Compilation of Chemical Kinetic Data for Combustion Chemistry.

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

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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)

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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

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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 (s^{-1})
2 ($cm^3\ mol^{-1}\ s^{-1}$)
3 ($cm^6\ mol^{-2}\ s^{-1}$)
1/1, 2/2 etc. (dimensionless)
2/1 ($cm^3\ mol^{-1}$), 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_6H_x-COMPOUND Reactions:

$C_6H_xO_y$-COMPOUND Reactions:

$C_6H_xS_y$-COMPOUND Reactions:

$C_6H_xN_y$-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:

$C_8H_xO_y$-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	EX	294-473	1.5(13)	0	2646±120	2	
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.							
$O + CH{\equiv}CH \rightarrow CO + CH_2$ (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	EX	295-1330	(1.6±0.5)(13)	0	1550	2	
$k_b + k_d$. 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.							
83 HOM/WEL2	EX	1000	2(12)			2	
k_b. Reaction of O atoms with CH≡CH, studied in a flow-reactor, with or without added H atoms. P(Total) = 2 Torr.							
$O + CH_2{=}CH_2 \rightarrow HCHO + CH_2$ (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	(3.78±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] = $(0.5\text{-}6.0)\times10^{14}$ molec.cm^{-3}. $[O]_o$ = $(0.2\text{-}1.2)\times10^{11}$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 + $CH_3CH{=}C{=}O$ → 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≡CC≡CH → 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 → N_2 + O, or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							
O + $CH{\equiv}CCH{=}CH_2$ → 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 → N_2 + O, or by decomposition of O_2 in a microwave-discharge. Mass-spectrometry. P(Total) = 2 torr.							
O + $CH_3CH_2C{\equiv}CH$ → 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 → 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 + $CH_3CH_2CH{=}C{=}O$ → products							
Oxygen atom + 1-Buten-1-one (Ethylketene)							
83 WAS/HAT 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.	EX	230-449	(3.23±0.50)(12)	0	224±47	2	
O + $(CH_3)_2C{=}C{=}O$ → products							
Oxygen atom + 1-Propen-1-one, 2-methyl- (Dimethylketene)							
83 WAS/HAT 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.	EX	230-449	(3.57±0.57)(12)	0	569±43	2	
O + $CH_3CH_2CH_2CH_2OH$ → OH + $CH_3CH_2CH_2CHOH$ (a) **→ OH + $[C_4H_8OH]$ (b)**							
Oxygen atom + 1-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	(1.35±0.39)(13)	0	1756+505	2	
($k_{overall}$) The O atom abstracts an H atom from any CH bond.	EX	298-606	2.99(13)	0	1780±190	2	1.17
[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)	EX	298-606	(3.06±0.49)(12)	0	1083±289	2	
The O atom abstracts an H atom only from a CH bond in position α to OH.							
($k_{overall}$)	EX	298-606	4.47(12)	0	1190±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 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)	EX	298-606	(1.39±0.18)(12)	0	1010±289	2	
The O atom abstracts an H atom only from the CH bond in position α to OH.							
($k_{overall}$)	EX	298-606	3.66(12)	0	1100±150	2	1.14
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.							
$O + (CH_3)_3COH \rightarrow OH + [C_4H_8OH]$							
Oxygen atom + 2-Propanol, 2-methyl-							
83 ROS	EX	298-606	4.99(12)	0	2190±270	2	1.22
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.							
$O_3 + SO \rightarrow O_2 + SO_2$							
Ozone + Sulfur monoxide							
83 BLA/SHA	EX	230-420	2.89(12)	0	1170±120	2	1.33
SO generated by ArF Laser-photodissociation of SO_2 at 193 nm.							
$P(SO_2)$ = 30 mtorr.							
$P(O_2)$ < 0.4 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_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.							
$[Ozone]_o$ = $(0.12\text{-}1.2)\times10^{13}$ 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.							
$[Ozone]_o$ = (0.12-1.2)x10^{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.							
$[Ozone]_o$ = (0.12-1.2)x10^{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.							
$[Ozone]_o$ = (0.12-1.2)x10^{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.							
$[Ozone]_o$ = (0.12-1.2)x10^{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.							
$[Ozone]_o$ = (0.12-1.2)x10^{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: $H + O_2 + M \rightarrow HO_2 + M$.							

