			2	
k_b. Discharge-flow. LMR-Spectrometry. P = 5.25 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(rel), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
79 TEM k_b. Flow-system. ESR-Spectrometry. LMR-spectrometry. HO_2 generated by the reaction: $H + O_2 + M \rightarrow HO_2 + M$.	EX	298	(4.4±1.0)(12)			2	
$H_2O + N_2O_5 \rightarrow HONO_2 + HONO_2$ Water + Nitrogen oxide (N_2O_5)							
83 TUA/ATK Reaction in Teflon environmental chambers. This value should be considered an upper limit to the homogeneous k.	EX	298	(7.83±1.20)(2)			2	
$H_2O + CH_3C(O)ONO_2 \rightarrow$ products Water + Peroxide, acetyl nitro							
76 PAT/ATK2 Reaction in a Teflon-lined aluminum tank. Gas-chromatography. Mass-spectrometry. IR-Absorption spectrometry. [Peroxide] = (7.6-8.3) ppm. $[H_2O]$ = (5900-12000) ppm.	EX	296	(1.34±0.20)(1)			2	
$SO + O_2 \rightarrow SO_2 + O$ Sulfur monoxide + Oxygen molecule							
83 BLA/SHA SO generated by ArF Laser-photodissociation of SO_2 at 193 nm. $P(SO_2)$ = 30 mtorr. $P(O_2)$ < 550 torr.	EX	230-420	1.45(11)	0	2370±250	2	2.0
83 GOE/SCH Static conditions. P(Total) = (1-200) mtorr.	EX	262-363	6.02(10)	0	2180±117	2	1.46
$SO + SO (+ M) \rightarrow SO_2 + S (+ M)$ Sulfur monoxide							
83 MAR/HER Discharge-flow reactor. SO generated by the reaction: $O + CS_2 \rightarrow SO + CS$. O atoms generated by passing a dilute N_2O/Ar mixture through a microwave-discharge.	EX	298	≃2.10(9)			2	4.0
$SO_2 + NO_2 \rightarrow SO_3 + NO$ Sulfur dioxide + Nitrogen oxide (NO_2)							
83 PEN/CAN Static reactor. Second derivative UV-spectrometry. $[SO_2] = (8.07\text{-}8.73)\times10^{18}$ molec.cm^{-3}. $[NO_2] = (0.78\text{-}4.40)\times10^{17}$ molec.cm^{-3}	EX	298	(1.4±0.1)(-2)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$SO_2 + CH_3C(O)ONO_2 \rightarrow$ products							
Sulfur dioxide + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	<8.10			2	
Reaction in a Teflon-lined aluminum tank. Gas-chromatography. Mass-spectrometry. IR-Absorption spectrometry. $[SO_2]$ = (1260-3540) ppm. [Peroxide] = 0.042 ppm.							
$SO_3 + NO_2 \rightarrow$ products							
Sulfur trioxide + Nitrogen oxide (NO_2)							
83 PEN/CAN	EX	298	(8.8±0.8)(4)			2	
Static reactor. Second derivative UV-spectrometry technique. $[SO_3]$ = $(5.72-0.64)x10^{16}$ $molec.cm^{-3}$. $[NO_2]$ = $2.53x10^{16}$ $molec.cm^{-3}$.							
$SH + O_2 \rightarrow$ products							
Mercapto + Oxygen molecule							
81 TIE/WAM	EX	298	≤1.93(9)			2	
Laser-induced fluorescence technique in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. Upper-limit k. $P(H_2S]$ = (30-100) mtorr. P(Ar) = (5-10) torr.							
$SH + SH \rightarrow H_2S + S$							
Mercapto							
81 TIE/WAM	EX	298	≤1.02(13)			2	
Laser-induced fluorescence technique in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. Upper-limit k. $P(H_2S)$ = (30-100) mtorr. P(Ar) = (5-10) torr.							
$SH + H_2S \rightarrow$ products							
Mercapto + Hydrogen sulfide							
81 TIE/WAM	EX	298	≤1.02(13)			2	
Laser-induced fluorescence technique in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. $P(H_2S)$ = (30-100) mtorr. P(Ar) = (5-10) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
SH + NO → products Mercapto + Nitrogen oxide (NO) → products							
81 TIE/WAM Laser-induced fluorescence technique in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. $P(H_2S)$ = (30-100) mtorr. [NO] = (0.5-40) torr. P(Ar) = (5-10) torr.	EX	298	3.37(11)			2	
SH + CH_2=CH_2 → products Mercapto + Ethene							
81 TIE/WAM Laser-induced fluorescence technique in the (320-330) nm. region. SH generated by H_2S photodissociation in Ar through an ArF excimer Laser, at 193 nm. Upper-limit k. $P(H_2S)$ = (30-100) mtorr. P(Ar) = (5-10) torr.	EX	298	≤1.39(9)			2	
N + OH → NO + H Nitrogen atom + Hydroxyl							
83 BRU/SCH2 Fast-flow reactor. Laser-magnetic Resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)	EX	298	(2.53±0.48)(13)			2	
N + HO_2 → products Nitrogen atom + Hydroperoxo							
83 BRU/SCH2 Fast-flow reactor. Laser-magnetic resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)	EX	298	(1.33±0.30)(13)			2	
$N + N_3 \rightarrow N_2(B^3\Pi_g) + N_2(X^1\Sigma_g^+)$ Nitrogen atom + Azide							
83 YAM/FUE Discharge-flow reactor. N atoms generated by dissociation of N_2 in a microwave-discharge. through a N_2/Ar mixture. N_3 generated by the reaction: $Cl + HN_3 \rightarrow HCl + N_3$.	EX	298	(9.64±6.63)(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$N + NH_2 \rightarrow NH + NH$ (a) **$\rightarrow N_2 + H$ (b)** Nitrogen atom + Amidogen							
83 WHY/PHI3 $(k_a + k_b)$ Fast-flow system. NH_2 generated by photolysis of NH_3 at 193 nm. N atoms generated by microwave discharge. Laser-induced Fluorescence. $[NH_3] \sim 3.0 \times 10^{14}$ molec.cm^{-3}.	EX	296	(7.29±0.84)(13)			2	
$N + CN(v{=}n) \rightarrow N_2 + C$ Nitrogen atom + Cyanogen							
83 WHY/PHI2 Fast-flow reactor. CN generated by the ArF Flash-photolysis of NCCN at 193 nm. N atom generated by microwave-discharge. Laser induced Fluorescence.	EX	300	(6.02±0.78)(13)			2	
$N + NCC \rightarrow CN + CN$ Nitrogen atom + Methylidyne, cyano-							
83 WHY/PHI2 (n = 0,1) Fast-flow reactor. N atom generated by microwave-discharge. NCC generated by reaction of C atom with NCCN. C atom generated by reacting CN with N atom. Laser induced fluorescence.	ES	300	6.02(13)			2	
$N_3 + N_3 \rightarrow N_2(B^3\Pi_g) + N_2X^1\Sigma_g^+) + N_2(X^1\Sigma_g^+)$ Azide							
83 YAM/FUE Discharge-flow reactor. N_3 generated by the reaction: $Cl + HN_3 \rightarrow HCl + N_3$	EX	298	8.43(11)			2	
$NO + NH_2 \rightarrow [NH_2NO] \rightarrow N_2 + H_2O\dagger$ Nitrogen oxide (NO) + Amidogen							
83 WHY/PHI3 Fast-flow system. NH_2 generated by the NH_3 photolysis at 193 nm. Laser-induced Fluorescence. $[NH_3] \sim 3.0 \times 10^{14}$ molec.cm^{-3}.	EX	297	(1.09±0.07)(13)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$NO + CH_3C(O)ONO_2 \rightarrow$ products							
Nitrogen oxide (NO) + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	(2.83±0.83)(-4)			1	
Reaction in a Teflon-lined aluminum tank.							
Gas-chromatography. Mass-spectrometry.							
IR-Absorption spectrometry.							
[Peroxide] = (4.1-17.6) ppm.							
[NO] = (26-211) ppm.							
$NO_2 + CH_3C(O)ONO_2 \rightarrow$ products							
Nitrogen oxide (NO_2) + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	(1.05±0.49)(3)			2	
Reaction in a Teflon-lined aluminum tank.							
Gas-chromatography. Mass-spectrometry.							
IR-Absorption spectrometry.							
[Peroxide] = (3.0-9.3) ppm.							
[NO_2] = (26-52) ppm.							
$NO_2 + (CH_3)_2NNH_2 \rightarrow HONO + (CH_3)_2NNH$							
Nitrogen oxide (NO_2) + Hydrazine, 1,1-dimethyl-							
→ Nitrous acid + Hydrazyl, 2,2-dimethyl-							
83 TUA/CAR2	EX	300	(1.39±0.12)(7)			2	
Postulated first step in the overall reaction:							
$2NO_2 + (CH_3)_2NNH_2$							
$\rightarrow 2HONO + 0.5[(CH_3)_2NN{=}NN(CH_3)_2]$							
Reaction in a Teflon vessel.							
FTIR-Spectrometry. P = 735 torr.							
[NO_2] = (0-4.66)x10^{14} molec.cm^{-3}.							
[1,1-Dimethylhydrazine] = (1.21-4.35)x10^{14} molec.cm^{-3}.							
$NO_2 + (CH_3)_3CNO + \rightarrow NO + (CH_3)_3CNO_2$							
Nitrogen oxide (NO) + Propane, 2-methyl-2-nitroso-							
83 JOH/MEC	EX	291-318	6.76(8)	0	23905±755	2	2.1
Static reactor. Mass-spectrometry.							
P = (1-3) torr.							
$N_2O (+ M) \rightarrow N_2 + O (+ M)$ (a)							
$\rightarrow$ any other products (b)							
Nitrogen oxide (N_2O)							
83 GON ($k_{overall}$)	EX	1600-2000	2.43(12)	0	18470	1	
Thermolysis of N_2O in a shock-tube.							
Time-of-flight Mass-spectrometry.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$NH + NH_2 \rightarrow NH_2NH$ (a)							
$\rightarrow$ any other products (b)							
Imidogen + Amidogen							
83 TEM ($k_{overall}$)	EX	296	(8.0±3.0)(13)			2	
Far-IR Laser-Magnetic-Resonance Spectrometry.							
$NH(a^1\Delta) + HN_3 \rightarrow NH_2 + N_3$ (a)							
$\rightarrow N_2 + NH{=}NH^*$ (b)							
Imidogen + Hydrazoic acid							
83 KOD1 (k_a)	RL	303	0.746			2/2	
83 KOD1 (k_b)	RL	303	1.23			2/2	
Photolysis of HN_3 in Xe, at 313 nm.							
Gas-chromatography. IR-Spectrometry.							
Rate constant ratios estimated on the basis of a proposed mechanism.							
k_{ref}: $NH(a^1\Delta) + HN_3 \rightarrow 2H + 2N_2$							
P(Xe) = (0-600) torr.							
P(HN_3) = 50 torr.							
$NH(a^1\Delta) + CH_2{=}CH_2 \rightarrow [CH_2{=}CHNH_2 =$ ]							
Imidogen + Ethene							
$\rightarrow$ [Ethenamine (Vinylamine) = Aziridine]							
83 KOD3	RL	303	1.64			2/2	
Photolysis of HN_3 vapor in presence of Ethene, at 313 nm.							
Rate constant ratio estimated on the basis of a proposed mechanism.							
Gas-chromatography. IR-Spectrometry.							
k_{ref}: $NH(a^1\Delta) + HN_3 \rightarrow$ products							
P(Ethene) = (0-188) torr.							
P(HN_3) = (0-105) torr.							
$NH(a^1\Delta) + CH_3CH_3 \rightarrow CH_3CH_2NH_2^*$							
Imidogen + Ethane							
83 KOD2	RL	303	3.34(-1)			2/2	
Photolysis of HN_3 vapor in presence of Ethane, at 313 nm.							
Gas-chromatography. IR-Spectrometry.							
Rate constant ratio estimated on the basis of a proposed mechenism.							
P(Ethane) = (0-450) torr.							
P(HN_3) = 50 torr.							
k_{ref}: $NH(a^1\Delta) + HN_3 \rightarrow$ products.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$NH_2 + O_2$ (+ M) → products							
Amidogen + Oxygen molecule							
83 HAC/KUR	EX	295	(4.8±1.0)(8)			2	
Discharge-flow reactor. M = He. NH_2 generated by reacting F atoms with NH_3. P(Total) = 3 torr.							
$NH_2 + NO_2 \rightarrow N_2O + H_2O$ (major channel)							
Amidogen + Nitrogen oxide (NO_2)							
83 WHY/PHI3	EX	297	(1.27±0.11)(13)			2	
Fast-flow system. NH_2 generated by the photolysis of NH_3 at 193 nm. Laser-induced Fluorescence. $[NH_3] \sim 3.0 \times 10^{14}$ molec.cm^{-3}.							
$NH_2 + NH_2$ (+ M) → $NH + NH_3$ (+ M) (a) **→ NH_2NH_2 (+ M) (b)** **→ any other products (b)**							
Amidogen							
83 TEM $(k_a/k_{overall})$	RL	296	≤2.0(-3)			2/2	
Far-IR-Laser-Magnetic-Resonance Spectroscopy.							
C + NCCN → CN + NCC							
Ethanedinitrile (Cyanogen, or Oxalonitrile) + Carbon atom							
83 WHY/PHI2	ES	300	≃1.81(13)			2	
Fast-flow reactor. C atom generated by reacting CN with N atom. CN generated by ArF Laser Flash-Photolysis of NCCN at 193 nm. N atom generated by microwave-discharge. Laser induced Fluorescence.							
$CO + O_2 \rightarrow CO_2 + O$							
Carbon monoxide + Oxygen molecule							
71 GAR/MCF	DE	1400-2500	3.1(11)	0	19124	2	
Incident shock-waves waves in $H_2/O_2/CO/Ar$ mixtures. Data-fit to induction time by computer simulation.							
83 THI/ROT	EX	1700-3500	5.06(13)	0	31800	2	
Reaction behind reflected shock-waves. Atomic-Resonance absorption Spectrophotometry. P(Total) = 1350 torr. $[O_2] = (0.02-4.92) \times 10^{17}$ molec.cm^{-3}. $[CO] = (0.12-2.46) \times 10^{17}$ molec.cm^{-3}.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CO + N_2O \rightarrow CO_2 + N_2$							
Carbon monoxide + Nitrogen oxide (N_2O)							
83 LOI/CAR	EX	1060-1220	5.01(13	0	22144±1510	2	
Reaction in a static cell.							
k determined by applying the thermal							
theory of explosion to the measurements							
of the critical ignition pressure.							
$CO + CH_3C(O)ONO_2 \rightarrow$ products							
Carbon monoxide + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	<8.10(1)			2	
Reaction in a Teflon-lined aluminum tank.							
Gas-chromatography. Mass-spectrometry.							
IR-Absorption spectrometry.							
[Peroxide] = 11 ppm.							
[CO] = 232 ppm.							
$CH(v{=}n) + O_2 \rightarrow CO + OH^*$							
Methylidyne + Oxygen molecule							
83 DUN/GUI (v = 0)	EX	298	(1.26±0.12)(12)			2	
(v = 1)	EX	298	(2.59±0.24)(12)			2	
Reaction in a cylindrical stainless cell,							
by using a crossed-beam CO_2 Laser pump							
and a tunable dye Laser.							
CH generated by IR multiphoton							
dissociation of CH_3OH.							
Laser-induced fluorescence.							
P(Methanol) = 30 mtorr.							
83 LIC/BER	EX	298	(4.82±1.81)(13)			2	
Reaction in Ar buffer, by chemiluminescence							
monitoring.							
P(Ar) = 20 torr.							
$CH(v{=}n) + N_2 \rightarrow HCN + N$							
Methylidyne + Nitrogen molecule							
83 DUN/GUI (v = 0)	EX	298	(4.28±0.36)(10)			2	
(v = 1)	EX	298	(1.81±0.30)(12)			2	
Reaction in a cylindrical stainless-steel							
cell, by using a crossed-beam CO_2 Laser							
pump and a tunable dye Laser.							
CH generated by IR multiphoton							
dissociation of CH_3OH.							
Laser-induced Fluorescence.							
P(Methanol) = 12 mtorr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH + N_2 (+ M) \rightarrow HCN_2 (+ M)$							
Methylidyne + Nitrogen molecule							
83 BER/LIN 1)	CO	297	(1.20±0.60)(13)			2	
Limiting high-pressure k. (RRKM calculation).							
83 BER/LIN 1)	ES	297	(1.02±0.18)(17)			3	
Extrapolated limiting low-pressure k.							
83 BER/LIN 1)	EX	297-675	(1.02±0.18)(10)		-981±65	2	
This weighted linear least-squares fit fails to adequately describe the data at the lowest and highest temperatures studied and is valid only over a limited T-range (probably 297-450 K.) At higher temperatures, the activation complex decomposes to give other products, probably HCN + N, which dominate above 1000 K.							
1) Reaction in Ar diluent. Laser-photolysis. Laser-induced fluorescence. CH generated by multiphoton dissociation of $CHBr_3$. P(Total) = (25-787) torr.							
$CH + NO \rightarrow CO + NH^*$							
Methylidyne + Nitrogen oxide (NO)							
83 LIC/BER	EX	298	(1.51±3.01)(14)			2	
Reaction in Ar buffer by chemilumninescence monitoring. P(Ar) = 20 torr.							
$CH(v=n) + CH_3OH \rightarrow$ products							
Methylidyne + Methanol							
83 DUN/GUI (v = 0)	ES	298	(6.38±0.36)(13)			2	
(v = 1)	ES	298	(2.02±0.15)(14)			2	
Reaction in a cylindrical stainless steel cell, by using a crossed-beam CO_2 Laser pump and a tunable dye laser. CH generated by IR multiple photon dissociation of CH_3OH. Laser-induced Fluorescence.							
$CH + CH{\equiv}CH \rightarrow$  $\rightarrow$ products							
Methylidyne + Ethyne							
83 BER/FLE	EX	171-657	(2.10±0.25)(14)	0	-61±36	2	
Reaction in a Laser-photolysis/Laser-induced Fluorescence apparatus. CH generated by multiphoton dissociation of $CHBr_3$ at 266 nm. P(Total) = 100 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH + CH_2{=}CH_2 \rightarrow$  $\rightarrow CH_2CH{=}CH_2$ (a) $\rightarrow$ any other products (b) Methylidyne + Ethene							
83 BER/FLE (k_a) Laser-photolysis/Laser-induced Fluorescence. CH generated by multiphoton dissociation of $CHBr_3$ at 266 nm. P(Total) = 100 torr.	EX	160-652	(1.34±0.16)(14)	0	-173±35	2	
$CH_2(a^1A_1) + O_2 \rightarrow$ products Methylene + Oxygen molecule							
83 LAN/PET Cw Laser resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.	EX	295	(4.46±0.30)(13)			2	
$CH_2(^1A_1) + H_2 \rightarrow$ products Methylene + Hydrogen molecule							
83 LAN/PET Cw Laser Resonance-Absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm. with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.	EX	295	(6.32±0,30)(13)			2	
$CH_2(a^1A_1) + N_2 \rightarrow$ products Methylene + Nitrogen molecule							
83 LAN/PET Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.	EX	295	(6.63±0.60)(12)			2	
$CH_2(a^1A_1) + NO \rightarrow$ products Methylene + Nitrogen oxide (NO)							
83 LAN/PET Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.	EX	295	(9.64±0.90)(13)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_2(a^1A_1) + CO \rightarrow$ products							
Methylene + Carbon monoxide							
83 LAN/PET	EX	295	(2.95±0.24)(13)			2	
CW Laser Resonance-absorption technique.							
$CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer.							
P(Ketene) = (0.1-0.2) torr.							
P(He) - (4-6) torr.							
$CH_2(a^1A_1) + CH_4 \rightarrow$ products							
Methylene + Methane							
83 LAN/PET	EX	295	(4.22±0.24)(13)			2	
Cw Laser Resonance-absorption technique.							
$CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer.							
P(Ketene) = (0.1-0.2) torr.							
P(He) = (4-6) torr.							
$CH_2(X^3B_1) + CH{\equiv}CH \rightarrow CH_2{=}C{=}CH_2$ (a)							
$\rightarrow CH_3C{\equiv}CH$ (b)							
$\rightarrow C_3H_2 + H_2$ (c)							
$\rightarrow C_3H_3 + H$ (d)							
Methylene + Ethyne							
83 HOM/WEL2 (k_c)	ES	295	8.5(10)			2	
(k_c)	ES	500	2.0(11)			2	
(k_c)	ES	1000	5.0(11)			2	
(k_d)	ES	295	1.8(12)			2	
(k_d)	ES	500	2.7(12)			2	
(k_d)	ES	1000	3.6(12)			2	
Estimations based on a suggested mechanism.							
High-temperature flow-reactor, with or without added H atoms.							
P = 2 torr.							
$CH_2(a^1A_1) + CH_2{=}CH_2 \rightarrow$ products							
Methylene + Ethene							
83 LAN/PET	EX	295	(9.03±0.36)(13)			2	
Cw Laser Resonance-absorption technique.							
$CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer.							
P(Ketene) = (0.1-0.2) torr.							
P(He) = (4-6) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_2(a^1A_1) + CH_3CH_3 \rightarrow$ products							
Methylene + Ethane							
83 LAN/PET	EX	295	(1.14±0.12)(14)			2	
Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. (He) = (4-6) torr.							
$CH_2(a^1A_1) + CH_2{=}C{=}O \rightarrow CH_2{=}CH_2 + CO$							
Methylene + Ethenone (Ketene)							
83 LAN/PET	EX	295	(1.63±0.12)(14)			2	
Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.							
$CH_2(a^1A_1) + CH_3CH_2CH_3 \rightarrow$ products							
Methylene + Propane							
83 LAN/PET	EX	295	(1.45±0.12)(14)			2	
Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a XCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.							
$CH_2(a^1A_1) + (CH_3)_2C{=}CH_2 \rightarrow$ products							
Methylene + 1-Propene, 2-methyl- (Isobutene)							
83 LAN/PET	EX	295	(1.45±0.12)(14)			2	
Reaction of $CH_2(a^1A_1)$ with Isobutene by using a Cw Laser Resonance-absorption technique. $CH_2(a^1A_1)$ generated by the photolysis of Ketene at 308 nm., with a HCl-excimer. P(Ketene) = (0.1-0.2) torr. P(He) = (4-6) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3 + O_2$ (+ M) → HCHO + O + H (+ M) (a) → CH_3O + O (+ M) (b) → CO + OH + H_2 (+ M) (c) → HCHO + OH (+ M) (d) → CH_3O_2 (+ M) (e) Methyl + Oxygen molecule							
83 HSU/SHA [1] (k_b) Rate constant determined by fitting the concentration time profiles data to a computer kinetic modeling mechanism. RRKM calculation.	DE	1150-1560	1.0(14)	0	15500±1100	2	
83 HSU/SHA [1] (k_b) Three-parameter curve-fitting of three sets of rate constant expressions from literature. The preexponential factor expressed as: $(T/298)^{-5.94}$. [1] Reaction of CH_3 with O_2 in incident shock-waves. CH_3 generated by decomposition of $CH_3N{=}NCH_3$ in excess O_2. Concentration time profile measured by using CO-Laser Resonance-Absorption. $[CH_3N{=}NCH_3]$ = 0.021% and 0.04% in O_2.	RE	1150-1560	4.42(19)	-5.94	21300	2	
83 SEL/BAY (k_e. M = Ar) P(Total) = 0.639 torr. $P_{max}(O_2)$ = 0.2426 torr.	EX	298	(4.82±0.36)(9)			2	
(k_e. M = Ar) P(Total) = 5.921 torr. $P_{max}(O_2)$ = 0.0730 torr.	EX	298	(3.68±0.40)(10)			2	
(k_e. M = N_2) P(Total) = 0.931 torr. $P_{max}(O_2)$ = 0.3552 torr.	EX	298	(6.81±0.36)(9)			2	
(k_e. M = N_2) P(Total) = 5.420 torr. $P_{max}(O_2)$ = 0.0743 torr.	EX	298	(3,50±0.17)(10)			2	
(k_e. M = He) P(Total) = 1.078 torr. $P_{max}(O_2)$ = 0.3431 torr.	EX	298	(5.54±0.48)(9)			2	
(k_e. M = He) P(Total) = 6.747 torr. $P_{max}(O_2)$ = 0.1234 torr. Photoionization Mass-spectrometry. CH_3 generated by Flash-photolysis of Methyl nitrite at 193 nm. P(Total) = (0.5-6.0) torr. Other rate constants given at various pressures within the indicated P-range. The rate constant increases with the pressure.	EX	298	(2.40±0.17)(10)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3 + H_2S \rightarrow CH_4 + SH$							
Methyl + Hydrogen sulfide							
83 ARI/ART2	EX	334-432	1.0(11)	0	1054±10	2	1.02
	SE	334-432	1.38(11)	0	1105±30	2	1.23
Best value by combining the present rate expression with the data found in the literature.							
Photolysis of Azomethane/H_2S mixtures in a cylindrical silica reaction vessel. Gas-chromatography. P(Azomethane) = 70 torr. P(H_2S) = 0.5 torr.							
$CH_3 + CH_3 (+ M) \rightarrow CH_3CH_2 + H (+ M)$ (a) **$\rightarrow CH_2{=}CH_2 + H_2 (+ M)$ (b)** **$\rightarrow CH_3CH_3 (+ M)$ (c)**							
Methyl							
81 SKI/ROG (k$_c$. Limiting high-pressure k.)	DE	298	2.75(13)			2	
Calculated on the basis of k = $k_{-1}K$.							
83 ART/ANA (k$_c$)	DE	308	1.90(13)			2	
Molecular modulation spectrometry. CH_3 generated by photolysis of Azomethane at 350 nm.							
Rate constant extracted from the data by computer-non-linear parameter estimation and numerical integration procedures.							
83 HAS/RIE (k$_c$)	DE	298	2.70(13)			2	
Flash-photolysis of Dimethyl oxalate. Gas-chromatography. k calculated by using a computer integration interaction program.							
83 MAC/PIL (k$_c$. M = Ar) Limiting high-pressure k.	EX	296-577	(1.67±0.11)(13)	0	-154±2	2	
(k$_c$. M = Ar) Limiting low-pressure k.	EX	296-577	(2.18±1.20)(19)	0	-1680±300	3	
Flash-photolysis. Absorption spectroscopy. CH_3 produced by laser-photolysis of Azomethane at 193 nm. P = (5-500) torr.							
$CH_3 + CH_4 \rightarrow CH_3CH_3 + H$ (a) **$\rightarrow CH_3CH_2 + H_2$ (b)**							
Methyl + Methane							
83 BAC	ES	802	≤6.3(1)			2	
k$_a$. Thermolysis of CH_4. P ~1000 torr. Upper-limit k.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3 + HCHO \rightarrow CH_4 + CHO$							
Methyl + Formaldehyde							
83 ANA2	EX	500-603	(8.43±0.60)(11)	0	3500±48	2	
CH_3 generated by photolysis of Acetone.							
[Acetone] = $1.0x10^{17}$ molec.cm^{-3}.							
[Formaldehyde] = $3.6x10^{16}$ molec.cm^{-3}.							
Total conc. = $5.4x10^{18}$ molec.cm^{-3}.							
Gas-chromatography.							
$CH_3 + CH_3O \rightarrow CH_4 + HCHO$ (a)							
$\rightarrow CH_3OCH_3$ (b)							
Methyl + Methoxy							
83 HAS/RIE (k_a)	DE	298	1.68(13)			2	
Flash-photolysis of Dimethyl oxalate.							
Gas-chromatography.							
k calculated by using a computer integration interaction program.							
$CH_3 + CH_3CH_2 \rightarrow CH_3CH_2CH_3$							
Methyl + Ethyl							
83 ART/ANA	DE	308	2.72(13)			2	
Molecular modulation spectrometry.							
CH_3 and CH_3CH_2 generated by photolysis of Azomethane and Azoethane at 350 nm.							
k extracted from the data by computer-based non-linear parameter estimation and numerical integration procedures.							
83 KAN/PUR1	DE	773-793	8.91(12)	0	-856	2	
CH_3 and CH_3CH_2 recombination. The radicals generated by the pyrolysis of Propane in a static reactor, in presence of Ethene.							
Determined from the reverse reaction and thermochemical data.							
P(Ethene) = (1.5-6.0)torr.							
P(Propane) = 200 torr.							
$CH_3 + CH_3OC(O) \rightarrow CH_3C(O)OCH_3$							
Methyl + Methyl, methoxyoxo-							
83 HAS/RIE	DE	298	1.64(13)			2	
Flash-photolysis of Dimethyl oxalate.							
Gas-chromatography.							
k calculated by using a computer integration interaction program.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3 + (CH_3)_2S \rightarrow CH_4 + CH_3SCH_2$							
Methyl + Methane, thiobis- (Dimethyl sulfide)							
76 ART/LEE	EX	393-488	4.17(11)	0	4613±82	2	1.20
Photolysis of $(CH_3)_2S$ in a silica reaction vessel.							
Gas-chromatography.							
$CH_3 + CH_3N{=}NCH_3 \rightarrow CH_4 + CH_3N{=}NCH_2$							
Methyl + Diazene, dimethyl- (Azomethane)							
83 ARI/ART1	EX	334-463	1.07(11)	0	3960±22	2	1.05
Photolysis of Azomethane in a silica reaction vessel.							
Gas-chromatography.							
P = (18-73) torr.							
$CH_3 + CH_2{=}C{=}CH_2 \rightarrow CH_2C(CH_3)C{=}CH_2$ (a) $\rightarrow CH_3CH_2C{=}CH_2$ (b)							
Methyl + 1,2-Propadiene (Allene)							
83 SCH/CLA 1) (k_b/k_{ref})	RL	573-595	6.76(-1)	0	-508±24	2/2	
k_{ref}: $CH_3 + CH_3N{=}NCH_3 \rightarrow CH_4 + CH_2N{=}NCH_3$							
83 SCH/CLA 1) (k_b)	RN	573-595	5.75(10)	0	3440±120	2	1.58
Put on an absolute basis using the k of the reference reaction.							
1) Addition of CH_3 to $CH_2{=}C{=}CH_2$ in a static system.							
CH_3 generated by decomposition of Azomethane.							
Gas-chromatography.							
Allene/Azomethane mixture = 1.5.							
P_o(Azomethane) = 29 torr.							
$CH_3 + (CH_3)_2CH \rightarrow CH_4 + CH_3CH{=}CH_2$ (a) $\rightarrow (CH_3)_3CH$ (b)							
Methyl + Ethyl, 1-methyl- (Isopropyl)							
83 ART/ANA	DE	308	2.20(13)			2	
Molecular modulation spectrometry.							
CH_3 and $(CH_3)_2CH$ generated by photolysis of Azomethane and Azoisopropane at 350 nm.							
k extracted from the data by computer-based non-linear parameter estimation and numerical integration procedures.							