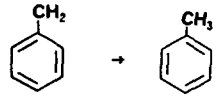
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$H + SH \rightarrow H_2 + S$							
Hydrogen atom + Mercapto							
81 TIE/WAM	EX	298	≤1.02(13)				2
Laser-induced Fluorescence in the (320-330) nm. region. SH generated by H_2S photodissociation 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 discharge. ESR-, and Mass-spectrometry. $[CH_3NH_2]_o = 6.0 \times 10^{17}$ 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 microwave 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 micro-wave-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.							
H +  → $[CH_2CH_2OH]\dagger$ → $CH_2{=}CH_2 + OH$ (a)							
→ $CH_2{=}CH + H_2O$ (b)							
→ H_2 + (c)							
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 → 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 → CH_2=C=CH_2 (a)							
→ CH_3C≡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≡CC≡CH → 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 → $CH_3CH_2CH_2CH_2$ (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 → $CH_3CH_2CHDCH_2$ (a)							
→ $CH_3CH_2CHCH_2D$ (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
H + cis-$CH_3CH=CHCH_3$ → H_2 + $CH_3CH=CHCH_2$ (a) **→ H_2 + $CH_3CHCH=CH_2$ (b)** **→ $CH_3CH_2CHCH_3$ (c)**							
Hydrogen atom + 2-Butene, (Z)-							
83 KYO/WAT k_c. Pulse-Radiolysis. Resonance-Absorption. H atoms generated by pulse-irradiation 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
D + cis-$CH_3CH=CHCH_3$ → $CH_3CHDCHCH_3$							
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
H + trans-$CH_3CH=CHCH_3$ → H_2 + $CH_3CH=CHCH_2$ (a) **→ H_2 + $CH_3CHCH=CH_2$ (b)** **→ $CH_3CH_2CHCH_3$ (c)**							
Hydrogen atom + 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
D + trans-$CH_3CH=CHCH_3$ → $CH_3CHDCHCH_3$							
Deuterium atom + 2-Butene, (E)-							
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	(1.40±0.14)(13)	0	1025±27		2
H + $(CH_3)_2C=CH_2$ (+ M) → $(CH_3)_3C$ (+ 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 + $(CH_3)_2C{=}CH_2$ → $(CH_3)_2CDCH_2$ (a) **→ $(CH_3)_2CCH_2D$ (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 → 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 → 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 → 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) → 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] = $(1.81\text{-}3.01)\times10^{12}$ molec.cm^{-3}. $[SO_2]$ ~2.1×10^{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: $k = (7.4\times10^{11})/(1+237/P)$ where P is in torr. and k is in $cm^3mol^{-1}s^{-1}$.							
OH + NO (+ M) → 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) → HO_2 + NO (+ M) (a)							
→ $HONO_2$ (+ 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 → H + CO_2 (a)							
→ 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: $k = 6.02 \times 10^{23} \exp(-30.03 \pm 1.22 \times 10^{-3} T)$ $cm^3 mol^{-1} s^{-1}$.							
OH + CH_4 → 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 → H + CO_2							
OH + CHO → 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] = 4.0×10^{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 → SH + COS (a)							
→ SOH + CS (b)							
→ any other products (c)							
Hydroxyl + Carbon disulfide							
83 BAR/BEC	EX	293	(1.63±0.36)(12)				2
$k_{overall}$. FTIR-Spectroscopy using photolytic and nonphotolytic competitive techniques. The effective k is dependent on T,P, and O_2 concentrations. P(Total) = 760 torr.							
OH + CH_3SH → products							
Hydroxyl + Methanethiol (Methyl mercaptan)							
83 LEE/TAN	EX	296	(1.54±0.27)(13)				2
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] = $(1.3\text{-}9.7)x10^{12}$ molec.cm^{-3}.							
83 MAC/POU	EX	293	(1.26±0.60)(12)				2
Discharge-flow. EPR-spectrometry.							
OH + CH_3ONO → products							
Hydroxyl + Nitrous acid methyl ester							
83 TUA/CAR1 [1])	RL	300	0.038±0.007				2/2
k_{ref}: OH + $CH_3(CH_2)_4CH_3$ → products							
83 TUA/CAR1 [1])	RN	300	(1.33±0.24(11)				2
Put on absolute basis by using the literature value of the rate constant for the reaction: OH + $CH_3(CH_2)_4CH_3$ → products.							
83 TUA/CAR1 [1])	RL	300	0.041±0.009				2/2
k_{ref}: OH + $(CH_3)_2O$ → products.							
83 TUA/CAR1 [1])	RN	300	(8.43±2.40(10)				2
Put on absolute basis by using the literature value of the rate constant for the reaction: OH + $(CH_3)_2O$ → products.							
83 TUA/CAR1 [1])	SE	300	1.08(11)				2
Average of the two normalized rate constants given above.							
[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≡CH → H + CH_2=C=O (a)							
→ H_2 + CH=C=O (b)							
→ CO + CH_3 (c)							
→ H + CH≡COH (d)							
→ [HO.CH≡CH]* (e)							
Hydroxyl + Ethyne							
83 TEM	EX	296	(9.4±2.0)(10)				2
$k_{overall}$. Reaction of OH with CH≡CH by Far-IR Laser-Magnetic-Resonance Spectrometry.							
OH + CH_2=CH_2 → CH_2CH_2OH → products (a)							
→ H_2O + CH_2+CH (b)							
Hydroxyl + Ethene							
83 TUL	EX	291-591	(1.05±0.32)(12)	0	-462±108		2
k_a. Reaction in a flow-reactor, in He diluent. OH generated by the 193 nm. photolysis of N_2O to $O(^1D)$ and N_2 and subsequent reaction of $O(^1D)$ with H_2O. Tunable dye Laser Fluorescence. P(He) = (50-600) torr.							
OH + CH_3CH_3 → H_2O + CH_3CH_2							
Hydroxyl + Ethane							
83 BAU/CRA [1]	RN	300-2000	1.11(12)	1.9	570		2/2
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 → H + CO_2							
83 TUL/RAV [1]	EX	297-800	3.41(12)	1.05	911		2
Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H_2O.							
[1] The preexponential factors expressed as: $(T/298)^n$.							
OH + OCHCHO → products							
Hydroxyl + Ethanedial (Glyoxal, or Diformyl)							
83 PLU/SAN	RN	298	(6.93±0.24)(12)				2
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.							

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 → 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 + $(CH_3)_2S$ → 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 → CO_2 + CH≡C=O (a) **→ 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 → 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 → products.							
OH + CH_3CH=CH_2 → products							
Hydroxyl + 1-Propene							
83 ATK/ASC2 [1]	RL	298	4.74±0.17				2/2
k_{ref}: OH + $CH_3(CH_2)_4CH_3$ → 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] = 2.38×10^{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] = $(0.07\text{-}8.51) \times 10^{13}$ 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. $[\text{Methyl nitrite}]_o = 2.38 \times 10^{13}$ 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
$k_{overall}$ placed on an absolute basis by using the k for OH + 1-Propene.							
OH + $CH_3C(O)CHO$ → 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] ~$2.4x10^{14}$ molec.cm^{-3}. [CH_3ONO] ~$(3-20)x10^{13}$ molec.cm^{-3}.							
OH + $(CH_3)_2CO$ → 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 + $CH_3(CH_2)_4CH_3$ → products.							
OH + CH_2=CHCH=CH_2 → 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=$CHCH_3$ → 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=$CHCH_3$ → 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 + $CH_3CH_2CH_2CH_3$ → H_2O + $CH_3CH_2CH_2CH_2$ (a)							
→ 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 + $CH_3(CH_2)_4CH_3$ → 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 → products							
Hydroxyl + 2-Butenal (Crotonaldehyde)							
83 ATK/ASC3 [1]	RL	299	1.39±0.16				2/2
k_{ref}: OH + CH_3CH=CH_2 → 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 → 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 → 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]$_o$ = 2.38×10^{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]$_o$ = 2.38×10^{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] = 2.38×10^{14} molec.cm^{-3}.							
83 MAC/JOU Discharge-flow reactor. OH generated by the reaction: H + NO → OH + N. OH atoms generated by dissociation of H_2 traces in He by a microwave-discharge. EPR-spectrometry. [OH]$_o$ = $(0.5\text{-}1.9) \times 10^{11}$atoms.cm^{-3}. [Thiophene]$_o$ = $(0.23\text{-}4.87) \times 10^{13}$ 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	RN	297	(2.19±0.08)(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(1,2-Pentadiene) ~ 1 mtorr.							
k determined relative to the reaction:							
OH + CH_2=CHCH=CH_2 → products.							
OH + cis-CH_2=CHCH=$CHCH_3$ → products							
Hydroxyl + 1,3-Pentadiene, (Z)-							
83 OHT	RN	297	(6.20±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(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.							
OH + CH_2=$CHCH_2CH$=CH_2 → products							
Hydroxyl + 1,4-Pentadiene							
83 OHT	RN	297	(3.05±0.08)(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(1,4-Pentadiene) ~ 1 mtorr.							
k determined relative to the reaction:							
OH + CH_3CH=CH_2 → products.							
OH + CH_2=C=C$(CH_3)_2$ → products							
Hydroxyl + 1,2-Butadiene, 3-methyl-							
83 OHT	RN	297	(3.49±0.11)(13)				2
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.							