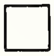
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3 + (CH_3)_2CO \rightarrow CH_4 + CH_2C(O)CH_3$ (a)							
$\rightarrow (CH_3)_3CO$ (b)							
$\rightarrow CH_3CH_2CH(CH_3)O$ (c)							
Methyl + 2-Propanone							
76 ART/LEE (k_a)	EX	393-488	4.07(11)	0	4869±55	2	1.12
Photolysis in a silica reaction nvessel.							
Gas-chromatography.							
83 ARI/ART1 (k_a)	EX	398-522	3.47(11)	0	4811±26	2	1.05
Photolysis in a silica reaction vessel.							
Gas-chromatography. P = (20-66) torr.							
$CH_3 + (CH_3)_3C \rightarrow (CH_3)_4C$							
Methyl + Ethyl, 1,1-dimethyl- (tert-Butyl)							
83 ART/ANA	DE	308	1.25(13)			2	
Molecular modulation spectrometry.							
CH_3 and $(CH_3)_3C$ generated by photolysis							
of Azomethane and Azo-t-butane at 350 nm.							
k extracted from the data by computer-							
based non-linear parameter estimation							
and numerical integration procedures.							
$CH_3 + (CH_3)_3CH \rightarrow CH_4 + (CH_3)_2CHCH_2$ (a)							
$\rightarrow CH_4 + (CH_3)_3C$ (b)							
Methyl + Propane, 2-methyl- (i-Butane)							
83 ANA1 ($k_a + k_b$)	EX	478-560	(3.73±0.66)(11)	0	4402±84	2	
Molecular modulation spectrometry.							
CH_3 generated by photolysis of Acetone.							
[Acetone] = 1.1×10^{17} molec.cm^{-3}.							
[Isopropane] = 6.9×10^{17} molec.cm^{-3}.							
Total conc. = 2.8×10^{18} molec.cm^{-3}.							
Gas-chromatography.							
83 MAR/SHA (k_a)	ES	504-640	1.58(13)	0	6616	2	
Pyrolysis of Isobutane sensitized by							
Azomethane in a static reactor.							
Gas-chromatography. P = (40-300) torr.							
$CH_4 (+ M) \rightarrow CH_3 + H (+ M)$ (a)							
$\rightarrow$ any other products (b)							
Methane							
83 KLO/DRO ($k_{overall}$)	EX	1600-2500	1.0(15)	0	50520	1	
Shock-tube. Pyrolysis of CH_4 in Ar,							
behind reflected shock-waves.							
[CH_4] = 1-9% in Ar.							
P = $(0.6-1.0)\times10^{6}$ Pa.							

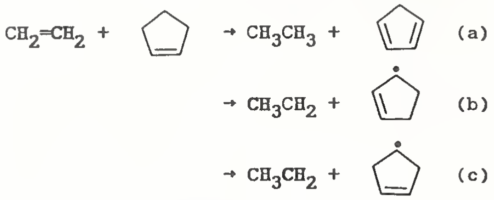
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CHO (+ M) → CO + H (+ M)							
Methyl, oxo-, (Formyl)							
(M = Ar)	EX	~1400	1.0(15)	0	7700	2	
Decomposition of CHO in premixed flames.							
Molecular-beam sampling. Mass-spectrometry.							
Unspecified T-range.							
P = (22.5-40) torr.							
CHO + O_2 (+ M) → CO + HO_2 (+ M) (a)							
→ CO_2 + OH (+ M) (b)							
→ HCO_3 (+ M) (c)							
Methyl, oxo-,(Formyl) + Oxygen molecule							
83 GUE/VAN (k_a)	EX	~1400	8.8(12)			2	
Reaction of CHO with O_2 in premixed flames.							
Molecular-beam sampling. Mass-spectrometry.							
Unspecified T-range.							
P = (22.5-40) torr.							
83 TEM (k_a)	EX	296	(3.2±0.7)(12)			2	
Reaction of CHO with O_2 by Far-IR Laser-Magnetic-Resonance Spectrometry.							
CHO + CHO → CO + CO + H_2 (a)							
→ HCHO + CO (b)							
→ OHCCHO (c)							
Methyl, oxo- (Formyl)							
83 TEM (k_a + k_b)	EX	296	(2.5±0.8)(13)			2	
Far-IR Laser-Magnetic-Resonance Spectrometry.							
HCHO (+ M) → H + CHO (+ M) (a)							
→ H_2 + CO (+ M) (b)							
Formaldehyde							
83 GUE/VAN (k_b. M = Ar)	EX	~1400	7.85(13)	0	12380	2	
Premixed flames. Molecular-beam sampling.							
Mass-spectrometry. Unspecified T-range.							
P = (22.5-40) torr.							
HC(O)OOH → H_2O + CO_2							
Methaneperoxoic acid (Performic acid)							
83 LEV/PRI	EX	403-513	2.14(11)	0	14266±1624	1	29.5
Thermolysis of Peracetic acid diluted in He or Ar, in a flow-type Teflon reactor.							
[Peracid] = 0.03-1.1vol% (in He, or Ar).							
P = 760 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3O + CH_3O \rightarrow HCHO + CH_3OH$ (a)							
$\rightarrow CH_3OOCH_3$ (b)							
Methoxy							
83 HAS/RIE (k_a)	DE	298	1.82(13)			2	
Flash-photolysis of Dimethyl oxalate. Gas-chromatography. k calculated by using a computer integration interaction program.							
$CH_3O + CH_3OC(O) \rightarrow HC(O)OCH_3 + HCHO$ (a)							
$\rightarrow CH_3OC(O)OCH_3$ (b)							
Methoxy + Methyl, methoxyoxo-							
83 HAS/RIE (k_a)	DE	298	8.80(12)			2	
(k_b)	DE	298	8.80(12)			2	
Flash-photolysis of Dimethyl oxalate. Gas-chromatography. k calculated by using a computer integration interaction program.							
CH_3O_2 (+ M) $\rightarrow CH_3 + O_2$ (+ M)							
Methyldioxy							
83 ANA/BLA ($M = N_2$)	RL	550	≤2.86(-11)			1/2	
Molecular Modulation Spectrometry. CH_3O_2 generated by photolysis of Acetone. k_{ref}: $CH_3 + O_2$ (+ M) $\rightarrow CH_3O_2$ (+ M).							
$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$ (a)							
$\rightarrow CH_3O + CH_3O + O_2$ (b)							
$\rightarrow CH_3OOCH_3 + O_2$ (c)							
Methyldioxy							
83 ANA/BLA (k_b/k_a)	RL	550	2.3			2/2	
(k_a)	ES	550	4.46(11)			2	
(k_b)	ES	550	1.03(11)			2	
Molecular Modulation Spectrometry. CH_3O_2 generated by photolysis of Acetone. k_b/k_a ratio based on extrapolation of data at lower temperature. Data-fit.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CS + O_2 \rightarrow COS + O$ (a) **$\rightarrow CO + SO$ (b)** Carbon monosulfide + Oxygen molecule							
75 RIC (k$_a$)	EX	290-500	1.58(8)	0	1862±453	2	
(k$_a$) Fast flow-reactor. CS generated by dissociation of CS_2 in an electric discharge. ESR-, and Mass-spectrometry. [Ar] = (1.0-5.0)x10^8 molec.cm^{-3}. [O_2] = (0.5-3.2)x10^8 molec.cm^{-3}. [CS] = (0.3-1.5)x10^8 molec.cm^{-3}. P = (0.39=8-1.58)torr.	EX	293	(2.7±1.0)(5)			2	
83 BLA/JUS (k$_a$ + k$_b$. M = He) Laser-induced Fluorescence. CS generated by Photodissociation of CS_2 at 193 nm. [O_2] = (99.6-99.99)% in He. P(CS_2) ~5mtorr.	EX	298	(1.75±0.24)(5)			2	
$CS + O_3 \rightarrow COS + O_2$ Carbon monosulfide + Ozone							
83 BLA/JUS (M = He) Laser-induced Fluorescence. CS generated by Photodissociation of CS_2 at 193 nm. P(CS_2) ~ 5 mtorr. P(He) = (50-300) torr.	EX	298	(1.81±0.24)(8)			2	
$CS + NO_2$ (+ M) $\rightarrow COS + NO$ (+ M) Carbon monosulfide + Nitrogen oxide (NO_2)							
83 BLA/JUS (M = He) Laser-induced Fluorescence. CS generated by Photodissociation of CS_2 at 193 nm. P(He) = 24 torr. P(CS_2) ~5 mtorr.	EX	298	(4.58±0.66)(7)			2	
$CH_3S + NO$ (+ M) $\rightarrow CH_3SNO$ (+ M) Methyl, mercapto- + Nitrogen oxide (NO)							
83 HAT/AKI Photooxidation of CH_3SH, CH_3SCH_3, or CH_3SSCH_3 with OH in air, in a quartz vessel. FTIR-Spectroscopy. Gas-chromatography. OH generated by photolysis of CH_3ONO, or CH_3CH_2ONO. Estimated ratio. k$_{ref}$: $CH_3S + O_2$ (+ M) $\rightarrow CH_3SO_2$ (+ M).	RL	303	2.0(3)			3/3	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CN(v=n) + O_2 → products							
Cyanogen + Oxygen molecule							
83 WHY/PHI2 (n = 0)	EX	300	(8.13±1.20)(12)			2	
(n = 1)	EX	300	(7.53±1.93)(12)			2	
Fast-flow reactor.							
CN generated by Flash-photolysis							
of NCCN at 193 nm.							
Dye-laser induced Fluorescence.							
CN + H_2 → HCN + H							
Cyanogen + Hydrogen molecule							
83 SZE/HAN1	ES	2700-3500	7.5(13)			2	1.36
Reaction in Ar, behind incident shock-waves.							
CN generated by NCCN dissociation.							
P = (230-420) torr.							
Best data-fit.							
CN + HCN → NCCN + H							
Cyanogen + Hydrocyanic acid							
83 SZE/HAN2	ES	2720-3070	1.0(13)			2	2.0
Reaction in Ar, behind incident shock-waves.							
CN generated by NCCN disociation.							
P = (323-518) torr.							
T-independent k.							
HCN (+ M) → H + CN (+ M)							
Hydrogen cyanide							
77 TAB/FUE	EX	2600-3600	(1.26±0.28)(16)	0	50171±700	2	
Thermolysis in Ar, behind incident							
shock-waves. Absorption-spectroscopy.							
[HCN] = (0.2-1.0) % in Ar.							
CH_2=C: + CH_4 → CH_2=CH + CH_3							
Ethenylidene (Vinylidene) + Methane							
83 LAU/YUN	DE	298	≃3.01(7)			2	
Calculated using the BSBL (Bond strength-							
Bond length) method of Berces and Dombi.							
CH_2=CH (+ M) → CH≡CH + H (+ M)							
Ethenyl							
83 KIE/KAP	DE	2300-3200	7.59(11)	0	2516	2	
Pyrolysis of 3% Ethene in Kr behind incident							
shock-waves.							
Data fit to a proposed mechanism.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_2{=}CH + O_2 \rightarrow CH{\equiv}CH + HO_2$							
Ethenyl (Vinyl) + Oxygen molecule							
83 TEM	EX	296	(1.5±0.7)(12)			2	
Reaction by Far-Infrared Laser-Magnetic-Resonance Spectrometry.							
$CH_2CH + CH_4 \rightarrow CH_2{=}CH_2 + CH_3$							
Ethenyl (Vinyl) + Methane							
83 LAU/YUN	DE	298	≃1.20(5)			2	
Calculated using the BSBL (Bond strength- Bond length) method of Berces and Dombi.							
$CH_2{=}CH_2\ (+ M) \rightarrow CH_2{=}CH + H\ (+ M)$ (a) **$\rightarrow CH{\equiv}CH + H_2\ (+ M)$ (b)**							
Ethene							
83 KIE/KAP (k$_a$)	DE	2300-3200	(1.4±0.3)(15)	0	41180	2	
(k$_b$)	DE	2300-3200	(1.5±0.3)(15)	0	27900	2	
Pyrolysis of 3% Ethene in Kr behind incident shock-waves. Data fit to a proposed mechanism.							
$CH_2{=}CH_2 + CH_2{=}CH_2 \rightarrow CH_2{=}CH + CH_3CH_2$ (a) →  **(b)**							
Ethene							
83 AYR/BAC (k$_a$)	RN	748-819	1.86(14)	0	32310±1007	2	4.0
Pyrolysis in a static system, with $(CH_3)_4$ and CH_3CH_3 as additives. Gas-chromatography. P(Ethene) = (100-300) torr.							
83 MAC/PAC (k$_a$)	DE	896	2.3(-1)			2	
Pyrolysis in a flow-system. Gas-chromatography. P = (23-78) torr. Estimation based on the relationships: $CH_3CH_2 + CH_3CH_2 \rightarrow CH_2{\rightarrow}CH_2 + CH_3CH_3$ (d) and $\rightarrow CH_3CH_2CH_2CH_3$ (r)							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Ethene + Cyclopentene							
→ Ethane + 1,3-Cyclopentadiene (a)							
→ Ethyl + 2-Cyclopenten-1-yl (b)							
→ Ethyl + 3-Cyclopenten-1-yl (c)							
80 BEN ($k_b + k_c$)	DE	650-770	2.0(13)	0	22295	2	
Estimation based on a proposed mechanism.							
$CH_3CH_2 + NO_2 \rightarrow$ products							
Ethyl + Nitrogen oxide (NO_2)							
83 PAR/GUT	EX	298	(2.71±0.06)(13)			2	
Reaction in a fast-flow system.							
CH_3CH_2 generated by the reaction:							
$CH_3CH_3 + Cl \rightarrow CH_3CH_2 + HCl$							
Cl atoms generated by dissociation of Cl_2 in a microwave-discharge.							
[Ethane] = ~$(5-50)x10^{13}$ molec.cm^{-3}.							
$[Cl]_o$ = $(0.5-1.5)x10^{11}$atom.cm^{-3}.							
P(Total) = (0.7-2.0) torr. (NO_2)							
$CH_3CH_2 + CH_2{=}CH_2 \rightarrow CH_3CH_3 + CH_2{=}CH$							
Ethyl + Ethene							
83 MAC/PAC	DE	896	8,0(7)			2	
Pyrolysis in a flow-system.							
Gas-chromatography.							
P = (23-78) torr.							
Estimation based on the relationships:							
$CH_3CH_2 + CH_3CH_2 \rightarrow CH_2{\rightarrow}CH_2 + CH_3CH_3$ (d) and							
$\rightarrow CH_3CH_2CH_2CH_3$ (r)							
$CH_3CH_2 + CH_3CH_2 \rightarrow CH_2{=}CH_2 + CH_3CH_3$ (a)							
$\rightarrow CH_3CH_2CH_2CH_3$ (b)							
Ethyl							
83 ART/ANA (k_b)	DE	308	8.77(12)			2	
Molecular modulation spectrometry. CH_3CH_2 generated by photolysis of Azoethane at 350 nm.							
k extracted from the data by computer-based non-linear parameter estimation and numerical integration procedures.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CH_3CH_3 (+ M) → CH_3 + CH_3 (+ M) (a) **→ $CH_2{=}CH_2$ + H_2 (+ M) (b)**							
Ethane							
81 SKI/ROG (k_a. 1% Ethane in Ar. P = 3 atm.	EX	1045-1172	3.98(15)	0	42728±1862	1	6.31
(k_a. 3% Ethane in Ar. P = 3 atm.)	EX	1007-1241	1.00(15)	0	41319±956	1	2.51
(k_a. 1% Ethane in Ar. P = 9 atm.)	EX	1000-1105	5.01(15)	0	42124±1963	1	6.31
(k_a. 3% Ethane in Ar. P = 9 atm.)	EX	1034-1126	3.16(16)	0	44338±2315	1	7.94
(k_a. Limiting high-pressure k.)	ES	1000-1300	1.58(17)	0	45798	1	
Thermolysis behind reflected shock-waves, in a single pulse shock-tube. Gas-chromatography. The limiting high-pressure expression is based on a RRKM extrapolation.							
83 KAN/PUR2 (k_a)	EX	841-913	3.31(16)	0	44238±886	1	2.75
(k_a)	SE	841-913	4.27(16)	0	44489±362	1	1.51
Pyrolysis in a static reactor, with or without N_2. P = (1-20) torr.							
$CH{=}C{=}O$ + $CH{\equiv}CH$ → CO + C_3H_3 (a) **→ any other products (b)**							
Ethenyl, 2-oxo- + Ethyne							
83 HOM/WEL2 (k_a)	DE	295	1.0(10)			2	
(k_a)	ES	500	1.0(10)			2	
(k_a)	ES	1000	1.0(10)			2	
Estimations based on a suggested mechanism for the reaction of Ethyne with O atoms, studied in a flow-reactor, with or without added H atoms. P(Total) = 2 torr.							
$CH_2{=}C{=}O$ (+ M) → CH_2 + CO (+ M)							
Ethenone (Ketene)							
71 WAG/ZAB (Low-pressure region k.)	EX	1300-2000	3.6(15)	0	29844±1007	2	
(Limiting high-pressure k.)	EX	1650	3.0(14)	0	35732	1	
Thermolysis of (0.01-0.5)% Ketene in Ar, behind reflected shock waves. Mass-spectrometry. M = Ar. [Ketene] = $(0.03-1.2)\times10^{21}$ molec.cm^{-3}.							
$CH_2{=}C{=}O$ + CH_3COOH → $CH_3C(O)OC(O)CH_3$							
Ethenone (Ketene) + Acetic acid							
71 BLA/DAV2	EX	379-488	6.46(8)	0	5564±29	2	1.12
Reaction in a static system.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_2{=}C{=}O + CH_3COSH \rightarrow CH_3C(O)SC(O)CH_3$							
Ethenone (Ketene) + Ethanethioic acid							
74 BLA/SPE	EX	401-501	2.69(+8)	0	4559±108	2	1.78
Reaction in a static system.							
$CH(O)CH_2 + O_2$ (+ M) → $CH(O)CH_2O_2$ (+ M)							
Ethyl, 2-oxo- (Vinoxy) + Oxygen molecule							
83 GUT/NEL (M = N_2. P(Total) = 1.5 torr.)	EX	295	(6.87±0.24)(10)			2	
(M = N_2. P(Total) = 100 torr.)	EX	476	(9.94±0.84)(10)			2	
(M = SF_6. P(Total) = 10 torr.)	EX	292	(1.13±0.04)(11)			2	
(M = SF_6. P(Total) = 90 torr.)	EX	473	(1.33±0.05)(11)			2	
Reaction in N_2, or SF_6 buffer gas. $CH(O)CH_2$ generated by reacting Cl atoms with Ethylene oxide. Cl atoms generated by the IR multiphoton dissociation of C_6H_5Cl. Other rate constants at various temperatures and pressures for M = N_2 and M = SF_6, are also given.							
$CH(O)CH_2$ + NO (+ M) → $CH(O)CH_2NO$ (+ M)							
Ethyl, 2-oxo- (Vinoxy) + Nitrogen oxide (NO)							
83 GUT/NEL (M = N_2. P(Total) = 2.5 torr.)	EX	295	(1.63±0.05)(11)			2	
(M = N_2. P(Total) = 300 torr.)	EX	295	(1.13±0.04)(13)			2	
(M = SF_6. P(Total) = 10 torr.)	EX	295	(4.18±0.15)(12)			2	
(M = SF_6. P(Total) = 40 torr.)	EX	295	(8.03±0.35)(12)			2	
(Limiting low-pressure k.)	EX	295	(2.37±0.31)(19)			3	
Data fit to Troe's semiempirical expression, by using a non-linear least-squares procedure.							
(Limiting high-pressure k.)	EX	295	(1.51±0.18)(13)			2	
Data fit to Troe's semiempirical expression, by using a non-linear least-squares procedure. Reaction of Vinoxy with NO in N_2, or SF_6 buffer gas. Vinoxy generated by reacting Cl atoms with Ethylene oxide. Cl atoms produced by the IR multiphoton dissociation of C_6H_5Cl. The limiting low-pressure and high-pressure expressions were obtained by data-fit to Troe's semiempirical relationship. Other rate constants at various pressures, for M = N_2, are also given.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3OC(O) + CH_3OC(O) \rightarrow CH_3OC(O)C(O)OCH_3$ Methyl, methoxyoxo-							
83 HAS/RIE	DE	298	1.73(13)			2	
Dimethyl oxalate Flash-photolysis. Gas-chromatography. k calculated using a computer integration interaction program.							
$CH_3CHO + CH_3C(O)ONO_2 \rightarrow$ products Acetaldehyde + Peroxide, acetyl nitro							
76 PAT/ATK2	EX	296	(4.45±0.81)(3)			2	
Reaction in a Teflon-lined aluminum tank. Gas-chromatography. Mass-spectrometry. IR-absorption spectrometry. [Peroxide] = (3.9-5.1) ppm. $[CH_3CHO]$ = (83-312) ppm.							
 $(+ M) \rightarrow CH_3CHO^{\dagger} (+ M) \rightarrow CH_3CHO (+ M)$ (a) $\rightarrow CH_3 + CHO (+ M)$ (b) $\rightarrow CH_4 + CO (+ M)$ (c) Oxirane → Acetaldehyde							
83 LIF/BEN (k_a. Limiting high-pressure k.)	ES	830-1200	~7.26(13)	0	28787	1	
(k_b. Limiting high-pressure k.)	ES	830-1200	~3.63(13)	0	28787	1	
(k_c. Limiting high-pressure k.)	ES	830-1200	~1.21(13)	0	28787	1	
Pyrolysis behind reflected shock-waves, in a single-pulse shock-tube. Gas-chromatography. P = (1.5-10) atm. M = Ar. Estimations based on a suggested mechanism which was fit to the experimentally determined product-distributions of the pyrolysis products.							
 $+ H \rightarrow CH_2CH_2OH^{\dagger} \rightarrow CH_2{=}CH_2 + OH$ (a) $\rightarrow CH_2{=}CH + H_2O$ (b) Oxirane (Ethylene oxide) + Hydrogen atom							
83 LIF/BEN (k_a)	ES	830-1200	9.5(10)	0	2516	2	
(k_b)	ES	830-1200	5.0(9)	0	2516	2	
Pyrolysis of Ethylene oxide diluted in Ar, behind reflected shock-waves, in a single-pulse shock-tube. Gas-chromatography. P = (1.5-10) atm. Estimations based on a suggested mechanism which was fit to the experimentally determined product- distributions of the pyrolysis products.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$HC(O)OCH_3 \rightarrow CH_3OH + CO$ (a)							
$\rightarrow HCHO + CO$ (b)							
$\rightarrow 2H_2 + 2CO$ (c)							
Fomic acid methyl ester (Methyl formate)							
83 DAV	EX	1180-1500	2.09(10)	0	25466±2617	1	6.17
Pyrolysis behind reflected shock-waves, in a single-pulse shock-tube.							
$CH_3C(O)OOH (+ M) \rightarrow CH_3 + CO_2 + OH (+ M)$							
Ethaneperoxoic acid (Peracetic acid)							
75 LEV/PRI	EX	403-488	4.04(13)	0	16960±277	1	1.70
	EX	403-513	1.15(13)	0	16383±1913	1	38.0
Thermolysis of Peracetic acid diluted in He, Ar, or N_2, in a flow-type Teflon reactor. [Peracid] = (0.03-1.1)vol% (in He, or Ar). P= 760 torr.							
$CH_3CH_2O_2 + CH_3CH_2O_2 \rightarrow CH_3CH_2O + CH_3CH_2O + O_2$ (a)							
$\rightarrow CH_3CHO + CH_3CH_2OH + O_2$ (b)							
$\rightarrow CH_3CH_2OOCH_2CH_3 + O_2$ (c)							
Ethyldioxy							
83 ANA/WAD (k_a/k_b)	RL	302	1.75±0.05			2/2	
(k_a/k_b)	RL	333	2.12±0.10			2/2	
(k_a/k_b)	RL	373	2.45±0.15			2/2	
(k_a)	ES	302-373	3.49(10)		316±167	2	1.65
(k_b)	ES	302-373	1.94(11)		683±24	2	1.08
Molecular Modulation Spectrometry. $CH_3CH_2O_2$ generated by photolysis of trans-Azoethane in presence of O_2 and N_2. Gas-chromatography. Mass-spectrometry. [trans-Azoethane] = 4.8 torr. $[N_2]$ = (410-550) torr. $[O_2]$ = (5-150) torr.							
$CH_3SCH_2 + CH_4 \rightarrow (CH_3)_2S + CH_3$							
Methyl, (methylthio)- + Methane							
76 ART/LEE	DE	393-488	6.31(11)	0	7662	2	
Calculated by using the k of the reverse reaction and thermochemical data.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3C(O)SH \rightarrow CH_2{=}C{=}O + H_2S$ (a) $\rightarrow CH_4 + COS$ (b) Ethanethioic acid (Thioacetic acid)							
83 TAY1 ($k_a + k_b$)	EX	529-655	3.16(12)	0	20978	1	
Thermolysis of $CH_3C(O)SH$ in a stainless-steel reactor. NMR-Spectroscopy. Thioacetic acid is either separately prepared, or produced by decomposition of Diacetyl sulfide. Channels (a) and (b) are the most likely paths.							
NCCN (+ M) → CN + CN (+ M) Ethanedinitrile (Cyanogen) (Oxalonitrile)							
71 SLA/FIS	EX	2700-4000	(4.58±0.40)(14)	0	34726±856	2	
71 SLA/FIS	SE	1750-4000	^{1})	^{1})	^{1})	2	
Thermolysis of 0.05-1% Cyanogen in Ar, behind incident shock waves. [Ar] = $(1.20-3.22)\times10^{18}$ molec.cm^{-3}. P_o = (5-40) mm.Hg. M = Ar. ^{1}) A combination of the above rate constant with the data of Tsang et al. is best fitted by the expression: $k = 3.71\times10^6 T^{0.5}(64771/T)^8 \exp(-64771/T)$ cm^{3}mol^{-1}s^{-1}.							
$CH_2CN + NO_2 \rightarrow$ products Methyl, cyano- + Nitrogen oxide (NO_2)							
83 PAR/GUT	EX	298	(1.16±0.05)(13)			2	
Reaction of CH_2CN with NO_2 in excess, in a fast-flow system. CH_2CN generated by the reaction: $CH_3CN + Cl \rightarrow CH_2CN + HCl$ Cl atoms generated by dissociation of Cl_2 in a microwave-discharge. $[CH_3CN] = \sim(5-50)\times10^{13}$ molec.cm^{-3}. $[Cl]_o = (0.5-1.5)\times10^{11}$atom.cm^{-3}. P(Total) = (0.7-2.0) torr. (NO_2)							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
[CH_2=$CHNH_2$ = ] → CH_2=CH + NH_2	(a)						
→ CH_3CN + H_2	(b)						
→ [CH_2=CHNH = ] + H	(c)						
→ CH_3 + CH_2CN	(d)						
[Ethenamine = Aziridine]							
83 KOD3 (k_a/k_d)	RL	303	7.34(-1)			1/1	
(k_b/k_d)	RL	303	1.02(-1)			1/1	
(k_c/k_d)	RL	303	5.64(-1)			1/1	
Photolysis of HN_3 vapor in presence of Ethene, at 313 nm. Gas-chromatography. IR-spectrometry. The reactant, [Ethenamine = Aziridine]†, formed by the reaction $NH(a^1\Delta)$ + CH_2=CH_2. P(Ethene) = (0-188) torr. P(HN_3) = (0-105) torr. Rate constant ratios estimated on the basis of the above proposed mechanism.							
CH_3N=NCH_3 → CH_3 + CH_3 + N_2 (a)							
→ CH_3CH_3 + N_2 (b)							
Diazene, dimethyl- (Azomethane)							
83 MAR/SHA (k_a)	EX	577-640	4.37(13)	0	22950±674	1	3.31
(k_a. Previous and present data)	SE	504-657	6.31(13)	0	23143±457	1	2.18
Thermolysis in a static system with four Pyrex glass reactors. Gas-chromatography. P = (4-300) torr.							
83 SCH/CLA	EX	573-595	7.08(15)	0	25897±1263	1	8.71
Thermolysis in a static system. Gas-chromatography. P(Azomethane) = 29 torr.							
$CH_3C(O)ONO_2$ + $(CH_3)_2C$=CH_2 → products							
Peroxide, acetyl nitro + 1-Propene, 2-methyl- (Isobutene)							
76 PAT/ATK2	EX	296	<4.05(2)			2	
Reaction in a Teflon-lined aluminum tank. IR-Absorption spectrometry. Gas-chromatography. Mass-spectrometry. [Peroxide] = 5.8 ppm. [CH_3CHO] = 51 ppm.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$C_3 + O_2 \rightarrow C_2(d^3\Pi,v=1) + CO + O$ (or CO_2) (a) $\rightarrow$ any other products (b)							
Carbon trimer + Oxygen molecule							
83 NEL/HEL	EX	520	≤1.20(8)			2	
$k_{overall}$. UV MUltiphoton -Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. Unreactive at 607 K and above. $P(O_2)$ = 90 torr.							
$C_3 + CH_4 \rightarrow$ products							
Carbon trimer + Methane							
83 NEL/HEL	EX	600	≤3.01(8)			2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. Unreactive at 607 K and above. $P(CH_4)$ = 90 torr.							
C_3 + CH–CH ≤ products							
Carbon trimer + Ethyne							
83 NEL/HEL	EX	296-610	(5.47÷1.61)(12)	0	4065÷161	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., bu using a KrF excimer Laser. P(CH-CH) = (0-30) torr.							
$C_3 + CH_2{=}CH_2$ ≤ products							
Carbon trimer + Ethene							
83 NEL/HEL	EX	296-610	(1.02÷0.31)(12)	0	3277÷168	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. $P(CH_2{=}CH_2)$ = (0-50) torr.							