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 → 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 → 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 → 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.							
[Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}							
OH + trans-CH_3CH=$CHCH_2CH_3$ → 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 → products.							
OH + $(CH_3)_2$C=$CHCH_3$ → 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 → products.							

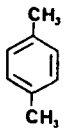
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + 1,3-Cyclohexadiene							
83 ATK/ASC5 [1])	RL	298	1.62±0.05				2/2
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1])	RN	298	(9.40±0.33)(13)				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]$_o$ = 2.38×10^{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]$_o$ = 2.38×10^{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=$CHCH_2CH_2CH$=CH_2 → products.							
OH + trans-CH_2=CHCH=$CHCH_2CH_3$ → 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.							

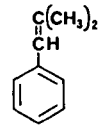
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
OH +  → products							
Hydroxyl + Cyclohexene							
83 ATK/ASC5 [1])	RL	298	(6.7±0.17)(-1)				2/2
k_{ref}: OH + CH_2=C(CH_3)CH=CH_2 → products.							
83 ATK/ASC5 [1])	RN	298	(3.87±0.10)(13)				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]$_o$ = 2.38x10^{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]$_o$ = 2.38x10^{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.							

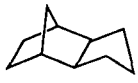
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
[1]) Irradiation of Cyclohexane/CH_3ONO/Air mixtures in a Teflon bag. OH generated by photolysis of CH_3ONO in Air. Gas-chromatography. P = 735 torr. [Methyl nitrite]$_o$ = 2.38×10^{13} molec.cm^{-3}.							
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=$CHCH_2CH_2$CH=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 + 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]$_o$ = 2.38×10^{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]$_o$ = 2.38×10^{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]) Placed on an absolute basis by using the k for OH + Cyclohexane.	RN	299	(8.91±0.60)(12)				2
[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]) Placed on an absolute basis by using the k for OH + Cyclohexane.	RN	299	(6.69±0.36)(12)				2
[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]) k_{ref}: OH +  → products.	RL	299	2.35±0.17				2/2
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.	RN	299	(6.87±0.24)(12)				2
[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.							
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.	RN	299	(1.39±0.13)(13)				2
[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.							
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]) 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.	RN	299	(1.21±0.08)(13)				2
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]) 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.	RN	299	(1.24±0.07)(13)				2
HO_2 + HO_2 (+ M) → H_2O_2 + O_2 (+ M)							
Hydroperoxo							
79 TSU/NAK 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.	EX	298	(2.8±0.3)(12)				2
HO_2 + NO (+ M) → O_2 + HNO (+ M) (a) **→ OH + NO_2 (+ M) (b)** **→ $HONO_2$ (+ M) (c)**							
Hydroperoxo + Nitrogen oxide (NO)							
78 HAC/KAU k_b. Discharge-flow. LMR-Spectrometry. P = 5.25 torr.	EX	296	(3.5±1.0)(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
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 + $CH_3C(O)ONO_2$ → 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 → 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 → 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 → 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 → 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	EX	298	3.37(11)				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. [NO] = (0.5-40) torr. P(Ar) = (5-10) torr.							
SH + CH_2=CH_2 → products							
Mercapto + Ethene							
81 TIE/WAM	EX	298	≤1.39(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.							
N + OH → NO + H							
Nitrogen atom + Hydroxyl							
83 BRU/SCH2	EX	298	(2.53±0.48)(13)				2
Fast-flow reactor. Laser-magnetic Resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)							
N + HO_2 → products							
Nitrogen atom + Hydroperoxo							
83 BRU/SCH2	EX	298	(1.33±0.30)(13)				2
Fast-flow reactor. Laser-magnetic resonance. Resonance-fluorescence. Resonance-absorption. P = (1-5) torr. (He, or Ar)							
N + N_3 → $N_2(B^3\Pi_g)$ + $N_2(X^1\Sigma_g^+)$							
Nitrogen atom + Azide							
83 YAM/FUE	EX	298	(9.64±6.63)(12)				2
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 → HCl + N_3.							

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 ($k_a + k_b$)	EX	296	(7.29±0.84)(13)				2
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}.							
$N + CN(v=n) \rightarrow N_2 + C$							
Nitrogen atom + Cyanogen							
83 WHY/PHI2	EX	300	(6.02±0.78)(13)				2
Fast-flow reactor. CN generated by the ArF Flash-photolysis of NCCN at 193 nm. N atom generated by microwave-discharge. Laser induced Fluorescence.							
$N + NCC \rightarrow CN + CN$							
Nitrogen atom + Methylidyne, cyano-							
83 WHY/PHI2 (n = 0,1)	ES	300	6.02(13)				2
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.							
$N_3 + N_3 \rightarrow N_2(B^3\Pi_g) + N_2X^1\Sigma_g^+) + N_2(X^1\Sigma_g^+)$							
Azide							
83 YAM/FUE	EX	298	8.43(11)				2
Discharge-flow reactor. N_3 generated by the reaction: $Cl + HN_3 \rightarrow HCl + N_3$							
$NO + NH_2 \rightarrow [NH_2NO] \rightarrow N_2 + H_2O$†							
Nitrogen oxide (NO) + Amidogen							
83 WHY/PHI3	EX	297	(1.09±0.07)(13)				2
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}.							