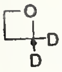
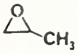
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
C_3 + $CH_3C{-}CH$ ≤ products Carbon trimer + 1-Propyne 83 NEL/HEL Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(1-Propyne) = (0-1) torr.	EX	296-610	(2.97÷0.28)(11)	0	121÷35	2	
C_3 + $CH_3CH{=}CH_2$ ≤ products Carbon trimer + 1-Propene 83 NEL/HEL Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(1-Propene) = (0-6.25) torr.	EX	296-610	(6.26÷0.36)(10)	0	159÷21	2	
C_3 + $CH_3CH_2CH{=}CH_2$ ≤ products Carbon trimer + 1-Butene 83 NEL/HEL Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(1-Butene) = (0-7) torr.	EX	296-610	(7.35÷0.30)(10)	0	139÷17	2	
C_3 + cis-$CH_3CH{=}CHCH_3$ ≤ products Carbon trimer + 2-Butene, (Z)- 83 NEL/HEL Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., bu using a KrF excimer Laser. P(cis-2-Butene) = (0-1) torr.	EX	296-610	(1.26÷0.06)(11)	0	-201÷19	2	

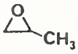
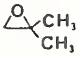
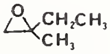
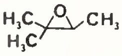
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$C_3 + (CH_3)_2C{=}CH_2 \le$ products							
Carbon trimer + 1-Propene, 2-methyl- (Isobutene)							
83 NEL/HEL	EX	296-610	(2.53÷0.10)(11)	0	-759÷15	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(Isobutene) = (0-0.08) torr.							
$C_3 + CH_3CH_2CH_2CH_3 \le$ products							
Carbon trimer + Butane							
83 NEL/HEL	EX	607	≤1.20(8)			2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., bu using a KrF excimer Laser. P(Butane) = 90 torr. Unreactive above 607 K.							
$C_3 + (CH_3)_2C{=}CHCH_3 \rightarrow$ products							
Carbon trimer + 2-Butene, 2-methyl-							
83 NEL/HEL	EX	296-610	(3.35±0.27)(11)	0	-1014±34	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(2-Methyl-2-Butene) = (0-0.1) torr.							
$C_3 + CH_3CH_2CH_2C{\equiv}CCH_3 \rightarrow$ products							
Carbon trimer + 2-Hexyne							
83 NEL/HEL	EX	296-610	(6.50±0.05)(11)	0	-695±24	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiophoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(2-Hexyne) = (0-0.07) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$C_3 + (CH_3)_2C{=}C(CH_3)_2 \rightarrow$ products Carbon trimer + 2-Butene, 2,3-dimethyl-							
83 NEL/HEL	EX	296-610	(1.26±0.11)(12)	0	-917±33	2	
Multiphoton UV-Photolysis/Laser-induced Fluorescence detection apparatus. C_3 generated by multiphoton UV-Photolysis of C_3H_6 at 249 nm., by using a KrF excimer Laser. P(2,3-Dimethyl-2-Butene) = (0-0.08) torr.							
$CH_2{=}CHCH_2 + NO\ (+ M) \rightarrow CH_2{=}CHCH_2NO\ (+ M)$ 2-Propenyl (Allyl) + Nitrogen oxide (NO)							
82 TUL/MAC	EX	295-404	(2.11±0.36)(12)	0	-403±12	2	
Reaction in an Laser-Flash-Photolysis system. Allyl generated by Flash-photolysis of 1,5-Hexadiene. [NO] = (50-100) torr. P(Total) = (50-500) torr. Limiting high-pressure k. The frequency factor: A = (2.11±0.36)x10(12)$cm^3.mol^{-1}.s^{-1}$, given above, is equivalent to: A = (3.35±0.10)x$10^{-12}cm^3$. molec.$^-$.s^{-1}. However, the authors give a value of: A = (3.35±0.10)x$10^{-11}cm^3$. molec.$^{-1}$.s^{-1}, which is probably a misprint.							
$CH_2{=}CHCH_2 + CH_2{=}CHCH_2 \rightarrow CH_2{=}CHCH_2CH_2CH{=}CHCH_2$ 2-Propenyl (Allyl)							
82 TUL/MAC	EX	293-571	(1.02±0.02)(13)	0	-132±12	2	
Recombination of Allyl in a Laser-Flash-Photolysis system. Allyl generated by Flash-photolysis of 1,5-Hexadiene. P(1,5-Hexadiene) = 182 mtorr. P(Ar) = 53 torr.							
 $(+ M) \rightarrow CH_3CH{=}CH_2\ (+ M)$ Cyclopropane							
78 LEW/GIE (Limiting high-pressure k.) (k_{ref} is k∞.)	RL	1038-1208	0.5±0.3			1	
(limiting high-pressure k.)	SE	1038-1208	1.58(15)	0	32713	1	
(Limiting high-pressure k.) (Second choice)	ES	1038-1208	2.82(15)	0	32964	1	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
Isomerization in Ar, or He diluent, in a single-pulse shock-tube, behind reflected shock-waves. Comparative-rate method with Cyclohexane decomposition taken as internal standard reaction. Gas-chromatography. P = (533-5097) torr.							
80 FUR/PAC Isomerization in a flow-reactor with quartz tubes. Gas-chromatography. P = 50 torr.	EX	897	1.72(-1)			1	
82 LEW/BOS Thermal isomerization in Ar, in presence of BCl_3, behind reflected shock-waves, in a single-pulse shock-tube. Gas-chromatography. [Cyclopropane] = 1% in Ar. $[BCl_3]$ = 1% in Ar. P = (2.5-3) atm.	EX	983-1333	2.24(11)	0	12823	1	
$(CH_3)_2CH \rightarrow H + CH_3CH{=}CH_2$ (a) **$\rightarrow CH_3 + CH_2{=}CH_2$ (b)** Ethyl, 1-methyl- (Isopropyl)							
75 SZI/MAR3 Static-, or flow-system. $(CH_3)_2CH$ generated by the pyrolysis of Azoisopropane. Mass-spectrometry. Determined relative to the reaction: $(CH_3)_2CH + (CH_3)_2CH \rightarrow (CH_3)_2CHCH(CH_3)_2$	RN	538-666	1.0(14)	0	18319±1057	1	6.31
$(CH_3)_2CH + (CH_3)_2CH \rightarrow (CH_3)_2CHCH(CH_3)_2$ (a) **$\rightarrow (CH_3)_2CHCH(CH_3)_2$ (b)** Ethyl, 1-methyl- (Isopropyl)							
83 ART/ANA (k_a) Molecular modulation spectrometry. $(CH_3)_2CH$ generated by photolysis of Azoisopropane at 350 nm. k extracted from the data by computer-based non-linear parameter estimation and numerical integration procedures.	ES	308	5.96(12)			2	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2CH_3$ (+ M) → CH_3 + CH_3CH_2 (+ M) (a)							
→ any other products (+ M) (b)							
Propane							
83 ALA/KIE (k_a)	EX	1400-1800	(7.74±1.55)(11)	0	28030	1	
(k_a. Limiting high-pressure k) (RRKM extrapolation.)	TH	1400-1700	1.48(17)	0	43500	1	
(k_a)	EX	1800-2300	(2.68±0.54)(17)	0	28280	2	
Pyrolysis in incident shock-waves.							
Laser-schlieren technique.							
P_o = (3-25) torr. M = Kr.							
(2-4)% Propane in Kr.							
83 KAN/PUR1 (k_a)	EX	773-793	5.13(16)	0	41973±981	1	3.47
Pyrolysis in a static reactor,							
in presence of Ethene.							
P(Propane) = 200 torr.							
P(Ethene) = (1.5-6.0) Tor.							
CH_2=$CHCH_2O_2$ → CH_2=$CHCH_2$ + O_2							
2-Propenyldioxy							
82 MOR/PIL	EX	413-427	(1.6±0.8)(10)	0	6411±192	1	
Laser Flash-photolysis system							
with a Xenon lamp.							
2-Propenyldioxy generated by the							
addition of O_2 to Allyl, in turn							
generated by the Flash-photolysis							
of 1,5-Hexadiene.							
Gas- chromatography.							
[O_2] = (0.49-1.38)x10^{17}molec.cm^{-3}.							
[Allyl] = 3x10^{13}particles cm^{-3}.							
P(Total) = 50 torr.							
 → $CH_2CH_2OCH_2$ → CH_2=CH_2 +HCHO (a)							
→ $CH_2CH_2CH_2O$ → CH_2=CH_2 + HCHO (b)							
Oxetane							
83 ZAL/HUN (k_a + k_b. Limiting high-pressure k)	ES	668-758	2.63(15)	0	31214±457	1	2.04
(k_a)	DE	673-758	1.3(15)	0	31515	1	
(k_b)	DE	673-758	9.2(14)	0	31755	1	
Thermolysis in a static vacuum system.							
Gas-chromatography.							
P = (0.075-52.5) torr.							
Data fit to RRKM theory.							

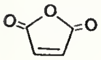
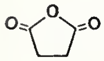
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_2CH_2OCD_2$ → $CH_2{=}CH_2$ +DCDO (a)							
→ $CH_2CH_2CD_2O$ → $CH_2{=}CH_2$ + DCDO (b)							
→ $CH_2CD_2OCH_2$ → $CH_2{=}CD_2$ + HCHO (c)							
→ $CD_2CH_2CH_2O$ → $CH_2{=}CD_2$ + HCHO (d)							
Oxetane-2,2-d_2							
83 ZAL/HUN (k$_{overall}$. Limiting high-pressure k)	ES	668-758	3.47(15)	0	31611±457	2	1.45
(k$_a$)	DE	~723	1.3(15)	0	31996	1	
(k$_b$)	DE	~723	9.2(14)	0	31755	1	
(k$_c$)	DE	~723	1.3(15)	0	31515	1	
(k$_d$)	DE	~723	9.2(14)	0	32236	1	
Thermolysis in a stativacuum system. Gas-chromatography. P = (0.075-52.5) torr. Data-fit to RRKM theory.							
 → CH_3CH_2CHO (a)							
→ $(CH_3)_2CO$ (b)							
→ $CH_2{=}CHCH_2OH$ (c)							
→ $CH_2{=}CHOCH_3$ (d)							
Oxirane, methyl-, → Propanal (a) → Propanone (b) → 2-Propen-1-ol (c) → Ethene, methoxy- (d)							
77 FLO (k$_a$)	EX	654-717	2.45(14)	0	29434±289	1	1.51
(k$_b$)	EX	654-717	1.51(14)	0	30131±289	1	1.51
(k$_b^\infty$. RRKM data-fit)	ES	656-717	1.70(14)	0	30552	1	
(k$_c$)	EX	656-717	7.94(12)	0	28760±241	1	1.41
(k$_d$)	EX	656-717	3.24(13)	0	29578±373	1	1.70
Thermal isomerization in a static vacuum-system, with packed and unpacked vessels, in presence or absence of NO. Gas-chromatography. P = (5-326) torr.							
$CH_3CH_2C(O)OOH$ → CH_3CH_2 + CO_2 + OH							
Propaneperoxoic acid (Perpropionic acid)							
83 LEV/PRI	EX	403-513	1.35(13)	0	16671±1708	1	30.2
Thermolysis in He or Ar, in a flow-type Teflon reactor. [Peracid] = 0.03-1.1vol% (in He, or Ar). P= 760 torr.							

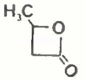
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$(CH_3)_2CHO_2 + CH_3CH{=}CH_2 \rightarrow (CH_3)_2CHO +$ 							
Ethyldioxy, 1-methyl- (Isopropylperoxo) + 1-Propene							
83 SWA/WAD	EX	303-408	8.31(11)	0	8143±301	2	2.29
Reaction in a Pyrex vessel. $(CH_3)_2CHO_2$ generated by photooxidation of trans-2,2'-Azopropane. P(1-Propene) = (200-400) torr. $P(O_2)$ = (300-500) torr. P(Total) = 750 torr.							
$(CH_3)_2CHO_2 + (CH_3)_2C{=}CH_2 \rightarrow (CH_3)_2CHO +$ 							
Ethyldioxy, 1-methyl- (Isopropylperoxo) + 1-Propene, 2-methyl- (Isobutene)							
83 SWA/WAD	EX	303-408	3.89(11)	0	7542±265	2	1.55
Reaction in a Pyrex vessel. $(CH_3)_2CH_2$ generated by photooxidation of trans-2,2'-Azopropane. P(Isobutene) = (50-200) torr. P(Total) = (700-750) torr. $P(O_2)$ = 450 torr.							
$(CH_3)_2CHO_2 + CH_3CH_2C(CH_3){=}CH_2 \rightarrow (CH_3)_2CHO +$ 							
Ethyldioxy, 1-methyl-, (Isopropylperoxo) + 1-Butene, 2-methyl-							
83 SWA/WAD	EX	303-408	3.89(11)	0	7542±265	2	1.55
Reaction in a Pyrex vessel. Isopropylperoxo generated by photooxidation of trans-2,2'-Azopropane. P(Isobutene) = 80 torr. $P(O_2)$ = (300-400) torr. P(Total) = 500 torr.							
$(CH_3)_2CHO_2 + (CH_3)_2CH{=}CHCH_3 \rightarrow (CH_3)_2CHO +$ 							
Ethyldioxy, 1-methyl-, (Isopropylperoxo) + 2-Butene, 2-methyl-							
83 SWA/WAD	EX	303-408	3.89(11)	0	7542±265	2	1.55

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
Reaction in a Pyrex reaction vessel.							
Isopropylperoxo generated by photooxidation of trans-2,2'-Azopropane.							
P(Isobutene) = 40 torr.							
P(Total) = 500 torr.							
$P(O_2)$ = 400 torr.							
$CH_3CH_2CN \rightarrow CH_3 + CH_2CN$ (a)							
$\rightarrow CH_2{=}CH_2 + HCN$ (b)							
$\rightarrow CH_2{=}CHCN + H_2$ (c)							
Propanenitrile							
83 TRE (k_a)	EX	789-850	3.16(15)	0	39607±478	1	2.0
Pyrolysis in a static reactor.							
P = (10-100) torr.							
$CH_3CH_2N{=}C{=}O \rightarrow CH_2CH_2 + HN{=}C{=}O$ (a)							
$\rightarrow CH_4 + HCN + CO$ (b)							
Ethane, isocyanato- (Ethyl Isocyanate)							
83 BLA/IJA (k_a. Unimolecular elimination)	EX	701-803	1.58(12)	0	28183±453	1	1.6
(k_a. Unimolecular elimination	EX	723	2.25(-5)			1	
(k_b. Chain decomposition)	EX	701-803	2.51(12)	0	26673±755	1	2.5
(k_b. Chain decomposition)	EX	723	9.33(-5)			1	
Thermolysis in carbon-coated, packed and unpacked reaction vessels.							
(Chains are quenched by inhibitors.)							
P = (29-204) torr.							
$CH_3CH_2CH_2OONO_2 \rightarrow CH_3CH_2CH_2O_2 + NO_2$							
Peroxynitric acid propyl ester							
79 EDN/SPE	DE	280-298	5.0(14)	0	9965	1	
Decomposition in a flow reactor, in air and in presence of NO.							
IR-spectrometry.							
P = 700 torr.							
E_a measured directly.							
The preexponential factor determined from E_a and the rate constant ratio of the reactions:							
$CH_3CH_2CH_2O_2 + NO \rightarrow CH_3CH_2CH_2O + NO_2$							
and							
$CH_3CH_2CH_2O_2 + NO_2 \rightarrow CH_3CH_2CH_2NO_2$							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (v=5,6) → $CH_2=CHCH=CH_2$							
Cyclobutene							
83 JAS/FRI (λ = 13346 cm^{-1})	EX	298	(3.5±0.8)(7)			1	
(λ = 16602 cm^{-1})	EX	298	(8.2±1.1)(8)			1	
Photoisomerization in a dye Laser.							
Photoacoustic spectrometry.							
s-chromatography.							
s-spectrometry.							
P = (0.1-60) torr.							
The rate constant, measured as a function of energy and overtone transition, is increasing with λ.							
$CH_3CH=CCH_3$ + H_2 → cis-$CH_3CH=CHCH_3$ + H							
1-Propenyl, 1-methyl-, + Hydrogen molecule							
83 COL/RIC	ES	773-794	1.26(13)	0	12179	2	
Thermal reaction in a static system.							
k determined from the experimental data on the basis of a suggested mechanism.							
cis-$CH_3CH=CHCH_3$ (+ M) → $CH_3CH=CHCH_2$ + H (+ M) (a)							
→ $CH_2=CHCH=CH_2$ + H_2 (+ M) (b)							
→ $CH_2=CHCH_2$ + CH_3 (+ M) (c)							
→ trans-$CH_3CH=CHCH_3$ (+ M) (d)							
2-Butene, (Z)-							
71 SPR/AKI (k_d)	EX	298-338	1.26(11)	0	6090±151	2	1.58
(k_d)	EX	298	(1.48±0.03)(2)			2	
Isomerization a glass reaction cell.							
Gas-chromatography. M = NO_2.							
P(cis-2-Butene) = (1-30) torr.							
P(NO_2) = (0.1-3.0) torr.							
$CH_3CH_2CHCH_3$ + H_2 → $CH_3CH_2CH_2CH_3$ + H							
Propyl, 1-methyl-, + Hydrogen molecule							
83 COL/RIC [1])	RL	773-794	7.8(2)			2/1	
k_{ref}: $CH_3CH_2CHCH_3$ → CH_3 + $CH_3CH=CH_2$							
Estimated ratio.							
83 COL/RIC [1])	ES	773-794	3.98(13)	0	8907	2	

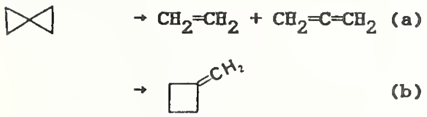
[1]) Thermal reaction in a static system.

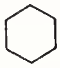
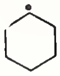
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2CHCH_3$ + cis-$CH_3CH{=}CHCH_3$							
$\rightarrow CH_3CH_2CH_2CH_3 + CH_3CH{=}CCH_3$							
Propyl, 1-methyl-, + 2-Butene, (Z)-							
83 COL/RIC 1)	RL	773-794	2.5(3)			2/1	
k_{ref}: $CH_3CH_2CHCH_3 \rightarrow CH_3 + CH_3CH{=}CH_2$							
Estimated ratio.							
83 COL/RIC 1)	ES	773-794	2.51(11)	0	4026	2	
1) Thermal reaction in a static system.							
$(CH_3)_3C + (CH_3)_3C \rightarrow (CH_3)_2CH{=}CH_2 + (CH_3)_3CH$ (a)							
$\rightarrow (CH_3)_3CC(CH_3)_3$ (b)							
Ethyl, 1,1-dimethyl- (t-Butyl)							
83 ART/ANA (k_b)	ES	308	4.31(12)			2	
Molecular modulation spectrometry. $(CH_3)_3C$ generated by photolysis of Azo-t-butane at 350 nm. k extracted from the data by computer-based non-linear parameter estimation and numerical integratiopn procedures.							
 $\rightarrow CO + CH{\equiv}CH + CO_2$							
2,5-Furandione (Maleic anhydride)							
81 BAC/PAR	EX	645-760	2.14(14)	0	30649±503	1	2.0
Thermolysis in a static system. Gas-chromatography. P = (0.7-20) torr.							
 $\rightarrow CO$ + other products (a)							
$\rightarrow CO_2$ + other products (b)							
2,5-Furandione, dihydro- (Succinic anhydride)							
83 YAM/BAC (k_a)	EX	625-775	3.98(11)	0	26673	1	
(k_b)	EX	625-775	3.16(5)	0	17111	1	
Thermolysis in packed, or unpacked vessels. P = (4-20) torr.							
$CH_3C(O)OCH{=}CH_2 \rightarrow (CH_3)_2CO + CO$ (a)							
$\rightarrow CH_3CHO + CH_2{=}C{=}O$ (b)							
Acetic acid ethenyl ester (Vinyl acetate)							
83 TAY3 ($k_a + k_b$)	EX	636-722	2.69(10)	0	21940	1	
(k_b)	EX	600	2.12(-6)			1	
Thermolysis in a static system.							

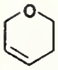
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_3CH{=}CH_2 + CO_2$							
2-Oxetanone, 4-methyl- (β-Butyrolactone)							
83 FRE/WAT	EX	482-523	2.45(14)	0	19655±120	1	1.26
Thermolysis in a static system. P = (0.1-10) torr.							
$CH_3C(O)OC(O)CH_3 \rightarrow CH_3COOH + CH_2{=}C{=}O$							
Acetic acid anhydride							
71 BLA/SPE	EX	470-643	1.86(11)	0	16202±226	1	1.55
Thermolysis in a static system.							
$CH_3CH_2OCH{=}CH_2 \rightarrow CH_2{=}CH_2 + CH_3CHO$							
Ethene, ethoxy- (Ethyl vinyl ether)							
82 MCE/TA	EX	617-677	6.65(11)	0	22363	1	
	EX	600	4.32(-5)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3C(O)OCH_2CH_3 \rightarrow CH_3COOH + CH_2{=}CH_2$							
Acetic acid ethyl ester							
83 LOU/TIN	EX	679-737	2.51(12)	0	24056±252	1	2.0
	EX	673	7.51(-4)			1	
Liquid phase thermolysis of Ethyl Acetate diluetd in Toluene or m-Xylene, in a microprocessor. Gas-chromatography.							
$CH_3OC(O)OCH_2CH_3 \rightarrow CH_3OH + CO_2 + CH_2{=}CH_2$							
Carbonic acid ethyl methyl ester							
83 TAY2	EX	626-682	1.59(12)	0	22547	1	
	EX	600	7.61(-5)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3CH_2CH_2C(O)OOH \rightarrow CH_3CH_2CH_2 + CO_2 + OH$							
Butaneperoxoic acid (Perbutyric acid)							
83 LEV/PRI	EX	403-513	9.55(12)	0	16527±2045	1	55.0
Thermolysis in He or Ar, in a flow-type Teflon reactor. P = 760 torr. [Peracid] = (0.03-1.1) vol% (in He, or Ar).							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$(CH_3)_2CHC(O)OOH \rightarrow (CH_3)_2CH + CO_2 + OH$							
Propaneperoxoic acid, 2-methyl- (Perisobutyric acid)							
83 LEV/PRI	EX	403-513	1.41(13)	0	16467±1888	1	42.7
Thermolysis in He or Ar, in a flow-type Teflon reactor.							
P = 760 torr.							
[Peracid] = (0.03-1.1) vol% (in He, or Ar).							
$(CH_3)_3CO$ (+ M) $\rightarrow (CH_3)_2CO + CH_3$ (+ M)							
Ethoxy, 1,1-dimethyl- (t-Butoxy)							
82 BAT/ROB	EX	402-443	3.98(14)	0	8002±604	1	3.98
(RRKM calculation.)	ES	402-443	7.94(14)	0	8354	1	
Thermolysis in a static system.							
$(CH_3)_3CO$ generated by the decomposition of di-t-Butyl peroxide diluted in NO.							
Gas-chromatography.							
Limiting high-pressure k.							
[t-BuO] = [NO] = $(0.72\text{-}1.20)\times10^{16}$ molec.cm^{-3}.							
$(CH_3)_3COOH(v{=}6) \rightarrow (CH_3)_3CO + OH$							
Hydroperoxide, 1,1-dimethyl ethyl- (t-Butyl hydroperoxide)							
82 RIZ/CRI	EX	298	(4.0±0.4)(6)			1	
Unimolecular decomposition of t-Butyl hydroperoxide excited to v = 6 (above the barrier for dissociation), with a YAG pumped dye-laser.							
Time-resolved Laser-induced fluorescence.							
P = (20-300) mtorr.							
Unreported T assumed to be 298 K.							
$CH_3C(O)SC(O)CH_3 \rightarrow CH_3C(O)SH + CH_2{=}C{=}O$							
Ethanethioic acid anhydrosulfide (Acetic thioanhydride, or Diacetyl sulfide)							
74 BLA/SPE	EX	459-526	1.05(11)	0	15757±770	1	4.68
Decomposition in a static system.							
83 TAY1	EX	569-600	6.92(11)	0	19125	1	
Thermolysis in a stainless-steel reactor.							
NMR-Spectroscopy.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_2{=}CHCH_2NC^{\dagger} \rightarrow CH_2{=}CHCH_2CN$							
1-Propene, 3-isocyano-, (Allyl isocyanide)							
→ 3-Butenenitryle (Allyl cyanide)							
79 RED/BER2 (λ = 746.4 nm.)	EX	300	≈6.0(5)			1	1.5
(λ = 532.2 nm.)	EX	300	4.6(8)			1	1.2
Photoisomerization with an intracavity Vibrationally excited Allyl isocianide formed from Allyl isocianide by a cw dye Laser.							
Photoacustic spectrometry.							
Gas-chromatography.							
P = (0-10) torr.							
k increases when λ decreases. (k values at intermediate wavelenghths are given in a table.)							
$(CH_3)_2CHNCO \rightarrow CH_3CH{=}CH_2 + HN{=}C{=}O$ (a)							
$\rightarrow CH_4 + CH_3CN + CO$ (b)							
Propane, 2-isocyanato- (Isopropyl isocyanate)							
72 BAR/MIR (k_a)	EX	686-771	5.13(12)	0	27831	2	
Unimolecular elimination.							
Thermolysis in a static reactor.							
Gas-chromatography.							
Mass-spectrometry.							
P = (70-433) torr.							
83 BLA/IJA (k_a)	EX	701-803	1.58(12)	0	26220±251	1	1.6
(k_a)	EX	723	3.53(-4)			1	
(k_b)	EX	701-803	2.51(10)	0	20533±2014	1	1.1
(k_b)	EX	723	1.73(-3)			1	
Thermolysis in carbon-coated, packed and unpacked reaction vessels.							
(Chains are quenched by inhibitors.)							
P = (29-204) torr.							
$CH_3C(O)NHC(O)CH_3 \rightarrow CH_3C(O)NH_2 + CH_2{=}C{=}O$							
Acetamide, N-acetyl-							
83 TAY1	EX	547-601	2.63(12)	0	19033	1	
	EX	600	4.37(-2)			1	
Thermolysis in a stainless-steel reactor.							
NMR-Spectroscopy.							

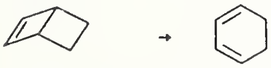
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[2.1.0]pent-2-ene → 1,3-Cyclopentadiene							
72 BAL/AND	EX	323	(1.39±0.02)(-4)			1	
Thermal isomerization in an aluminum column. Gas-chromatography.							
							
Cyclopentene							
73 KNE	EX	753-803	(6.3±0.1)(12)	0	29089	1	
Thermolysis in a Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. UV-Spectrometry. P = (4-34) torr.							
							
Cyclopentene-d_8							
73 KNE	EX	753-803	(9.9±0.2)(12)	0	30347	1	
Thermolysis in a Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. UV-Spectrometry. P = (4-34) torr.							
							
Spiropentane → Ethene + 1,2-Propadiene (a) → Cyclobutane, methylene- (b)							
72 FLO/GIB (k_a)	DE	663	7.94(13)	0	27932	1	
(k_b. Isomerization)	EX	663	1.58(15)	0	27932	1	
Thermolysis in a static system, with or without CF_2ClF_2Cl. Gas-chromatography. RRKM fit to the data, on the basis of a proposed mechanism. P(Spiropentane) = (0.9-335) torr. P(CF_2ClCF_2Cl) = (0-721) torr.							
73 KNE (k_a)	EX	753-803	(9.9±0.2)(12)	0	30347	1	
Thermolysis in a Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. UV-Spectrometry. P = (4-34) torr.							

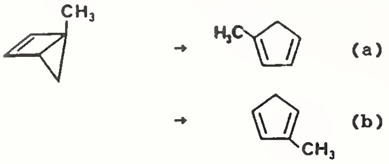
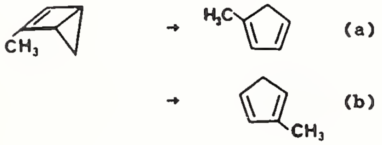
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → CH_2=$CHCH_2CH_2CH_2$							
Cyclopentyl → 4-Pentenyl							
74 CAR/TAR2	DE	298	1.0(14)	0	17413±302	1	2.51
Decyclization of Cyclopentyl in a Pyrex reaction vessel. Cyclopentyl generated by reacting Cyclopentene with H atom, wich was itself generated by the Hg-photosensitized decomposition of H_2. k calculated by fitting the data to a model mechanism. P = (0-11.1) torr.							
 + NO_2 → products							
Cyclopentyl + Nitrogen oxide (NO_2)							
83 PAR/GUT	EX	298	(2.23±0.06)(13)			2	
Reaction in a fast-flow system. Cyclopentyl generated by the reaction: Cl +  → HCl +  Cl atoms generated by dissociation of Cl_2 in a microwave-discharge. [Cyclohexane] = ~(5-50)x10^{13} molec.cm^{-3}. $[Cl]_o$ = (0.5-1.5)x10^{11} atom.cm^{-3}. P(Total) = (0.7-2.0) torr. (NO_2)							
 → $CH_3CH_2CH_2CH$=CH_2 (a) → CH_2=CH_2 +  (b)							
Cyclopentane							
79 KAL/SHV ($k_{overall}$)	RL	978-1143	5.3±1.2	0	0	1/1	
Pyrolysis of Cyclopentane-Pentane mixtures in a flow-reactor. Gas-chromatography. [Cyclopentane] = (3.5-26.4) % [Pentane] = (4.9-44.9) %. P ~ 1 torr. k_{ref}: CH_3CH_3 → products.							

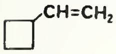
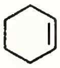
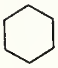
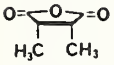
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2CH_2CH_3CH_3$ → products							
Pentane							
79 KAL/SHV	RL	978-1143	1.3±0.1	0	0	1/1	
Pyrolysis of Pentane-Cyclopentane mixtures in a flow-reactor. Gas-chromatography. [Cyclopentane] = (3.5-26.4)% [Pentane] = (4.9-44.9)% P ~ 1 torr.							
k_{ref}:  → products							
$(CH_3)_4C$ (+ M) → $(CH_3)_3C$ + CH_3 (+ M)							
Propane, 2,2-dimethyl- (Neopentane)							
83 BER/SKI (M = Ar)	EX	1140-1300	1.7(17)	0	42677	1	2.0
Pyrolysis behind reflected shock-waves. Resonance-absorption Spectroscopy. Gas-chromatography. [Neopentane] = $(1.19-4.76)x10^{14}$ $molec.cm^{-3}$.							
 → CH_2=$CHCH$=CH_2 + HCHO							
2H-Pyran, 3,6-dihydro-							
79 FRE/LOD	EX	602-647	2.86(14)	0	25254±221	1	1.42
Thermolysis in Pyrex, packed or unpacked reaction vessels. Gas-chromatography.							
$(CH_3)_2CHOCH$=CH_2 → CH_3CH=CH_2 + CH_3CHO							
Propane, 2-(ethenyloxy)- (Ethyl isopropyl ether)							
82 MCE/TAY	EX	617-677	3.37(12)	0	21960	1	
	EX	600	4.32(-4)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3CH_2OC(O)OCH_2CH_3$ → CH_2=CH_2 + CO_2 + CH_3CH_2OH							
Carbonic acid diethyl ester (Diethyl carbonate)							
83 FAR/BEC	EX	540-620	(1.94±1.33)(13)	0	23524±375	1	
Thermolysis in sealed Pyrex tubes. Gas-chromatography. Arrhenius expression calculated from the reported experimental data.							

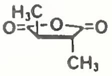
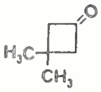
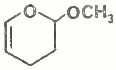
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2OC(O)OCD_2CD_3 \rightarrow CH_2{=}CH_2 + CO_2 + CD_3CD_2OH$ (a)							
$\rightarrow CD_2{=}CD_2 + CO_2 + CH_3CH_2OD$ (b)							
Carbonic acid ethyl ethyl-d_5 ester							
(Diethyl carbonate-1,1,2,2-d_5)							
83 FAR/BEC ($k_a + k_b$)	EX	540-620	(1.59±1.03)(13)	0	23572±369	1	
(Calculated from the reported experimental data.)							
(k_a/k_b)	RL	540-620	(0.80±0.18)	0	574±131	1/1	
(k_a/k_b)	RL	300	5.42			1/1	
Thermolysis in sealed Pyrex tubes.							
Gas-chromatography.							
$CH_3OC(O)OCH(CH_3)_2 \rightarrow CH_3OH + CO_2 + CH_3CH_2{=}CH_2$							
Carbonic acid methyl 1-methylethyl ester							
(Isopropyl methyl carbonate)							
83 TAY2	EX	595-661	1.09(13)	0	21668	1	
	EX	600	2.23(-3)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3C(O)OCH(CH_3)CN \rightarrow CH_3COOH + CH_2{=}CHCN$							
Propanenitrile, 2-(acetyloxy)-							
83 HER/CHU	EX	583-683	7.59(12)	0	24454±313	1	1.95
Thermolysis in a static system.							
P = (39-313) torr.							
$(CH_3)_3CNCO \rightarrow (CH_3)_2C{=}CH_2 + HN{=}C{=}O$							
Propane, 2-isocyanato-2-methyl- (-t-Butyl isocyanate)							
72 BAR/MIR	EX	683-693	3.89(13)	0	26371	2	
Thermolysis in a static system.							
Gas-chromatography.							
Mass-spectrometry.							
P = (70-433) torr.							
83 BLA/IJA	EX	701-803	2.51(13)	0	25969±151	1	1.26
	EX	723	5.74(-3)			1	
Thermolysis in carbon-coated, packed and unpacked reaction vessels.							
P = (29-204) torr.							
$(CH_3)_2NC(O)OCH_2CH_3 \rightarrow (CH_3)_2NH + CO_2 + CH_2{=}CH_2$							
Carbamic acid, dimethyl- ethyl ester							
72 DAL/ZIO	EX	643-703	1.26(12)	0	22315±201	1	
Thermolysis in a static system.							
Unreported, assumed T-range.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
trans-CH_2=CHCH=CHCH=CH_2 → cis-CH_2=CHCH=CHCH=CH_2 1,3,5-Hexatriene, (E)-, → 1,3,5-Hexatriene, (Z)-							
74 ORC/THR	EX	588-640	(4.5±1.5)(12)	0	21808±241	1	
(Limiting high-pressure k.)	EX	640	7.08(-3)			1	
Thermal isomerization in a static system. P = (1-20) mtorr.							
							
1,3-Cyclohexadiene							
74 ORC/THR	EX	719-824	(4.7±2.2)(13)	0	31033±481	1	
Thermolysis in a static system. P = (1-20) mTorr.							
							
1,3-Cyclopentadiene, 1-methyl- → 1,3-Cyclopentadiene, 2-methyl							
72 BAL/AND	EX	323	8.2(-6)			1	
Thermal isomerization in an aluminum column. Gas-chromatography.							
							
1,3-Cyclopentadiene, 2-methyl- → 1,3-Cyclopentadiene, 1-methyl-							
72 BAL/AND	EX	323	5.8(-6)			1	
Thermal isomerization in an aluminum column. Gas-chromatography.							
							
Bicyclo[2.2.0]hex-2-ene → 1,3-Cyclohexadiene							
76 GOL/LEI	EX	376-425	(7.4±0.8)(13)	0	16583±45	1	
Thermal rearrangement. P = (240-420) torr.							

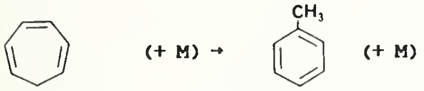
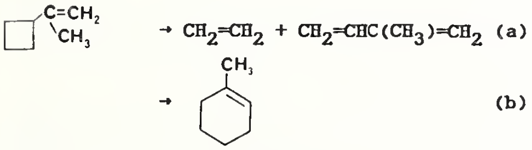
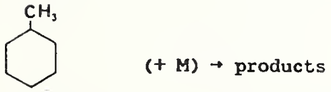
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[2.1.0]pent-2-ene, 1-methyl- → 1,3-Cyclopentene, 1-methyl- (a) → 1,3-Cyclopentene, 2-methyl- (b)							
72 BAL/AND (k_a)	EX	323	1.94(-4)			1	
(k_b)	EX	323	1.2(-4)			1	
Thermal isomerization in an aluminum column. Gas-chromatography.							
							
Bicyclo[2.1.0]pent-2-ene, 2-methyl- → 1,3-Cyclopentadiene, 1-methyl (a) → 1,3-Cyclopentadiene, 2-methyl (b)							
72 BAL/AND (k_a)	EX	323	3.6(-5)			1	
(k_b)	EX	323	4.64(-5)			1	
Thermal isomerization in an aluminum column. Gas-chromatography.							
 (+ M) → $CH_2=CHCH=CH_2$ + $CH_2=CH_2$ (+ M)							
Cyclohexene							
78 LEW/GIE (Limiting high-pressure k.)	SE	1038-1208	1.41(15)	0	33488	1	
(Limiting high-pressure k.)	ES	1038-1208	2.00(15)	0	33689	1	
Decomposition in a single-pulse shock-tube, behind reflected shock-waves. Calibration experiments. Gas-chromatography. M = Ar, or He. P = (533-5097) torr.							
81 SKI/ROG (P = 3 atm.)	EX	1000-1241	1.00(16)	0	33518±1007	1	3.16
(P = 9 atm.)	EX	1000-1341	2,51(15)	0	33719±1359	1	3.16
Thermolysis behind reflected shock-waves, in a single pulse shock-tube. M = Ar (with added CH_4). Calibration experiments. Gas-chromatography. [Cyclohexene] = 0.9 % in Ar. [Methane] = 0.9 % in Ar.							

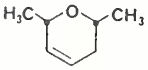
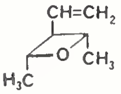
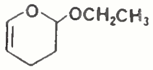
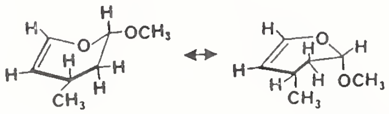
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_2{=}CH_2$ + $CH_2{=}CHCH{=}CH_2$ (a)							
→  (b)							
Cyclobutane, ethenyl- → Ethene + 1,3-Butadiene (a)							
→ Cyclohexene (b)							
78 FRE/POT (k_a)	EX	569-639	7.41(14)	0	25529±91	1	1.16
(k_b)	EX	569-639	7.14(13)	0	24480±183	1	1.35
(k_a + k_b)	EX	569-639	5.25(14)	0	25059±79	1	1.14
Thermolysis in a static system.							
Gas-chromatography. P = (1-13.5) torr.							
 (+ M) → $CH_2{=}CHCH_2CH_2CH_2CH_3$ (+ M) (a)							
→ any other products (b)							
Cyclohexane							
81 SAT/KAL ($k_{overall}$)	EX	993-1103	8.91(18)	0	44741±1761	1	5.01
Pyrolysis in a tubular quartz reactor.							
M = Ar. P(Ar) = 760 torr.							
P(Cyclohexane) = 80 torr.							
83 ZYC/BAC ($k_{overall}$)	EX	1023-1123	7.8(16)	0	41378±481	1	
Thermolysis in a flow-reactor.							
Gas-chromatography. P = 760 torr.							
$CH_3(CH_2)_4CH_3$ → products							
Hexane							
83 EBE/EDE	EX	650-840	8.32(13)	0	31310	1	
Thermolysis in a static reactor.							
Gas-chromatography.							
83 ZYC/BAC	EX	953-1033	5.4(11)	0	26463±241	1	
Thermolysis flow-reactor.							
Gas-chromatography. P = 760 torr.							
 → CO + other products (a)							
→ CO_2 + other products (b)							
2,5-Furandione, dihydro-3,4-dimethyl-, cis-							
(Succinic anhydride, 2,3-dimethyl-, cis)							
83 YAM/BAC (k_a)	EX	625-775	2.51(10)	0	23956	1	
(k_b)	EX	625-775	≈1.58(8)	0	21137	1	
Thermolysis in packed, or unpacked vessels.							
P = (4-13) torr.							

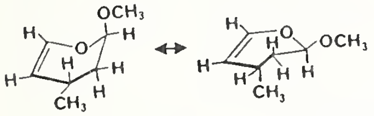
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → CO + other products (a) → CO_2 + other products (b)							
2,5-Furandione, dihydro-3,4-dimethyl-, trans-							
(Succinic anhydride, 2,3-dimethyl-, trans-)							
83 YAM/BAC (k_a)	EX	625-775	3.54(9)	0	21798	1	
(k_b)	EX	625-775	≈1.58(8)	0	21137	1	
Thermolysis in packed, or unpacked vessels.							
P = (4-13) torr.							
 → $CH_2=C(CH_3)_2$ + $CH_2=C=O$							
Cyclobutanone, 3,3-dimethyl-							
77 FRE/SMI	EX	534-586	3.74(14)	0	23186±101	1	1.20
Thermolysis in a static system, with packed or unpacked vessels. Gas-chromatography.							
P_o = (0.5-8.0) torr.							
 → $CH_3OCH=CH_2$ + $CH_2=CHCHO$							
2H-Pyran, 3,4-dihydro-2-methoxy- → Ethene, methoxy-, + 2-Propenal							
72 FRE/HOP	EX	569-626	2.63(14)	0	24430±54	1	1.10
Thermolysis in a Pyrex vessel with vacuum system. Gas-chromatography.							
P = (1-9) torr.							
$CH_3CH_2C(O)OC(O)CH_2CH_3$ → CH_3CH_2COOH + $CH_3CH=C=O$							
Propanoic acid anhydride							
76 BLA/CRA	EX	493-567	2.40(11)	0	16888±391	1	2.09
Thermolysis in a static system, with packed or unpacked vesels.							
$CH_3C(O)OCH(CH_3)C(O)CH_3$ → CH_3COOH + $CH_2=CHC(O)CH_3$							
2-Butanone, 3-(acetyloxy)-							
83 HER/CHU	EX	583-683	2.51(13)	0	24394±123	1	1.58
Thermolysis in a static system.							
P = (39-313) torr.							
83 LOU/TIN	EX	711-793	1.58(12)	0	22899±252	1	2.0
	EX	673	2.51(-3)			1	
Liquid phase Thermolysis in Toluene or m-Xylene, in a microreactor. Gas-chromatography.							