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 + $CH_3C(O)ONO_2$ → 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 + $CH_3C(O)ONO_2$ → 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 + $(CH_3)_2NNH_2$ → 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 + $(CH_3)_3CNO$ + → 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) → N_2 + O (+ M) (a)							
→ 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.							
$NH(a^1\Delta) + CH_2{=}CH_2 \rightarrow [CH_2{=}CHNH_2 = \text{  }]$							
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	≃1.91(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 → 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 Spectro-photometry. P(Total) = 1350 torr. $[O_2] = (0.02\text{-}4.92) \times 10^{17}$ molec.cm^{-3}. $[CO] = (0.12\text{-}2.46) \times 10^{17}$ molec.cm^{-3}.							

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
$CO + N_2O \rightarrow CO_2 + N_2$							
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.							

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 → △ → CH_2CH=CH_2 (a)							
→ any other products (b)							
Methylidyne + Ethene							
83 BER/FLE (k_a)	EX	160-652	(1.34±0.16)(14)	0	-173±35		2
Laser-photolysis/Laser-induced Fluorescence. CH generated by multiphoton dissociation of $CHBr_3$ at 266 nm. P(Total) = 100 torr.							
$CH_2(a^1A_1)$ + O_2 → products							
Methylene + Oxygen molecule							
83 LAN/PET	EX	295	(4.46±0.30)(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.							
$CH_2(^1A_1)$ + H_2 → products							
Methylene + Hydrogen molecule							
83 LAN/PET	EX	295	(6.32±0,30)(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.							
$CH_2(a^1A_1)$ + N_2 → products							
Methylene + Nitrogen molecule							
83 LAN/PET	EX	295	(6.63±0.60)(12)				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.							
$CH_2(a^1A_1)$ + NO → products							
Methylene + Nitrogen oxide (NO)							
83 LAN/PET	EX	295	(9.64±0.90)(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
$CH_2(a^1A_1)$ + CO → 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 → 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≡CH → CH_2=C=CH_2 (a)							
→ CH_3C≡CH (b)							
→ C_3H_2 + H_2 (c)							
→ 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 → 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)	DE	1150-1560	1.0(14)	0	15500±1100		2
Rate constant determined by fitting the concentration time profiles data to a computer kinetic modeling mechanism. RRKM calculation.							
83 HSU/SHA [1] (k_b)	RE	1150-1560	4.42(19)	-5.94	21300		2
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.							
83 SEL/BAY (k_e. M = Ar)	EX	298	(4.82±0.36)(9)				2
P(Total) = 0.639 torr.							
$P_{max}(O_2)$ = 0.2426 torr.							
(k_e. M = Ar)	EX	298	(3.68±0.40)(10)				2
P(Total) = 5.921 torr.							
$P_{max}(O_2)$ = 0.0730 torr.							
(k_e. M = N_2)	EX	298	(6.81±0.36)(9)				2
P(Total) = 0.931 torr.							
$P_{max}(O_2)$ = 0.3552 torr.							
(k_e. M = N_2)	EX	298	(3,50±0.17)(10)				2
P(Total) = 5.420 torr.							
$P_{max}(O_2)$ = 0.0743 torr.							
(k_e. M = He)	EX	298	(5.54±0.48)(9)				2
P(Total) = 1.078 torr.							
$P_{max}(O_2)$ = 0.3431 torr.							
(k_e. M = He)	EX	298	(2.40±0.17)(10)				2
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.							

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] = 1.0×10^{17} molec.cm^{-3}.							
[Formaldehyde] = 3.6×10^{16} molec.cm^{-3}.							
Total conc. = 5.4×10^{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 = $(0.6\text{-}1.0) \times 10^6$ 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)	EX	293	(2.7±1.0)(5)				2
Fast flow-reactor. CS generated by dissociation of CS_2 in an electric discharge. ESR-, and Mass-spectrometry. $[Ar] = (1.0\text{-}5.0)\times10^8$ molec.cm^{-3}. $[O_2] = (0.5\text{-}3.2)\times10^8$ molec.cm^{-3}. $[CS] = (0.3\text{-}1.5)\times10^8$ molec.cm^{-3}. P = (0.39=8-1.58)torr.							
83 BLA/JUS ($k_a + k_b$. M = He)	EX	298	(1.75±0.24)(5)				2
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.							
$CS + O_3 \rightarrow COS + O_2$							
Carbon monosulfide + Ozone							
83 BLA/JUS (M = He)	EX	298	(1.81±0.24)(8)				2
Laser-induced Fluorescence. CS generated by Photodissociation of CS_2 at 193 nm. $P(CS_2)$ ~ 5 mtorr. P(He) = (50-300) torr.							
$CS + NO_2$ (+ M) $\rightarrow COS + NO$ (+ M)							
Carbon monosulfide + Nitrogen oxide (NO_2)							
83 BLA/JUS (M = He)	EX	298	(4.58±0.66)(7)				2
Laser-induced Fluorescence. CS generated by Photodissociation of CS_2 at 193 nm. P(He) = 24 torr. $P(CS_2)$ ~5 mtorr.							
$CH_3S + NO$ (+ M) $\rightarrow CH_3SNO$ (+ M)							
Methyl, mercapto- + Nitrogen oxide (NO)							
83 HAT/AKI	RL	303	2.0(3)				3/3
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).							