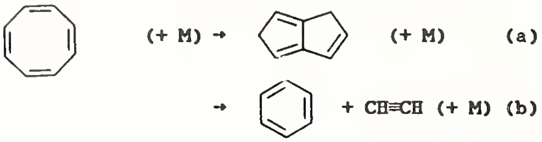
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3C(O)OCH(CH_3)C(O)OCH_3 \rightarrow CH_3COOH + CH_2{=}CHC(O)OCH_3$							
Propanoic acid, 2-(acetyloxy)-, methyl ester							
83 HER/CHU	EX	583-683	2.82(13)	0	25200±60	1	1.12
Thermolysis in a static system.							
P = (39-313) torr.							
83 LOU/TIN	EX	725-790	2.00(13)	0	25516±252	1	2.0
	EX	673	6.30(-4)			1	
Liquid phase thermolysis in Toluene or m-Xylene, in a microreactor.							
Gas-chromatography.							
$CH_3C(O)OCH_2CH_2C(O)OCH_3 \rightarrow CH_3COOH + CH_2{=}CHC(O)OCH_3$							
Propanoic acid, 3-(acetyloxy)-, methyl ester							
81 TAY	EX	632-683	1.00(11)	0	19240	1	
$CH_3C(O)OCH_2CH_2OC(O)CH_3 \rightarrow CH_3C(O)OCH{=}CH_2 + CH_3COOH$							
1,2-Ethanediol diacetate (1,2-Diacetoxyethane)							
83 TAY3	EX	683	2.4(-4)			1	
	EX	691	3.6(-4)			1	
Thermolysis in a static system with a stainless-steel reactor.							
$CH_3CH_2CH_2CH_2OCH{=}CH_2 \rightarrow CH_3CH_2CH{=}CH_2 + CH_3CHO$							
Butane, 1-(ethenyloxy)- (n-Butyl vinyl ether)							
82 MCE/TAY	EX	650-681	1.92(11)	0	21367	1	
	EX	600	6.57(-5)			1	
Thermolysis in a stainless-steel reactor.							
$(CH_3)_3COCH{=}CH_2 \rightarrow (CH_3)_2C{=}CH_2 + CH_3CHO$							
Propane, 2-(ethenyloxy)-2-methyl- (t-Butyl vinyl ether)							
82 MCE/TAY	EX	595-651	1.48(12)	0	19733	1	
	EX	600	7.68(-3)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3C(O)OC(CH_3)_3 \rightarrow CH_3COOH + CH_2{=}C(CH_3)_2$							
Acetic acid 1,1-dimethylethyl ester (t-Butyl acetate)							
83 LOU/VER	EX	582-627	1.91(14)	0	21050	1	
Pyrolysis in a microreactor, or in a Pyrex glass macroreactor.							
Gas-chromatography.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH(OH)CH_2C(O)OCH_2CH_3 \rightarrow CH_3CHO + CH_3C(O)OCH_2CH_3$							
Butanoic acid, 3-hydroxy-, ethyl ester							
71 YAT/RAM	EX	583-613	9.54(10)	0	19980	1	
Thermolysis in capilary glass tubes.							
Gas-chromatography.							
$(CH_3)_2C(OH)CH_2C(O)OCH_3 \rightarrow (CH_3)_2CO + CH_3C(O)OCH_3$							
Butanoic acid, 3-hydroxy-3-methyl-, methyl ester							
71 YAT/RAM	EX	563-593	2.19(11)	0	19678	1	
Thermolysis in capilary glass tubes.							
Gas-chromatography.							
$CH_3OC(O)OC(CH_3)_3 \rightarrow CH_3OH + CO_2 + (CH_3)_2C{=}CH_2$							
Carbonic acid 1,1-dimethyl methyl ester							
83 TAY2	EX	546-598	8.65(12)	0	18772	1	
	EX	600	2.22(-1)			1	
Thermolysis in a stainless-steel reactor.							
$CH_3C(O)CH_2SCH_2CH{=}CH_2 \rightarrow CH_3C(O)CHS + CH_3CH{=}CH_2$							
2-Propanone, 1-(2-propenylthio)- (Acetonyl allyl sulfide) → Propanethyal, 2-oxo- + 1-Propene							
83 MAR/ROP	EX	586-625	8.91(9)	0	15036±361	1	1.95
Pyrolysis in a stirred-flow-reactor.							
Mass-spectrometry. P = (3-13) torr.							
$(CH_3)_2CHN{=}NCH(CH_3)_2 \rightarrow (CH_3)_2CH + (CH_3)_2CH + N_2$							
Diazene, bis(1-methylethyl)- (Azoisopropane)							
75 SZI/MAR2	EX	494-546	2.51(15)	0	22446±252	1	1.58
Thermolysis in a static system.							
Gas-chromatography.							
$CH_3C(O)OC(CN)(CH_3)_2 \rightarrow CH_3COOH + CH_2{=}C(CN)CH_3$							
Propanenitrile, 2-(acetyloxy)-2-methyl-							
83 LOU/TIN	EX	640-713	7.94(11)	0	20232±252	1	2.0
	EX	673	6.30(-2)			1	
Liquid phase thermolysis in Toluene or m-Xylene, in a microreactor.							
Gas-chromatography.							
$(CH_3)_2NC(O)OCH(CH_3)_2 \rightarrow (CH_3)_2NH + CO_2 + CH_3CH{=}CH_2$							
Carbamic acid, dimethyl-, 1-methylethyl ester							
72 DAL/ZIO	EX	643-703	1.10(13)	0	21797±201	1	
Thermolysis in a static system. Assumed T-range.							

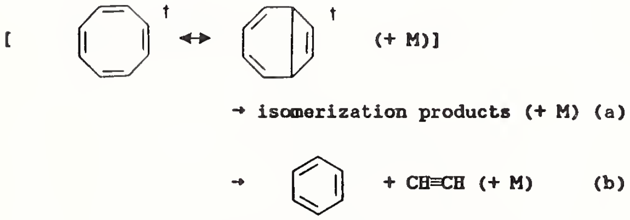
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (+ M) → (+ M)							
1,3,5-Cycloheptatriene → Benzene, methyl- (Toluene)							
76 GAY/GIL	EX	990-1250	3.98(13)	0	25741±1203	1	2.0
Thermal isomerization behind shock-waves. [1,3,5-Cycloheptatriene] = (0.01-0.1) % in Ar. P_o = 98-190 torr. P = (300-600) torr.							
76 GAY/GIL	EX	800-1130	3.98(13)	0	26186±253	1	1.26
Thermal isomerization by VLPP-Technique. Mass-spectrometry. P ~2 mtorr.							
79 AST/TRO (M = Ar)	EX	900-1300	2.69(13)	0	25079±722	1	1.58
(M = Ar. Limiting high-pressure k) (Extrapolation)	ES	600-1400	1.25(14)	0	26523	1	
Isomerization behind incident and reflected shock-waves. [Ar] = 4.46×10^{13} molec.cm^{-3}.							
 → $CH_2{=}CH_2 + CH_2{=}CHC(CH_3){=}CH_2$ (a) → (b)							
Cyclobutane, (1-methylethenyl)- → Ethene + 1,3-Butadiene, 2-methyl- (a) → Cyclohexene, 1-methyl- (b)							
78 FRE/POT (k_a)	EX	574-624	1.66(15)	0	26345±213	1	1.42
(k_b)	EX	574-624	5.77(13)	0	24636±278	1	1.58
($k_a + k_b$)	EX	574-624	9.08(14)	0	25699±152	1	1.29
Thermolysis in a static system, with packed or unpacked Pyrex vessels. Gas-chromatography. P = (1-13.5) torr.							
 (+ M) → products							
Cyclohexane, methyl-							
81 SAT/KAL	EX	988-1073	9.12(17)	0	40765±1711	1	5.01
Pyrolysis in a quartz reactor. M = Ar. P(Methylcyclohexane) = 80 torr. P(Ar) = 760 torr.							
83 ZYC/BAC	EX	993-1083	1.2(16)	0	38130±722	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 750 torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → + CH_2=C=O							
Bicyclo[3.2.0]hept-2-en-6-one → 1,3-Cyclopentadiene + Ethenone (Ketene)							
72 EGG/COC2 Pyrolysis in a static reactor, in Propene diluent. Gas-chromatography. P(substrate) = (148-223) torr. P(Propene) = (132-500) torr. P_o = (15-485) torr.	EX	471-534	1.45(13)	0	18888±126	1	1.29
 → trans-CH_3CH=CHCH=CH_2 + CH_3CHO							
2H-Pyran, 3,6-dihydro-2,6-dimethyl-, cis- → 1,3-Pentadiene, (E)- + Acetaldehyde							
79 FRE/POT Thermolysis in a static system. Gas-chromatography. P = (3-7) torr.	EX	573-624	8.13(13)	0	23612±144	1	1.26
 → CH_3CHO + CH_2=CHCH=$CHCH_3$ (major pathway)							
Oxetane, 3-ethenyl-2,4-dimethyl-, (2α,3β,4α)- → Acetaldehyde + 1,3-Pentadiene							
80 CAR/MAI Thermolysis static system. P = (3.5-30) torr.	EX	599-657	2.63(13)	0	24093±902	1	3.98
 → CH_3CH_2OCH=CH_2 + CH_2=CHCHO							
2H-Pyran, 2-ethoxy-3,4-dihydro-							
77 BAI/FRE Thermolysis in a static system. Gas-chromatography. P = (1-13) torr.	EX	561-628	2.92(14)	0	24308±75	1	1.14
 → CH_3OCH=CH_2 + CH_3CH=CHCHO							
2H-Pyran, 3,4-dihydro-2-methoxy-4-methyl-, cis							
75 COL/FRE Thermolysis in a static system. P = (4-12) torr.	EX	560-618	9.08(13)	0	23576±84	1	1.15

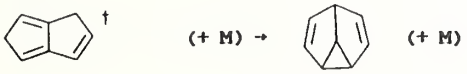
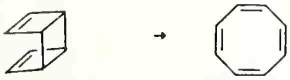
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 $\rightarrow CH_3OCH{=}CH_2 + CH_3CH{=}CHCHO$							
2H-Pyran, 3,4-dihydro-2-methoxy-4-methyl-, trans-							
75 COL/FRE	EX	560-618	1.76(14)	0	24233±144	1	1.28
Thermolysis in a static system. P = (4-12) torr.							
$(CH_3)_2CHCH_2C(O)OCH_2CH_3 \rightarrow (CH_3)_2CHCH_2COOH + CH_2{=}CH_2$							
Butanoic acid, 3-methyl-, ethyl ester							
83 CHU/MAR	EX	633-693	5.01(12)	0	24538±529	1	1.29
Pyrolysis in a static system. P = (71-286) torr.							
$CH_3C(O)OCH_2CH_2CH_2CH_2OCH_3 \rightarrow CH_3OOH + CH_2{=}CHCH_2CH_2OCH_3$							
1-Butanol, 4-methoxy-, acetate							
78 CHU/ROT	EX	643-693	2.34(13)	0	25200±349	1	1.70
Pyrolysis in a static system.. P = (67-216) torr.							
$CH_3CH(OH)CH(CH_3)C(O)OCH_2CH_3$ $\rightarrow CH_3CHO + CH_3CH_2C(O)OCH_2CH_3$							
Butanoic acid, 3-hydroxy-2-methyl-, ethyl ester							
71 YAT/RAM	EX	573-603	1.78(11)	0	19628	1	
Thermolysis in capilary glass tubes. Gas-chromatography.							
$(CH_3)_2C(OH)CH_2C(O)OCH_2CH_3 \rightarrow (CH_3)_2CO$							
Butanoic acid, 3-hydroxy-3-methyl-, ethyl ester							
71 YAT/RAM	EX	563-693	1.58(11)	0	19376	1	
Thermolysis in capilary glass tubes. Gas-chromatography.							
$CH_3C(O)OCH(CH_3)CH_2N(CH_3)_2 \rightarrow CH_3COOH + CH_2{=}CHCH_2N(CH_3)_2$							
2-Propanol, 1-(dimethylamino)-, acetate ester							
83 HER/CHU	EX	583-683	4.57(12)	0	22361±301	1	1.16
Thermolysis in a static system. P = (39-313) torr.							
$(CH_3)_2NC(O)OC(CH_3)_3 \rightarrow (CH_3)_2NH + CO_2 + CH_2{=}C(CH_3)_2$							
Carbamic acid, dimethyl-, 1,1-dimethylethyl ester							
72 DAL/ZIO	EX	643-703	7.41(12)	0	18993±201	1	
Thermolysis in a static system. Assumed T-range.							

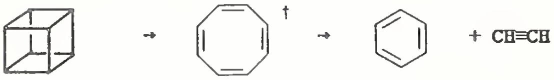
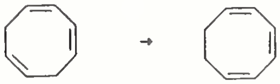
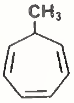


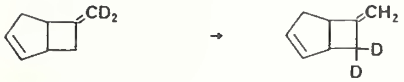
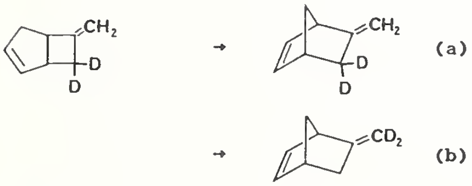
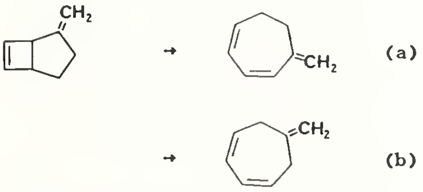
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
1,3,5,7-Cyclooctatetraene → Peentalene, 1,5-dihydro- (a) → Benzene + Ethyne (b)							
79 DUD/GLA1 ($k_a + k_b$)	EX	1000-1400	1.58(13)	0	24177±601	1	1.58
(k_a)	EX	1000-1400	3.98(12)	0	23095	1	
(k_b)	EX	1000-1400	6.31(13)	0	26944	1	
Pyrolysis behind reflected shock-waves. UV-, and IR-Absorption Spectrometry. M = Ar. [Ar] = $(0.06\text{-}1.2)\times10^{20}$ molec.cm^{-3}.							
83 MAR/PFO ($k_a + k_b$)	EX	646-666	6.31(14)	0	27932±755	1	3.16
Thermolysis in a static system. P = 0.3 torr.							

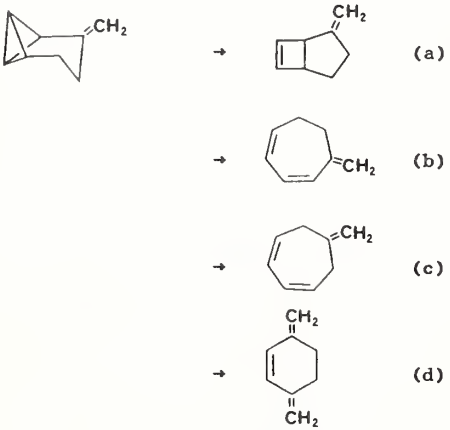
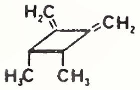
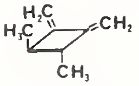


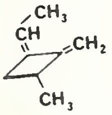
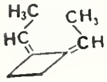
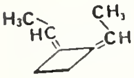
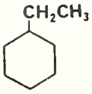
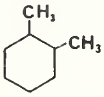
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
[1,3,5,7-Cyclooctatetraene – Bicyclo[4.2.0]octa-2,4,7-triene] → isomerization products (a) → Benzene + Ethyne (b)							
79 DUD/GLA2 ($k_a + k_b$) λ = 311.8 nm. <E> = 94.168 kcal.$mol.^{-1}$ M = 1,3,5,7-Cyclooctatetraene.	EX	298	1.1(6)			1	
($k_a + k_b$) λ = 247.4 nm. <E> = 118.045 kcal.$mol.^{-1}$. M = 1,3,5,7-Cyclooctatetraene.	EX	298	2.7(7)			1	
($k_a + k_b$. M = He) λ = 282 nm. <E> = 103.872 kcal.mol^{-1}.	EX	298	4.5(6)			1	
($k_a + k_b$. M = He) λ = 245 nm. <E> = 119.168 kcal.mol^{-1}.	EX	298	3.0(7)			1	
Isomerization and decomposition of Cyclooctatetraene by both, steady-state Photolysis and Laser Flash-photolysis.							

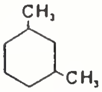
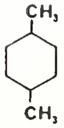
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
1,5-Dihydropentalene → Benzene, ethenyl- (Styrene)							
79 DUD/GLA1 Pyrolysis behind incident or reflected shock-waves. M = Ar. UV-, and IR-Absorption spectrometry. [Ar] = (0.06-0.12)x10^{19} molec.cm^{-3}.	EX	1200-1600	1.26(13)	0	29109±962	1	2.0
							
(main primary product)							
1,5-Dihydropentalene → Cyclopropa[cd]pentalene, 2a,2b,4a,4b-tetrahydro- (Semibullvalene)							
79 DUD/GLA2 <E> = 118.714 kcal.mol.$^{-1}$ at 246 nm. M = 1,5-Dihydropentalene. Isomerization by steady-state photolysis.	EX	298	1.5(7)			1	
							
Cyclopropa[cd]pentalene, 2a,2b,4a,4b-tetrahydro- (Semibullvalene) → 1,5-Dihydropentalene							
79 DUD/GLA1 Pyrolysis behind incident or reflected shock-waves. M = Ar. UV-, and IR-Absorption Spectrometry. [Ar] = (1.2-3.0)x10^{19} molec.cm^{-3}.	EX	740-900	6.31(14)	0	20689±1203	1	2.51
							
Tricyclo[4.2.0.0^{2,5}]octa-3,7-diene, (1α,2α,5α,6α)- (syn form) → 1,3,5,7-Cyclooctatetraene							
74 CAS/DEW	EX	1)	2.29(13)	0	14494±171	1	2.19
	EX	370	2.75(-4)			1	
1) Temperature range not given.							
75 FRE/MAR Gas-chromatography.	EX	363-394	1.66(14)	0	15345±81	1	1.23

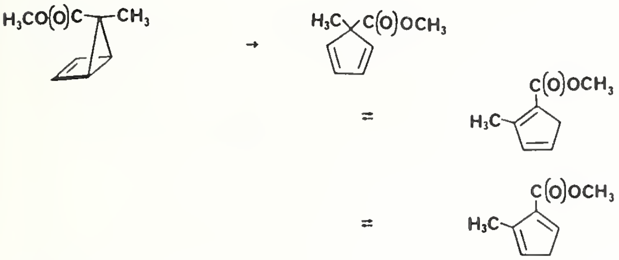
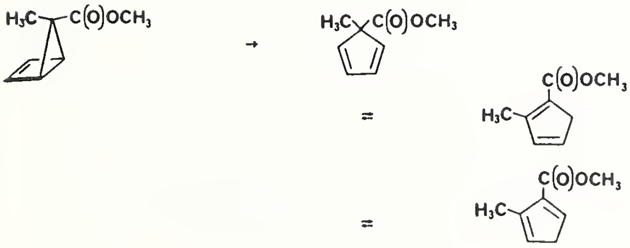
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Tricyclo[4.2.0.0^{2,5}]octa-3,7-diene, (1α,2β,5β,6α)- (anti form) → 1,3,5,7-Cyclooctatetraene							
74 CAS/DEW	EX	1)	1.51(14)	0	16306±453	1	3.63
	EX	370	1.40(-5)			1	
1) Temperature range not given.							
75 FRE/MAR	EX	385-419	1.02(14)	0	16402±86	1	1.23
Gas-chromatography.							
							
Pentacyclo[4.2.0.0^{2,5}0^{3,8}0^{4,7}]octane (Cubane) → 1,3,5,7-Cyclooctatetraene → Benzene + Ethyne							
83 MAR/PFO	EX	507-521	7.94(14)	0	21943±352	1	2.0
Thermolysis of Cubane in static system. P = 0.3 torr.							
							
1,3,6-Cyclooctatriene → 1,3,5-Cyclooctatriene							
83 GRE/ORC	EX	390-490	8.51(10)	0	13941±84	1	1.20
Static system. Gas-chromatography.							
 (+ M) → products							
1,3,5-Cycloheptatriene, 7-methyl-							
79 AST/TRO	EX	900-1400	1.79(13)	0	24478±601	1	1.58
(Limiting high-pressure k)	ES	600-1400	9.77(13)	0	26030	1	
(Extrapolation.)							
Isomerization behind incident and reflected shock-waves. M = Ar. [Ar] = 4.81x10^{17}-1.20x10^{20} molec.cm^{-3}.							
							
Bicyclo[2.2.1]hept-2-ene, 5-methylene-d$_2$- → Bicyclo[2.2.1]hept-2-ene-5,5-d$_2$, 6-methylene-							
72 HAS	EX	530-561	3.16(13)	0	23100±151	1	1.26
Static reactor. P = 1 torr.							

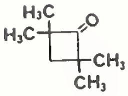
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[3.2.0]hept-2-ene, 6-methylene- → Bicyclo[.2.2.1]hept-2-ene, 5-methylene-							
72 HAS	EX	459-491	5.01(13)	0	19930±50	1	1.58
Static reactor. P = 1 torr.							
							
Bicyclo[3.2.0]hept-2-ene, 6-methylene-d_2- → Bicyclo[3.2.0]hept-2-ene-7,7-d_2, 6-methylene-							
73 HAS	EX	468-499	2.51(13)	0	20584±201	1	1.58
Static reactor. NMR-spectrometry. P = 1 torr.							
							
Bicyclo[3.2.0]hept-2-ene-7,7-d_2, 6-methylene- → Bicyclo[2.2.1]hept-2-ene-5,5-d_2, 6-methylene- (a) → Bicyclo[2.2.1]hept-2-ene, 5-methylene-d_2- (b)							
($k_a + k_b$)	EX	468-499	6.31(13)	0	20081±50	1	1.26
Static reactor. NMR-spectrometry. P = 1 torr.							
							
Bicyclo[3.2.0]hept-6-ene, 2-methylene- → 1,3-Cycloheptadiene, 5-methylene- (a) → 1,3-Cycloheptadiene, 6-methylene- (b)							
80 HAS/LOO ($k_a + k_b$)	EX	436-481	4.07(13)	0	19024±81	1	1.20
Static reactor. P = (0.075-5.25) torr. k is P-independent within this range.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[4.2.0]octa-2,4-diene → 1,3,5-Cyclooctatriene							
83 GRE/ORC	EX	330-475	2.40(12)	0	12858±180	1	1.70
Static reactor. Gas-chromatography.							
							
Tricyclo[4.1.0.$0^{2,7}$]heptane, 3-methylene- → Bicyclo[3.2.0]hept-6-ene, 2-methylene- (a) → 1,3-Cycloheptadiene, 5-methylene- (b) → 1,3-Cycloheptadiene, 6-methylene- (c) → Cyclohexene, 3,6-bis(methylene)- (d)							
80 HAS/LOO ($k_{overall}$)	EX	396-446	3.02(12)	0	16376±221	1	1.70
Static reactor. P = (0.075-3.75) torr. k is P-independent within this range.							
 → products							
Cyclobutane, 1,2-dimethyl-3-4-bis(methylene)-, cis- → products							
72 GAJ/SHI	EX	511	2.9(-5)			1	
	EX	528	(1.20±0.05)(-4)			1	
Pyrolysis in a static reactor. P <10 torr.							
 → products							
Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, trans- → products							
72 GAJ/SHI	EX	511	4.2(-5)			1	
	EX	528	(1.50±0.05)(-4)			1	
Pyrolysis in a static reactor. P <10 torr.							

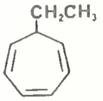
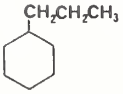
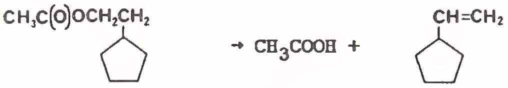
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → products							
Cyclobutane, 1-ethylidene-3-methyl-2-methylene-, (Z)- → products							
72 GAJ/SHI	EX	528	(1.10±0.05)(-3)			1	
Pyrolysis in a static reactor. P <10 torr.							
 → products							
Cyclobutane, 1,2-diethylidene, (Z,Z)- → products							
72 GAJ/SHI	EX	528	(5.6±0.1)(-4)			1	
Pyrolysis in a static reactor. P <10 torr.							
 → products							
Cyclobutane, 1,2-diethylidene, (E,Z)- → products							
72 GAJ/SHI	EX	528	(3.9±0.1)(-4)			1	
Pyrolysis in a static reactor. P <10 torr.							
 (+ M) → products							
Cyclohexane, ethyl-							
81 SAT/KAL	EX	993-1093	7.08(19)	0	44741±1711	1	5.25
Pyrolysis in a quartz reactor. M = Ar. P(Ethylcyclohexane) = 80 torr. P(Ar) = 760 torr.							
83 ZYC/BAC	EX	953-1083	9.6(13)	0	31996±241	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 760 torr.							
 (+ M) → products							
Cyclohexane, 1,2-dimethyl-							
81 SAT/KAL	EX	953-1073	5.50(12)	0	27730±2365	1	7.94
Pyrolysis in a quartz reactor. M = Ar. P(1,2-Dimethylcyclohexane) = 80 torr. P(Ar) = 760 torr.							

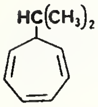
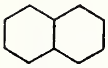
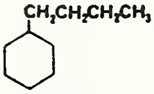
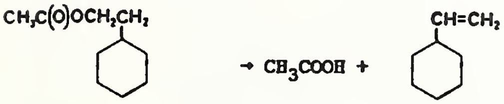
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (+ M) → products							
Cyclohexane, 1,3-dimethyl-							
81 SAT/KAL	EX	993-1098	6.92(12)	0	28183±2365	1	5.01
Pyrolysis in a quartz reactor. M = Ar. P(1,3-Dimethylcyclohexane) = 80 torr. P(Ar) = 760 torr.							
 (+ M) → products							
Cyclohexane, 1,4-dimethyl-							
81 SAT/KAL	EX	963-1103	7.08(15)	0	35682±1409	1	3.98
Pyrolysis in a quartz reactor. M = Ar. P(1,4-Dimethylcyclohexane) = 80 torr. P(Ar) = 760 torr.							
$CH_3(CH_2)_6CH_3$ (+ M) → products							
Octane							
83 DOO/MAC	EX	1100-1400	7.41(11)	0	27064±1202	1	2.69
(Theoretical fit) (Based on a proposed mechanism.)	DE	1100-1400	4.57(11)	0	26463	1	
Pyrolysis in a single-pulse shock-tube, behind reflected shock-waves. Gas-chromatography. M = Ar, or H_2.							
 (a) → $CH_2{=}CHCH_2CH{=}CHC(CH_3){=}C(O)$ → products (b)							
Bicyclo[3.2.0]hept-3-en-6-one, 5-methyl- → Bicyclo[2.2.1]hept-5-en-2-one, 5-methyl- (a) → 1,3,6-Heptatrien-1-one, 2-methyl- (b)							
73 COC/EGG2 $(k_a + k_b)$	EX	489-565	3.16(14)	0	22108±337	1	1.91
Pyrolysis in a static system. Gas-chromatography. P = (2.7-20) torr. The product of the channel (b), 2-Methyl-1,3,6-hexatrien-1-one, undergoes rapid secondary reactions, to give two major products: 3-Methyl-bicyclo[3.2.0]hept-3-en-6-one and 5-Methyl-1,3-Cyclohexadiene-1-carboxaldehyde, as well as two minor products: 3-Methyl-benzaldehyde and Toluene.							

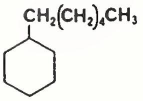
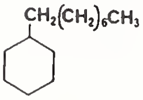
Reaction, Reference Code, Notes		Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
								
Bicyclo[2.1.0]pent-2-ene-5-carboxylic acid, 5-methyl-, methyl ester (1α,4α,5α)- (exo form) → 2,4-Cyclopentadiene-1-carboxylic acid, 1-methyl-, methyl ester = 1,3-Cyclopentadiene-1-carboxylic acid, 2-methyl-, methyl ester = 1,4-Cyclopentadiene-1-carboxylic acid, 5-methyl-, methyl ester								
83 KLA/ADA	(P = 0.4 torr.)	EX	322	(1,77±0.07)(-4)			1	
	(P = 19.4 torr.)	EX	322	(2.31±0.03)(-4)			1	
	Gas-phase Thermolysis in a Pyrex vessel. k increases with the pressure. P = (0.4-20) torr.							
		EX	304-343	1.22(14)	0	13191±96	1	
	Liquid-phase Thermolysis, 0.5 Vol.% in Hexane.							
								
Bicyclo[2.1.0]pent-2-ene-5-carboxylic acid, 5-methyl-, methyl ester (1α,4α,5β)- (endo form) → 2,4-Cyclopentadiene-1-carboxylic acid, 1-methyl-, methyl ester = 1,3-Cyclopentadiene-1-carboxylic acid, 2-methyl-, methyl ester = 1,4-Cyclopentadiene-1-carboxylic acid, 5-methyl-, methyl ester								
83 KLA/ADA	(P = 0.4 torr.)	EX	322	(1.45±0.07)(-4)			1	

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
83 KLA/ADA (P = 18.3 torr) Gas-phase Thermolysis in a Pyrex vessel. k increases with the pressure. P = (0.4-20) torr.	EX	322	(1.98±0.01)(-4)			1	
Liquid-phase Thermolysis, 0.5 Vol.% in Hexane.	EX	304-343	5.07(13)	0	12974±55	1	
 → $(CH_3)_2C=CH_2 + (CH_3)_2C=C=O$ (a) (major pathway) →  + CO (b) (minor pathway) Cyclobutanone, 2,2,4,4-tetramethyl- → 1-Propane, 2-methyl- + 1-Propenone, 2-methyl- (a) → Cyclopropane, 1,1,2,2-tetramethyl- + Carbon monoxide (b)							
(k_a)	EX	637-700	7.23(14)	0	28156±47	1	1.10
(k_b)	EX	637-700	7.36(14)	0	29988±47	1	1.10
($k_a + k_b$) Thermolysis in a static system. IR-, and NMR-Spectrometry. Gas-chromatography. P_o = (6-8) torr. Rate constants are P-independent within this range.	EX	637-700	8.91(14)	0	28269±47	1	1.07
$(CH_3)_2CHC(O)OC(O)CH(CH_3)_2 \rightarrow (CH_3)CHCOOH + (CH_3)_2C=C=O$ Propanoic acid, 2-methyl-, anhydride							
76 BLA/CRA Thermolysis in a static system with packed and unpacked vessels.	EX	519-556	6.45(11)	0	18223±366	1	1.95
$CH_3C(O)OCH_2CH_2CH(CH_3)CH_2CH_3$ $CH_3COOH + CH_2=CHCH(CH_3)CH_2CH_3$ 1-Pentanol, 3-methyl-, acetate							
81 MAR/CHU Pyrolysis in a static system. P = (34-377) torr.	EX	633-693	4.17(13)	0	25488±144	1	1.23

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3C(O)OCH_2CH_2CH_2CH(CH_3)_2 \rightarrow CH_3COOH + CH_2{=}CHCH_2CH(CH_3)_2$							
1-Pentanol, 4-methyl-, acetate							
81 MAR/CHU	EX	633-693	6.61(12)	0	24430±72	1	1.12
Pyrolysis in a static system. P = (34-377) torr.							
$CH_3C(O)OCH(CH_3C(CH_3)_3 \rightarrow CH_3COOH + CH_2{=}CHC(CH_3)_3$ + other minor products							
2-Butanol, 3,3-dimethyl-, acetate							
72 CHU/MAR	EX	578-653	3.16(12)	0	22174±302	1	1.66
Pyrolysis in a static system. P = (25-300) torr. The rate constant is P-independent within the given range.							
$(CH_3)_3CCH_2C(O)OCH_2CH_3 \rightarrow (CH_3)_3CCH_2COOH + CH_2{=}CH_2$							
Butanoic acid, 3,3-dimethyl-, ethyl ester							
83 CHU/MAR	EX	633-693	1.10(13)	0	24911±120	1	1.20
Pyrolysis in a static system. P = (71-286) torr.							
$(CH_3)_3COOC(CH_3)_3 \rightarrow (CH_3)_3CO + (CH_3)_3CO$ (a) $\rightarrow (CH_3)_2CO + (CH_3)_2CO + CH_3 + CH_3$ (b)							
Peroxide, bis(1,1-dimethylethyl)- (tert-Butyl peroxide)							
82 BAT/ROB k_a)	EX	402-443	3.16(15)	0	18621±503	1	3.39
Thermolysis in a static system, in presence of NO. Gas-chromatography. [tert-Butyl peroxide] = (0.72-1.20)x10^{16} molec.cm^{-3}. [NO] = (0.72-1.20)x10^{16} molec.cm^{-3}.							
$(CH_3)_3CSSC(CH_3)_3 \rightarrow (CH_3)_2C{=}CH_2 + HSSH$ + other products							
Disulfide, bis(1,1-dimethylethyl)-							
76 MAR/BAR	EX	603-673	3.98(14)	0	22132±481	1	2.51
Thermolysis in a stirred-flow system.							
76 MAR/BAR	EX	519-573	3.98(13)	0	21290±241	1	1.58
Thermolysis in a static system.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (+ M) → products							
1,3,5-Cycloheptatriene, 7-ethyl-							
79 AST/TRO	EX	940-1350	1.38(13)	0	24141±601	1	1.58
(Limiting high-pressure k, model A_1) (Extrapolated)	ES	900-1400	9.12(13)	0	25741	1	
(Limiting high-pressure k, model A_2) (Extrapolated)	ES	900-1400	3.89(13)	0	24947	1	
Unimolecular isomerization behind incident and reflected shock waves. M = Ar. [Ar] = 1.81×10^{19} molec.cm^{-3}.							
 → products							
Cyclohexane, propyl-							
83 ZYC/BAC	EX	933-1073	8.8(12)	0	28989±241	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 760 torr.							
							
Cyclopentaneethanol acetate → Acetic acid + Cyclopentane, ethenyl-							
81 MAR/CHU	EX	633-693	1.58(13)	0	24947±385	1	1.82
Pyrolysis in a static system. P = (34-377) torr.							
$CH_3C(O)OC(CH_3)_2C(CH_3)_3 \rightarrow CH_3COOH + CH_2{=}C(CH_3)C(CH_3)_3$							
2-Butanol, 2,3,3-trimethyl acetate (1,1,2,2-Tetramethylpropyl acetate)							
83 LOU/VER	EX	538-582	1.66(14)	0	19847	1	
Pyrolysis in a microreactor, or in a Pyrex macroreactor. Gas-chromatography.							
$CH_3C(O)OCH(CH_2CH_3)C(CH_3)_3$ $\rightarrow CH_3COOH + cis\text{-}CH_3CH{=}CHC(CH_3)_3$ (a) $\rightarrow CH_3COOH + trans\text{-}CH_3CH{=}CHC(CH_3)_3$ (b)							
3-Pentanol, 2,2-dimethyl-, acetate							
72 CHU/MAR ($k_a + k_b$)	EX	578-653	1.15(13)	0	22572±393	1	1.23
Thermolysis in a static system. P = (25-300) torr. k is P-independent within the given range.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$(CH_3)_3COC(O)OC(CH_3)_3 \rightarrow (CH_3)_3COH + CO_2 + (CH_3)_2C{=}CH_2$							
Carbonic acid bis(1,1-dimethylethyl) ester							
83 TAY2	EX	546-595	8.51(12)	0	18653	1	
	EX	600	2.68(-1)			1	
Thermolysis in a stainless-steel reactor.							
 (+ M) → products							
1,3,5-Cycloheptatriene, 7-(1-methylethyl)-							
79 AST/TRO	EX	960-1340	8.51(12)	0	23648±962	1	2.24
(Limiting high-pressure k, model A_1)	ES	900-1400	2.19(14)	0	26402	1	
(Extrapolated)							
(Limiting high-pressure k, model A_2)	ES	900-1400	2.29(13)	0	24394	1	
(RExtrapolated)							
Unimolecular isomerization behind incident and reflected shock waves in Ar. $[Ar] = 1.81x10^{19}$ molec.cm^{-3}.							
 → products							
Naphthalene, decahydro-, (Decalin) (Unspecified form)							
79 POP/PET	EX	900-975	4.966(11)	0	26162	1	
Thermolysis of Decalin/Dodecane mixtures in presence of H_2O vapor, in a static reactor. Mass-spectrometry. Gas-chromatography. P(Hydrocarbons) = 0.75 torr.							
 → products							
Cyclohexane, butyl-							
83 ZYC/BAC	EX	923-1023	7.4(12)	0	28628±722	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 760 torr.							
							
Cyclohexaneethanol acetate → Acetic acid + Cyclohexane, ethenyl-							
81 MAR/CHU	EX	633-693	2.0(13)	0	25031±409	1	1.91
Pyrolysis in a static system. P = (34-377) torr.							

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3C(O)OCHCH(CH_3)_2C(CH_3)_3$ → $CH_3COOH + (CH_3)_2C{=}CHC(CH_3)_3 + CH_2{=}C(CH_3)CHC(CH_3)_3$ (+ other minor products)							
3-Pentanol, 2,2,4-trimethyl-, acetate							
72 CHU/MAR	EX	578-653	1.31(13)	0	23452±116	1	1.20
Thermolysis in a static system. P = (25-300) torr. k is P-independent within the given range.							
$CH_3C(O)OC(CH_3)[CH(CH_3)_2]_2$ → $CH_3COOH + (CH_3)_2C{=}C(CH_3)CH(CH_3)_2$							
3-Pentanol, 2,3,4-trimethyl acetate (1-Isopropyl-1,2-dimethylpropyl acetate)							
83 LOU/VER	EX	525-590	7.94(13)	0	19366	1	
Pyrolysis in a microreactor, or in a Pyrex glass macroreactor. Gas-chromatography.							
 → products							
Cyclohexane, hexyl-							
83 ZYC/BAC	EX	923-1053	5.7(12)	0	28147±361	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 760 torr.							
$CH_3(CH_2)_{10}CH_3$ → products							
Dodecane							
79 POP/PET	EX	900-975	3.715(10)	0	23167	1	
Thermolysis of Dodecane-Decalin mixtures in presence of H_2O vapor, in a reactor with a 75 cm^3 vessel. Mass-spectrometry. Gas-chromatography. P(Hydrocarbons) = 0.75 torr.							
 → products							
Cyclohexane, octyl-							
83 ZYC/BAC	EX	923-1003	1.7(12)	0	26703±962	1	
Thermolysis in a flow-reactor. Gas-chromatography. P = 760 torr.							

5. References to the Table

71 BLA/DAV2 Blake, P. G., and Davies, H. H., "Reaction of Keten. Part I. Kinetics of the Gas-phase Reaction with Acetic Acid," J. Chem. Soc. B, 1727 (1971).

71 BLA/SPE Blake, P. G., and Speis, A., "Kinetics of Thermal Decomposition of Acetic Anhydride in Flow and Static Systems," J. Chem. Soc. B, 1877 (1971).

71 GAR/MCF Gardiner, W. C., McFarland, M., Morinaga, K., Takeyama, T., and Walker, B. F., "Initiation Rate for Shock-Heated Hydrogen-Oxygen-Carbon Monoxide-Argon Mixtures as Determined by OH Induction Time Measurements," J. Phys. Chem. **75**, 1504 (1971).

71 SLA/FIS Slack, M. W., Fishburne, E. S., and Johnson, A. R., "Kinetics and Thermodynamics of the CN Molecule. II. The Dissociation of C_2N_2," J. Chem. Phys. **54**, 1652 (1971).

71 SPR/AKI Sprung, J. L., Akimoto, H., and Pitts, J. N., Jr., "Nitrogen Dioxide Catalyzed Cis-Trans Isomerization of cis-2-Butene," J. Amer. Chem. Soc. **93**, 4358 (1971).

71 WAG/ZAB Wagner, H. Gg., and Zabel, F., "Zum thermischen Zerfall von Keten in der Gasphase," Ber. Bunsenges. Phys. Chem. **71**, 114 (1971).

71 YAT/RAM Yates, B. L., Ramirez, A., and Velasquez, O., "The Thermal Decomposition of β-Hydroxy Esters," J. Org. Chem. **36**, 3579 (1971).

72 BAL/AND Baldwin, J. E., and Andrews, G. D., "The Thermal Gas-Phase Partitioning of 1-Methyl- and 2-Methylbicyclo[2.1.0]pent-2-ene," J. Am. Chem. Soc. **94**, 1775 (1972).

72 BAR/MIR Barroeta, N., and Miralles, A., "Thermal Reactions of Alkyl Isocyanates. I.," J. Org. Chem. **37**, 2255 (1972).

72 CHU/MAR Chuchani, G., Martin, G., Barroeta, N., and Maccoll, A., "Pyrolyses of Some Highly Branched Secondary Acetates," J. Chem. Soc., Perkin Trans. 2, 2239 (1972).

72 DAL/ZIO Daly, N. J., and Ziolkowski, F., "Thermolyses of NN-Dimethylcarbamates and the Implications for Thermal β-Elimination Reaction Mechanisms," J. Chem. Soc., Chem. Commun. 911 (1972).

72 EGG/COC Egger, K. W., and Cocks, A. T., "Kinetics of the Four-centre Elimination of Keten from Bicyclo[3.2.0]hept-2-en-6-one in the Gas Phase," J. Chem. Soc., Perkin Trans. 2, 211 (1972).

72 FLO/GIB Flowers, M. C., and Gibbons, A. R., "Application of the RRKM Theory of Unimolecular Reactions to the Thermal Reactions of Spiropentane," J. Chem. Soc., Perkin Trans. 2, 548 (1972).

72 FRE/HOP Frey, H. M., Hopkins, R. G., and Isaacs, N. S., "The Thermal Unimolecular Decomposition of 2-Methoxy-3,4-dihydro-2H-pyran," J. Chem. Soc., Perkin 2, 2082 (1972).

72 GAJ/SHI Gajewski, J. J., and Shih, C. N., "Hydrocarbon Thermal Degenerate Rearrangements. V. Stereochemistry of the 1,2-Dimethylenecyclobutane Self-Interconversion and Its Relation to the Allene Dimerization and the Rearrangements of Other C_6H_8 Isomers," J. Am. Chem. Soc. **94**, 1675 (1972).

72 HAS Hasselmann, D., "Degenerierte Thermische Umlagerung von 5-Methylen-Bicyclo[2,2,1]Hepten-(2)," Tetrahedron Letters No. 33, 3465 (1972).

73 BLU/WAG Blumenberg, B., and Wagner, H. Gg., "Die Reaktion von Methylamin mit Wasserstoffatomen," Ber. Bunsenges. Phys. Chem. 77, 253 (1973).

73 COC/EGG2 Cocks, A. T., and Egger, K. W., "The Gas-phase Thermal Reactions of 1-Methylbicyclo[3.2.0]hept-2-en-7-one," J. Chem. Soc. Perkin Trans. 2, 835 (1973).

73 FRE/HOP Frey, H. M., and Hopf, H., "The Thermal Unimolecular Decomposition of 2,2,4,4-Tetramethylcyclobutanone," J. Chem. Soc. Perkin Trans 2, 2016 (1973).

73 HAS Hasselmann, D., "Entartete Umlagerung eines Bicyclischen Methylen-cyclobutans: 6-Methylen-Bicyclo[3.2.0]Hepten-(2) Mechanismus Seiner Isomerisierung zu 5-Methylen-Bicyclo[2.2.1]-Hepten-(2)," Tetrahedron Lett. 3739 (1973).

73 KNE Knecht, D. A., "Thermal Decomposition of Cyclopentene and Cyclopentene-d_8 in the Gas Phase," J. Amer. Chem. Soc. **95**, 7933 (1973).

73 ORC/THR Orchard, S. W., and Thrush, B. A., "Unimolecular Isomerisation of Hexa-1, trans-3,5-triene and Symmetry-forbidden Pyrolysis of Cyclohexa-1,3-diene," J. Chem. Soc., Chem. Commun. 16 (1973).

74 BLA/SPE Blake, P. G., and Speis, A., "Reactions of Keten. Part IV. Kinetics and Thermodynamics of the Gas-phase Reaction: Thioacetic Acid + Keten → Acetic Thioanhydride," J. Chem. Soc. Perkin Trans. 2, 1879 (1974).

74 CAR/TAR2 Carter, W. P. L., and Tardy, D. C., "Ring Opening of Chemically Activated Cyclopentyl and Methylcyclobutyl Radicals," J. Phys. Chem. **78**, 1573 (1974).

74 CAS/DEW Case, R. S., Dewar, M. J. S., Kirschner, St., Petit, R., and Slegeir, W., "Possible Intervention of Triplet States in Thermal Reactions of Hydrocarbons. A Study of the Rearrangements of Cyclobutadiene Dimers and Analogous Compounds," J. Amer. Chem. Soc. **96**, 7581 (1974).

74 ORC/THR Orchard, S. W., and Thrush, B. A., "Photochemical Studies of Unimolecular Processes. VI. The Unimolecular Reactions of C_6H_8 Isomers and the Interpretation of their Photolyses," Proc. R. Soc. Lond. A 337, 257 (1974); Supersedes 73 ORC/THR.

75 COL/FRE Collins, J. F., Frey, H. M., and Isaacs, N. S., "The Thermal Decomposition of cis- and trans-2-Methoxy-4-methyl-3,4-dihydro-2H-pyran," J. Chem. Soc. Perkin Trans. 2, 1 (1975).

75 FRE/MAR Frey, H. M., Martin, H.-D., and Hekman, M., "Thermolysis of syn- and anti-Dimers of Cyclobutadiene," J. Chem. Soc., Chem. Commun. 204 (1975).

75 LEV/PRI Levush, S. S., Prisyazhnyuk, Z. P., Shevchuk, U. V., and Garbuzyuk, I. A., "Kinetics of Thermal Decomposition of Peracetic Acid in the Gas Phase," Kinet. Catal. 16, 16 (1975); tr. of Kinet. Katal. 16, 26 (1975).

75 LUU/GLA Luu, S. H., Glanzer, K., and Troe, J., "Thermal Isomerization in Shock Waves and Flash Photolysis of Cycloheptatriene, III," Ber. Bunsenges. Phys. Chem. 79, 855 (1975).

75 RIC Richardson, R. J., "CS-O_2 Flame Reaction Chemistry," J. Phys. Chem. **79**, 1153 (1975).

75 SZI/MAR2 Szirovicza, L., and Marta, F., "Thermal Decomposition of Azoisopropane," React. Kinet. Catal. Lett. **2**, 383 (1975).

75 SZI/MAR3 Szirovicza, L., and Marta, F., "Thermal Isomerization of Isopropenyl Radicals," React. Kinet. Catal. Lett. 3, 155 (1975).

76 ART/LEE Arthur, N. L., and Lee, M.-S., "Reactions of Methyl Radicals. I. Hydrogen Abstraction from Dimethyl Sulphide," Aust. J. Chem. **29**, 1483 (1976).

76 BLA/CRA Blake, P. G., Craggs, A., and Vayjooee, M. B., "The Thermal Decomposition of Propanoic and 2-Methylpropanoic Anhydrides in the Gas Phase," J. Chem. Soc. Perkin 2, 986 (1976).

76 GAY/GIL Gaynor, B. J., Gilbert, R. G., King, K. D., and Mackie, J. C., "The Isomerization of cycloheptatriene at High Temperatures," Int. J. Chem. Kinet. **8**, 695 (1976).

76 GOL/LEI Goldstein, M. J., Leight, R. S., and Lipton, M. S., "Thermolysis of Bicyclo[2.2.0]hex-2-ene," J. Amer. Chem. Soc. 98, 5717 (1976).

76 HAC/PIL Hack, W., Pilz, C., and Wagner, H. G., "Measurements of the rate Constants of the Reaction of Atomic Hydrogen and Hydroxy Radicals with Carbon Suboxide in the 295 to 480 K Temperature Range," Ber.- Max-Planck-Inst. Stroemungsforsch. 1976, (6), 28 pp. (Ger); Chem. Abstr. 85:149615a (1976).

76 MAR/BAR Martin, G., and Barroeta, N., "Gas-phase Thermolysis of Sulphur Compounds. Part 1. Di-t-butyl Disulphide," J. Chem. Soc. Perkins 2, 1421 (1976).

76 PAT/ATK2 Pate, C. T., Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Gas Phase Reaction of Peroxyacetyl Nitrate with Selected Atmospheric Constituents," J. Environ. Sci. Health - Environ. Sci. Eng., A11(1), 19 (1976).

77 BAI/FRE Bailey, I. M., and Frey, H. M., "Thermal Unimolecular Decomposition of 2-Ethoxy-3,4-dihydro-2H-pyran," J. Chem. Soc. Perkins Trans. 2, 1976 (1977).

77 FLO Flowers, M. C., "Kinetics of the Thermal Gas-Phase Decomposition of 1,2-Epoxypropane," J. Chem. Soc., Faraday Trans. 1 71, 1927 (1977).

77 FRE/SMI Frey, H. M., and Smith, R. A., "Thermal Decomposition of 3,3-Dimethylcyclobutanone," J. Chem. Soc. Perkin 2, 752 (1977).

77 RED/BER Reddy, K. V., and Berry, M. J., "Intracavity CW Dye Laser Photoactivation of Unimolecular Reactants: Isomerization of State-selected Methyl Isocyanide," Chem. Phys. Lett. 52, 111 (1977).

77 SAL/THR Salter, L. F., and Thrush, B. A., "Reaction of Oxygen Atoms with Methyl and Ethyl Nitrates," J. Chem. Soc. Trans. 1 73, 1098 (1977).

77 TAB/FUE Tabayashi, K., Fueno, T., Takasa, K., Kajimoto, O., and Okada, K., "Thermal Decomposition of Hydrogen Cyanide in Shock Waves," Bull. Chem. Soc. Jpn. 50, 1754 (1977).

78 CAM/HAN Campbell, I. M., and Handy, B. J., "Studies of Reactions of Atoms in a Discharge Flow Stirred Reactor. Part 2. – O + H_2 + CO System," J. Chem. Faraday Trans. 2 74, 316 (1978).

78 CHU/ROT Chuchani, G., and Rotinov, A., "Assessment of the Methoxy Substituent Effect in the Gas Phase Elimination of Methoxyalkyl Acetates," React. Kinet. Catal. Lett. 9, 359 (1978).

78 FRE/POT Frey, H. M., and Pottinger, R., "Thermal Unimolecular Reactions of Vinylcyclobutane and Isopropenylcyclobutane," J. Chem. Soc. Faraday Trans. 1 74, 1827 (1978).

78 HAC/KAU Hack, W., Kaufman, F., Preuss, A. W., and Wagner, H. G., "Measurement of the Rate of the Reaction Nitric Oxide + Hydroperoxyl radical → Hydroxyl radical + Nitrogen Dioxide Using Laser Magnetic Resonance," Ber.-Max-Planck-Inst. Stroemungsforsch. 1978 (8), 28 pp. (Ger); Chem. Abstr. 89:200860e (1978).

78 HIP/LUT Hippler, H., Luther, K., Troe, J., and Walsh, R., "Ultraviolet-Laser Study of Specific Rate Constants for Unimolecule Isomerization of Substituted Cycloheptatrienes," J. Chem. Phys. 68, 323 (1978).

78 LEW/GIE Lewis, D. K., Giesler, S. E., and Brown, M. S., "Further Study of of Cyclopropane Structural Isomerization behind Reflected Shock Waves," Int. J. Chem. Kinet. 10, 277 (1978).

79 AST/TRO Astholz, D. C., Troe, J., and Wieters, W., "Unimolecular Processes in Vibrationally Highly Excited Cycloheptatrienes. I. Thermal Isomerization in Shock Waves," J. Chem. Phys. 70, 5107 (1979).

79 DUD/GLA1 Dudek, D., Glänzer, K., and Troe, J., "Pyrolysis of 1.3.5.7-Cyclooctatetraene, Semibullvalene, and 1.5-Dihydropentalene in Shock Waves and in a Flow System (Part I)," Ber. Bunsenges. Phys. Chem. 83, 776 (1979).

79 DUD/GLA2 Dudek, D., Glänzer, K., and Troe, J., "Photolysis of 1.3.5.7-Cyclooctatetraene and 1.5-Dihydropentalene by Steady State and by Laser Flash Irradiation (Part II)," Ber. Bunsenges. Phys. Chem. 83, 788 (1979).

79 EDN/SPE Edney, E. O., Spence, J. W., and Hanst, P. L., "Synthesis and Thermal Stability of Peroxy Alkyl Nitrates," J. Air Poll. Control Assoc. 29, 741 (1979).

79 FRE/LOD Frey, H. M., and Lodge, S. P., "Thermal Decomposition of 3,6-Dihydro-2H-pyran," J. Chem. Soc. Perkin Trans. 2, 1463 (1979).

79 FRE/POT Frey, H. M., Pottinger, R., Carless, H. A. J., and Lingley, D. J., "The Thermal Decomposition of cis-2,6-Dimethyl-3,6-dihydro-2H-pyran,"J. Chem. Soc. Perkin Trans. 2, 1460 (1979).