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) $\rightarrow$ □ (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
$CH_2{=}CH_2$ +  → CH_3CH_3 +  (a)							
→ CH_3CH_2 +  (b)							
→ CH_3CH_2 +  (c)							
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 → 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 → 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 + $CH_2{=}CH_2$ → 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 → $CH_2{=}CH_2$ + CH_3CH_3 (d) and							
→ $CH_3CH_2CH_2CH_3$ (r)							
CH_3CH_2 + CH_3CH_2 → $CH_2{=}CH_2$ + CH_3CH_3 (a)							
→ $CH_3CH_2CH_2CH_3$ (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≡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)x10^{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 → $CH_3C(O)SC(O)CH_3$							
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) → $CH_3CHO^{\dagger}$ (+ M) → CH_3CHO (+ M) (a)** → CH_3 + CHO (+ M) (b) → 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 → $CH_2CH_2OH^{\dagger}$ → CH_2=CH_2 + OH (a)** → 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] = $(1.20\text{-}3.22)\times10^{18}$ 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: $k = 3.71\times10^{6}T^{0.5}(64771/T)^{8}\exp(-64771/T)$ $cm^3mol^{-1}s^{-1}$.							
$CH_2CN + NO_2$ → 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. $[CH_3CN] = \sim(5\text{-}50)\times10^{13}$ molec.cm^{-3}. $[Cl]_o = (0.5\text{-}1.5)\times10^{11}$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
$[CH_2{=}CHNH_2 = \overset{H}{\underset{\triangle}{N}}\dagger]$ → $CH_2{=}CH + NH_2$	(a)						
→ $CH_3CN + H_2$	(b)						
→ $[CH_2{=}CHNH = \underset{\triangle}{\dot{N}}] + H$	(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.							
$CH_3N{=}NCH_3 \rightarrow CH_3 + CH_3 + N_2$ (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.							
$C_3 + CH_2{=}CH_2 \leq$ 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 + $CH_3C{\equiv}CH$ ≤ products							
Carbon trimer + 1-Propyne							
83 NEL/HEL	EX	296-610	(2.97÷0.28)(11)	0	121÷35		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(1-Propyne) = (0-1) torr.							
C_3 + $CH_3CH{=}CH_2$ ≤ products							
Carbon trimer + 1-Propene							
83 NEL/HEL	EX	296-610	(6.26÷0.36)(10)	0	159÷21		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(1-Propene) = (0-6.25) torr.							
C_3 + $CH_3CH_2CH{=}CH_2$ ≤ products							
Carbon trimer + 1-Butene							
83 NEL/HEL	EX	296-610	(7.35÷0.30)(10)	0	139÷17		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(1-Butene) = (0-7) torr.							
C_3 + cis-$CH_3CH{=}CHCH_3$ ≤ products							
Carbon trimer + 2-Butene, (Z)-							
83 NEL/HEL	EX	296-610	(1.26÷0.06)(11)	0	-201÷19		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(cis-2-Butene) = (0-1) torr.							

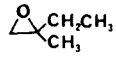
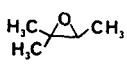
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
C_3 + $(CH_3)_2C{=}CH_2$ ≤ products							
Carbon trimer + 1-Propene, 2-methyl- (Isobutene)							
83 NEL/HEL	EX	296-610	(2.53÷0.10)(11)	0	-759÷15		2
'Multiphoton UV-Photolysis/Laser-induced							
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 + $CH_3CH_2CH_2CH_3$ ≤ 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 + $(CH_3)_2C{=}CHCH_3$ → 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 + $CH_3CH_2CH_2C{\equiv}CCH_3$ → 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 + $(CH_3)_2C{=}C(CH_3)_2$ → 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) → $CH_2{=}CHCH_2NO$ (+ 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.							
$CH_2{=}CHCH_2$ + $CH_2{=}CHCH_2$ → $CH_2{=}CHCH_2CH_2CH{=}CHCH_2$							
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) → $CH_3CH{=}CH_2$ (+ 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	EX	897	1.72(-1)			1	
Isomerization in a flow-reactor with quartz tubes. Gas-chromatography. P = 50 torr.							
82 LEW/BOS	EX	983-1333	2.24(11)	0	12823	1	
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.							
$(CH_3)_2CH \rightarrow H + CH_3CH{=}CH_2$ (a)							
$\rightarrow CH_3 + CH_2{=}CH_2$ (b)							
Ethyl, 1-methyl- (Isopropyl)							
75 SZI/MAR3	RN	538-666	1.0(14)	0	18319±1057	1	6.31
Static-, or flow-system. $(CH_3)_2CH$ generated by the pyrolysis of Azoisopropane. Mass-spectrometry. Determined relative to the reaction: $(CH_3)_2CH + (CH_3)_2CH \rightarrow (CH_3)_2CHCH(CH_3)_2$							
$(CH_3)_2CH + (CH_3)_2CH \rightarrow (CH_3)_2CHCH(CH_3)_2$ (a)							
$\rightarrow (CH_3)_2CHCH(CH_3)_2$ (b)							
Ethyl, 1-methyl- (Isopropyl)							
83 ART/ANA (k_a)	ES	308	5.96(12)			2	
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.							

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.							

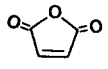
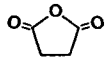
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_2CH_2OCD_2$ → $CH_2{=}CH_2$ +DCDO (a)							
→ $CH_2CH_2CD_2O$ → $CH_2{=}CH_2$ + DCDO (b)							
→ $CH_2CD_2OCH_2$ → $CH_2{=}CD_2$ + HCHO (c)							
→ $CD_2CH_2CH_2O$ → $CH_2{=}CD_2$ + HCHO (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^∞. 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.							
$CH_3CH_2C(O)OOH \rightarrow CH_3CH_2 + CO_2 + OH$							
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.							
-spectrometry.							
= (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.							

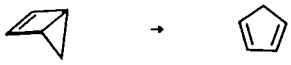
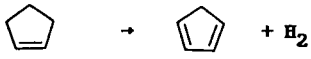
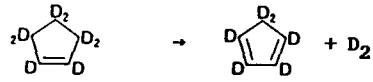
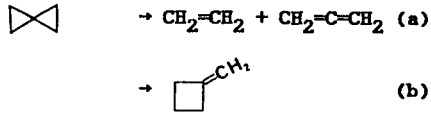
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

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
$CH_3CH_2CHCH_3$ + cis-CH_3CH=$CHCH_3$ → $CH_3CH_2CH_2CH_3$ + CH_3CH=CCH_3							
Propyl, 1-methyl-, + 2-Butene, (Z)-							
83 COL/RIC [1]	RL	773-794	2.5(3)			2/1	
k_{ref}: $CH_3CH_2CHCH_3$ → 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.							
$(CH_3)_3C$ + $(CH_3)_3C$ → $(CH_3)_2CH$=CH_2 + $(CH_3)_3CH$ (a)							
→ $(CH_3)_3CC(CH_3)_3$ (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.							
 → CO + CH≡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.							
 → CO + other products (a)							
→ 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 → $(CH_3)_2CO$ + CO (a)							
→ 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=$CHCH_2NC^{\dagger}$ → 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.)							
$(CH_3)_2CHNCO$ → CH_3CH=CH_2 + HN=C=O (a) → 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.							
$CH_3C(O)NHC(O)CH_3$ → $CH_3C(O)NH_2$ + 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.							