79 KAL/SHV Kalinenko, R. A., Shvedova, S. G., and Nametkin, N. S., "Kinetics of the Pyrolysis of Mixtures of Cyclopentane with Paraffin Hydrocarbons," Neftekhimiya 19, 415 (1979); Chem. Abstr. 91:123197f (1979).

79 POP/PET Pop, G., Petre, K., Ivanus, G., and Tomi, P., "Kinetics of the Thermal Decomposition of n-Dodecane-Decalin Binary Mixtures in the Presence of Water Vapor," Neftekhimiya 19, 535 (1979); Chem. Abstr. 91:192556j (1979).

79 RED/BER1 Reddy, K. V., and Berry, M. J., "Reaction Dynamics of State-Selected Unimolecular Reactants. Energy Dependence of the Rate Coefficient for Methyl Isocyanide Isomerization," Faraday Dis cuss. Chem. Soc. pg. 188 (No. 67) (1979).

79 RED/BER2 Reddy, K. V., and Berry, M. J., "A Nonstatistical Unimolecular Chemical Reaction: Isomerization of State-Selected Allyl Isocyanide," Chem. Phys. Lett. 66, 223 (1979).

79 TEM Temps, F., "Investigation of reactions of the hydroperoxyl radical by a Combined Electron Spin Resonance-Laser Magnetic Resonance Spectrometer," Ber.-Max-Planck-Inst. Stroemungsforsch. 1979 (16) 79 pp. (Ger); Chem. Abstr. 92:65334f (1980).

79 TSU/NAK Tsughiya, A., and Nakamura, T., "Lifetime Measurement of HO_2 Radical," Bull. Chem. Soc. Jpn. 52, 1527 (1979).

80 BEN Benson, S. W., "On the Reaction between Ethylene and Cyclopentene, A Radical Mechanism," Int. J. Chem. Kinet. 12, 755 (1980).

80 CAN/CRI Cannon, B. D., and Crim, F. F., "Direct Observation of Unimolecular Reaction in State Selected Tetramethyldioxetane," J. Chem. Phys. 73, 3013 (1980).

80 CAR/MAI Carless, H. A. J., Maitra, A. K., Pottinger, R., and Frey, H. M., "Thermal Decomposition of cis-2,4-Dimethyl-trans-3-vinyloxetan," J. Chem. Soc. Faraday 1 76, 1849 (1980).

80 FUR/PAC Furue, H., and Pacey, P. D., "Performance of Cylindrical Flow Reactors in a Kinetic Study of the Isomerization of Cyclopropane," J. Phys. Chem. 84, 3139 (1980).

80 HAS/LOO Hasselmann, D., and Loosen, K., "New C_8H_{10} Isomers: 2-Methylene-bicyclo[3.2.0]hept-6-ene and 3-Methylenetricyclo[4.1.0.$0^{2,7}$]heptane – Thermal and Metal-Catalyzed Rearrangements," Angew. Chem. Int. Ed. Engl. 19, 634 (1980).

81 BAC/PAR Back, R. A., and Parson, J. M., "The Thermal and Photochemical Decomposition of Maleic Anhydride in the Gas Phase," Can. J. Chem. 59, 1342 (1981).

81 CAN/CRI1 Cannon, B. D., and Crim, F. F., "Kinetics of Gas Phase Tetramethyldioxetane Decomposition and Chemiluminescence," J. Am. Chem. Soc. 103, 6722 (1981).

81 CAN/CRI2 Cannon, B. D., and Crim, F. F., "Local Mode Excitation and Direct Unimolecular Reaction Rate Measurements in Tetramethyldioxetane," J. Chem. Phys. 75, 1752 (1981).

81 MAR/CHU Martin, I., and Chuchani, G., "Steric Acceleration in the Pyrolysis Kinetics of 2-Substituted Ethyl Acetates," J. Phys. Chem. 85, 3902.

81 SAT/KAL Satanova, R. B., Kalinenko, R. A., and Nametkin, N. S., "Kinetic Relationships in Pyrolysis of Dimethylcyclohexanes," Kinet. Catal. 21, 986 (1981); tr. of Kinet. Katal. 21, 1390 (1980).

81 SKI/ROG Skinner, G. B., Rogers, D., and Patel, K. B., "Consistency of Theory and Experiment in the Ethane-Methyl Radical System," Int. J. Chem. Kinet. 13, 481 (1981).

81 TAY Taylor, R., "The Mechanism of Ester Pyrolysis. Part 10. The Effect of the β-Methoxycarbonyl Group in Pyrolysis of Methyl 3-Acetoxypropionate," J. Chem. Res. (S), 250 (1981).

81 TIE/WAM Tiee, J. J., Wampler, F. B., Oldenborg, R. C., and Rice, W. W., "Spectroscopy and Reaction Kinetics of HS Radicals," Chem. Phys. Lett. 82, 80 (1981).

82 BAT/ROB Batt, L., and Robinson, G. N., "Decomposition of the t-Butoxy Radical," Comm. Eur. communities [Rep] EUR 1982, EUR 7624, Phys. Chem. Behav. Atmos. Pollut., 172-80 (Eng); Chem. Abstr.96:217074u (1982).

82 LEW/BOS Lewis, D. K., Bosch, H. W., and Hossenlopp, J. M., "Thermal Isomerization of Cyclopropane to Propene in the Presence of Boron Trichloride at T ~ 1000-1300 K," J. Phys. Chem. 86, 803 (1982).

82 MCE/TAY McEwen, I., and Taylor, R., "The Mechanisms of Thermal Eliminations. Part 12. Relative Rates of Pyrolysis of Ethyl, Isopropyl, t-Butyl, and n-Butyl Vinyl Ethers: Rate Spread as an Index of Elimination Mechanisms," J. Chem. Soc. Perkin Trans. 2, 1179 (1982).

82 MOR/PIL Morgan, C. A., Pilling, M. J., and Tulloch, J. M., "Direct Determination of the Equilibrium Constant and Thermodynamic Parameters for the Reaction $C_3H_5 + O_2 \rightarrow C_3H_5O_2$," J. Chem. Soc., Faraday Trans. 2 78, 1323 (1982).

82 RIZ/CRI Rizzo, T. R., and Crim, F. F., "State-to-State Unimolecular Reaction of t-Butylhydroperoxide," J. Chem. Phys. 76, 2754 (1982).

82 TUL/MAC Tulloch, J. M., Macpherson, M. T., Morgan, C. A., and Pilling, M. J., "Flash Photolysis Studies of Free-Radical Reactions: $C_3H_5 + C_3H_5$ (298-691 K) and C_3H_5 + NO (295-400 K)," J. Phys. Chem. 86, 3819 (1982).

83 ALA/KIE Al-Alami, M. Z., and Kiefer, J. H., "Shock-Tube Study of Propane Pyrolysis. Rate of Initial Dissociation from 1400 to 2300 K," J. Phys. Chem. 87, 499 (1983).

83 AMA/YAM Amano, A., Yamada, M., Hashimoto, K., and Sugiura, K., "Kinetic Feature of the Reaction between Methanethiol and Hydrogen Atoms," Nippon Kagaku Kaishi, 385 (1983).

83 ANA1 Anastasi, C., "Study of the Methyl-Isobutane Reaction in the Range $478 \leq T/K \leq 560$," J. Chem. Soc., Faraday Trans. I 79, 741 (1983).

83 ANA2 Anastasi, C., "Reaction of Methyl Radicals with Formaldehyde in the Range $500 \leq T/K \leq 603$," J. Chem. Soc., Faraday Trans. I 79, 749 (1983).

83 ANA/BLA Anastasi, C., Blackmore, D. K., and Hancock, D. U., "A Study of the Mutual Reaction and Thermochemistry of the CH_3O_2 Radical at 550K," Bull. Soc. Chim. Belg. 92, 645 (1983).

83 ANA/WAD Anastasi, C., Waddington, D. J., and Woolley, A., "Reactions of Oxygenated Radicals in the Gas Phase. Part 10. – Self-reactions of Ethylperoxy Radicals," J. Chem. Soc. Faraday Trans I 79, 505 (1983).

83 ARI/ART1 Arican, H., and Arthur, N. L., "Reactions of Methyl Radicals. IV. Hydrogen Abstraction from Tetramethylsilane by Methyl Radicals Produced by the Photolysis of both Acetone and Azomethane," Aust. J. Chem. 36, 2185 (1983).

83 ARI/ART2 Arican, H., and Arthur, N. L., "Reactions of Methyl Radicals. V. Hydrogen Abstraction from Hydrogen Sulfide," Aust. J. Chem. 36, 2195 (1983).

83 ART/ANA Arthur, N. L., and Anastasi, C., "Rate Constants for the Reaction of CH_3 Radicals with C_2H_5, i-D_3H_7 and t-C_4H_9 Radicals," Bull. Soc. Chim. Belg. 92, 647 (1983).

83 ATK/ASC1 Atkinson, R., Aschmann, S. M., and Carter, W. P. L., "Rate Constants for the Gas-Phase Reactions of OH Radicals with a Series of Bi- and Tricycloalkanes at 299 ± 2 K: Effects of Ring Strain," Int. J. Chem. Kinet. 15, 37 (1983).

83 ATK/ASC2 Atkinson, R., Aschmann, S. M., and Carter W. P. L., "Kinetics of the Reactions of O738 and OH Radicals with Furan and Thiophene at 298 ± 2 K," Int. J. Chem. Kinet. 15, 51 (1983).

83 ATK/ASC3 Atkinson, R., Aschmann, S. M., and Pitts, J. N., Jr., "Kinetics of the Gas-Phase Reactions of OH Radicals with a Series of α,β-Unsaturated Carbonyls at 299 ± 2 K," Int. J. Chem. Kinet. 15, 75 (1983).

83 ATK/ASC4 Atkinson, R., Aschmann, S. M., Carter, W. P. L., and Pitts, J. N., Jr., "Effects of Ring Strain on Gas-Phase Rate Constants. I. Ozone Reactions with Cycloalkenes," Int. J. Chem. Kinet. 15, 721 (1983).

83 ATK/ASC5 Atkinson, R., Aschmann, S. M., and Carter, W. P., "Effects of Ring Strain on Gas-Phase Rate Constants. 2. OH Radical Reactions with Cycloalkenes," Int. J. Chem. Kinet. 15, 1161 (1983).

83 AYR/BAC Ayranci, G., and Back, M. H., "Kinetics of the Reaction: $2C_2H_4 \rightarrow C_2H_5 + C_2H_3$. Heat of Formation of the Vinyl Radical," Int. J. Chem. Kinet. 15, 83 (1983).

83 BAC Back, R. A., "A Search for a Gas-Phase Free-Radical Inversion Displacement Reaction at a Saturated Carbon Atom," Can. J. Chem. 61, 916 (1983).

83 BAR/BEC Barnes, I., Becker, K. H., Fink, E. H., Reimer, A., and Zabel, F., "Rate Constants and Products of the Reaction CS_2 + OH in the Presence of O_2," Int. J. Chem. Kinet. 15, 631 (1983).

83 BAU/CRA Baulch, D. L., Craven, R. J. B., Din, M., Drysdale, D. D., Grant, S., Richardson, D. J., Walker, A., and Watling, G., "Rates of Hydroxy Radical Reactions with Methane, Ethane and Propane over the Temperature Range 403-696 K," J. Chem. Soc., Faraday Trans. I 79, 689 (1983).

83 BER Bernfeld, D. L., "1. Tests of the Coupled Shock Tube/Mass Spectrometer Technique. 2. The Pyrolysis of Neopentane by Atomic Resonance Absorption Spectrophotometry," Diss. Abstr. Int. 44, 180–B (1983); superseded by 83 BER/SKI.

83 BER/FLE Berman, M. R., Fleming, J. W., Harvey, A. B., and Lin, M. C., "Temperature Dependence of the Reactions of CH Radicals with Unsaturated Hydrocarbons," Chem. Phys. 73, 27 (1983).

83 BER/LIN Berman, M. R., and Lin, M. C., "Kinetics and Mechanism of the CH + N_2 Reaction. Temperature- and Pressure-Dependence Studies and Transition-State-Theory Analysis," J. Phys. Chem. 87, 3933 (1983).

83 BER/SKI Bernfeld, D., and Skinner, G. B., "Formation of Hydrogen Atoms in Pyrolysis of 2,2-Dimethylpropane behind Shock Waves," J. Phys. Chem. 87, 3732 (1983).

83 BLA/IJA Blake, P. G., and Ijadi-Maghsoodi, S., "The Kinetics and Mechanism of Thermal Decomposition of

Alkyl Isocyanates," Int. J. Chem. Kinet. **15**, 609 (1983).

83 BLA/JUS Black, G., Jusinski, L. E., and Slanger, T. G., "Rate Coefficients for CS Reactions with O_2, O_3 and NO_2 at 298 K," Chem. Phys. Lett. **102**, 64 (1983).

83 BLA/SHA Black, G., Sharpless, R. L., and Slanger, T. C., "Stratospheric Reactions of SO - A Source or Sink for Odd Oxygen?," Bull. Soc. Chim. Belg. **92**, 629 (1983).

83 BRU/SCH1 Brune, W., Schwab, J., Friedl, R., and Anderson, J., "Laboratory Studies of HO_2, OH and SH," Bull. Soc. Chim. Belg. **92**, 624 (1983). Superseded by 83 BRU/SCH2.

83 BRU/SCH2 Brune, W. H., Schwab, J. J., and Anderson, J. G., "Laser Magnetic Resonance, Resonance fluorescence, and Resonance Absorption Studies of the Reaction Kinetics of O + OH → H + O_2, O + HO_2 → OH + O_2, N + OH → H + NO, and N + HO_2 → Products at 300 K between 1 and 5 torr," J. Phys. Chem. **87**, 4503 (1983).

83 BUR/WAL Burrows, J. P., Wallington, T. J., and Wayne, R. P., "Kinetics of the Gas-phase Reactions of OH with NO_2 and with NO," J. Chem. Soc. Faraday Trans. **79**, 111 (1983).

83 CHI/BIG Chiorboli, C., Bignozzi, C. A., Maldotti, A., Giardini, P. F., Rossi, A., and Carassiti, V., "Rate Constants for the Gas-Phase Reactions of OH Radicals with β-Dimethylstyrene and Acetone. Mechanism of β-Dimethylstyrene NO_x-Air Photooxidation," Int. J. Chem. Kinet. **15**, 579 (1983).

83 CHU/MAR Chuchani, G., and Martin, I., "The Pyrolysis Kinetics of Ethyl Esters in the Gas Phase. The Alkyl Substituent Effect at the Acyl Carbon," Int. J. Chem. Kinet. **15**, 455 (1983).

83 COL/RIC Collongues, C., Richard, C., and Martin, R., "Thermal Reaction of Hydrogen-Butene-2-cis Mixtures at 500°C: Hydrogenation, Hydrogenolysis, and Thermal Reaction of the Olefin," Int. J. Chem. Kinet. **15**, 5 (1983).

83 DAV Davis, C. P., Jr., "The Pyrolysis of Methyl Formate in Shock Waves," Diss. Abstr. Int. **44**, 803–B (1983).

83 DOO/MAC Doolan, K. R., and Mackie, J. C., "Kinetics of Pyrolysis of Octane in Argon-Hydrogen Mixtures," Combust. Flame **50**, 29 (1983).

83 DUN/GUI Duncanson, J. A., Jr., and Guillory, W. A., "The State-Selective Reactions of Vibrationally Excited CH($X^2\Pi$) with Oxygen and Nitrogen," J. Chem. Phys. **78**, 4958 (1983).

83 EBE/EDE Ebert, K. H., Ederer, H. J., and Isbarn, G., "The Thermal Decomposition of n-Hexane," Int. J. Chem. Kinet. **15**, 475 (1983).

83 FAR/BEC Farneth, W. E., and Beck, T. L., "Intramolecular Hydrogen Isotope Effect in the Pyrolysis of Diethyl Carbonate-1,1,1,2,2-d_5," Int. J. Chem. Kinet. **15**, 461 (1983).

83 FON/MAE Fonderie, V., Maes, D., and Peeters, J., "The Kinetic Coefficient of the C_2H_4 + O Reaction over Extended Pressure and Temperature Ranges," Bull. Soc. Chim. Belg. **92**, 641 (1983).

83 FRE/WAT Frey, H. M., and Watis, H. P., "Thermal Unimolecular Decomposition of β-Butyrolactone (4-Methyloxetan-2-one)," J. Chem. Soc. Faraday Trans. I **79**, 1659 (1983).

83 GON Gonzalez, F. S., "A Shock Tube Study of the Pyrolysis of Nitric & Nitrous Oxides," Diss. Abstr. Int. **44**, 1184–B (1983).

83 GOE/SCH Goede, H-J., and Schurath, U., "Temperature Dependence of the Reactions SO + O_3 and SO + O_2," Bull. Soc. Chim. Belg. **92**, 661 (1983).

83 GRE/ORC Greathead, J. M., and Orchard, S. W., "Kinetic and Equilibrium Study of Gas-Phase Interconversions of 1,3,6-Cyclooctatriene and Bicyclo[4.2.0]octa-2,4-diene," Int. J. Chem. Kinet. **15**, 1069 (1983).

83 GUE/VAN de Guertechin, L. O., Vandooren, J., and Van Tiggelen, P. J., "Radical Reactions in Formaldehyde Flames," Bull. Soc. Chim. Belg. **92**, 663 (1983).

83 GUT/NEL Gutman, D., and Nelson, H. H., "Gas-Phase Reactions of the Vinoxy Radical with O_2 and NO," J. Phys. Chem. **87**, 3902 (1983).

83 HAC/KUR Hack, W., Kurzke, H., and Wagner, H. G., "Elementary Reactions of NH_2-Radicals in the Gas Phase. III.," Ber.-Max-Planck-Inst. Stroemungsforsch., 29 (1983) (Eng); Chem. Abstr. 99:146913r (1983).

83 HAG/LOR Hägele, J., Lorenz, K., Rhäsa, D., and Zellner, R., "Rate Constants and CH_3O Product Yield of the Reaction OH + CH_3OH → Products," Ber. Bunsenges. Phys. Chem. **87**, 1023 (1983).

83 HAS/RIE Hassinen, E., Riepponen, P., Blomqvist, K., Kalliorinne, K., and Koskikallio, J., "Rates of Reactions between Methoxycarbonyl, Methyl and Methoxy Radicals Formed in Flash Photolysis of Dimethyl Oxalate in Gas Phase," Bull. Soc. Chim. Belg. **92**, 847 (1983).

83 HAT/AKI Hatakeyama, S., and Akimoto, H., "Reactions of OH Radicals with Methanethiol, Dimethyl Sulfide, and Dimethyl Disulfide in Air," J. Phys. Chem. **87**, 2387 (1983).

83 HER/CHU Hernández A., J. A., and Chuchani, G., "Gas-Phase Elimination Kinetics of 1-Substituted Ethyl Acetates. Effect of Polar Substituents at the α Carbon of Secondary Acetates," Int. J. Chem. Kinet. **15**, 205 (1983).

83 HIP/LUT Hippler, H., Luther, K., Troe, J., and Wendelken, H. J., "Unimolecular Processes in Vibrationally Highly Excited Cycloheptatrienes. III. Direct k(E) Measurements after Laser Excitation," J. Chem. Phys. **79**, 239 (1983).

83 HOM/WEL1 Homann, K. H., and Wellmann, Ch., "Arrhenius Parameters for the Reactions of O Atoms with Some Alkynes in the Range 300-1300 K," Ber. Bunsenges. Phys. Chem. **87**, 527 (1983).

83 HOM/WEL2 Homann, K. H., and Wellmann, Ch., "Kinetics and Mechanism of Hydrocarbon Formation in the system C_2H_2/O/H at Temperatures up to 1300 K," Ber. Bunsenges. Phys. Chem. **87**, 609 (1983).

83 HOR/BAU Horie, O., Bauer, W., Meuser, R., Schmidt, V. H., and Becker, K. H., "The Rate of the Reactions of C_2O Radicals with H and H_2," Chem. Phys. Lett. **100**, 251 (1983).

83 HSU/SHA Hsu, D. S. Y., Shaub, W. M., Creamer, T., Gutman, D., and Lin, M. C., "Kinetic Modeling of CO Production from the Reaction of CH_3 with O_2 in Shock Waves," Ber. Bunsenges. Phys. Chem. **87**, 909 (1983).

83 JAS/FRI Jasinski, J. M., Frisoli, J. K., and Moore, C. B., "High Vibrational Overtone Photochemistry of Cyclobutene," J. Chem. Phys. **79**, 1312 (1983).

83 JOH/MEC Johnson, C. A. F., and Mechie, C. M., "Kinetics of the Reaction between Nitrogen Dioxide and 2-Methyl-2-Nitrosopropane," J. Chem. Res. (S), 212 (1983).

83 KAN/PUR1 Kanan, K., Purnell, H., and Smith, E., "Induced Heterogeneity, a Novel Technique for the Study of Gas-Phase Reactions. Part I. Determination of the Arrhenius Parameters for C-C Bond Scission in Propane," Int. J. Chem. Kinet. **15**, 63 (1983).

83 KAN/PUR2 Kanan, K., Purnell, H., and Sepherad, A., "Induced Heterogeneity, a Novel Technique for the Study of Gas-Phase Reactions. 2. Direct Study of C-C Bond Scission in Ethane," Int. J. Chem. Kinet. **15**, 845 (1983).

83 KEY	Keyser, L. F., "Relative Rate Constants for the Reactions of Atomic Oxygen with HO_2 and OH Radicals," J. Phys. Chem. **87**, 837 (1983).
83 KIE/KAP	Kiefer, J. H., Kapsalis, S. A., Al-Alami, M. Z., and Budach, K. A., "The Very High Temperature Pyrolysis of Ethylene and the Subsequent Reactions of Product Acetylene," Combust. Flame **51**, 79 (1983).
83 KLA/ADA	Klärner, F.-G., and Adamsky, F., "Synthese und Umlagerung substituierter Bicyclo[2.1.0]pent-2-ene. Eine Thermische "walk" Umlagerung," Chem. Ber. **116**, 299 (1983).
83 KLO/DRO	Klotz, H.-D., Drost, H., und Schulz, G., "Zum Einfluss der Stosswellenreflexion auf die Hochtemperaturpyrolyse von Kohlenwasserstoffen im Stosswellenrohr," Exper. Techn. Phys. **31**, 125 (1983) (Ger).
83 KOD1	Kodama, S., "Reactions of NH Radicals. I. Photolysis of HN_3 Vapor at 313 nm," Bull. Chem. Soc. Jpn. **56**, 2348 (1983).
83 KOD2	Kodama, S., "Reactions of NH Radicals. II. Photolysis of HN_3 in the Presence of C_2H_6 at 313 nm," Bull. Chem. Soc. Jpn. **56**, 2355 (1983).
83 KOD3	Kodama, S., "Reactions of NH Radicals. III. Photolysis of HN_3 in the Presence of C_2H_4 at 313 nm," Bull. Chem. Soc. Jpn. **56**, 2363 (1983).
83 KYO/WAT	Kyogoku, T., Watanabe, T., Tsunashima, S., and Sato, S., "Arrhenius Parameters for the Reactions of Hydrogen and Deuterium Atoms with Four Butenes," Bull. Chem. Soc. Jpn. **56**, 19 (1983).
83 LAM/MOL	Lamb, J. J., Molina, L. T., Smith, C. A., and Molina, M. J., "Rate Constant of the $OH + H_2O_2 \rightarrow HO_2 + H_2O$ Reaction," J. Phys. Chem. **87**, 4467 (1983).
83 LAN/PET	Langford, A. O., Petek, H., and Moore, C. B., "Collisional Removal of $CH_2(^1A_1)$: Absolute Rate Constants for Atomic and Molecular Collisional Partners at 298 K," J. Chem. Phys. **78**, 6650 (1983).
83 LAU/YUN	Laufer, A. H., and Yung, Y. L., "Equivalence of Vinylidene and C_2H_2: Calculated Rate Constant for Vinylidene Abstraction from CH_4," J. Phys. Chem. **87**, 181 (1983).
83 LEE/TAN	Lee, J. H., and Tang, I. N., "Absolute Rate Constants for the Hydroxyl Radical Reactions with CH_3SH and C_2H_5SH at Room Temperatures," J. Chem. Phys. **78**, 6646 (1983).
83 LEV/PRI	Levush, S. S., Prisyazhnyuk, Z. P., and Kovalskaya, A. M., "Kinetics of the Thermal Gas Phase Decomposition of C_1-C_4 Organic Peracids," Kinet. Catal. **24**, 1098 (1983); tr. of Kinet. Katal. **24**, 1294 (1983).
83 LIC/BER	Lichtin, D. A., Berman, M. R., and Lin, M. C., "Kinetic Studies of Initiated Reactions of CH and CN Radicals," Bull. Soc. Chim. Belg. **92**, 656 (1983).
83 LIF/BEN	Lifshitz, A., and Ben-Hamou, H., "Thermal Reactions of Cyclic Ethers at High Temperatures. 1. Pyrolysis of Ethylene Oxide Behind Reflected Shocks," J. Phys. Chem. **87**, 1782 (1983).
83 LOI/CAR	Loirat, H., Caralp, F., and Destriau, M., "Rate Constant and Activation Energy of the Exchange Reaction $CO + N_2O \rightarrow CO_2 + N_2$ in the Temperature Range 1060-1220 K. Application of the Thermal Explosion Theory to a System with Two Parallel Reactions," J. Phys. Chem. **87**, 2455 (1983).
83 LOU/TIN	Louw, R., Tinkelenberg, A., and Werner, E. S. E., "Thermolytic Reactions of Esters. Part XIII. The Effect of Electron Attracting α-substituents in Alkyl Acetates," Recl. Trav. Chim. Pays-Bas **102**, 519 (1983).
83 LOU/VER	Louw, R., Vermeeren, H. P. W., and Vogelzang, M., "Thermolytic Reactions of Esters. Part 12. Steric versus Polar Effects on Pyrolytic β-Elimination of Acetic Acid fron (Tertiary) Alkyl Acetates," J. Chem. Soc. Perkin Trans. II, 1875 (1983).
83 MAC/JOU	MacLeod, H., Jourdain, J. L., and Le Bras, G., "Absolute Rate Constant for the Reaction of OH with Thiophene between 293 and 473 K," Chem. Phys. Lett. **98**, 381 (1983).
83 MAC/PAC	MacKenzie, A. L., Pacey, P. D., and Wimalasena, J. H., "Induction Periods in the Formation of Ethane fromn the Pyrolysis of Ethylene," Can. J. Chem. **61**, 2033 (1983).
83 MAC/PIL	MacPherson, M. T., Pilling, M. J., and Smith, M. J. C., "The Pressure and Temperature Dependence of the Rate Constant for Methyl Radical Recombination over the Temperature Range 296-577 K," Chem. Phys. Lett. **94**, 430 (1983).
83 MAC/POU	MacLeod, H., Poulet, G., and Le Bras, G., "Etude Cinetique des Reactions du Radical OH Avec CH_3SCH_3, CH_3SH et C_2H_5SH," J. Chim. Phys. Phys.-Chim. Biol. **80**, 287 (1983).
83 MAR/HER	Martinez, R. I., and Herron, J. T., "Methyl Thiirane: Kinetic Gas-Phase Titration of Sulfur Atoms in S_xO_y Systems," Int. J. Chem. Kinet. **15**, 1127 (1983).
83 MAR/PFO	Martin, H.-D., Pföhler, P., Urbanek, T., and Walsh, R., "Thermolyse von Ansaran, Ansaren und Cuban," Chem. Ber. **16**, 1415 (1983).
83 MAR/ROP	Martin, G., and Ropero, M., "Gas Phase Thermolysis of Acetonyl Allyl Sulfide," React. Kinet. Catal. Lett. **22**, 171 (1983).
83 MAR/SHA	Marshall, R. M., and Shahkar, G., "The Molecular Component in the Thermal Decomposition of Azomethane," J. Chem. Soc. Faraday Trans. I **79**, 1891 (1983).
83 NEL/HEL	Nelson, H. H., Helvajian, H., Pasternack, L., and McDonald, J. R., "Temperature Dependence of $C_3(X^1\Sigma_g^+)$ Reactions with Alkenes and Alkynes, 295-610 K," Chem. Phys. **73**, 431 (1983).
83 NIK/MAK	Niki, H., Maker, P. D., Savage, C. M., and Breitenbach, L. P., "A Fourier Transform Infrared Study of the Kinetics and Mechanism for the Reaction $HO + CH_3OOH$," J. Phys. Chem. **87**, 2190 (1983).
83 OHT	Ohta, T., "Rate Constants for the Reactions of Diolefins with OH Radicals in the Gas Phase. Estimate of the Rate Constants from Those for Monoolefins," J. Phys. Chem. **87**, 1209 (1983).
83 PAR/GUT	Park, J.-Y., and Gutman, D., "Reactions of Ethyl, Cyclopentyl, and Cyanomethyl Radicals with Nitrogen Dioxide," J. Phys. Chem. **87**, 1844 (1983).
83 PAR/SIN	Paraskevopoulos, G., Singleton, D. L., and Irwin, R. S., "Rates of OH Radical Reactions. The Reaction $OH + SO_2 + N_2$†," Chem. Phys. Lett. **100**, 83 (1983).
83 PEN/CAN	Penzhorn, R.-D., and Canosa, C. E., "Second Derivative UV Spectroscopy Study of the Thermal and Photochemical Reaction of NO_2 with SO_2 and SO_3," Ber. Bunsenges. Phys. Chem. **87**, 648 (1983).
83 PLU/SAN	Plum, C. N., Sanhueza, E., Atkinson, R., Carter, W. P. L., and Pitts, J. N., Jr., "OH Radical Rate Constants and Photolysis Rates of α-Dicarbonyls," Environ. Sci. Technol. **17**, 479 (1983).
83 PRA/WOO	Pratt, G. L., and Wood, S. W., "Stoichiometry and Rate of Reaction of Hydrogen Atoms with Oxygen," J. Chem. Soc., Faraday Trans. I **79**, 2597 (1983).
83 RAV/THO	Ravishankara, A. R., and Thompson, R. L., "Kinetic Study of the Reaction of OH with CO from 250 to 1040 K," Chem. Phys. Lett. **99**, 377 (1983).
83 RAV/WIN	Ravishankara, A. R., Wine, P. H., and Nicovich, J. M., "Pulsed Laser Photolysis Study of the Reaction between $O(^3P)$ and HO_2," J. Chem. Phys. **78**, 6629 (1983).
83 ROS	Roscoe, J. M., "The Reactions of $O(^3P)$ with the Butanols," Can. J. Chem. **62**, 2716 (1983).

83 SCH	Schwab, J. J., "Spectroscopy and Reaction Kinetics of Halogen-, Hydrogen-, and Oxygen-Containing Free Radicals," Diss. Abstr. Int. **44**, 1344-B (1983).
83 SCH/CLA	Scherzer, K., Claus, P., and Dabbagh, M., "Kinetische Untersuchungen der Reaktionen von Methylradikalen mit Allen," J. Prakt. Chem. **325**, 680 (1983).
83 SCH/KOH	Schieferstein, M., Kohse-Höinghaus, K., and Stuhl, F., "Temperature Dependence of the Rate Constants of the Reaction $O + NO + M \rightarrow NO_2 + M$ ($M = He, NO, N_2, CH_4$)," Ber. Bunsenges. Phys. Chem. **87**, 361 (1983).
83 SCH/MEU	Schmidt, V. H., Meuser, R., Horie, O., Bauer, W., and Becker, K. H., "The Reaction of C_2O Radicals with H Atoms," Bull. Soc. Chim. Belg. **92**, 655 (1983).
83 SEL/BAY	Selzer, E. A., and Bayes, K. D., "Pressure Dependence of the Rate of Reaction of Methyl Radicals with O_2," J. Phys. Chem. **87**, 392 (1983).
83 SMI	Smith, R. H., "Rate Constant for the Gaseous Reaction between Hydroxyl and Propene," J. Phys. Chem. **87**, 1596 (1983).
83 SRI/KAU	Sridharan, U. C., and Kaufman, F., "Primary Products of the $O + C_2H_4$ Reaction," Chem. Phys. Lett. **102**, 45 (1983).
83 SWA/WAD	Sway, M. I., and Waddington, D. J., "Reactions of Oxygenated Radicals in the Gas Phase. Part 12. The Reactions of Isopropylperoxyl Radicals and Alkenes," J. Chem. Soc. Perkin Trans. II, 139 (1983).
83 SZE/HAN1	Szekely, A. Hanson, R. K., and Bowman, C. T., "High-Temperature Determination of the Rate Coefficient for the Reaction $H_2 + CN \rightarrow H + HCN$," Int. J. Chem. Kinet. **15**, 915 (1983).
83 SZE/HAN2	Szekely, A., Hanson, R. K., and Bowman, C. T., "Shock-Tube Determination of the Rate Coefficient for the Reaction $CN + HCN \rightarrow C_2N_2 + H$," Int. J. Chem. Kinet. **15**, 1237 (1983).
83 TAY1	Taylor, R., "The Mechanism of Thermal Elimination. Part 14. Pyrolysis of Diacetamide, 2-Acetoxypyridine, Diacetyl Sulphide, and Thioacetic Acid: Possible Involvement of Enol Forms in Gasphase Eliminations," J. Chem. Soc. Perkin Trans. II, 89 (1983).
83 TAY2	Taylor, R., "The Mechanism of Thermal Eliminations. Part 15. Abnormal Rate Spread in Pyrolysis of Alkyl Methyl Carbonates and S-Alkyl O-Methyl Carbonates due to Enhanced Nucleophilicity of the Carbonyl Group," J. Chem. Soc. Perkin Trans. II, 291 (1983).
83 TAY3	Taylor, R., "The Mechanism of Thermal Elimination. Part 17. Rate Data for Pyrolysis of Vinyl Acetate and 1,2-Diacetoxyethane," J. Chem. Soc. Perkin Trans. II, 1157 (1983).
83 TEM	Temps, F., "Study of Radical-Radical Reactions using a FIR-LMR Spectrometer," Ber. -Max-Planck-Inst. Stroemungsforsch., 140 pp. (1983) (Ger); Chem. Abstr. 100:127433g (1984).
83 THI/ROT	Thielen, K., and Roth, P., "Stosswellenuntersuchungen zum Start der Reaktion $CO + O_2$," Ber. Bunsenges. Phys. Chem. **87**, 920 (1983).
83 TRE	Trenwith, A. B., "Pyrolysis of Propionitrile and the Resonance Stabilisation Energy of the Cyanomethyl Radical," J. Chem. Soc. Far. Trans. I **79**, 2755 (1983).
83 TUA/ATK	Tuazon, E. C., Atkinson, R., Plum, C. N., Winer, A. M., and Pitts, J. N., Jr., "The Reaction of Gas Phase N_2O_5 with Water Vapor," Geophys. Res. Lett. **10**, 953 (1983).
83 TUA/CAR1	Tuazon, E. C., Carter, W. P. L., Atkinson, R., and Pitts, J. N., Jr., "The Gas-Phase Reaction of Hydrazine and Ozone: A Nonphotolytic Source of OH Radicals for Measurement of Relative OH Radical Rate Constants," Int. J. Chem. Kinet. **15**, 619 (1983).
83 TUA/CAR2	Tuazon, E. C., Carter, W. P. L., Brown, R. V., Winer, A. M., and Pitts, J. N., Jr., "Gas-Phase Reaction of 1,1-Dimethylhydrazine with Nitrogen Dioxide," J. Phys. Chem. **87**, 1600 (1983).
83 TUL	Tully, F. P., "Laser Photolysis/Laser-Induced Fluorescence Study of the Reaction of Hydroxyl Radical with Ethylene," Chem. Phys. Lett. **96**, 148 (1983).
83 TUL/RAV	Tully, F. P., Ravishankara, A. R., and Carr, K., "Kinetic Study of the Reactions of the Hydroxyl Radical with Ethane and Propane," Int. J. Chem. Kinet. **15**, 1111 (1983).
83 WAS/HAT	Washida, N., Hatakeyama, S., Takagi, H., Kyogoku, T., and Sato, S., "Reaction of Ketenes with Atomic Oxygen," J. Chem. Phys. **78**, 4533 (1983).
83 WHY/PHI1	Whyte, A. R., and Phillips, L. F., "Rate of Reaction of $CN(\nu=0,1)$ with N Atoms," Bull. Soc. Chim. Belg. **92**, 635 (1983); superseded by 83 WHY/PHI2.
83 WHY/PHI2	Whyte, A. R., and Phillips, L. F., "Rate of Reaction of N with $CN(\nu=0,1)$," Chem. Phys. Lett. **98**, 590 (1983).
83 WHY/PHI3	Whyte, A. R., and Phillips, L. F., "Rates of Reaction of NH_2 with N, NO and NO_2," Chem. Phys. Lett. **102**, 451 (1983).
83 WIN/NIC	Wine, P. H., Nicovich, J. M., Thompson, R. J., and Ravishankara, A. R., "Kinetics of $O(^3P_j)$ Reactions with H_2O_2 and O_3," J. Phys. Chem. **87**, 3948 (1983).
83 YAM/BAC	Yamamoto, S., and Back, R. A., "The Thermal and Photochemical Decompositions of Succinic Anhydride and 2,3-Dimethyl Succinic Anhydride in the Gas Phase," Can. J. Chem. **61**, 2790 (1983).
83 YAM/FUE	Yamasaki, K., Fueno, T., and Kajimoto, O., "Studies on the Reaction $N + N_3 \rightarrow N_2(B^3\Pi_g) + N_2(X^1\Sigma_g^+)$," Chem. Phys. Lett. **94**, 425 (1983).
83 ZAL/HUN	Zalotai, L., Hunyadi-Zoltán, Zs., Bérces, T., and Márta, F., "Kinetics of Gas Phase Decomposition of Oxetan and Oxetan-2,2-d_2," Int. J. Chem. Kinet. **15**, 505 (1983).
83 ZYC/BAC	Zychlinski, W., Bach, G., Glauch, B., and Zimmermann, G., "Kinetische Untersuchungen zur Pyrolyse von Mono-n-alkyl-cyclohexanen," J. f. prakt. Chemie **315**, 66 (1983).

6. Conversion Factors for Rate Constants

Equivalent second order rate constants

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

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

Table adapted from High Temperature Reaction Rate Data No. 5, The University, Leeds (1970).

Equivalent third order rate constants

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

See note to table for second order rate constants.

7. ERRATUM

to

NSRDS-NBS 73, Part 1

Compilation of Chemical Kinetic Data for Combustion Chemistry.

Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)

Page No.	Line No.	
55	12 (from top)	For entry 80 TOB/ULL, the reference reaction is: k_{ref}: $O + CO \rightarrow CO_2$.
94	10 (from top)	Instead of: $O + CH{=}CHCH_2CH_2CH_2 \rightarrow$ products it should be: $O +$ cy-$CH{=}CHCH_2CH_2CH_2 \rightarrow$ products
112	7 (from bottom)	The first product of the reaction O + 1-Pentanethiol is not OOH, but OH.
188	8 (from top)	For entry 71 COW/KEI the data type is not RL, but RN.
192	18 (from top)	Step (a) of the reaction is not $H + (CH_3)_2CHCHCH{=}CH_2$, but $(CH_3)_2CHCH{=}CH_2$.
201	16 (from top)	For the second entry 73 DAY/THO, the reference reaction is: k_{ref}: $OH + CO \rightarrow H + CO_2$.
201	5 (from bottom)	For entry 76 BRA/CAP the units are not 2, but 2/2.
203	12 (from top)	Reaction $OH + HD \rightarrow HDO + H$ is valid only for the last two entries under this heading, namely: 72 DIX with $k = (9.6\pm0.5)(11)$, and 73 DAY/THO with the same k. For the first two entries, 72 DIX with $k/k_{ref} = 2.8\pm0.42$, and 72 DIX, with $k/k_{ref} = 2.4\exp(155/T)$, the reaction is: $OH + H_2 \rightarrow H_2O + H$.
242	1 (from bottom)	The reference reaction is not $OH + CH_3CH_2CH_2CH_2 \rightarrow$ products, but $OH + CH_3CH_2CH_2CH_3 \rightarrow$ products.
252	14 (from bottom)	For the first entry 74 GOR/VOL, the reference reaction is: k_{ref}: $OH + CO \rightarrow H + CO_2$.
269	26 (from top)	For entry 82 ATK/ASC2, the reference reaction is not $OH + CH_3(CH_2)CH_3$, but $OH + CH_3(CH_2)_4CH_3$.
269	19 (from top)	For first entry 74 GOR/VOL, the reference reaction is: k_{ref}: $OH + CO \rightarrow H + CO_2$.
276	20 (from top)	The formula for 2,6-dimethyl-4-heptanone, incorrectly written, should be: $(CH_3)_2CH_2CHC(O)CHCH_2(CH_3)_2$.
278	3 (from top)	For the second entry 77 HAM/LII, the products of the reference reaction are not $H_2O_2 + O_2$, but $D_2O_2 + O_2$.
280	1 (from bottom)	After this line, just before the page number, the definition of footnote 2 should be indicated: $^{2})$ k_b. (All the entries marked with footnote 2 refer to step (b) of reaction $HO_2 + N$ (+ M)).

Page No.	Line No.	
287	4 (from top)	For entry 71 BAL/LAN, the reference reaction is not CH_3CH_3 + HCHO → products, but HO_2 + HCHO → H_2O_2 + CHO.
287	5 (from bottom)	For first entry 71 BAL/LAN, the value of the rate ratio is not 7.8(-2), but 8.8(-2).
287	3 (from bottom)	For the same entry, the reference reaction is not HCHO + $CH_3CH_2CH_3$ → products, but HO_2 + HCHO → H_2O_2 + CHO.
287	2 (from bottom)	For the second entry 71 BAL/LAN, the rate constant is not k = 7.86(7), but k = 7.57(7).
289	6 (from top)	For entry 71 BAL/LAN, the reference reaction is not HCHO + $(CH_3)_3CH$ → products, but HO_2 + HCHO → H_2O_2 + CHO.
386	9 (from bottom)	The product of step (a) is not $CH_3CH_2CH(CH_3)C(CH_3)_{23}$ but $CH_3CH_2CH(CH_3)C(CH_3)_2$.
394	1 (from bottom)	The first reactant of the reference reaction is not CH_3, but CH_3O.
399	8 (from top)	The second product of the reaction CH_3O + $(CH_3)_3CH$, is not $(CH_3)C$, but $(CH_3)_3C$.
407	1 (from top)	The second product of the reaction CH_3O_2 + $(CH_3)_2CHO_2$ should be written $(CH_3)_2CO$.
410	3 (from bottom)	In the reaction of Mercaptomethyl + Thiirane, the reactants are not CH_3S + #172, but CH_3 + cy-CH_2CH_2S.
412	19 (from top)	The first product of the reaction CN + CO_2 is not CNO, but NCO (Cyanato free radical).
415	14 (from top)	The systematic name of NH_2CO is not Amidogen, formyl-, but Methyl, aminooxo- (or Carbamyl).
432	9 (from bottom)	The products of the reference reaction are not $CH_3CH_3CH_3CH_2CO$, but CH_3CH_3 + CH_3CH_2CO.
468	1 (from top)	The product of step (a) is not $CH_2CH{=}CH_3$, but $CH_3CH{=}CH_2$.
497	11 (from top)	The reactants of the reference reaction are not $(CH_3)_3$ + H_2, but $(CH_3)_3C$ + H_2.
550	7 (from bottom)	The first product of the reaction is the free radical $CH_3C{\equiv}CCH(\cdot)CH_3$.

NBS-114A (REV. 2-80)

U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** *(See instructions)*	1. PUBLICATION OR REPORT NO. NBS/NSRDS-73/2	2. Performing Organ. Report No.	3. Publication Date December 1987

4. TITLE AND SUBTITLE

Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 2. Non-Aromatic C, H, O, N, and S Containing Compounds. (1983)

5. AUTHOR(S)

Francis Westley, John T. Herron, and R. J. Cvetanović

6. PERFORMING ORGANIZATION *(If joint or other than NBS, see instructions)*

NATIONAL BUREAU OF STANDARDS
U.S. DEPARTMENT OF COMMERCE
GAITHERSBURG, MD 20899

7. Contract/Grant No.

8. Type of Report & Period Covered
1983

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS *(Street, City, State, ZIP)*

Same as item 6.

10. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 87-20244

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

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

Chemical kinetic data for reactions of importance in combustion chemistry are compiled. Experimental, theoretical, evaluated, or estimated rate constants are given for reactions of O, O_3, H, H_2, OH, HO_2, H_2O, N, N_3, NO, NO_2, N_2O, NH, NH_2, SH, H_2S, SO, SO_2, and the aliphatic, alicyclic, and heterocyclic saturated and unsaturated C_1 to C_{15} hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides, and their free radicals. The data were taken from the literature published in 1983. Data omitted from Part 1 of this series, covering the period 1971 to 1982, are also included. The data are reported as rate constants or in terms of the parameters A, n, and B of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$, where $B = E/R$. Data are given for 434 reactions.

12. KEY WORDS *(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)*

Arrhenius parameters; carbon; chemical kinetics; combustion; compilation; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

13. AVAILABILITY

☒ Unlimited
☐ For Official Distribution. Do Not Release to NTIS
☒ Order From Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.
☐ Order From National Technical Information Service (NTIS), Springfield, VA. 22161

14. NO. OF PRINTED PAGES
142

15. Price

USCOMM-DC 6043-P80

Announcement of New Publications in National Standard Reference Data Series

Superintendent of Documents,
Government Printing Office,
Washington, D.C. 20402

Please add my name to the announcement list of new publications to be issued in the series: National Standard Reference Data Series—National Bureau of Standards.

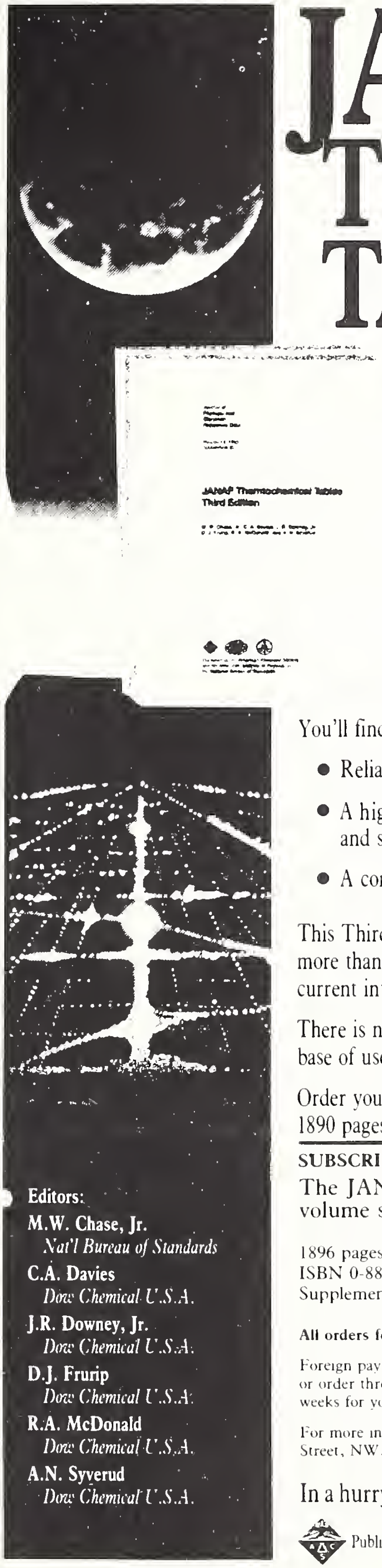
Name____

Company____

Address____

City________________State______________Zip Code______________

(Notification Key N-519)



JUST PUBLISHED!

JANAF THERMOCHEMICAL TABLES

Third Edition

A Major Supplement from JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA

Presenting Reliable Data Utilized by Chemists, Chemical Engineers, and Materials Scientists from Around the World for Over 25 Years

JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA is very pleased to publish the Third Edition of the JANAF THERMOCHEMICAL TABLES.

Since the first version appeared 25 years ago, the JANAF THERMOCHEMICAL TABLES have been among the most widely used data tables in science and engineering.

You'll find:

- Reliable tables of thermodynamic properties of substances of wide interest
- A highly professional approach with critical evaluations of the world's thermochemical and spectroscopic literature
- A concise and easy-to-use format

This Third Edition presents an extensive set of tables including thermodynamic properties of more than 1800 substances, expressed in SI units. The notation has been made consistent with current international recommendations.

There is no other reference source of thermodynamic data that satisfies the needs of such a broad base of users.

Order your 2-volume set of the JANAF THERMOCHEMICAL TABLES today! You'll get over 1890 pages of valuable information that is crucial to your research—in two hardback volumes.

Editors:
M.W. Chase, Jr.
Nat'l Bureau of Standards
C.A. Davies
Dow Chemical U.S.A.
J.R. Downey, Jr.
Dow Chemical U.S.A.
D.J. Frurip
Dow Chemical U.S.A.
R.A. McDonald
Dow Chemical U.S.A.
A.N. Syverud
Dow Chemical U.S.A.

SUBSCRIPTION INFORMATION

The JANAF THERMOCHEMICAL TABLES, THIRD EDITION is a two-volume supplement of *Journal of Physical and Chemical Reference Data.*

1896 pages, 2 volumes, hardcover
ISBN 0-88318-473-7
Supplement Number 1 to Volume 14, 1985

U.S. & Canada	**$130.00**
All Other Countries	**$156.00**
(Postage included.)	

All orders for supplements must be prepaid.

Foreign payment must be made in U.S. currency by international money order, UNESCO coupons, U.S. bank draft, or order through your subscription agency. For rates in Japan, contact Maruzen Co., Ltd. Please allow four to six weeks for your copy to be mailed.

For more information, write **American Chemical Society,** Marketing Communications Department, 1155 Sixteenth Street, NW, Washington, DC 20036.

In a hurry? Call TOLL FREE 800-424-6747 and charge your order!

Published by the **American Chemical Society** and the **American Institute of Physics** for the **National Bureau of Standards**

* U.S. Government Printing Office: 1987 0-201-490 (60198)

NBS Technical Publications

Periodical

Journal of Research—The Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. Issued six times a year.

Nonperiodicals

Monographs—Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications—Include proceedings of conferences sponsored by NBS, NBS annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396).
NOTE: The Journal of Physical and Chemical Reference Data (JPCRD) is published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements are available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

Building Science Series—Disseminates technical information developed at the Bureau on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

Technical Notes—Studies or reports which are complete in themselves but restrictive in their treatment of a subject. Analogous to monographs but not so comprehensive in scope or definitive in treatment of the subject area. Often serve as a vehicle for final reports of work performed at NBS under the sponsorship of other government agencies.

Voluntary Product Standards—Developed under procedures published by the Department of Commerce in Part 10, Title 15, of the Code of Federal Regulations. The standards establish nationally recognized requirements for products, and provide all concerned interests with a basis for common understanding of the characteristics of the products. NBS administers this program as a supplement to the activities of the private sector standardizing organizations.

Consumer Information Series—Practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

Order the **above** *NBS publications from: Superintendent of Documents, Government Printing Office, Washington, DC 20402.*

Order the **following** *NBS publications—FIPS and NBSIR's—from the National Technical Information Service, Springfield, VA 22161.*

Federal Information Processing Standards Publications (FIPS PUB)—Publications in this series collectively constitute the Federal Information Processing Standards Register. The Register serves as the official source of information in the Federal Government regarding standards issued by NBS pursuant to the Federal Property and Administrative Services Act of 1949 as amended, Public Law 89-306 (79 Stat. 1127), and as implemented by Executive Order 11717 (38 FR 12315, dated May 11, 1973) and Part 6 of Title 15 CFR (Code of Federal Regulations).

NBS Interagency Reports (NBSIR)—A special series of interim or final reports on work performed by NBS for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Service, Springfield, VA 22161, in paper copy or microfiche form.

U.S. Department of Commerce
National Bureau of Standards
Gaithersburg, MD 20899