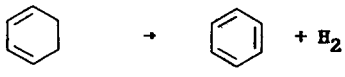
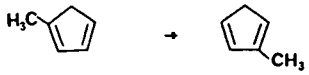
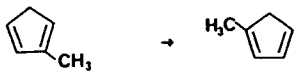
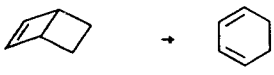
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[2.1.0]pent-2-ene → 1,3-Cyclopentadiene							
72 BAL/AND	EX	323	(1.39±0.02)(-4)				1
Thermal isomerization in an aluminum column. Gas-chromatography.							
							
Cyclopentene							
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.							

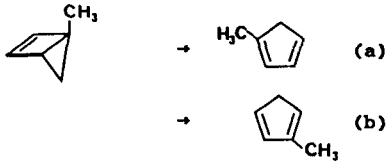
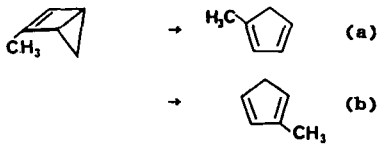
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → CH_2=$CHCH_2CH_2CH_2$							
Cyclopentyl → 4-Pentenyl							
74 CAR/TAR2	DE	298	1.0(14)	0	17413±302	1	2.51
Decyclization of Cyclopentyl in a Pyrex reaction vessel. Cyclopentyl generated by reacting 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.							

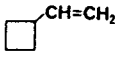
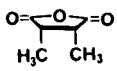
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2CH_2CH_3CH_3$ → products							
Pentane							
79 KAL/SHV	RL	978-1143	1.3±0.1	0	0	1/1	
Pyrolysis of Pentane-Cyclopentane mixtures in a flow-reactor. Gas-chromatography. [Cyclopentane] = (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.							
$(CH_3)_2$CHOCH=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.							

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

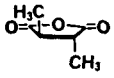
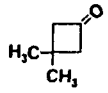
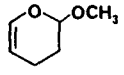
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH_2OC(O)OCD_2CD_3 \rightarrow CH_2{=}CH_2 + CO_2 + CD_3CD_2OH$ (a)							
$\rightarrow CD_2{=}CD_2 + CO_2 + CH_3CH_2OD$ (b)							
Carbonic acid ethyl ethyl-d_5 ester							
(Diethyl carbonate-1,1,2,2-d_5)							
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.							

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 rearangement. 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
 (a) (b)							
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.							
 (a) (b)							
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.							

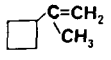
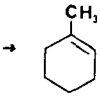
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_2{=}CH_2$ + $CH_2{=}CHCH{=}CH_2$ (a)							
 (b)							
Cyclobutane, ethenyl- → Ethene + 1,3-Butadiene (a)							
→ Cyclohexene (b)							
78 FRE/POT (k_a)	EX	569-639	7.41(14)	0	25529±91	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.							

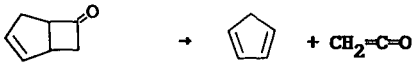
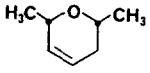
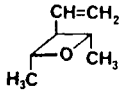
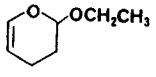
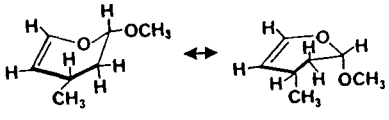
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

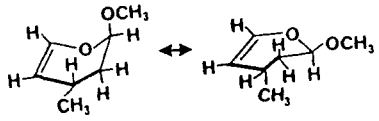
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → CO + other products (a)							
→ CO_2 + other products (b)							
2,5-Furandione, dihydro-3,4-dimethyl-, trans-							
(Succinic anhydride, 2,3-dimethyl-, trans-)							
83 YAM/BAC (k_a)	EX	625-775	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.							
$CH_3CH_2C(O)OC(O)CH_2CH_3 \rightarrow CH_3CH_2COOH + CH_3CH=C=O$							
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.							
$CH_3C(O)OCH(CH_3)C(O)CH_3 \rightarrow CH_3COOH + CH_2=CHC(O)CH_3$							
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.							

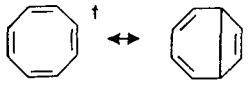
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3C(O)OCH(CH_3)C(O)OCH_3 \rightarrow CH_3COOH + CH_2{=}CHC(O)OCH_3$							
Propanoic acid, 2-(acetyloxy)-, methyl ester							
83 HER/CHU	EX	583-683	2.82(13)	0	25200±60	1	1.12
Thermolysis in 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.							

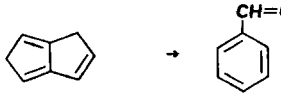
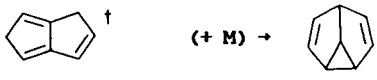
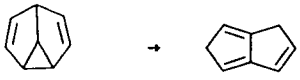
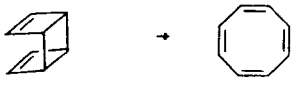
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$CH_3CH(OH)CH_2C(O)OCH_2CH_3 \rightarrow CH_3CHO + CH_3C(O)OCH_2CH_3$							
Butanoic acid, 3-hydroxy-, ethyl ester							
71 YAT/RAM	EX	583-613	9.54(10)	0	19980	1	
Thermolysis in capilary glass 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.							

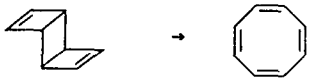
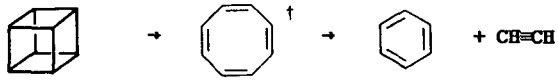
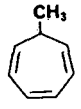
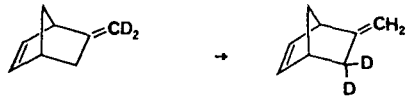
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (+ M) →  (+ M)							
1,3,5-Cycloheptatriene → Benzene, methyl- (Toluene)							
76 GAY/GIL	EX	990-1250	3.98(13)	0	25741±1203	1	2.0
Thermal isomerization behind shock-waves. [1,3,5-Cycloheptatriene] ≈ (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.							

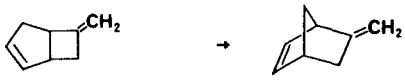
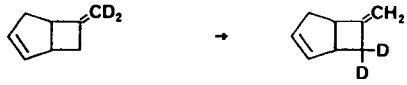
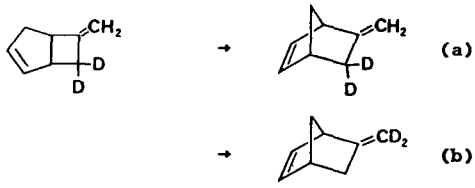
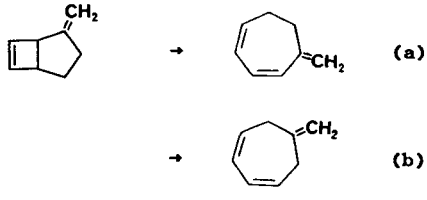
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[3.2.0]hept-2-en-6-one → 1,3-Cyclopentadiene + Ethenone (Ketene)							
72 EGG/COC2	EX	471-534	1.45(13)	0	18888±126	1	1.29
Pyrolysis in a static reactor, in Propene diluent. Gas-chromatography.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

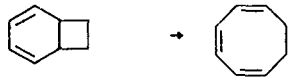
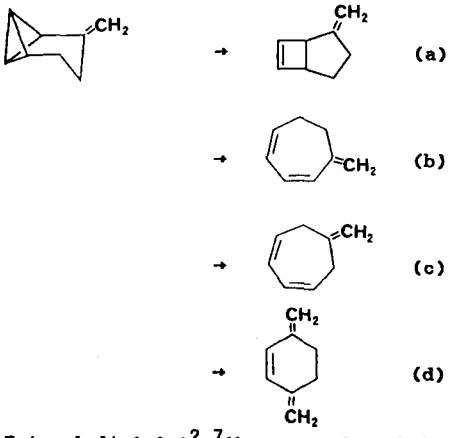
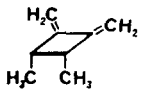
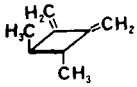
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 → $CH_3OCH{=}CH_2 + CH_3CH{=}CHCHO$							
2H-Pyran, 3,4-dihydro-2-methoxy-4-methyl-, trans-							
75 COL/FRE	EX	560-618	1.76(14)	0	24233±144	1	1.28
Thermolysis in a static system.							
P = (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.							

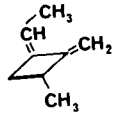
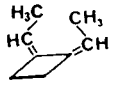
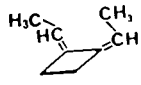
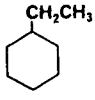
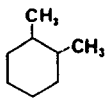
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 (+ M) →  (+ M) (a)							
→  + CH≡CH (+ M) (b)							
1,3,5,7-Cyclooctatetraene → Peentalene, 1,5-dihydro- (a)							
→ Benzene + Ethyne (b)							
79 DUD/GLA1 ($k_a + k_b$)	EX	1000-1400	1.58(13)	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] = (0.06-1.2)x10^{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.							
[ (+ M)]							
→ isomerization products (+ M) (a)							
→  + CH≡CH (+ M) (b)							
[1,3,5,7-Cyclooctatetraene - Bicyclo[4.2.0]octa-							
2,4,7-triene] → isomerization products (a)							
→ Benzene + Ethyne (b)							
79 DUD/GLA2 ($k_a + k_b$)	EX	298	1.1(6)			1	
λ = 311.8 nm.							
<E> = 94.168 kcal.$mol.^{-1}$							
M = 1,3,5,7-Cyclooctatetraene.							
($k_a + k_b$)	EX	298	2.7(7)			1	
λ = 247.4 nm.							
<E> = 118.045 kcal.$mol.^{-1}$.							
M = 1,3,5,7-Cyclooctatetraene.							
($k_a + k_b$. M = He)	EX	298	4.5(6)			1	
λ = 282 nm.							
<E> = 103.872 kcal.mol^{-1}.							
($k_a + k_b$. M = He)	EX	298	3.0(7)			1	
λ = 245 nm.							
<E> = 119.168 kcal.mol^{-1}.							
Isomerization and decomposition of							
Cyclooctatetraene by both, steady-state							
Photolysis and Laser Flash-photolysis.							

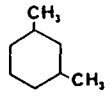
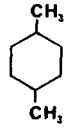
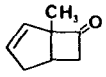
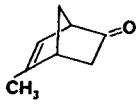
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
1,5-Dihydropentalene → Benzene, ethenyl- (Styrene)							
79 DUD/GLA1	EX	1200-1600	1.26(13)	0	29109±962	1	2.0
Pyrolysis behind incident or reflected shock-waves. M = Ar. UV-, and IR-Absorption spectrometry. [Ar] = (0.06-0.12)x10^{19} molec.cm^{-3}.							
							
(main primary product)							
1,5-Dihydropentalene → Cyclopropa[cd]pentalene, 2a,2b,4a,4b-tetrahydro- (Semibullvalene)							
79 DUD/GLA2	EX	298	1.5(7)			1	
<E> = 118.714 kcal.$mol.^{-1}$ at 246 nm. M = 1,5-Dihydropentalene. Isomerization by steady-state photolysis.							
							
Cyclopropa[cd]pentalene, 2a,2b,4a,4b-tetrahydro- (Semibullvalene) → 1,5-Dihydropentalene							
79 DUD/GLA1	EX	740-900	6.31(14)	0	20689±1203	1	2.51
Pyrolysis behind incident or reflected shock-waves. M = Ar. UV-, and IR-Absorption Spectrometry. [Ar] = (1.2-3.0)x10^{19} molec.cm^{-3}.							
							
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	EX	363-394	1.66(14)	0	15345±81	1	1.23
Gas-chromatography.							

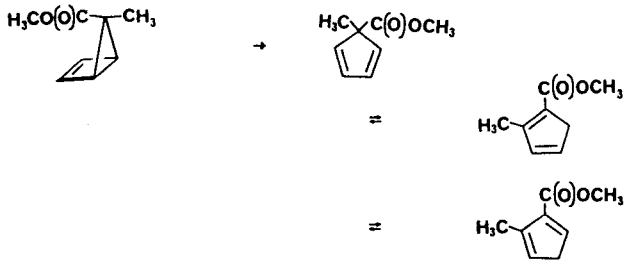
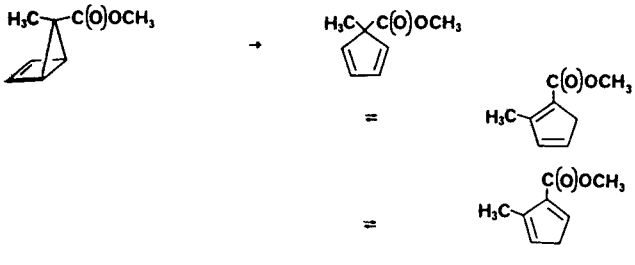
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Tricyclo[4.2.0.$0^{2,5}$]octa-3,7-diene, (1α,2β,5β,6α)- (anti form) → 1,3,5,7-Cyclooctatetraene							
74 CAS/DEW	EX	[1])	1.51(14)	0	16306±453	1	3.63
	EX	370	1.40(-5)			1	
[1]) Temperature 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] = 4.81×10^{17}-1.20×10^{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.							

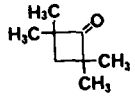
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
							
Bicyclo[4.2.0]octa-2,4-diene → 1,3,5-Cyclooctatriene							
83 GRE/ORC	EX	330-475	2.40(12)	0	12858±180	1	1.70
Static reactor. Gas-chromatography.							
 (a) (b) (c) (d)							
Tricyclo[4.1.0.0^{2,7}]heptane, 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.							

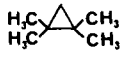
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 **(+ M) → products**							
Cyclohexane, 1,3-dimethyl-							
81 SAT/KAL	EX	993-1098	6.92(12)	0	28183±2365	1	5.01
Pyrolysis in a quartz reactor. M = Ar. P(1,3-Dimethylcyclohexane) = 80 torr. P(Ar) = 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)	DE	1100-1400	4.57(11)	0	26463	1	
(Based on a proposed mechanism.)							
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
($k_a + k_b$)	EX	637-700	8.91(14)	0	28269±47	1	1.07

Thermolysis in a static system.
IR-, and NMR-Spectrometry.
Gas-chromatography.
P_o = (6-8) torr.
Rate constants are P-independent within this range.

$(CH_3)_2CHC(O)OC(O)CH(CH_3)_2$ → $(CH_3)CHCOOH$ + $(CH_3)_2C{=}C{=}O$

Propanoic acid, 2-methyl-, anhydride

76 BLA/CRA	EX	519-556	6.45(11)	0	18223±366	1	1.95

Thermolysis in a static system with packed and unpacked vessels.

$CH_3C(O)OCH_2CH_2CH(CH_3)CH_2CH_3$

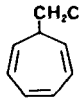
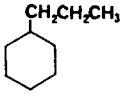
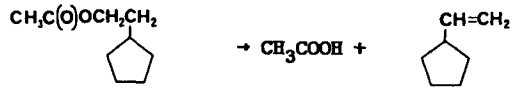
CH_3COOH + $CH_2{=}CHCH(CH_3)CH_2CH_3$

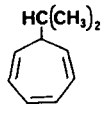
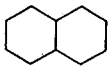
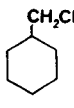
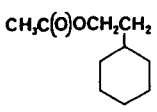
1-Pentanol, 3-methyl-, acetate

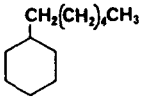
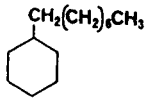
81 MAR/CHU	EX	633-693	4.17(13)	0	25488±144	1	1.23

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
$CH_3C(O)OCH_2CH_2CH_2CH(CH_3)_2 \rightarrow CH_3COOH + CH_2{=}CHCH_2CH(CH_3)_2$							
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)	ES	900-1400	9.12(13)	0	25741	1	
(Extrapolated)							
(Limiting high-pressure k, model A_2)	ES	900-1400	3.89(13)	0	24947	1	
(Extrapolated)							
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.							
$CH_3C(O)OCH(CH_2CH_3)C(CH_3)_3$ → CH_3COOH + cis-$CH_3CH{=}CHC(CH_3)_3$ (a) → CH_3COOH + trans-$CH_3CH{=}CHC(CH_3)_3$ (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] = 1.81×10^{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.							

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6. Conversion Factors for Rate Constants

Equivalent second order rate constants

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

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

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

Equivalent third order rate constants

A \ B	$cm^6\ mol^{-2}\ s^{-1}$	$dm^6\ mol^{-2}\ s^{-1}$	$m^6\ mol^{-2}\ s^{-1}$	$cm^6\ molecule^{-2}\ s^{-1}$	$(mm\ Hg)^{-2}\ s^{-1}$	$atm^{-2}\ s^{-1}$	$ppm^{-2}\ min^{-1}$	$m^4\ kN^{-2}\ s^{-1}$
1 $cm^6\ mol^{-2}\ s^{-1}$ =	1	10^{-6}	10^{-12}	2.76×10^{-48}	$2.57 \times 10^{-10}\ T^{-2}$	$1.48 \times 10^{-4}\ T^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-8}\ T^{-2}$
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 $cm^6 molecule^{-2}\ s^{-1}$ =	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	1.623×10^6
1 $m^1\ kN^{-2}\ s^{-1}$ =	$6.91 \times 10^7\ T^2$	$69.1\ T^2$	$6.91 \times 10^{-5}\ T^2$	$1.904 \times 10^{-40}\ T^2$	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 $H + (CH_3)_2CHCH{=}CH_2$, but $(CH_3)_2CH{=}CH_2$.
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±0.5)(11), and 73 DAY/THO with the same k. For the first two entries, 72 DIX with k/k_{ref} = 2.8±0.42, 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 $CH_3C{\equiv}CCH(\cdot)CH_3$.

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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.

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